IMPLICIT BIAS OF MSE GRADIENT OPTIMIZATION IN UNDERPARAMETERIZED NEURAL NETWORKS

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ABSTRACT

We study the dynamics of a neural network in function space when optimizing the mean squared error via gradient flow. We show that in the underparameterized regime the network learns eigenfunctions of an integral operator T_K determined by the Neural Tangent Kernel (NTK) at rates corresponding to their eigenvalues. For example, for uniformly distributed data on the sphere S^{d-1} and rotation invariant weight distributions, the eigenfunctions of T_K are the spherical harmonics. Our results can be understood as describing a spectral bias in the underparameterized regime. The proofs use the concept of "Damped Deviations" where deviations of the NTK matter less for eigendirections with large eigenvalues. Aside from the underparameterized regime, the damped deviations point-of-view allows us to extend certain results in the literature in the overparameterized setting.

1 INTRODUCTION

A surprising but well established empirical fact is that neural networks optimized by gradient descent can find solutions to the empirical risk minimization (ERM) problem that generalize. This is surprising from an optimization point-of-view because the ERM problem induced by neural networks is nonconvex (Sontag & Sussmann, 1989; 1991) and can even be NP-Complete in certain cases (Blum & Rivest, 1993). Perhaps even more surprising is that the discovered solution can generalize even when the network is able to fit arbitrary labels (Zhang et al., 2017), rendering traditional complexity measures such as Rademacher complexity inadequate. How does deep learning succeed in the face of pathological behavior by the standards of classical optimization and statistical learning theory?

Towards addressing generalization, a modern line of thought that has emerged is that gradient descent performs implicit regularization, limiting the solutions one encounters in practice to a favorable subset of the model's full capacity (see, e.g., Neyshabur et al., 2015; 2017; Gunasekar et al., 2017; Wu et al., 2017). An empirical observation is that neural networks optimized by gradient descent tend to fit the low frequencies of the target function first, and only pick up the higher frequencies later in training (Rahaman et al., 2019; Ronen et al., 2019; Basri et al., 2020; Xu et al., 2019). A closely related theme is gradient descent's bias towards smoothness for regression problems (Williams et al., 2019; Jin & Montúfar, 2021). For classification problems, in suitable settings gradient descent provably selects max-margin solutions (Soudry et al., 2018; Ji & Telgarsky, 2019). Gradient descent is not impartial, thus understanding its bias is an important program in modern deep learning.

Generalization concerns aside, the fact that gradient descent can succeed in a nonconvex optimization landscape warrants attention on its own. A brilliant insight made by Jacot et al. (2018) is that in function space the neural network follows a kernel gradient descent with respect to the "Neural Tangent Kernel" (NTK). This kernel captures how the parameterization biases the trajectory in function space, an abstraction that allows one to largely ignore parameter space and its complications. This is a profitable point-of-view, but there is a caveat. The NTK still depends on the evolution of the network parameters throughout time, and thus is in general time-dependent and complicated to analyze. However, under appropriate scaling of the parameters in the infinite-width limit it remains constant (Jacot et al., 2018). Once the NTK matrix has small enough deviations to remain strictly positive definite throughout training, the optimization dynamics start to become comparable to that of a linear model (Lee et al., 2019). For wide networks (quadratic or higher polynomial dependence on the number of training data samples n and other parameters) this property holds and this has been used by a variety of works to prove global convergence guarantees for the optimization (Du

et al., 2019b; Oymak & Soltanolkotabi, 2020; Du et al., 2019a; Allen-Zhu et al., 2019a;b; Zou et al., 2020; Zou & Gu, 2019; Song & Yang, 2020; Dukler et al., 2020)[1] and to characterize the solution throughout time (Arora et al., 2019; Basri et al., 2020). The NTK has been so heavily exploited in this setting that it has become synonymous with polynomially wide networks where the NTK is strictly positive definite throughout training, the so called "NTK Regime". This begs the question, to what extent is the NTK informative outside the NTK regime?

While the NTK has hitherto been associated with the heavily overparameterized regime, we demonstrate that refined analysis is possible in the underparameterized setting. The NTK regime is highly profitable and deserves to be studied, however if we are to understand practical neural networks on their own terms we must push the theory to allow for moderate widths relative to the number of samples. Our theorems primarily concern a one-hidden layer network, however unlike many NTK results appearing in the literature our network has *biases* and *both* layers are trained. In fact, the machinery we build is strong enough to extend some existing results in the overparameterized regime appearing in the literature to the case of training both layers.

1.1 Related Work

There has been a deluge of works on the Neural Tangent Kernel since it was introduced by Jacot et al. (2018), and thus we do our best to provide a partial list. Global convergence guarantees for the optimization, and to a lesser extent generalizeation, for networks polynomially wide in the number of training samples n and other parameters has been addressed in several works (Du et al., 2019b; Oymak & Soltanolkotabi, 2020; Du et al., 2019a; Allen-Zhu et al., 2019a;b; Zou et al., 2020; Zou & Gu, 2019; Song & Yang, 2020; Arora et al., 2019). To our knowledge, for the regression problem with arbitrary labels, quadratic overparameterization $m \gtrsim n^2$ is state-of-the art (Oymak & Soltanolkotabi, 2020; Song & Yang, 2020; Nguyen & Mondelli, 2020). Weinan E (2020) gave a fairly comprehensive study of optimization and generalization of shallow networks trained under the standard parameterization. Under the standard parameterization, changes in the outer layer weights are more significant, whereas under the NTK parameterization both layers have roughly equal effect. Since we study the NTK parameterization in this work, we view the analysis as complementary.

Our work is perhaps most closely connected with Arora et al. (2019). In Theorem 4.1 in that work they showed that for a shallow network in the polynomially overparameterized regime $m \gtrsim n^7$, the training error along eigendirections of the NTK matrix decay linearly at rates that correspond to their eigenvalues. Our main Theorem 3.5 can be viewed as an analogous statement for the actual risk (not the empirical risk) in the underparameterized regime: eigenfunctions of the NTK integral operator T_K are approximately learned linearly at rates that correspond to their eigenvalues. In contrast with Arora et al. (2019), we have that the requirements on width m and number of samples n required to learn eigenfunctions with large eigenvalues are smaller compared to those with small eigenvalues. Surprisingly the machinery we build is also strong enough to prove in our setting the direct analog of Theorem 4.1. Our overparameterization requirement ignoring logarithmic factors is is smaller by a factor of $\frac{n^2}{d\delta^4}$ where n is the number of input samples, d is the input dimension, and δ is the failure probability. Note that Arora et al. (2019) train the hidden layer of a ReLU network via gradient descent, whereas we are training both layers with biases for a network with smooth activations via gradient flow. Due to the different settings, the results are not directly comparable.

Although it was not our focus, the tools to prove Theorem 3.5 are enough to prove analogs of Theorem 4 and Corollary 2 in the work of Su & Yang (2019). Again in this work they train the hidden layer of a ReLU network via gradient descent, whereas we are training both layers with biases for a network with smooth activations via gradient flow. Theorem 4 and Corollary 2 of Su & Yang (2019) are empirical risk guarantees that show that for target functions that participate mostly in the top eigendirections of the NTK integral operator T_K, moderate overparameterization is possible. In our results the bounds and requirements are comparable to Su & Yang (2019), with neither appearing better. Again due to the different settings, we emphasize the results are not directly comparable. Nevertheless we think it is important to demonstrate that these results hold for training both layers with biases, and we hope our "Damped Deviations" approach will simplify the interpretation of the aforementioned works.

[1] Not all these works explicitly use that the NTK is positive definite. However, they all operate in the regime where the weights do not vary much and thus are typically associated with the NTK regime.

1.2 OUR CONTRIBUTIONS

The key idea for our work is the concept of "Damped Deviatons", the fact that for the squared error deviations of the NTK are softened by a damping factor, with large eigendirections being damped the most. This enables the following results.

- In Theorem 3.5 we characterize the bias of the neural network to learn the eigenfunctions of the integral operator T_K associated with the Neural Tangent Kernel (NTK) at rates proportional to the corresponding eigenvalues.
- In Theorem 3.7 we show that in the overparameterized setting the training error along different dynamics can be sharply characterized, showing that Theorem 4.1 in Arora et al. (2019) holds when training both layers with a smaller overparameterization requirement.
- In Theorem 3.8 and Corollary 3.9 we show that moderate overparameterization is sufficient for solving the ERM problem when the target function has a compact representation in terms of eigenfunctions of T_K. This extends the results in Su & Yang (2019) to the setting of training both layers with smooth activations.

2 GRADIENT DYNAMICS AND DAMPED DEVIATIONS

2.1 NOTATIONS

We will use $\|\bullet\|_2$ and $\langle \bullet, \bullet \rangle_2$ to denote the L^2 norm and inner product respectively (for vectors or for functions depending on context). For a matrix A, $\|A\|_{op} := \sup_{\|x\|_2 \leq 1} \|Ax\|_2$ is the operator norm induced by the Euclidean norm. We will let $\langle \bullet, \bullet \rangle_{\mathbb{R}^n}$ denote the standard inner product on $\mathbb{R}^n$ normalized by $\frac{1}{n}$, namely $\langle x, y \rangle_{\mathbb{R}^n} = \frac{1}{n}\langle x, y \rangle_2 = \frac{1}{n}\sum_{i=1}^n x_i y_i$. We will let $\|x\|_{\mathbb{R}^n} = \sqrt{\langle x, x \rangle_{\mathbb{R}^n}}$ be the associated norm. This normalized inner product has the convenient property that if $v \in \mathbb{R}^n$ such that $v_i = O(1)$ for each i then $\|v\|_{\mathbb{R}^n} = O(1)$, where by contrast $\|v\|_2 = O(\sqrt{n})$. This is convenient as we will often consider what happens when $n \to \infty$. $\|\bullet\|_\infty$ will denote the supremum norm with associated space L^∞. We will use the standard big O and Ω notation with $\tilde{O}$ and $\tilde{\Omega}$ hiding logarithmic terms.

2.2 GRADIENT DYNAMICS AND THE NTK INTEGRAL OPERATOR

We will let $f(x; \theta)$ denote our neural network taking input $x \in \mathbb{R}^d$ and parameterized by $\theta \in \mathbb{R}^p$. The specific architecture of the network does not matter for the purposes of this section. Our training data consists of n input-label pairs $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. We focus on the setting where the labels are generated from a fixed target function f^*, i.e. $y_i = f^*(x_i)$. We will concatenate the labels into a label vector $y \in \mathbb{R}^n$, i.e. $y_i = f^*(x_i)$. We will let $\hat{r}(\theta) \in \mathbb{R}^n$ be the vector whose ith entry is equal to $f(x_i; \theta) - f^*(x_i)$. Hence $\hat{r}(\theta)$ is the residual vector that measures the difference between our neural networks predictions and the labels. We will be concerned with optimizing the squared loss

$$\Phi(\theta) = \frac{1}{2n} \|\hat{r}(\theta)\|_2^2 = \frac{1}{2} \|\hat{r}(\theta)\|_{\mathbb{R}^n}^2 .$$

Optimization will be done by gradient flow

$$\partial_t \theta_t = -\partial_\theta \Phi(\theta),$$

which is the continuous time analog of gradient descent. We will denote the residual at time t, $\hat{r}(\theta_t)$, as $\hat{r}_t$ for the sake of brevity. We will let $r_t(x) := f(x; \theta_t) - f^*(x)$ denote the residual off of the training set for an arbitrary input x.

We quickly recall some facts about the Neural Tangent Kernel and its connection to the gradient dynamics. For a comprehensive tutorial we suggest Jacot et al. (2018). The analytical NTK is the kernel given by

$$K^\infty(x, x') := \mathbb{E}\left[\left\langle \frac{\partial f(x;\theta)}{\partial \theta}, \frac{\partial f(x';\theta)}{\partial \theta} \right\rangle_2 \right],$$

where the expectation is taken with respect to the parameter initialization for θ. We associate K^∞ with the integral operator $T_K : L^2 \to L^2$ defined by

$$T_K f(x) := \int_X K^\infty(x,s) f(s) d\rho(s),$$

where X is our input space with probability measure ρ. Our training data $x_i \in X$ are distributed according to this measure $x_i \sim \rho$. By Mercer's theorem we can decompose

$$K^\infty(x,x') = \sum_{i=1}^{\infty} \sigma_i \phi_i(x) \phi_i(x'),$$

where $\{\phi_i\}_{i=1}^n$ is an orthonormal basis of L^2, $\{\sigma_i\}_{i=1}^\infty$ is a nonincreasing sequence of positive values, and each ϕ_i is an eigenfunction of T_K with eigenvalue $\sigma_i > 0$. When $X = S^{d-1}$ is the unit sphere, ρ is the uniform distribution, and the weights of the network are from a rotation invariant distribution (e.g. standard Gaussian), $\{\phi_i\}_{i=1}^\infty$ are the spherical harmonics (which in $d = 2$ is the Fourier basis) due to K^∞ being rotation-invariant (see Bullins et al., 2018, Theorem 2.2). We will let $\kappa := \max_{x \in X} K^\infty(x,x)$ which will be a relevant quantity in our later theorems. The training data inputs $\{x_1, \ldots, x_n\}$ induce a discretization of the integral operator T_K, namely $T_n : C(X) \to C(X)$

$$T_n f(x) := \frac{1}{n} \sum_{i=1}^n K^\infty(x, x_i) f(x_i) = \int_X K^\infty(x,s) f(s) d\rho_n(s),$$

where $\rho_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ is the empirical measure. We recall the definition of the time-dependent NTK[2],

$$K_t(x,x') := \left\langle \frac{\partial f(x;\theta_t)}{\partial \theta}, \frac{\partial f(x';\theta_t)}{\partial \theta} \right\rangle_2.$$

We can look at the version of T_n corresponding to K_t, namely

$$T_n^t f(x) := \frac{1}{n} \sum_{i=1}^n K_t(x, x_i) f(x_i) = \int_X K_t(x,s) f(s) d\rho_n(s).$$

We recall that the residual $r_t(x) := f(x;\theta) - f^*(x)$ follows the update rule

$$\partial_t r_t(x) = -\frac{1}{n} \sum_{i=1}^n K_t(x, x_i) r_t(x_i) = -T_n^t r_t.$$

We will let $(H_t)_{i,j} := K_t(x_i, x_j)$ and $H^\infty_{i,j} := K^\infty(x_i, x_j)$ denote the Gram matrices induced by these kernels and we will let $G_t := \frac{1}{n} H_t$ and $G^\infty := \frac{1}{n} H^\infty$ be their normalized versions[3]. Throughout we will let $u_1, \ldots, u_n$ denote the eigenvectors of G^∞ with corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$. The $u_1, \ldots, u_n$ are chosen to be orthonormal with respect to the inner product $\langle \bullet, \bullet \rangle_{\mathbb{R}^n}$. When restricted to the training set we have the update rule

$$\partial_t \hat{r}_t = -\frac{1}{n} H_t \hat{r}_t = -G_t \hat{r}_t.$$

2.3 Damped Deviations

The concept of damped deviations comes from the very simple lemma that follows (the proof is provided in Appendix D). The lemma compares the dynamics of the residual $\hat{r}(t)$ on the training set to the dynamics of an arbitrary kernel regression $\exp(-Gt)\hat{r}(0)$:

Lemma 2.1. *Let $G \in \mathbb{R}^{n \times n}$ be an arbitrary positive semidefinite matrix G_s the time dependent NTK matrix at time s. Then*

$$\hat{r}_t = \exp(-Gt)\hat{r}_0 + \int_0^t \exp(-G(t-s))(G - G_s)\hat{r}_s ds.$$

[2]The NTK is an overloaded term. To help ameliorate the confusion, we will use NTK to describe K^∞ and NTK (italic font) to describe the time-dependent version K_t.

[3]G_t and G^∞ are the natural matrices to work with when working with the mean squared error as opposed to the unnormalized squared error. Also G^∞'s spectra concentrates around the spectrum of the associated integral operator T_K and is thus a more convenient choice in our setting.

Let's specialize the lemma to the case where $G = G^\infty$. In this case the first term is $\exp(-G^\infty t)\hat{r}_0$, which is exactly the dynamics of the residual in the exact NTK regime when $G_t = G^\infty$ for all t. The second term is a correction term that weights the NTK deviations $(G^\infty - G_s)$ by the damping factor $\exp(-G^\infty(t-s))$. We see that damping is largest along the large eigendirections of G^∞. The equation becomes most interpretable when projected along a specific eigenvector. Fix an eigenvector u_i of G^∞ corresponding to eigenvalue λ_i. Then the equation along this component becomes

$$\langle \hat{r}_t, u_i \rangle_{\mathbb{R}^n} = \exp(-\lambda_i t)\langle \hat{r}_0, u_i \rangle_{\mathbb{R}^n} + \int_0^t \langle \exp(-\lambda_i(t-s))(G^\infty - G_s)\hat{r}_s, u_i \rangle_{\mathbb{R}^n} ds.$$

The first term above converges to zero at rate λ_i. The second term is a correction term that weights the deviatiations of the NTK matrix G_s from G^∞ by the damping factor $\exp(-\lambda_i(t-s))$. The second term can be upper bounded by

$$\begin{aligned} \left| \int_0^t \langle \exp(-\lambda_i(t-s))(G^\infty - G_s)\hat{r}_s, u_i \rangle_{\mathbb{R}^n} ds \right| &\leq \int_0^t \exp(-\lambda_i(t-s)) \left\| G^\infty - G_s \right\|_{op} \left\| \hat{r}_s \right\|_{\mathbb{R}^n} ds \\ &\leq \frac{[1-\exp(-\lambda_i t)]}{\lambda_i} \sup_{s\in[0,t]} \left\| G^\infty - G_s \right\|_{op} \left\| \hat{r}_0 \right\|_{\mathbb{R}^n}, \end{aligned}$$

where we have used the property $\|\hat{r}_s\|_{\mathbb{R}^n} \leq \|\hat{r}_0\|_{\mathbb{R}^n}$ from gradient flow. When $f^* = O(1)$ we have that $\|\hat{r}_0\|_{\mathbb{R}^n} = O(1)$, thus whenever $\|G^\infty - G_s\|_{op}$ is small relative to λ_i this term is negligible. It has been identified that the NTK matrices tend to have a small number of outlier large eigenvalues and exhibit a low rank structure (Oymak et al., 2020; Arora et al., 2019). In light of this, the dependence of the above bound on the magnitude of λ_i is particularly interesting. We reach following important conclusion.

Observation 2.2. *The dynamics in function space will be similar to the NTK regime dynamics along eigendirections whose eigenvalues are large relative to the deviations of the time-dependent NTK matrix from the analytical NTK matrix.*

The equation in Lemma 2.1 concerns the residual restricted to the training set, but we will be interested in the residual for arbitrary inputs. Recall that $r_t(x) = f(x;\theta_t) - f^*(x)$ denotes the residual at time t for an arbitrary input. Then more generally we have the following damped deviations lemma for the whole residual (proved in Appendix C.3).

Lemma 2.3. *Let $[T_K h](\bullet) = \int_X K^\infty(\bullet, s)h(s)d\rho(s)$ be the integral operator associated with K^∞ and let $[T_n^s h](\bullet) = \frac{1}{n}\sum_{i=1}^n K_s(\bullet, x_i)h(x_i)$ denote the time-dependent operator associated with K_s. Then*

$$r_t = \exp(-T_K t)r_0 + \int_0^t \exp(-T_K(t-s))(T_K - T_n^s)r_s ds,$$

where the equality is in the L^2 sense.

Here T_K and T_n^s are the operator analogs of G^∞ and G_s respectively. From this statement the same concepts holds as before, the dynamics of r_t will be similar to that of $\exp(-T_K t)r_0$ along eigendirections whose eigenvalues are large relative to the deviations $(T_K - T_n^s)$. In the underparameterized regime we can bound the second term and make it negligible (Theorem 3.5) and thus demonstrate that the eigenfunctions ϕ_i of T_K with eigenvalues σ_i will be learned at rate σ_i. When the input data are distributed uniformly on the sphere S^{d-1} and the network weights are from a rotation-invariant distribution, the eigenfunctions of T_K are the spherical harmonics (which is the Fourier basis when $d = 2$). In this case the network is biased towards learning the spherical harmonics that correspond to large eigenvalues of T_K. It is in this vein that we will demonstrate a spectral bias.

3 Main Results

Our theorems will concern the shallow neural network

$$f(x;\theta) = \frac{1}{\sqrt{m}}\sum_{\ell=1}^m a_\ell \sigma(\langle w_\ell, x\rangle_2 + b_\ell) + b_0 = \frac{1}{\sqrt{m}} a^T \sigma(Wx + b) + b_0,$$

where $W \in \mathbb{R}^{m\times d}$, $a, b \in \mathbb{R}^m$ and $b_0 \in \mathbb{R}$ and $w_\ell = W_{\ell,:}$ denotes the ℓth row of W and $\sigma : \mathbb{R} \to \mathbb{R}$ is applied entry-wise. $\theta = (a^T, vec(W)^T, b^T, b_0)^T \in \mathbb{R}^p$ where $p = md + 2m + 1$ is the total number

of parameters. Here we are utilizing the NTK parameterization (Jacot et al., 2018). For a thorough analysis using the standard parameterization we suggest Weinan E (2020). We will consider two parameter initialization schemes. The first initializes $W_{i,j}(0) \sim \mathcal{W}$, $b_\ell(0) \sim \mathcal{B}$, $a_\ell(0) \sim \mathcal{A}$, $b_0 \sim \mathcal{B}'$ i.i.d., where $\mathcal{W}, \mathcal{B}, \mathcal{A}, \mathcal{B}'$ represent zero-mean unit variance subgaussian distributions. In the second initialization scheme we initialize the parameters according to the first scheme and then perform the following swaps $W(0) \to \begin{bmatrix} W(0) \\ W(0) \end{bmatrix}$, $b(0) \to \begin{bmatrix} b(0) \\ b(0) \end{bmatrix}$, $a(0) \to \begin{bmatrix} a(0) \\ -a(0) \end{bmatrix}$, $b_0 \to 0$ and replace the $\frac{1}{\sqrt{m}}$ factor in the parameterization with $\frac{1}{\sqrt{2m}}$. This is called the "doubling trick" (Chizat et al., 2019; Zhang et al., 2020) and ensures that the network is identically zero $f(x;\theta_0) \equiv 0$ at initialization. We will explicitly state where we use the second scheme and otherwise will be using the first scheme.

The following assumptions will persist throughout the rest of the paper:

Assumption 3.1. *σ is a C^2 function satisfying $\|\sigma'\|_\infty, \|\sigma''\|_\infty < \infty$.*

Assumption 3.2. *The inputs satisfy $\|x\|_2 \leq M$.*

Assumption 3.3. *T_K is strictly positive, i.e., $\langle f, T_K f\rangle_2 > 0$ for $f \neq 0$.*

Most activation functions other than ReLU satisfy Assumption 3.1, such as Softplus $\sigma(x) = \ln(1 + e^x)$, Sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$, and Tanh $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$. Assumption 3.2 is a mild assumption which is satisfied for instance for RGB images and has been commonly used (Du et al., 2019b;a; Oymak & Soltanolkotabi, 2020). Assumption 3.3 is again a mild assumption that is satisfied for a broad family of parameter initializations (e.g. Gaussian) anytime σ is not a polynomial function, as we will show in Appendix G. Assumption 3.3 is not strictly necessary but it simplifies the presentation by ensuring T_K has no zero eigenvalues.

We will track most constants that depend on parameters of our theorems such as M, the activation function σ, and the target function f^*. However, constants appearing in concentration inequalities such as Hoeffding's or Bernstein's inequality or constants arising from $\delta/2$ or $\delta/3$ arguments will not be tracked. We will reserve $c, C > 0$ for untracked constants whose precise meaning can vary from statement to statement. In the proofs in the appendix it will be explicit which constants are involved.

3.1 Uniform NTK Deviation Bound

The key technical innovation that we will use to prove our main result (Theorem 3.5) is an NTK deviation bound that is uniform over *all* inputs, and allows us to vary the width m independently from the number of samples n. Existing works (e.g. Huang & Yau, 2020; Du et al., 2019b;a) focus on the setting where the number of samples n is fixed and the width m is allowed to vary, and only give bounds on the kernel restricted to the training set. In Appendix B we prove the following result (Theorem B.26) which provides uniform deviation bounds for the NTK.

Theorem 3.4. *(Informal) For some $\Gamma > 1$ we have with high probability over the sampling of θ_0*

$$\sup_{(x,x') \in B_M \times B_M} |K_t(x,x') - K^\infty(x,x')| = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 \|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right).$$

Theorem 3.4 is technical to prove, but once one has this bound it can be combined with the damped deviations Lemmas 2.1 and 2.3 to describe the dynamics in function space of the network both on and off the training set. We think this NTK deviation bound is of independent interest and can potentially be used to prove further results in the setting of training both layers with biases.

3.2 Underparameterized Regime

Our main result compares the dynamics of the residual $r_t(x) = f(x;\theta_t) - f^*(x)$ to that of $\exp(-T_K t) r_0$ in the underparameterized setting. Note that $\langle \exp(-T_K t) r_0, \phi_i\rangle_2 = \exp(-\sigma_i t)\langle r_0, \phi_i\rangle_2$, thus $\exp(-T_K t) r_0$ learns the eigenfunctions ϕ_i of T_K at rate σ_i. Therefore $\exp(-T_K t) r_0$ exhibits a bias to learn the eigenfunctions of T_K corresponding to large eigenvalues more quickly. To our knowledge no one has been able to rigorously relate the dynamics in function space of the residual r_t to $\exp(-T_K t) r_0$, although that seems to be what is suggested by Ronen

et al. (2019); Basri et al. (2020). The existing works we are aware of (Arora et al., 2019; Basri et al., 2020; Cao et al., 2020) characterize the bias of the empirical residual in the heavily overparameterized regime. By contrast, we characterize the bias of the whole residual in the underparameterized regime.

Theorem 3.5. *Let P_k be the orthogonal projection in L^2 onto span$\{\phi_1, \ldots, \phi_k\}$ and let $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$. If we are doing the doubling trick set $S' = 0$ and otherwise set $S' = O(\sqrt{d\log(CM\tilde{O}(\sqrt{m})) + \log(c/\delta)}) = \tilde{O}(\sqrt{d})$, $\quad S = \|f^*\|_\infty + S'$. Also let $\Gamma > 1, T > 0$. Assume*

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta) + \tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta) + \tilde{O}(d))\right\}.$$

Then with probability at least $1-\delta$ we have that for all $t \leq T$ and $k \in \mathbb{N}$

$$\|P_k(r_t - \exp(-T_K t)r_0)\|_2 \leq \frac{1-\exp(-\sigma_k t)}{\sigma_k}\tilde{O}\left(S\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 S\right] + \frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right)$$

and

$$\|r_t - \exp(-T_K t)r_0\|_2 \leq t\tilde{O}\left(S\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 S\right] + \frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right).$$

If we are performing the doubling trick the hypothesis $m \geq \frac{4D^2 O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}$ can be removed and the same conclusion holds.

Theorem 3.5 will be proved in Appendix C. The proof uses the uniform deviation bounds for the NTK to bound $T_n - T_n^s$ and tools from empirical process theory to show convergence of T_n to T_K uniformly over a class of functions corresponding to networks with bounded parameter norms.

To interpret the results, we observe that to track the dynamics for eigenfunctions corresponding to eigenvalue σ_k and above, the expression under the $\tilde{O}$ needs to be small relative to $\frac{1}{\sigma_k}$. Thus the bias towards learning the eigenfunctions corresponding to large eigenvalues appears more pronounced. When $t = \log(\|r_0\|_2/\epsilon)/\sigma_k$, we have that $\|P_k \exp(-T_k t)r_0\|_2 \leq \epsilon$. Thus by applying this stopping time we get that to learn the eigenfunctions corresponding to eigenvalue σ_k and above, $\frac{1}{\sqrt{m}}$ and $\frac{\sqrt{p}}{\sqrt{n}}$ need to be small relative to $\frac{1}{\sigma_k^2}$. In typical NTK works the width m needs to be polynomially large relative to the number of samples n, where by contrast here the width depends on the inverse of the eigenvalues for the relevant components of the target function. From an approximation point-of-view this makes sense; the more complicated the target function the more expressive the model must be. We believe these are first steps towards adopting more precise requirements on the width m that do not require growth relative to the number of samples n.

We can apply Theorem 3.5 for an appropriate early stopping time t to get a bound on the test error:

Corollary 3.6. *Suppose that $f^* = O(1)$ and assume we are performing the doubling trick where $f_0 \equiv 0$ so that $r_0 = -f^*$. Let $k \in \mathbb{N}$ and let P_k be the orthogonal projection onto span$\{\phi_1, \ldots, \phi_k\}$. Set $t = \frac{\log(\sqrt{2}\|P_k f^*\|_2/\epsilon^{1/2})}{\sigma_k}$ Then we have that $m = \tilde{\Omega}(\frac{d}{\epsilon\sigma_k^4})$ and $n = \tilde{\Omega}\left(\frac{\sigma_1\kappa p}{\sigma_k^4\epsilon}\right)$ suffices to ensure with probability at least $1-\delta$*

$$\frac{1}{2}\|r_t\|_2^2 \leq 2\epsilon + 2\|(I-P_k)f^*\|_2^2.$$

If one specialized to the case where f^* is a finite sum of eigenfunctions of T_K (when the data is uniformly distributed on the sphere S^{d-1} and the network weights are from a rotation invariant distribution this corresponds to a finite sum of spherical harmonics, which in $d = 2$ is equivalently a bandlimited function) one can choose k such that $\|(I-P_k)f^*\|_2^2 = 0$. In this case σ_k can be treated as a constant that depends on the target function f^*. Since κ, σ_1 depend only on K^∞ which is fixed, we may consider them as constants. In this case to achieve ϵ test error it suffices to set $m = \tilde{\Omega}(\frac{d}{\epsilon})$ and $n = \tilde{\Omega}(\frac{p}{\epsilon})$. In the classic paper by Barron (1994) in approximation theory the estimated neural

network achieves test error $O(\frac{C_{f^*}}{m}) + O(\frac{p}{n}\log n)$, where C_{f^*} is a constant that depends on the decay in frequency domain of the target function. Thus in Barron's paper to achieve ϵ test error one requires $m = \Omega(C_{f^*}/\epsilon)$ and $n = \Omega(p/\epsilon)$. Thus in this special case gradient flow with early stopping achieves essentially the same rates (up to constants and logarithms) as Barron (1994). Barron (1994) has no gradient optimization, rather they study the performance of an empirical risk minimizer with an explicit regularizer that ensures bounded parameter norms. For us the gradient based optimization leads to bounded parameter norms which enables a similar covering number argument provided in Section C.4. The additional benefit of Theorem 3.5 is that one has control of the training dynamics along different components and does not merely ensure a test error bound. It is also interesting to note that the approximation results by Barron (1994) depend on the decay in frequency domain of the target function f^* via C_{f^*}, and similarly for us the constant $1/\sigma_k^4$ grows with the bandwidth of the target function in the case of uniform distribution on the sphere S^2 which we mentioned parenthetically above.

3.3 Overparameterized Regime

We now demonstrate how Theorem 3.4 can be combined with the damped deviations equation (Lemma 2.1) to describe the dynamics of the empirical risk in the overparameterized setting. The following is the analog of Theorem 4.1 from Arora et al. (2019) in our setting, proved in Appendix E. The result demonstrates that when the network is heavily overparameterized, the dynamics of the residual $\hat{r}_t$ follow the NTK regime dynamics $\exp(-G^\infty t)\hat{r}_0$.

Theorem 3.7. *Assume $m = \tilde{\Omega}(dn^5\epsilon^{-2}\lambda_n(H^\infty)^{-4})$ and $m \geq O(\log(c/\delta) + \tilde{O}(d))$ and $f^* = O(1)$. Assume we are performing the doubling trick so that $\hat{r}_0 = -y$. Let $v_1, \ldots, v_n$ denote the eigenvectors of G^∞ normalized to have unit L2 norm $\|v_i\|_2 = 1$. Then with probability at least $1-\delta$*

$$\hat{r}_t = \exp(-G^\infty t)(-y) + \delta(t),$$

where $\sup_{t\geq 0}\|\delta(t)\|_2 \leq \epsilon$. In particular

$$\|\hat{r}_t\|_2 = \sqrt{\sum_{i=1}^{n}\exp(-2\lambda_i t)|\langle y, v_i\rangle_2|^2} \pm \epsilon.$$

In the work of Arora et al. (2019) the requirement is $m = \Omega(\frac{n^7}{\lambda_n(H^\infty)^4\kappa^2\delta^4\epsilon^2})$ and $\kappa = O(\frac{\epsilon\delta}{\sqrt{n}})$ where $w_\ell \sim N(0, \kappa^2 I)$ (not to be confused with our definition of $\kappa := \max_x K^\infty(x,x)$). By contrast we are using $\kappa = 1$. They require κ to be small to ensure the neural network is small in magnitude at initializeation. To achieve the same effect we can perform antisymmetric initializeation to ensure the network is equivalently 0 at initializeation. Our overparameterization requirement ignoring logarithmic factors is smaller by a factor of $\frac{n^2}{d\delta^4}$. Again due to the different settings we do not claim superiority over this work.

The following is our analog of Theorem 4 by Su & Yang (2019) proved in Appendix F. This shows that when the target has a compact representation in terms of eigenfunctions of T_K, a more moderate overparametrization is sufficient to approximately solve the ERM problem.

Theorem 3.8. *Assume $m = \tilde{\Omega}\left(\epsilon^{-2}dT^2\|f^*\|_\infty^2(1+T\|f^*\|_\infty)^2\right)$ where $T > 0$ is a time parameter and $m \geq O(\log(c/\delta) + \tilde{O}(d))$ and $n \geq \frac{128\kappa^2\log(2/\delta)}{(\sigma_k-\sigma_{k+1})^2}$ Also assume $f^* \in L^\infty(X) \subset L^2(X)$ and let P^{T_K} be the orthogonal projection onto the eigenspaces of T_K corresponding to the eigenvalue $\alpha \in \sigma(T_K)$ and higher. Assume that $\left\|(I-P^{T_K})f^*\right\|_\infty \leq \epsilon'$ for some $\epsilon' > 0$. Pick k so that $\sigma_k = \alpha$ and $\sigma_{k+1} < \alpha$, i.e. k is the index of the last repeated eigenvalue corresponding to α in the ordered sequence $\{\sigma_i\}_i$. Also assume we are performing the doubling trick so that $\hat{r}(0) = -y$. Then we have with probability at least $1-3\delta$ over the sampling of $x_1, \ldots, x_n$ and θ_0 that for $t \leq T$*

$$\|\hat{r}_t\|_{\mathbb{R}^n} \leq \exp(-\lambda_k t)\|y\|_{\mathbb{R}^n} + \frac{4\kappa\|f^*\|_2\sqrt{10\log(2/\delta)}}{(\sigma_k-\sigma_{k+1})\sqrt{n}} + 2\epsilon' + \epsilon.$$

Su & Yang (2019) have $\|f^*\|_2 \leq \|f^*\|_\infty \leq 1$, $\kappa \leq \frac{1}{2}$ and they treat d as a constant. Taking these into account we do not see the overparameterization requirements or bounds of either work being

superior to the other. From Theorem 3.8, setting $\epsilon = \frac{4\kappa\|f^*\|_2\sqrt{10\log(2/\delta)}}{(\sigma_k-\sigma_{k+1})\sqrt{n}}$ and $\epsilon' = 0$ we immediately get the analog of Corollary 2 in the work of Su & Yang (2019). This explains how in the special case that the target function is a finite sum of eigenfunctions of T_K, the width m and the number of samples n can grow at the same rate, up to logarithms, and still solve the ERM problem. This is an ERM guarantee for $m = \tilde{\Omega}(n)$ and thus attains moderate overparameterization.

Corollary 3.9. *Assume* $m = \tilde{\Omega}\left(\frac{n(\sigma_k-\sigma_{k+1})^2 d\|f^*\|_\infty^2(1+\lambda_k^{-1}\|f^*\|_\infty)^2}{\kappa^2\|f^*\|_2^2\lambda_k^2}\right) \quad m \geq O(\log(c/\delta) + \tilde{O}(d))$ $n \geq \frac{128\kappa^2\log(2/\delta)}{(\sigma_k-\sigma_{k+1})^2}$. *Let* f^*, P^{T_K}, *and* k *be the same as in the hypothesis of Theorem 3.8. Furthermore assume that* $\left\|(I-P^{T_K})f^*\right\|_\infty = 0$. *Also assume we are performing the doubling trick so that* $\hat{r}(0) = -y$. *Set* $T = \log(\sqrt{n}\,\|\hat{r}(0)\|_{\mathbb{R}^n})/\lambda_k$. *Then we have with probability at least* $1-3\delta$ *over the sampling of* $x_1,\ldots,x_n$ *and* θ_0 *that for* $t \leq T$

$$\|\hat{r}_t\|_{\mathbb{R}^n} \leq \exp(-\lambda_k t)\,\|y\|_{\mathbb{R}^n} + \frac{8\kappa\,\|f^*\|_2\sqrt{10\log(2/\delta)}}{(\sigma_k-\sigma_{k+1})\sqrt{n}}.$$

Note Su & Yang (2019) are training only the hidden layer of a ReLU network by gradient descent, by contrast we are training both layers with biases of a network with smooth activations by gradient flow. For Corollary 2 by Su & Yang (2019) they have the overparameterization requirement $m \gtrsim n\log n\left(\frac{1}{\lambda_k^4} + \frac{\log^4 n\log^2(1/\delta)}{(\lambda_k-\lambda_{k+1})^2 n^2\lambda_k^4}\right)$. Thus both bounds scale like $\frac{n}{\lambda_k^4}$. Our bound has the extra factor $(\sigma_k-\sigma_{k+1})^2$ in front which could make it appear smaller at first glance but their Theorem 4 is strong enough to include this factor in the corollary they just chose not to. Thus we view both overparameterization requirements as comparable with neither superior to the other.

4 Conclusion and Future Directions

We demonstrated that in the underparameterized regime a two-layer neural network learns eigenfunctions of the NTK integral operator at rates corresponding to their eigenvalues. In our results the width m of the network doesn't need to be large relative to the number of samples n, otherwise we could not operate in the underparameterized regime. Rather for our results the width needs to be large relative to the inverse of the eigenvalues for the eigenfunctions/eigenvectors one wishes to approximate. We suspect future works that make assumptions about the target function can adopt refined requirements on the width that do not depend on n. We believe these are first steps towards NTK based analysis outside the NTK regime. Aside from the underparameterized regime, we extended two existing results in the literature to the case where all parameters are trained using our NTK deviation bound and the damped deviations equation. Since many NTK results become much easier once NTK deviation bounds are in-hand, we suspect our NTK deviation bounds can be used to prove further results.

An open question is what are appropriate assumptions on the target function that lead to a profitable convergence and generalization theory. In this paper the relevant assumption for things to work nicely is that the target function has a compact representation in terms of eigenfunctions of the NTK integral operator. This is only one such possible assumption, but we suspect there are many others, many of which will not involve the NTK at all.

The concept of damped deviations we introduced is not particular to a shallow network. If one were to prove uniform NTK deviation bounds for deep networks, then the results of this paper could be extended to deep networks, and it could open the door to future analysis for deep networks outside the NTK regime. We suspect that this may be possible, at least for certain initialization schemes, and we hope the community or us can address this in later works.

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APPENDIX

A NOTATIONS

We let $[k] := \{1, 2, 3, \ldots, k\}$. For a set A we let $|A|$ denote its cardinality. $\|\bullet\|_2$ and $\langle \bullet, \bullet \rangle_2$ denote the L^2 norm and inner product respectively (for vectors or for functions depending on context), $\|\bullet\|_F$ denotes the Frobenius norm for matrices, $\|\bullet\|_\infty$ is the supremum norm, $\|A\|_{op} := \sup_{\|x\|_2 \leq 1} \|Ax\|_2$ is the operator norm induced by the Euclidean norm. For two matrices $A, B \in \mathbb{R}^{n \times m}$ we will let $\langle A, B \rangle = Tr(A^T B) = \sum_{i=1}^n \sum_{j=1}^m A_{i,j} B_{i,j}$ denote the Frobenius or entry-wise inner product. $\langle \bullet, \bullet \rangle_{\mathbb{R}^n} = \langle \bullet, \bullet \rangle_2 / n$ is the normalized Euclidean inner product with associated norm $\|\bullet\|_{\mathbb{R}^n}$. We will track most constants such as constants that depend on parameters of our theorems such as M, σ, and the target function f^*. However, constants appearing in concentration inequalities such as Hoeffding or Bernstein's inequality or constants arising from $\delta/2$ or $\delta/3$ arguments will not be tracked. We will reserve $c, C > 0$ for untracked constants whose precise meaning can vary from statement to statement. We will use the standard big O and Ω notation with $\tilde{O}$ and $\tilde{\Omega}$ hiding logarithmic terms.

B NTK DEVIATION AND PARAMETER NORM BOUNDS

Let $\Gamma > 1$. At the end of this section we will prove a high probability bound of the form

$$\sup_{(x,x') \in B_M \times B_M} |K_t(x, x') - K^\infty(x, x')| = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}} \left[1 + t\Gamma^3 \|\hat{r}(0)\|_{\mathbb{R}^n} \right] \right).$$

Ideally we would like to use the results in Huang & Yau (2020) where they prove for a deep feed-forward network without biases:

$$\sup_{1 \leq i,j \leq n} |K_t(x_i, x_j) - K^\infty(x_i, x_j)| = \tilde{O}\left(\frac{t^2}{m} + \frac{1}{\sqrt{m}} \right).$$

However there are three problems that prevent this. The first is that the have a constant under the $\tilde{O}$ above that depends on the training data. Specifically their Assumption 2.2 requires that the smallest singular value of the data matrix $[x_{\alpha_1}, \ldots, x_{\alpha_r}]$ is greater than $c_r > 0$ where $1 \leq \alpha_1, \ldots, \alpha_r \leq n$ are arbitrary distinct indices. As you send the number of samples to infinity you will have $c_r \to 0$,

thus it is not clear how the bound will scale in the large sample regime. The second is that their bound only holds on the training data, whereas we need a bound that is uniform over all inputs. The final one is their network does not have biases. In the following section we will overcome these issues. The main difference between our argument and theirs is how we prove convergence at initialization. In their argument for convergence at initialization they make repeated use of a Gaussian conditioning lemma as they pass through the layers, and this relies on their Assumption 2.2. By contrast we will use Lipschitzness of the NTK and convergence over an ϵ net to prove convergence at initialization. As we see it, our deviation bounds for the time derivative $\partial_t K_t$ are proved in a very similar fashion and the rest of the argument is very much inspired by their approach.

This section is conceptually simple but technical. We will take care to outline the high level structure of each section to prevent the technicalities from obfuscating the overall simplicity of the approach. Our argument runs through the following steps:

- Control parameter norms throughout training.
- Bound the Lipschitz constant of the NTK with respect to spatial inputs.
- Use concentration of subexponential random variables (Bernstein's inequality) to show that $|K^\infty(z') - K_0(z')| = \tilde{O}(1/\sqrt{m})$ (roughly) for all z' in an ϵ net of the spatial domain. Combine with the Lipschitz property of the NTK to show convergence over *all* inputs, namely $\sup_{z\in B_M} |K^\infty(z) - K_0(z)| = \tilde{O}(1/\sqrt{m})$ (roughly).
- Produce the bound $\sup_{z\in B_M\times B_M} |\partial_t K_t(z)| = \tilde{O}(1/\sqrt{m})$ (roughly).
- Conclude that $\sup_{z\in B_M\times B_M} |K_t(z) - K_0(z)| = \tilde{O}(t/\sqrt{m})$ (roughly).

B.1 Important Equations

The following list contains the equations that are relevant for this section. We found it easier to read the following proofs by keeping these equations on a separate piece of paper or in a separate tab. We write $a\otimes x = ax^T$. Throughout this section, to free up a letter we will use $y \in \mathbb{R}^d$ to denote an input and not the labels as described in the introduction. Since the labels do not appear in this section we hope this will not cause confusion. Also throughout this section the training data will be considered fixed and thus the randomness of the inputs is not relevant to this section. The randomness will come entirely from the parameter initialization θ_0.

$$f(x;\theta) = \frac{1}{\sqrt{m}} a^T \sigma(Wx+b) + b_0$$

$$x^{(1)} := \frac{1}{\sqrt{m}} \sigma(Wx+b)$$

$$\sigma_1'(x) := diag(\sigma'(Wx+b))$$

$$\sigma_1''(x) := diag(\sigma''(Wx+b))$$

$$\partial_a f(x;\theta) = \frac{1}{\sqrt{m}} \sigma(Wx+b) = x^{(1)}$$

$$\partial_W f(x;\theta) = \frac{1}{\sqrt{m}} \sigma_1'(x) a \otimes x$$

$$\partial_b f(x;\theta) = \frac{1}{\sqrt{m}} \sigma_1'(x) a$$

$$\partial_{b_0} f(x;\theta) = 1$$

$$\partial_t a = -\frac{1}{n}\sum_{i=1}^n \hat{r}_i x_i^{(1)}$$

$$\partial_t W = -\frac{1}{n}\sum_{i=1}^n \hat{r}_i \frac{1}{\sqrt{m}} \sigma_1'(x_i) a \otimes x_i$$

$$\partial_t b = -\frac{1}{n}\sum_{i=1}^n \hat{r}_i \frac{1}{\sqrt{m}} \sigma_1'(x_i) a$$

$$\partial_t b_0 = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i$$

$$\partial_t x^{(1)} = \partial_t \frac{1}{\sqrt{m}}\sigma(Wx+b) = \frac{1}{\sqrt{m}}\sigma_1'(x)[\partial_t W x + \partial_t b]$$
$$= -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \left[\frac{1}{\sqrt{m}}\sigma_1'(x)\sigma_1'(x_i)\frac{a}{\sqrt{m}}\right][\langle x, x_i\rangle_2 + 1]$$

$$\partial_t \sigma_1'(x) = \partial_t \sigma'(Wx+b) = \sigma_1''(x) diag(\partial_t W x + \partial_t b)$$
$$= -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \frac{1}{\sqrt{m}}\sigma_1''(x)\sigma_1'(x_i) diag(a)[\langle x, x_i\rangle_2 + 1]$$

B.2 A Priori Parameter Norm Bounds

In this section we will provide bounds for the following quantities:

$$\xi(t) = \max\{\frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2, \frac{1}{\sqrt{m}}\|a\|_2, 1\}$$
$$\tilde{\xi}(t) = \max\{\max_{\ell\in[m]}\|w_\ell\|_2, \|a\|_\infty, \|b\|_\infty, 1\}.$$

Here $w_\ell = W_{\ell,:} \in \mathbb{R}^d$ is the vector of input weights to the ℓth unit. These quantities appear repeatedly throughout the rest of the proofs of this section and thus need to be controlled. The parameter norm bounds will also be useful for the purpose of the covering number argument in Section C.6. This section is broken down as follows:

- Prove Lemma B.1
- Bound $\xi(t)$
- Bound $\tilde{\xi}(t)$

The time derivatives throughout will repeatedly be of the form $\frac{1}{n}\sum_{i=1}^{n}\hat{r}_i(t)v_i$. The next Lemma B.1 provides a simple bound that we will use over and over again.

Lemma B.1. *Let $\|\bullet\|$ be any norm over a vector space V. Then for any $v_1, \ldots, v_n \in V$ we have*

$$\left\|\frac{1}{n}\sum_{i=1}^{n}\hat{r}_i(t)v_i\right\| \le \max_{i\in[n]}\|v_i\|\,\|\hat{r}(t)\|_{\mathbb{R}^n} \le \max_{i\in[n]}\|v_i\|\,\|\hat{r}(0)\|_{\mathbb{R}^n}.$$

Proof. Note that

$$\left\|\frac{1}{n}\sum_{i=1}^{n}\hat{r}_i(t)v_i\right\| \le \frac{1}{n}\sum_{i=1}^{n}|\hat{r}_i(t)|\,\|v_i\| \le \max_{i\in[n]}\|v_i\|\,\frac{1}{n}\sum_{i=1}^{n}|\hat{r}_i(t)|$$
$$\le \max_{i\in[n]}\|v_i\|\,\frac{1}{\sqrt{n}}\|\hat{r}(t)\|_2 = \max_{i\in[n]}\|v_i\|\,\|\hat{r}(t)\|_{\mathbb{R}^n} \le \max_{i\in[n]}\|v_i\|\,\|\hat{r}(0)\|_{\mathbb{R}^n},$$

where the last inequality follows from $\|\hat{r}(t)\|_{\mathbb{R}^n} \le \|\hat{r}(0)\|_{\mathbb{R}^n}$ from gradient flow. □

We now proceed to bound $\xi(t)$.

Lemma B.2. *Let $\xi(t) = \max\{\frac{1}{\sqrt{m}}\|W(t)\|_{op}, \frac{1}{\sqrt{m}}\|b(t)\|_2, \frac{1}{\sqrt{m}}\|a(t)\|_2, 1\}$ and*

$$D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}.$$

Then for any initial conditions $W(0)$, $b(0)$, $a(0)$ we have for all t

$$\xi(t) \le \exp\left(\frac{D}{\sqrt{m}}\int_0^t \|\hat{r}(s)\|_{\mathbb{R}^n}\,ds\right)\xi(0) \le \exp\left(\frac{D}{\sqrt{m}}\|\hat{r}(0)\|_{\mathbb{R}^n}\,t\right)\xi(0).$$

Proof. Recall that

$$\partial_t a = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i x_i^{(1)}$$

$$\partial_t W = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \frac{1}{\sqrt{m}}\sigma_1'(x_i) a \otimes x_i$$

$$\partial_t b = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \frac{1}{\sqrt{m}}\sigma_1'(x_i) a.$$

We will show that each of the above derivatives is $\lesssim \|\hat{r}(t)\|_{\mathbb{R}^n} \xi(t)$ then apply Grönwall's inequality. By Lemma B.1 it suffices to show that the terms multiplied by $\hat{r}_i$ in the above sums are $\lesssim \xi(t)$. First we note that

$$\left\|x_i^{(1)}\right\|_2 = \left\|\frac{1}{\sqrt{m}}\sigma(Wx_i + b)\right\|_2 \leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \|Wx_i + b\|_2$$
$$\leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\|W\|_{op}\|x_i\|_2 + \|b\|_2\right] \leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\|W\|_{op} M + \|b\|_2\right]$$
$$\leq D\xi.$$

Second we have that

$$\left\|\frac{1}{\sqrt{m}}\sigma_1'(x_i) a \otimes x_i\right\|_{op} = \left\|\frac{1}{\sqrt{m}}\sigma_1'(x_i) a\right\|_2 \|x_i\|_2 \leq M\|\sigma'\|_\infty \frac{1}{\sqrt{m}}\|a\|_2 \leq D\xi.$$

Finally we have that

$$\left\|\frac{1}{\sqrt{m}}\sigma_1'(x_i) a\right\| \leq \|\sigma'\|_\infty \frac{1}{\sqrt{m}}\|a\|_2 \leq D\xi.$$

Thus by Lemma B.1 and the above bounds we have

$$\|\partial_t W(t)\|_{op}, \|\partial_t a(t)\|_2, \|\partial_t b(t)\|_2 \leq D\|\hat{r}(t)\|_{\mathbb{R}^n}\xi(t).$$

Let $v(t)$ be a placeholder for one of the functions $\frac{1}{\sqrt{m}}a(t)$, $\frac{1}{\sqrt{m}}W(t)$, $\frac{1}{\sqrt{m}}b(t)$ with corresponding norm $\|\bullet\|$. Then we have that

$$\|v(t)\| \leq \|v(0)\| + \|v(t) - v(0)\| = \|v(0)\| + \left\|\int_0^t \partial_s v(s) ds\right\|$$
$$\leq \|v(0)\| + \int_0^t \|\partial_s v(s)\| ds \leq \xi(0) + \int_0^t \frac{\|\hat{r}(s)\|_{\mathbb{R}^n}}{\sqrt{m}} D\xi(s) ds.$$

This inequality holds for any of the three choices of v thus we get that

$$\xi(t) \leq \xi(0) + \int_0^t \frac{\|\hat{r}(s)\|_{\mathbb{R}^n}}{\sqrt{m}} D\xi(s) ds.$$

Therefore by Grönwall's inequality we get that

$$\xi(t) \leq \exp\left(\frac{D}{\sqrt{m}}\int_0^t \|\hat{r}(s)\|_{\mathbb{R}^n} ds\right)\xi(0) \leq \exp\left(\frac{D}{\sqrt{m}}\|\hat{r}(0)\|_{\mathbb{R}^n} t\right)\xi(0).$$

□

We will now bound $\tilde{\xi(t)}$ using essentially the same argument as in the previous lemma.

Lemma B.3. *Let* $\tilde{\xi}(t) = \max\{\max_{\ell\in[m]}\|w_\ell(t)\|_2, \|a(t)\|_\infty, \|b(t)\|_\infty, 1\}$ *and*

$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}.$$

Then for any initial conditions $W(0)$, $b(0)$, $a(0)$ *we have for all* t

$$\tilde{\xi}(t) \leq \exp\left(\frac{D}{\sqrt{m}}\int_0^t \|\hat{r}(s)\|_{\mathbb{R}^n} ds\right)\tilde{\xi}(0) \leq \exp\left(\frac{D}{\sqrt{m}}\|\hat{r}(0)\|_{\mathbb{R}^n} t\right)\tilde{\xi}(0).$$

Proof. The proof is basically the same as Lemma B.2. We have that

$$\partial_t w_\ell = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \frac{a_\ell}{\sqrt{m}} \sigma'(\langle w_\ell, x_i\rangle_2 + b_\ell) x_i.$$

Now note

$$\left\| \frac{a_\ell}{\sqrt{m}} \sigma'(\langle w_\ell, x_i\rangle_2 + b_\ell) x_i \right\|_2 \leq \frac{1}{\sqrt{m}} \|a\|_\infty \|\sigma'\|_\infty M \leq \frac{D}{\sqrt{m}} \tilde{\xi}.$$

Thus by Lemma B.1 we have that

$$\|\partial_t w_\ell(t)\|_2 \leq \frac{D}{\sqrt{m}} \|\hat{r}(t)\|_{\mathbb{R}^n} \tilde{\xi}(t).$$

On the other hand

$$\partial_t a = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i x_i^{(1)}$$

with

$$\begin{aligned}\left\| x_i^{(1)} \right\|_\infty = \left\| \frac{1}{\sqrt{m}} \sigma(W x_i + b) \right\|_\infty &\leq \frac{1}{\sqrt{m}} \left[|\sigma(0)| + \|\sigma'\|_\infty \|W x_i + b\|_\infty \right] \\ &\leq \frac{1}{\sqrt{m}} \left[|\sigma(0)| + \|\sigma'\|_\infty \left(M \max_\ell \|w_\ell\|_2 + \|b\|_\infty \right) \right] \leq \frac{D}{\sqrt{m}} \tilde{\xi}.\end{aligned}$$

Thus again by Lemma B.1 we have

$$\|\partial_t a(t)\|_\infty \leq \frac{D}{\sqrt{m}} \|\hat{r}(t)\|_{\mathbb{R}^n} \tilde{\xi}(t).$$

Finally we have

$$\partial_t b = -\frac{1}{n}\sum_{i=1}^{n} \hat{r}_i \frac{1}{\sqrt{m}} \sigma_1'(x_i) a$$

with

$$\left\| \frac{1}{\sqrt{m}} \sigma_1'(x_i) a \right\|_\infty \leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|a\|_\infty \leq \frac{D}{\sqrt{m}} \tilde{\xi}.$$

Again applying Lemma B.1 one last time we get

$$\|\partial_t b(t)\|_\infty \leq \frac{D}{\sqrt{m}} \|\hat{r}(t)\|_{\mathbb{R}^n} \tilde{\xi}(t).$$

Therefore by the same argument as in Lemma B.2 using Grönwall's inequality we get that

$$\tilde{\xi}(t) \leq \exp\left(\frac{D}{\sqrt{m}} \int_0^t \|\hat{r}(s)\|_{\mathbb{R}^n} \, ds \right) \tilde{\xi}(0) \leq \exp\left(\frac{D}{\sqrt{m}} \|\hat{r}(0)\|_{\mathbb{R}^n} \, t \right) \tilde{\xi}(0).$$

□

B.3 NTK Is Lipschitz With Respect To Spatial Inputs

The NTK being Lipschitz with respect to spatial inputs is essential to our proof. The Lipschitz property means that to show convergence uniformly for *all* inputs it suffices to show convergence on an ϵ net of the spatial domain. Since the parameters are changing throughout time, the Lipschitz constant of the NTK will change throughout time. We will see that the Lipschitz constant depends on the quantities $\xi(t)$ and $\tilde{\xi}(t)$ from the previous Section B.2.

The NTK $K_t(x, x')$ is a sum of terms of the form $g(x)^T g(x')$ where g is one of the derivatives $\partial_a f(x;\theta_t), \partial_b f(x;\theta_t), \partial_W f(x;\theta_t), \partial_{b_0} f(x;\theta_t)$. Since $\partial_{b_0} f(x;\theta_t) \equiv 1$ this term can be ignored for the rest of the section. The upcomming Lemma B.4 shows that if g is Lipschitz and bounded then $(x, x') \mapsto g(x)^T g(x')$ is Lipschitz. This lemma guides the structure of this section:

- Prove Lemma B.4

- Show that $\partial_a f(x;\theta), \partial_b f(x;\theta), \partial_W f(x;\theta)$ are bounded and Lipschitz
- Conclude the NTK is Lipschitz

Lemma B.4. *Let $g : \mathbb{R}^k \to \mathbb{R}^l$ be L-Lipschitz with respect to the 2-norm, i.e.*

$$\|g(x) - g(z)\|_2 \leq L \|x - z\|_2$$

and satisfy $\|g(x)\|_2 \leq M$ for all x in some set $\mathcal{X}$. Then $K_g : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

$$K_g(x, x') := g(x)^T g(x')$$

is ML-Lipschitz with respect to the norm

$$\|(x, x')\| := \|x\|_2 + \|x'\|_2 .$$

Proof. We have

$$\begin{aligned}
|K_g(x,x') - K_g(z,z')| &= |g(x)^T g(x') - g(z)^T g(z')| \\
&= |g(x)^T (g(x') - g(z'))| + |(g(x) - g(z))^T g(z')| \\
&\leq \|g(x)\|_2 \|g(x') - g(z')\|_2 + \|g(x) - g(z)\|_2 \|g(z')\|_2 \\
&\leq ML \|x' - z'\|_2 + ML \|x - z\|_2 \leq ML \|(x,x') - (z,z')\| .
\end{aligned}$$

□

By the previous Lemma B.4, to show that the NTK is Lipschitz it suffices to show that $\partial_a f(x;\theta), \partial_b f(x;\theta), \partial_W f(x;\theta), \partial_{b_0} f(x;\theta)$ are bounded and Lipschitz. The following lemma bounds the norms of the derivatives $\partial_a f(x;\theta), \partial_W f(x;\theta), \partial_b f(x;\theta)$.

Lemma B.5. *Let $D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$ and*

$$\xi = \max\{\frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2, \frac{1}{\sqrt{m}}\|a\|_2, 1\}.$$

Then

$$\|\partial_a f(x;\theta)\|_2, \|\partial_W f(x;\theta)\|_F, \|\partial_b f(x;\theta)\|_2 \leq D\xi.$$

Proof. We have

$$\begin{aligned}
\|\partial_a f(x;\theta)\|_2 = \left\|\frac{1}{\sqrt{m}}\sigma(Wx+b)\right\|_2 &\leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \|Wx+b\|_2 \\
&\leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\|W\|_{op}\|x\|_2 + \|b\|_2\right] \\
&\leq |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\|W\|_{op} M + \|b\|_2\right] \leq D\xi,
\end{aligned}$$

$$\|\partial_W f(x;\theta)\|_F = \left\|\frac{1}{\sqrt{m}}\sigma_1'(x) a \otimes x\right\|_F = \left\|\frac{1}{\sqrt{m}}\sigma_1'(x) a\right\|_2 \|x\|_2 \leq \frac{M}{\sqrt{m}}\|\sigma'\|_\infty \|a\|_2 \leq D\xi,$$

$$\|\partial_b f(x;\theta)\|_2 = \left\|\frac{1}{\sqrt{m}}\sigma_1'(x) a\right\|_2 \leq \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \|a\|_2 \leq D\xi.$$

□

The following lemma demonstrates that $\partial_a f(x;\theta)$, $\partial_W f(x;\theta)$, and $\partial_b f(x;\theta)$ are Lipschitz as functions of the input x.

Lemma B.6. *Let*

$$\xi = \max\{\frac{1}{\sqrt{m}} \|W\|_{op}, \frac{1}{\sqrt{m}} \|b\|_2, \frac{1}{\sqrt{m}} \|a\|_2, 1\},$$

$$\tilde{\xi} = \max\{\max_{\ell \in [m]} \|w_\ell\|_2, \|a\|_\infty, \|b\|_\infty, 1\},$$

$$D' = \max\{\|\sigma'\|_\infty, M \|\sigma''\|_\infty, \|\sigma''\|_\infty\},$$

$$L = 2\xi\tilde{\xi}D'.$$

Then $\partial_a f(x;\theta)$, $\partial_b f(x;\theta)$, $\partial_W f(x;\theta)$ are all L-Lipschitz with respect to the Euclidean norm $\|\bullet\|_2$. In symbols:

$$\|\partial_a f(x;\theta) - \partial_a f(y;\theta)\|_2 \leq L \|x-y\|_2$$

$$\|\partial_W f(x;\theta) - \partial_W f(y;\theta)\|_F \leq L \|x-y\|_2$$

$$\|\partial_b f(x;\theta) - \partial_b f(y;\theta)\|_2 \leq L \|x-y\|_2$$

Proof. We have

$$\|\partial_a f(x;\theta) - \partial_a f(y;\theta)\|_2 = \left\| \frac{1}{\sqrt{m}} (\sigma(Wx+b) - \sigma(Wy+b)) \right\|_2$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|W(x-y)\|_2 \leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|W\|_{op} \|x-y\|_2 \leq L \|x-y\|_2,$$

$$\|\partial_W f(x;\theta) - \partial_W f(y;\theta)\|_F = \left\| \frac{1}{\sqrt{m}} \sigma_1'(x) a \otimes x - \frac{1}{\sqrt{m}} \sigma_1'(y) a \otimes y \right\|_F$$
$$\leq \left\| \frac{1}{\sqrt{m}} \sigma_1'(x) a \otimes [x-y] \right\|_F + \left\| \frac{1}{\sqrt{m}} [\sigma_1'(x) a - \sigma_1'(y) a] \otimes y \right\|_F$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma_1'(x) a\|_2 \|x-y\|_2 + \frac{1}{\sqrt{m}} \|[\sigma_1'(x) - \sigma_1'(y)] a\|_2 \|y\|_2$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|a\|_2 \|x-y\|_2 + \frac{1}{\sqrt{m}} \|\sigma'(Wx+b) - \sigma'(Wy+b)\|_\infty \|a\|_2 M$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|a\|_2 \|x-y\|_2 + \frac{1}{\sqrt{m}} \|\sigma''\|_\infty \|W(x-y)\|_\infty \|a\|_2 M$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma'\|_\infty \|a\|_2 \|x-y\|_2 + \frac{1}{\sqrt{m}} \|\sigma''\|_\infty \max_{\ell \in [m]} \|w_\ell\|_2 \|x-y\|_2 \|a\|_2 M$$
$$\leq L \|x-y\|_2,$$

$$\|\partial_b f(x;\theta) - \partial_b f(y;\theta)\|_2 = \left\| \frac{1}{\sqrt{m}} \sigma_1'(x) a - \frac{1}{\sqrt{m}} \sigma_1'(y) a \right\|_2$$
$$= \frac{1}{\sqrt{m}} \|\sigma'(Wx+b) - \sigma'(Wy+b)\|_\infty \|a\|_2$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma''\|_\infty \|W(x-y)\|_\infty \|a\|_2$$
$$\leq \frac{1}{\sqrt{m}} \|\sigma''\|_\infty \max_{\ell \in [m]} \|w_\ell\|_2 \|x-y\|_2 \|a\|_2 \leq L \|x-y\|_2.$$

□

Finally we can prove that the Neural Tangent Kernel is Lipschitz.

Theorem B.7. *Consider the Neural Tangent Kernel*

$$K(x,y) = \langle \partial_a f(x;\theta), \partial_a f(y;\theta)\rangle_2 + \langle \partial_b f(x;\theta), \partial_b f(y;\theta)\rangle_2 + \langle \partial_W f(x;\theta), \partial_W f(y;\theta)\rangle + 1$$

and let

$$\xi = \max\{\frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2, \frac{1}{\sqrt{m}}\|a\|_2, 1\},$$
$$\tilde{\xi} = \max\{\max_{\ell\in[m]}\|w_\ell\|_2, \|a\|_\infty, \|b\|_\infty, 1\},$$
$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$$
$$D' = \max\{\|\sigma'\|_\infty, M\|\sigma''\|_\infty, \|\sigma''\|_\infty\}.$$

Then the Neural Tangent Kernel is Lipschitz with respect to the norm

$$\|(x,y)\| := \|x\|_2 + \|y\|_2$$

with Lipschitz constant $L := 6DD'\xi^2\tilde{\xi}$. In symbols:

$$|K(x,y) - K(x',y')| \leq L\|(x,y) - (x',y')\|.$$

Proof. By Lemma B.5, we have that the gradients are bounded

$$\|\partial_a f(x;\theta)\|_2, \|\partial_W f(x;\theta)\|_F, \|\partial_b f(x;\theta)\|_2 \leq D\xi.$$

Also by Lemma B.6 the gradients are Lipschitz with Lipschitz constant $2\xi\tilde{\xi}D'$. Thus these two facts combined with Lemma B.4 tell us that each of the three terms $\langle \partial_a f(x;\theta), \partial_a f(y;\theta)\rangle$, $\langle \partial_b f(x;\theta), \partial_b f(y;\theta)\rangle$, and $\langle \partial_W f(x;\theta), \partial_W f(y;\theta)\rangle$ are individually Lipschitz with constant $(D\xi)\cdot(2\xi\tilde{\xi}D')$. Thus the Lipschitz constant of the NTK itself is bounded by the sum of the 3 Lipschitz constants, for a total of $6DD'\xi^2\tilde{\xi}$. □

Using that the NTK at time zero $K_0(x,y)$ is Lipschitz we can prove that the analytical NTK $K^\infty = \mathbb{E}[K_0(x,y)]$ is Lipschitz. We will use this primarily as a qualitative statement, meaning that the estimate that we derive for the Lipschitz constant will not be used as it is not very explicit. Rather, in theorems where we use the fact that K^∞ is Lipschitz we will simply take the Lipschitz constant of K^∞ as an external parameter.

Theorem B.8. *Assume that $W_{i,j}(0) \sim \mathcal{W}$, $b_\ell(0) \sim \mathcal{B}$, $a_\ell(0) \sim \mathcal{A}$ are all i.i.d. zero-mean, unit variance subgaussian random variables. Let*

$$\xi(0) = \max\{\frac{1}{\sqrt{m}}\|W(0)\|_{op}, \frac{1}{\sqrt{m}}\|b(0)\|_2, \frac{1}{\sqrt{m}}\|a(0)\|_2, 1\},$$
$$\tilde{\xi}(0) = \max\{\max_{\ell\in[m]}\|w_\ell(0)\|_2, \|a(0)\|_\infty, \|b(0)\|_\infty, 1\},$$
$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\},$$
$$D' = \max\{\|\sigma'\|_\infty, M\|\sigma''\|_\infty, \|\sigma''\|_\infty\}.$$

Then the analytical Neural Tangent Kernel $K^\infty(x,y) = \mathbb{E}[K_0(x,y)]$ is Lipschitz with respect to the norm

$$\|(x,y)\| := \|x\|_2 + \|y\|_2$$

with Lipschitz constant $\leq 6DD'\mathbb{E}[\xi^2\tilde{\xi}] < \infty$. If one instead does the doubling trick then the same conclusion holds.

Proof. First assume we are not doing the doubling trick. We note that

$$|K^\infty(x,y) - K^\infty(x',y')| = |\mathbb{E}[K_0(x,y)] - \mathbb{E}[K_0(x',y')]|$$
$$\leq \mathbb{E}|K_0(x,y) - K_0(x',y')| \leq 6DD'\mathbb{E}[\xi^2\tilde{\xi}]\|(x,y) - (x',y')\|$$

where the last line follows from the Lipschitzness of K_0 provided by Theorem B.7. Using that $\|W(0)\|_{op} \leq \|W(0)\|_F$ and the fact that the Euclidean norm of a vector with i.i.d. subgaussian entries is subgaussian (Vershynin, 2018, Theorem 3.1.1), we have that $\xi(0)$ and $\tilde{\xi}(0)$ are maximums of subgaussian random variables. Since a maximum of subgaussian random variables is subgaussian, we have that $\xi(0)$ and $\tilde{\xi}(0)$ are subgaussian. From the inequality $ab \leq \frac{1}{2}(a^2+b^2)$ we get $\mathbb{E}[\xi^2\tilde{\xi}] \leq \frac{1}{2}\mathbb{E}[\xi^4] + \frac{1}{2}\mathbb{E}[\tilde{\xi}^2] < \infty$ since moments of subgaussian random variables are all finite. Since the doubling trick does not change the distribution of K_0, the same conclusion holds under that initialization scheme. □

B.4 NTK CONVERGENCE AT INITIALIZATION

In this section we prove that $\sup_{z \in B_M \times B_M} |K_0(z) - K^\infty(z)| = \tilde{O}(1/\sqrt{m})$. Our argument traces the following steps:

- Show that K_0 is sum of averages of m independent subexponential random variables
- Use subexponential concentration to show that $\sup_{z' \in \Delta} |K_0(z') - K^\infty(z')| = \tilde{O}(1/\sqrt{m})$ for all z' in an ϵ net Δ of $B_M \times B_M$
- Use that K_0 is Lipschitz and convergence over the epsilon net Δ to show that

$$\sup_{z \in B_M \times B_M} |K_0(z) - K^\infty(z)| = \tilde{O}(1/\sqrt{m}) \text{ (roughly)}$$

We recall the following definitions 2.5.6 and 2.7.5 from Vershynin (2018).

Definition B.9. *(Vershynin 2018) Let Y be a random variable. Then we define the subgaussian norm of Y to be*

$$\|Y\|_{\psi_2} = \inf\{t > 0 : \mathbb{E}\exp(Y^2/t^2) \leq 2\}$$

If $\|Y\|_{\psi_2} < \infty$, then we say Y is subgaussian.

Definition B.10. *(Vershynin 2018) Let Y be a random variable. Then we define the subexponential norm of Y to be*

$$\|Y\|_{\psi_1} = \inf\{t > 0 : \mathbb{E}\exp(|Y|/t) \leq 2\}$$

If $\|Y\|_{\psi_1} < \infty$, then we say Y is subexponential.

We also recall the following useful lemma Vershynin (2018, Lemma 2.7.7).

Lemma B.11. *(Vershynin 2018) Let X and Y be subgaussian random variables. Then XY is subexponential. Moreover*

$$\|XY\|_{\psi_1} \leq \|X\|_{\psi_2} \|Y\|_{\psi_2}$$

We recall one last definition Vershynin (2018, Definition 3.4.1)

Definition B.12. *(Vershynin 2018) A random vector $Y \in \mathbb{R}^k$ is called subgaussian if the one dimensional marginals $\langle Y, x \rangle$ are subgaussian random variables for all $x \in \mathbb{R}^k$. The subgaussian norm of Y is defined as*

$$\|Y\|_{\psi_2} = \sup_{x \in S^{k-1}} \|\langle Y, x \rangle\|_{\psi_2}$$

The typical example of a subgaussian random vector is a random vector with independent subgaussian coordinates. The following lemma demonstrates that the NTK at initializeation is a sum of terms that are averages of independent subexponential random variables, which will enable us to use concentration arguments later.

Theorem B.13. *Let w_ℓ, b_ℓ, a_ℓ all be independent subgaussian random variables with subgaussian norms satisfying $\|\bullet\|_{\psi_2} \leq K$. Furthermore assume $\|1\|_{\psi_2} \leq K$. Also let*

$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}.$$

Then for fixed x, y, each of the following

$$\langle \partial_a f(x;\theta), \partial_a f(y;\theta) \rangle, \langle \partial_b f(x;\theta), \partial_b f(y;\theta) \rangle, \langle \partial_W f(x;\theta), \partial_W f(y;\theta) \rangle$$

is an average of m independent subexponential random variables with subexponential norms bounded by D^2K^2.

Proof. We first observe that

$$\begin{aligned}\langle \partial_a f(x;\theta), \partial_a f(y;\theta) \rangle_2 &= \frac{1}{m}\langle \sigma(Wx+b), \sigma(Wy+b) \rangle_2 \\ &= \frac{1}{m}\sum_{\ell=1}^m \sigma(\langle w_\ell, x \rangle_2 + b_\ell)\sigma(\langle w_\ell, y \rangle_2 + b_\ell),\end{aligned}$$

$$\langle \partial_b f(x;\theta), \partial_b f(y;\theta)\rangle_2 = \langle \frac{1}{\sqrt{m}}\sigma_1'(x)a, \frac{1}{\sqrt{m}}\sigma_1'(y)a\rangle_2$$
$$= \frac{1}{m}\sum_{\ell=1}^{m} a_\ell^2 \sigma'(\langle w_\ell, x\rangle_2 + b_\ell)\sigma'(\langle w_\ell, y\rangle_2 + b_\ell),$$

$$\langle \partial_W f(x;\theta), \partial_W f(y;\theta)\rangle = \langle \frac{1}{\sqrt{m}}\sigma_1'(x)a \otimes x, \frac{1}{\sqrt{m}}\sigma_1'(y)a \otimes y\rangle_2$$
$$= \frac{1}{m}\langle \sigma_1'(x)a, \sigma_1'(y)a\rangle_2 \langle x, y\rangle_2 = \frac{\langle x, y\rangle_2}{m}\sum_{\ell=1}^{m} a_\ell^2 \sigma'(\langle w_\ell, x\rangle_2 + b_\ell)\sigma'(\langle w_\ell, y\rangle_2 + b_\ell).$$

Note that
$$|\sigma(\langle w_\ell, x\rangle_2 + b_\ell)| \le |\sigma(0)| + \|\sigma'\|_\infty [|\langle w_\ell, x\rangle| + |b_\ell|].$$
Thus
$$\begin{aligned}\|\sigma(\langle w_\ell, x\rangle_2 + b_\ell)\|_{\psi_2} &\le |\sigma(0)| \|1\|_{\psi_2} + \|\sigma'\|_\infty [\||\langle w_\ell, x\rangle|\|_{\psi_2} + \||b_\ell|\|_{\psi_2}] \\ &\le |\sigma(0)| \|1\|_{\psi_2} + \|\sigma'\|_\infty [M \|w_\ell\|_{\psi_2} + \||b_\ell|\|_{\psi_2}] \\ &\le 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty\} K \le DK.\end{aligned}$$
Also
$$|a_\ell \sigma'(\langle w_\ell, x\rangle_2 + b_\ell)| \le |a_\ell| \|\sigma'\|_\infty \le D|a_\ell|,$$
therefore
$$\|a_\ell \sigma'(\langle w_\ell, x\rangle_2 + b_\ell)\|_{\psi_2} \le D\|a_\ell\|_{\psi_2} \le DK.$$
Finally
$$\left\| |\langle x, y\rangle_2|^{1/2} a_\ell \sigma'(\langle w_\ell, x\rangle_2 + b_\ell)\right\|_{\psi_2} \le M\|\sigma'\|_\infty \|a_\ell\|_{\psi_2} \le DK.$$
It follows by Lemma B.11 that each of $\langle \partial_a f(x;\theta), \partial_a f(y;\theta)\rangle$, $\langle \partial_W f(x;\theta), \partial_W f(y;\theta)\rangle$, and $\langle \partial_b f(x;\theta), \partial_b f(y;\theta)\rangle$ is an average of m independent subexponential random variables with subexponential norm $\|\bullet\|_{\psi_1} \le D^2K^2$. □

We now recall the following Theorem from Vershynin (2012, Theorem 5.39) which will be useful.

Lemma B.14 (Vershynin 2012)**.** *Let A be an $N \times n$ matrix whose rows A_i are independent subgaussian isotropic random vectors in $\mathbb{R}^n$. Then for every $t \ge 0$, with probability at least $1 - 2\exp(-ct^2)$ one has the following bounds on the singular values*
$$\sqrt{N} - C\sqrt{n} - t \le s_{min}(A) \le s_{max}(A) \le \sqrt{N} + C\sqrt{n} + t.$$
Here $C = C_K > 0$ depends only on the subgaussian norms $K = \max_i \|A_i\|_{\psi_2}$ of the rows.

Also the following special case of Vershynin (2012, Lemma 5.5) will be useful for us.

Lemma B.15 (Vershynin 2012)**.** *Let Y be subgaussian. Then*
$$\mathbb{P}(|Y| > t) \le C\exp(-ct^2/\|Y\|_{\psi_2}^2).$$

It will be useful to remind the reader that $C, c > 0$ denote absolute constants whose meaning will vary from statement-to-statement, as this abuse of notation becomes especially prevalent during the concentration of measure arguments of the rest of the section. The following lemma provides a concentration inequality for the maximum of subgaussian random variables which will be useful for bounding ξ and $\tilde{\xi}$ later which is necessary for bounding the Lipschitz constant of K_0.

Lemma B.16. *Let $Y_1, \ldots, Y_n$ be subgaussian random variables with $\|Y_i\|_{\psi_2} \le K$ for $i \in [n]$. Then there exists absolute constants $c, c', C > 0$ such that*
$$\mathbb{P}\left(\max_{i\in[n]} |Y_i| > t + K\sqrt{c'\log n}\right) \le C\exp(-ct^2/K^2).$$

Proof. Since each Y_i is subgaussian we have for any $t \geq 0$ (Lemma B.15)

$$\mathbb{P}\left(|Y_i| > t\right) \leq C \exp\left(-ct^2 / \|Y_i\|_{\psi_2}^2\right).$$

By the union bound,

$$\begin{aligned}\mathbb{P}\left(\max_{i\in[n]} |Y_i| > t + K\sqrt{c^{-1}\log n}\right) &\leq \sum_{i=1}^{n} \mathbb{P}\left(|Y_i| > t + K\sqrt{c^{-1}\log n}\right) \\ &\leq nC \exp\left(-c\left[t + K\sqrt{c^{-1}\log n}\right]^2 / K^2\right) = C\exp(-ct^2/K^2).\end{aligned}$$

Thus by setting $c' := c^{-1}$ we get the desired result. □

We now introduce a high probability bound for ξ.

Lemma B.17. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let*

$$\xi = \max\{\frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2, \frac{1}{\sqrt{m}}\|a\|_2\}$$

Then with probability at least $1-\delta$

$$\xi \leq 1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}$$

Proof. Note that by setting $t = \sqrt{c^{-1}\log(2/\delta)}$ in Lemma B.14 we have that with probability at least $1-\delta$

$$\frac{1}{\sqrt{m}}\|W\|_{op} \leq 1 + \frac{C\sqrt{d}}{\sqrt{m}} + \frac{\sqrt{c^{-1}\log(2/\delta)}}{\sqrt{m}}$$

Also by Theorem 3.1.1 in (Vershynin, 2018)

$$\left\|\|a\|_2 - \sqrt{m}\right\|_{\psi_2} \leq CK^2$$

$$\left\|\|b\|_2 - \sqrt{m}\right\|_{\psi_2} \leq CK^2$$

Thus by Lemma B.15 and a union bound we have with probability at least $1-2\delta$

$$\frac{1}{\sqrt{m}}\|a\|_2, \frac{1}{\sqrt{m}}\|b\|_2 \leq 1 + \frac{C}{\sqrt{m}}K^2\sqrt{\log(c/\delta)}$$

Thus by replacing every δ in the above arguments with $\delta/3$ and using the union bound we have with probability at least $1-\delta$

$$\xi \leq 1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}.$$

□

Similarly we now introduce a high probability bound for $\tilde{\xi}$.

Lemma B.18. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let*

$$\tilde{\xi} = \max\{\max_{\ell\in[m]}\|w_\ell\|_2, \|a\|_\infty, \|b\|_\infty\}$$

Then with probability at least $1-\delta$ we have

$$\tilde{\xi} \leq \sqrt{d} + CK^2\left[\sqrt{\log(c/\delta)} + \sqrt{\log m}\right]$$

Proof. By Theorem 3.1.1 in (Vershynin, 2018) we have

$$\left\| \|w_\ell\|_2 - \sqrt{d} \right\|_{\psi_2} \leq CK^2$$

Well then by Lemma B.16 there is a constant $c' > 0$ so that

$$\mathbb{P}\left(\max_{\ell \in [m]} \|w_\ell\|_2 - \sqrt{d} > t + CK^2\sqrt{c' \log m} \right)$$
$$\leq \mathbb{P}\left(\max_{\ell \in [m]} \left| \|w_\ell\|_2 - \sqrt{d} \right| > t + CK^2\sqrt{c' \log m} \right) \leq C\exp(-ct^2/K^4).$$

Thus by setting $t = CK^2\sqrt{\log(c/\delta)}$ we have with probability at least $1-\delta$

$$\max_{\ell \in [m]} \|w_\ell\|_2 \leq \sqrt{d} + CK^2\sqrt{\log(c/\delta)} + CK^2\sqrt{\log m}$$

where we have absorbed the constant $\sqrt{c'}$ into C. Similarly by Lemma B.16 and a union bound we get with probability at least $1-2\delta$ that

$$\|a\|_\infty, \|b\|_\infty \leq CK\sqrt{\log(c/\delta)} + CK\sqrt{\log m}$$

Thus by replacing each δ with $\delta/3$ in the above arguments and using the union bound we get with probability at least $1-\delta$

$$\tilde{\xi} \leq \sqrt{d} + CK^2\left[\sqrt{\log(c/\delta)} + \sqrt{\log m}\right]$$

□

We are now finally ready to prove the main theorem of this section.

Theorem B.19. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let*

$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}.$$
$$D' = \max\{\|\sigma'\|_\infty, M\|\sigma''\|_\infty, \|\sigma''\|_\infty\}$$

Define

$$\rho(M, \sigma, d, K, \delta, m) :=$$
$$CDD'\left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2 \left\{\sqrt{d} + CK^2\left[\sqrt{\log(c/\delta)} + \sqrt{\log m}\right]\right\}$$

Let $L(K^\infty)$ denote the Lipschitz constant of K^∞. If

$$m \geq C[\log(c/\delta) + 2d\log(CM\max\{\rho, L(K^\infty)\}\sqrt{m})]$$

then with probability at least $1-\delta$

$$\sup_{z \in B_M \times B_M} |K_0(z) - K^\infty(z)| \leq \frac{1}{\sqrt{m}}\left[1 + CD^2K^2\sqrt{\log(c/\delta) + 2d\log(CM\max\{\rho, L(K^\infty)\}\sqrt{m})}\right]$$

If one instead does the doubling trick then the same conclusion holds.

Proof. First assume we are not doing the doubling trick. Recall that by Theorem B.7 that K_0 is Lipschitz with constant at most

$$CDD'\xi(0)^2\tilde{\xi(0)}$$

where ξ and $\tilde{\xi}$ are defined as in the theorem. Well then by Lemmas B.17, B.18 and a union bound we have with probability at least $1-2\delta$

$$\xi(0)^2\tilde{\xi}(0) \leq \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2 \left\{\sqrt{d} + CK^2\left[\sqrt{\log(c/\delta)} + \sqrt{\log m}\right]\right\}.$$

Let $L(K_0), L(K^\infty)$ denote the Lipschitz constant of K_0 and K^∞ respectively. Then assuming the above inequality holds we have that

$$L(K_0) \leq \rho(M, \sigma, d, K, \delta, m). \tag{1}$$

For conciseness from now on we will suppress the arguments of ρ. Now set

$$\gamma := \frac{1}{2\max\{\rho, L(K^\infty)\}\sqrt{m}}.$$

Let $\mathcal{N}_\gamma(B_M)$ be the cardinality of a maximal γ-net of the ball $B_M = \{x : \|x\|_2 \leq M\}$ with respect to the L2 norm $\|\bullet\|_2$. By a standard volume argument we have that

$$\mathcal{N}_\gamma(B_M) \leq \left(\frac{CM}{\gamma}\right)^d.$$

By taking the product of two $\gamma/2$ nets of B_M it follows that we can choose a γ net of $B_M \times B_M$, say Δ, with respect to the norm

$$\|(x, y)\| = \|x\|_2 + \|y\|_2.$$

such that

$$|\Delta| \leq \left|\mathcal{N}_{\gamma/2}(B_M)\right|^2 \leq \left(\frac{CM}{\gamma}\right)^{2d} =: \mathcal{M}_\gamma$$

By Theorem B.13 for $(x, y) \in B_M \times B_M$ fixed each of the following

$$\langle \partial_a f(x;\theta), \partial_a f(y;\theta)\rangle_2, \langle \partial_b f(x;\theta), \partial_b f(y;\theta)\rangle_2, \langle \partial_W f(x;\theta), \partial_W f(y;\theta)\rangle$$

is an average of m subexponential random variables with subexponential norm at most D^2K^2. Therefore separately from the randomness discussed before by Bernstein's inequality Vershynin (2018, Theorem 2.8.1) and a union bound we have

$$\mathbb{P}(|K_0(x, y) - K^\infty(x, y)| > t) \leq 3 \times 2\exp\left(-c\min\left\{\frac{mt^2}{D^4K^4}, \frac{mt}{D^2K^2}\right\}\right).$$

Thus for $t \leq D^2K^2$ we have

$$\mathbb{P}(|K_0(x, y) - K^\infty(x, y)| > t) \leq 6\exp\left(-c\frac{mt^2}{D^4K^4}\right).$$

Then by a union bound and the previous inequality we have that for $t \leq D^2K^2$

$$\mathbb{P}\left(\max_{z'\in\Delta} |K_0(z') - K^\infty(z')| > t\right) \leq 6\mathcal{M}_\gamma \exp\left(-c\frac{mt^2}{D^4K^4}\right).$$

Thus by setting $t = CD^2K^2\frac{\sqrt{\log(c/\delta)+\log\mathcal{M}_\gamma}}{\sqrt{m}}$ (note that the condition on m in the hypothesis ensures that $t \leq D^2K^2$) we get that with probability $1 - \delta$

$$\max_{z'\in\Delta} |K_0(z') - K^\infty(z')| \leq t.$$

Now fix $z \in B_M \times B_M$ and choose $z' \in \Delta$ such that $\|z - z'\| \leq \gamma$. Then

$$\begin{aligned} |K_0(z) - K^\infty(z)| &\leq |K_0(z) - K_0(z')| \\ &+ |K_0(z') - K^\infty(z')| + |K^\infty(z') - K^\infty(z)| \\ &\leq 2\max\{L(K_0), L(K^\infty)\}\gamma + t. \end{aligned} \tag{2}$$

Note that this argument runs through for any $z \in B_M \times B_M$ therefore

$$\sup_{z\in B_M\times B_M} |K_0(z) - K^\infty(z)| \leq 2\max\{L(K_0), L(K^\infty)\}\gamma + t.$$

Well by replacing δ with $\delta/3$ in the previous arguments by taking a union bound we can assume that equations (1) and (2) hold simultaneously. In which case

$$\begin{aligned} &\sup_{z\in B_M\times B_M} |K_0(z) - K^\infty(z)| \leq 2\max\{L(K_0), L(K^\infty)\}\gamma + t \leq 2\max\{\rho, L(K^\infty)\}\gamma + t \\ &\leq \frac{1}{\sqrt{m}} + CD^2K^2\frac{\sqrt{\log(c/\delta) + \log\mathcal{M}_\gamma}}{\sqrt{m}} = \frac{1}{\sqrt{m}} + CD^2K^2\frac{\sqrt{\log(c/\delta) + 2d\log(CM/\gamma)}}{\sqrt{m}} \\ &= \frac{1}{\sqrt{m}}\left[1 + CD^2K^2\sqrt{\log(c/\delta) + 2d\log(CM\max\{\rho, L(K^\infty)\}\sqrt{m})}\right] \end{aligned}$$

where we have used the definition of $\mathcal{M}_\gamma$ in the second-to-last equality and the definition of γ in the last equality. Since the doubling trick does not change the distribution of K_0, the same conclusion holds under that initialization scheme. □

We immediately get the following corollary.

Corollary B.20. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Then*

$$m \geq C[\log(c/\delta) + \tilde{O}(d)]$$

suffices to ensure that with probability at least $1-\delta$

$$\sup_{z \in B_M \times B_M} |K_0(z) - K^\infty(z)| = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\right)$$

If one instead does the doubling trick then the same conclusion holds.

B.5 Control of Network At Initialization

Many of our previous results depend on the quantity $\|\hat{r}(0)\|_{\mathbb{R}^n}$ which depends on the network at initialization. Before we proceed we must control the infinity norm of the network at initialization and work out a few consequences of this. The following lemma controls $\|f(\bullet;\theta_0)\|_\infty$.

Lemma B.21. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$, $b_0 \sim \mathcal{B}'$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let*

$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}.$$

$$L(m,\sigma,d,K,\delta) := \sqrt{m}\|\sigma'\|_\infty \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2$$

Assume that

$$m \geq C[\log(c/\delta) + d\log(CML)].$$

Then with probability at least $1-\delta$

$$\sup_{x \in B_M} |f(x;\theta_0)| \leq CDK^2\sqrt{d\log(CML) + \log(c/\delta)} = \tilde{O}(\sqrt{d})$$

Proof. First we note that

$$\left|\frac{a^T}{\sqrt{m}}\sigma(Wx+b) - \frac{a^T}{\sqrt{m}}\sigma(Wy+b)\right| \leq \frac{\|a\|_2}{\sqrt{m}}\|\sigma(Wx+b) - \sigma(Wy+b)\|_2$$
$$\leq \frac{\|a\|_2}{\sqrt{m}}\|\sigma'\|_\infty\|W(x-y)\|_2 \leq \frac{\|a\|_2}{\sqrt{m}}\|\sigma'\|_\infty\|W\|_{op}\|x-y\|_2 \leq \sqrt{m}\|\sigma'\|_\infty\xi(0)^2\|x-y\|_2$$

where $\xi(0)$ is defined as in Lemma B.17. Thus $f(\bullet;\theta_0)$ is Lipschitz with constant $L = \sqrt{m}\|\sigma'\|_\infty\xi(0)^2$. Well then by Lemma B.17 we have with probability at least $1-\delta$

$$\xi(0)^2 \leq \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2 \tag{3}$$

When the above holds we have that $f(\bullet;\theta_0)$ is Lipschitz with constant

$$L := \sqrt{m}\|\sigma'\|_\infty \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2$$

On the other hand note that

$$|\sigma(\langle w_\ell, x\rangle_2 + b_\ell)| \leq |\sigma(0)| + \|\sigma'\|_\infty[|\langle w_\ell, x\rangle_2| + |b_\ell|].$$

Thus

$$\begin{aligned}\|\sigma(\langle w_\ell, x\rangle_2 + b_\ell)\|_{\psi_2} &\leq |\sigma(0)|\|1\|_{\psi_2} + \|\sigma'\|_\infty[\||\langle w_\ell, x\rangle_2|\|_{\psi_2} + \||b_\ell|\|_{\psi_2}] \\ &\leq |\sigma(0)|\|1\|_{\psi_2} + \|\sigma'\|_\infty[M\|w_\ell\|_{\psi_2} + \||b_\ell|\|_{\psi_2}] \\ &\leq 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty\}K \leq DK\end{aligned}$$

Therefore by Lemma B.11 we have

$$\|a_\ell \sigma(\langle w_\ell, x\rangle_2 + b_\ell)\|_{\psi_1} \leq DK^2$$

Thus for each x fixed we have by Bernstein's inequality Vershynin (2018, Theorem 2.8.1)

$$\mathbb{P}\left(\left|\sum_{\ell=1}^m a_\ell \sigma(\langle w_\ell, x\rangle_2 + b_\ell)\right| > t\sqrt{m}\right) \leq 2\exp\left(-c\min\left[\frac{t^2}{[DK^2]^2}, \frac{t\sqrt{m}}{DK^2}\right]\right)$$

Thus for $t \leq \sqrt{m}DK^2$ this simplifies to

$$\mathbb{P}\left(\left|\sum_{\ell=1}^m a_\ell \sigma(\langle w_\ell, x\rangle_2 + b_\ell)\right| > t\sqrt{m}\right) \leq 2\exp\left(-c\frac{t^2}{D^2K^4}\right)$$

Let Δ be a γ net of the ball $B_M = \{x : \|x\|_2 \leq M\}$ with respect to the Euclidean $\|\bullet\|_2$ norm. Then by a standard volume argument we have that

$$|\Delta| \leq \left(\frac{CM}{\gamma}\right)^d =: \mathcal{M}_\gamma$$

Thus by a union bound we have for $t \leq \sqrt{m}DK^2$

$$\mathbb{P}\left(\max_{x\in\Delta}\left|\sum_{\ell=1}^m a_\ell \sigma(\langle w_\ell, x\rangle_2 + b_\ell)\right| > t\sqrt{m}\right) \leq 2\mathcal{M}_\gamma \exp\left(-c\frac{t^2}{D^2K^4}\right)$$

Thus by setting $t = CDK^2\sqrt{\log(c\mathcal{M}_\gamma/\delta)}$ assuming $t \leq \sqrt{m}DK^2$ we have with probability at least $1-\delta$

$$\max_{x\in\Delta}\left|\sum_{\ell=1}^m \frac{a_\ell}{\sqrt{m}} \sigma(\langle w_\ell, x\rangle_2 + b_\ell)\right| \leq t \tag{4}$$

On the other hand by Lemma B.15 our prior definition of t is large enough (up to a redefinition of the constants c, C) to ensure that with probability at least $1-\delta$

$$|b_0| \leq t \tag{5}$$

When Equations 4 and 5 hold simultaneously we have that $\max_{x'\in\Delta}|f(x', \theta_0)| \leq 2t$. By a union bound we have with probability at least $1-3\delta$ that Equations 3, 4, 5 hold simultaneously. Well then for any $x \in B_M$ we may choose $x' \in \Delta$ so that $\|x - x'\|_2 \leq \gamma$. Then

$$|f(x;\theta_0)| \leq |f(x';\theta_0)| + |f(x;\theta_0) - f(x';\theta_0)| \leq 2t + L\gamma$$

Therefore

$$\sup_{x\in B_M} |f(x;\theta_0)| \leq 2t + L\gamma$$

and this argument runs through for any $\gamma > 0$. We will set $\gamma = 1/L$. Note that for this choice of γ the hypothesis on m ensures that $t \leq \sqrt{m}DK^2$. Thus the preceding argument goes through in this case. Thus by replacing δ with $\delta/3$ in the previous argument we get the desired conclusion up to a redefinition of c, C. □

We quickly introduce the following lemma.

Lemma B.22.

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \leq \|f(\bullet;\theta_0)\|_\infty + \|y\|_{\mathbb{R}^n}$$

Proof. Let $\hat{y} \in \mathbb{R}^n$ be the vector whose ith entry is equal to $f(x_i;\theta_0)$. Well then note that $\|\hat{y}\|_{\mathbb{R}^n} \leq \|f(\bullet;\theta_0)\|_\infty$. Therefore

$$\|\hat{r}(0)\|_{\mathbb{R}^n} = \|\hat{y} - y\|_{\mathbb{R}^n} \leq \|\hat{y}\|_{\mathbb{R}^n} + \|y\|_{\mathbb{R}^n} \leq \|f(\bullet;\theta_0)\|_\infty + \|y\|_{\mathbb{R}^n}.$$

□

Finally we prove one last lemma that will be useful later.

Lemma B.23. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$, $D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$,*

$$L(m, \sigma, d, K, \delta) := \sqrt{m}\|\sigma'\|_\infty \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2,$$

$$\rho := CDK^2\sqrt{d\log(CML) + \log(c/\delta)} = \tilde{O}(\sqrt{d}).$$

Suppose

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2\rho^2T^2}{[\log(\Gamma)]^2}, \left(\frac{\rho}{DK^2}\right)^2\right\}$$

then with probability at least $1 - \delta$

$$\max_{t \leq T} \xi(t) \leq \Gamma\xi(0) \quad \max_{t \leq T} \tilde{\xi}(t) \leq \Gamma\tilde{\xi}(0)$$

where $\xi(t)$ and $\tilde{\xi}(t)$ are defined as in Lemmas B.2 and B.3. If one instead does the doubling trick the second hypothesis on m can be removed and the conclusion holds with probability 1.

Proof. First assume we are not doing the doubling trick. Well from the condition $m \geq \left(\frac{\rho}{DK^2}\right)^2$ we have by Lemma B.21 that with probability at least $1 - \delta$

$$\sup_{x \in B_M} |f(x; \theta_0)| \leq CDK^2\sqrt{d\log(CML) + \log(c/\delta)} =: \rho.$$

Also by Lemma B.22 and the above bound we have

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \leq \|y\|_{\mathbb{R}^n} + \rho$$

Well in this case

$$\frac{D\|\hat{r}(0)\|_{\mathbb{R}^n} t}{\sqrt{m}} \leq \frac{D[\|y\|_{\mathbb{R}^n} + \rho]t}{\sqrt{m}} \leq \frac{2D\max\{\|y\|_{\mathbb{R}^n}, \rho\}t}{\sqrt{m}} \leq \log(\Gamma)$$

where we have used the hypothesis on m in the last inequality. Therefore by Lemmas B.2, B.3 we have in this case that

$$\max_{t \leq T} \xi(t) \leq \Gamma\xi(0) \quad \max_{t \leq T} \tilde{\xi}(t) \leq \Gamma\tilde{\xi}(0)$$

Now assume we are performing the doubling trick so that $f(\bullet; \theta_0) \equiv 0$. Then ρ in the previous argument can simply be replaced with zero and the same argument runs through, except using Lemma B.21 is no longer necessary (and thus the second hypothesis on m is not needed). Without using Lemma B.21 the whole argument is deterministic so that the conclusion holds with probability 1. □

B.6 NTK Time Deviations Bounds

In this section we bound the deviations of the NTK throughout time. This section runs through the following steps

- Bound $\sup_{(x,y) \in B_M \times B_M} |\partial_t K_t(x, y)|$
- Bound $\sup_{(x,y) \in B_M \times B_M} |K_t(x, y) - K_0(x, y)|$

In the following lemma we will provide an upper bound on the NTK derivative $\sup_{x,y \in B_M \times B_M} |\partial_t K_t(x, y)|$

Lemma B.24. *Let*

$$\xi(t) = \max\{\frac{1}{\sqrt{m}}\|W(t)\|_{op}, \frac{1}{\sqrt{m}}\|b(t)\|_2, \frac{1}{\sqrt{m}}\|a(t)\|_2, 1\},$$

$$\tilde{\xi}(t) = \max\{\max_{\ell \in [m]}\|w_\ell(t)\|_2, \|a(t)\|_\infty, \|b(t)\|_\infty, 1\}$$

$$D = 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$$
$$D' := \left[\max\{\|\sigma'\|_\infty, \|\sigma''\|_\infty\}^2[M^2+1] + D\|\sigma'\|_\infty\right]\max\{1, M\}$$

Then for any initial conditions $W(0)$, $b(0)$, $a(0)$ we have for all t

$$\sup_{x,y\in B_M\times B_M}|\partial_t K_t(x,y)| \le \frac{CDD'}{\sqrt{m}}\xi(t)^2\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

Proof. We need to bound the following time derivatives

$$\partial_t\partial_a f(x;\theta) = \partial_t x^{(1)} = -\frac{1}{n}\sum_{i=1}^n \hat{r}_i\left[\frac{1}{\sqrt{m}}\sigma_1'(x)\sigma_1'(x_i)\frac{a}{\sqrt{m}}\right][\langle x, x_i\rangle_2 + 1]$$

$$\partial_t\partial_W f(x;\theta) = \partial_t\frac{1}{\sqrt{m}}\sigma_1'(x)a\otimes x$$
$$= \frac{1}{\sqrt{m}}[(\partial_t\sigma_1'(x))a + \sigma_1'(x)(\partial_t a)]\otimes x$$

$$\partial_t\partial_b f(x;\theta) = \partial_t\frac{1}{\sqrt{m}}\sigma_1'(x)a = \frac{1}{\sqrt{m}}\left([\partial_t\sigma_1'(x)]a + \sigma_1'(x)\partial_t a\right)$$

Note that

$$\left\|\frac{1}{\sqrt{m}}\sigma_1'(x)\sigma_1'(x_i)\frac{a}{\sqrt{m}}[\langle x, x_i\rangle_2+1]\right\|_2 \le \frac{1}{\sqrt{m}}\|\sigma'\|_\infty^2\frac{1}{\sqrt{m}}\|a\|_2[M^2+1]$$

Thus by Lemma B.1

$$\|\partial_t\partial_a f(x;\theta)\|_2 \le \frac{1}{\sqrt{m}}\|\sigma'\|_\infty^2\frac{1}{\sqrt{m}}\|a\|_2[M^2+1]\|\hat{r}(t)\|_{\mathbb{R}^n}$$
$$\le \frac{\|\sigma'\|_\infty^2[M^2+1]]}{\sqrt{m}}\xi(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

On the other hand

$$[\partial_t\sigma_1'(x)]a = -\frac{1}{n}\sum_{i=1}^n\hat{r}_i\frac{1}{\sqrt{m}}\sigma_1''(x)\sigma_1'(x_i)diag(a)a[\langle x, x_i\rangle_2+1].$$

Well

$$\frac{1}{\sqrt{m}}\|\sigma_1''(x)\sigma_1'(x_i)diag(a)a[\langle x, x_i\rangle_2+1\| \le \frac{1}{\sqrt{m}}\|\sigma''\|_\infty\|\sigma'\|_\infty\|a\|_\infty\|a\|_2[M^2+1]$$
$$\le \|\sigma''\|_\infty\|\sigma'\|_\infty[M^2+1]\xi(t)\tilde{\xi}(t)$$

Thus by Lemma B.1 we have that

$$\|[\partial_t\sigma_1'(x)]a\| \le \|\sigma''\|_\infty\|\sigma'\|_\infty[M^2+1]\xi(t)\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

Finally we have

$$\sigma_1'(x)\partial_t a = -\frac{1}{n}\sum_{i=1}^n\hat{r}_i\sigma_1'(x)x_i^{(1)}.$$

Well

$$\left\|\sigma_1'(x)x_i^{(1)}\right\| \le \|\sigma'\|_\infty\left\|x_i^{(1)}\right\|_2 = \|\sigma'\|_\infty\frac{1}{\sqrt{m}}\|\sigma(Wx_i+b)\|_2$$
$$\le \|\sigma'\|_\infty\left[|\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty(\|W\|_{op}M + \|b\|_2)\right]$$
$$\le \|\sigma'\|_\infty\left[|\sigma(0)| + M\|\sigma'\|_\infty + \|\sigma'\|_\infty\right]\xi(t) \le \|\sigma'\|_\infty D\xi(t)$$

Thus we finally by Lemma B.1 again we get that

$$\|\sigma_1'(x)\partial_t a\| \leq \|\sigma'\|_\infty D\xi(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

It follows that

$$\|\partial_t\partial_b f(x;\theta)\| \leq \frac{1}{\sqrt{m}}\left[\|\sigma''\|_\infty \|\sigma'\|_\infty [M^2+1] + \|\sigma'\|_\infty D\right]\xi(t)\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

and similarly

$$\|\partial_t\partial_W f(x;\theta)\| \leq \frac{M}{\sqrt{m}}\left[\|\sigma''\|_\infty \|\sigma'\|_\infty [M^2+1] + \|\sigma'\|_\infty D\right]\xi(t)\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

Thus in total we can say

$$\|\partial_t\partial_a f(x;\theta)\|_2, \|\partial_t\partial_b f(x;\theta)\|_2, \|\partial_t\partial_w f(x;\theta)\|_F \leq \frac{D'}{\sqrt{m}}\xi(t)\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

It thus follows by the chain rule and Lemma B.5 that

$$\sup_{(x,y)\in B_M\times B_M}|\partial_t K_t(x,y)| \leq \frac{CDD'}{\sqrt{m}}\xi(t)^2\tilde{\xi}(t)\|\hat{r}(t)\|_{\mathbb{R}^n}$$

□

Using the previous lemma we can now bound the deviations of the NTK.

Theorem B.25. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$ and $T > 0$ be positive constants,*

$$D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\},$$

$$D' := \left[\max\{\|\sigma'\|_\infty, \|\sigma''\|_\infty\}^2[M^2+1] + D\|\sigma'\|_\infty\right]\max\{1, M\},$$

and assume

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta)+\tilde{O}(d))\right\}.$$

Then with probability at least $1-\delta$

$$\sup_{(x,y)\in B_M\times B_M}|K_t(x,y) - K_0(x,y)| \leq$$

$$t\Gamma^3\frac{CDD'}{\sqrt{m}}\|\hat{r}(0)\|_{\mathbb{R}^n}\left\{1 + C\frac{\sqrt{d}+K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2\left\{\sqrt{d}+CK^2\left[\sqrt{\log(c/\delta)}+\sqrt{\log m}\right]\right\}.$$

If one instead does the doubling trick then the second condition on m can be removed from the hypothesis and the same conclusion holds.

Proof. First assume we are not doing the doubling trick. By Lemmas B.17, B.18 and a union bound we have with probability at least $1-\delta$

$$\xi(0)^2\tilde{\xi}(0) \leq \left\{1 + C\frac{\sqrt{d}+K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2\left\{\sqrt{d}+CK^2\left[\sqrt{\log(c/\delta)}+\sqrt{\log m}\right]\right\}. \quad (6)$$

Note that ρ as defined in Lemma B.23 satisfies $\rho^2 = O(\log(c/\delta)+\tilde{O}(d))$. Thus the hypothesis on m is strong enough to apply Lemma B.23, therefore by applying this lemma we have with probability at least $1-\delta$

$$\max_{t\leq T}\xi(t) \leq \Gamma\xi(0) \quad \max_{t\leq T}\tilde{\xi}(t) \leq \Gamma\tilde{\xi}(0) \quad (7)$$

Thus by replacing δ with $\delta/2$ and taking a union bound we have that with probability at least $1-\delta$ Equations 6 and 7 hold simultaneously. Then using Lemma B.24 and the fact that $\|\hat{r}(t)\|_{\mathbb{R}^n} \leq \|\hat{r}(0)\|_{\mathbb{R}^n}$ we have for $t \leq T$

$$\sup_{(x,y)\in B_M\times B_M} |\partial_t K_t(x,y)| \leq \Gamma^3 \frac{CDD'}{\sqrt{m}} \xi(0)^2 \tilde{\xi}(0) \|\hat{r}(0)\|_{\mathbb{R}^n}.$$

Therefore by the fundamental theorem of calculus for $t \leq T$

$$\sup_{(x,y)\in B_M\times B_M} |K_t(x,y) - K_0(x,y)| \leq t\Gamma^3 \frac{CDD'}{\sqrt{m}} \xi(0)^2 \tilde{\xi}(0) \|\hat{r}(0)\|_{\mathbb{R}^n}$$

$$\leq t\Gamma^3 \frac{CDD'}{\sqrt{m}} \|\hat{r}(0)\|_{\mathbb{R}^n} \left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2 \left\{\sqrt{d} + CK^2\left[\sqrt{\log(c/\delta)} + \sqrt{\log m}\right]\right\}.$$

Now consider if one instead does the doubling trick where one does the following swaps $W(0) \to \begin{bmatrix} W(0) \\ W(0) \end{bmatrix}$, $b(0) \to \begin{bmatrix} b(0) \\ b(0) \end{bmatrix}$, $a(0) \to \begin{bmatrix} a(0) \\ -a(0) \end{bmatrix}$ and $m \to 2m$ where $W(0)$, $b(0)$, and $a(0)$ are initialized as before. Then $\xi(0)$ and $\tilde{\xi}(0)$ do not change. We can then run through the same exact proof as before except when we apply Lemma B.23 the second hypothesis on m is no longer needed. □

Theorem B.26. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$ and $T > 0$ be positive constants and let $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$. Assume*

$$m \geq \frac{4D^2\|y\|^2_{\mathbb{R}^n} T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta) + \tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta) + \tilde{O}(d))\right\}.$$

Then with probability at least $1-\delta$ we have for $t \leq T$

$$\sup_{(x,y)\in B_M\times B_M} |K_t(x,y) - K^\infty(x,y)| = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

If one instead does the doubling trick then one can remove the assumption $m \geq \frac{4D^2 O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}$ and have the same conclusion hold.

Proof. The condition $m \geq O(\log(c/\delta) + \tilde{O}(d))$ is sufficient to satisfy the hypothesis of Theorem B.19. The condition on m also immediately satisfies the hypothesis of Theorem B.25. The desired result then follows from a union bound. □

Theorem B.27. *Under the same assumptions as Theorem B.26 we have that with probability at least $1-\delta$ for all $t \leq T$*

$$\|H^\infty - H_t\|_{op} \leq n\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

$$\sup_{s\leq T}\|G^\infty - G_t\|_{op} \leq \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

Proof. Recall that for a matrix $A \in \mathbb{R}^{m\times n}$ $\|A\|_{op} \leq \sqrt{mn}\max_{i,j}|A_{i,j}|$. Thus by Theorem B.26 with probability at least $1-\delta$

$$\|H^\infty - H_t\|_{op} \leq n\max_{i,j}|H^\infty_{i,j} - (H_t)_{i,j}| \leq n\sup_{(x,y)\in B_M\times B_M}|K_t(x,y) - K^\infty(x,y)|$$

$$= n\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right).$$

The second bound follows from $G_s = \frac{1}{n}H_s$ and $G^\infty = \frac{1}{n}H^\infty$. □

C UNDERPARAMETERIZED REGIME

In this section we build the tools to study the NTK in the underparameterized case. Our ultimate goal is prove Theorem 3.5.

Outline of this section

- Review operator theory
- Prove damped deviations equation
- Bound $\|(T - T_n^s)r_t\|_2$
  - Bound $\|(T_n - T_n^s)r_t\|_2$ using NTK deviation results (comparatively easy)
  - Bound $\|(T - T_n)r_t\|_2$
    - Derive covering number for a class of functions $\mathcal{C}$
    - Use covering number to bound $\sup_{g\in\mathcal{C}} \|(T - T_n)g\|$
    - Show that r_t is in class $\mathcal{C}$
- Prove Theorem 3.5

C.1 RKHS AND MERCER'S THEOREM

We recall some facts about Reproducing Kernel Hilbert Spaces (RKHS) and Mercer's Theorem. For additional background we suggest Berlinet & Thomas-Agnan (2004). Let $X \subset \mathbb{R}^d$ be a compact space equipped with a strictly positive (regular Borel) probability measure ρ. Let $K : X \times X \to \mathbb{R}$ be a continuous, symmetric, positive definite function. We define the integral operator $T_K : L^2(X) \to L^2(X)$

$$T_K f(x) := \int_X K(x,s)f(s)d\rho(s).$$

In this setting T_K is a compact, positive, self-adjoint operator. By the spectral theorem there is a countable nonincreasing sequence of nonnegative values $\{\sigma_i\}_{i=1}^\infty$ and an orthonormal set $\{\phi_i\}_{i=1}^\infty$ in L^2 such that $T_K\phi_i = \sigma_i\phi_i$. We will assume that T_K is strictly positive, i.e. $\langle f, T_K f\rangle_2 > 0$ for $f \neq 0$, so that we have further that $\{\phi_i\}_{i=1}^\infty$ is an orthonormal basis of L^2 and $\sigma_i > 0$ for all i. Moreover since K is continuous we may select the ϕ_i so that they are continuous functions, i.e. $\phi_i \in C(X)$ for each i. Then by Mercer's theorem we can decompose

$$K(x,y) = \sum_{i=1}^\infty \sigma_i\phi_i(x)\phi_i(y)$$

where the convergence is uniform. Furthermore the RKHS $\mathcal{H}$ associated with K is given by the set of functions

$$\mathcal{H} = \left\{ f \in L^2 : \sum_{i=1}^\infty \frac{|\langle f, \phi_i\rangle_2|^2}{\sigma_i} < \infty \right\}$$

where the inner product on $\mathcal{H}$ is given by

$$\langle f, g\rangle_{\mathcal{H}} = \sum_{i=1}^\infty \frac{\langle f, \phi_i\rangle_2 \langle g, \phi_i\rangle_2}{\sigma_i}.$$

Note that in this setting $\{\sqrt{\sigma_i}\phi_i\}_{i=1}^\infty$ is an orthonormal basis of $\mathcal{H}$. Define $K_x := K(\bullet, x)$. Recall the RKHS has the defining properties

$$K_x \in \mathcal{H} \quad \forall x \in X$$

$$h(x) = \langle h, K_x\rangle_{\mathcal{H}} \quad \forall (x,h) \in X \times \mathcal{H}$$

We will let $\kappa := \sup_{x\in X} K(x,x) < \infty$. From this we will have the useful inequality: for $h \in \mathcal{H}$

$$\begin{aligned} |h(x)| = |\langle h, K_x\rangle_{\mathcal{H}}| \leq \|h\|_{\mathcal{H}} \|K_x\|_{\mathcal{H}} = \|h\|_{\mathcal{H}} \sqrt{\langle K_x, K_x\rangle_{\mathcal{H}}} = \|h\|_{\mathcal{H}} \sqrt{K(x,x)} \\ \leq \kappa^{1/2} \|h\|_{\mathcal{H}}. \end{aligned}$$

Furthermore the elements of $\mathcal{H}$ are bounded continuous functions and $\mathcal{H}$ is seperable.

C.2 HILBERT-SCHMIDT AND TRACE CLASS OPERATORS

We will recall some definitions from (Rosasco et al., 2010). A bounded operator on a separable Hilbert space with associated norm $\|\bullet\|$ is called *Hilbert-Schmidt* if

$$\sum_{i=1}^{\infty} \|Ae_i\|^2 < \infty$$

for some (any) orthonormal basis $\{e_i\}_i$. For such an operator we define its Hilbert-Schmidt norm $\|A\|_{HS}$ to be the square root of the above sum. The Hilbert-Schmidt norm is the analog of the Frobenius norm for matrices. It is useful to note that every Hilbert-Schmidt operator is compact. The space of Hilbert-Schmidt operators is a Hilbert space with respect to the inner product

$$\langle A, B\rangle = \sum_j \langle Ae_j, Be_j\rangle.$$

A stronger notion is that of a *trace class* operator. We say a bounded operator on a separable Hilbert space is *trace class* if

$$\sum_{i=1}^{\infty} \langle \sqrt{A^*A}e_i, e_i\rangle < \infty$$

for some (any) orthonormal bases $\{e_i\}_i$. For such an operator we may define

$$Tr(A) := \sum_{i=1}^{\infty} \langle Ae_i, e_i\rangle.$$

By Lidskii's theorem the above sum is also equal to the sum of the eigenvalues of A repeated by multiplicity. The space of trace class operators is a Banach space with the norm $\|A\|_{TC} = Tr(\sqrt{A^*A})$. The following inequalities will be useful

$$\|A\| \leq \|A\|_{HS} \leq \|A\|_{TC}.$$

Furthermore if A is Hilbert-Schmidt and B is bounded we have

$$\|BA\|_{HS}, \|AB\|_{HS} \leq \|A\|_{HS} \|B\|.$$

Note that in our setting we have

$$\kappa \geq \int_X K(x,x)d\rho(x) = \int_X \sum_{i=1}^{\infty} \sigma_i |\phi_i(x)|^2 d\rho(x) = \sum_{i=1}^{\infty} \sigma_i \int_X |\phi_i(x)|^2 d\rho(x)$$
$$= \sum_{i=1}^{\infty} \sigma_i = Tr(T_K)$$

where the interchange of integration and summation is justified by the monotone convergence theorem. Thus T_K is a trace class operator and we have the inequality

$$\kappa \geq \sum_{i=1}^{\infty} \sigma_i$$

which will prove useful later.

C.3 DAMPED DEVIATIONS

Let $x \mapsto g_s(x) \in L^2$ for each $s \in [0,t]$ such that $s \mapsto \langle \phi_i, g_s\rangle_2$ is measureable for each i and $\int_0^t \|g_s\|_2^2 < \infty$. Then we define the integral

$$\int_0^t g_s ds$$

coordinatewise, meaning that $\int_0^t g_s ds$ is the L^2 function h such that

$$\langle h, \phi_i\rangle_2 = \int_0^t \langle g_s, \phi_i\rangle_2 ds.$$

Using this definition, we can now prove the "Damped Deviations" lemma.

Lemma 2.3. *Let* $[T_K h](\bullet) = \int_X K^\infty(\bullet, s)h(s)d\rho(s)$ *be the integral operator associated with* K^∞ *and let* $[T_n^s h](\bullet) = \frac{1}{n}\sum_{i=1}^n K_s(\bullet, x_i)h(x_i)$ *denote the time-dependent operator associated with* K_s*. Then*

$$r_t = \exp(-T_K t)r_0 + \int_0^t \exp(-T_K(t-s))(T_K - T_n^s)r_s ds,$$

where the equality is in the L^2 *sense.*

Proof. We have that

$$\partial_s r_s(x) = -\frac{1}{n}\sum_{i=1}^n K_s(x, x_i)r_s(x_i) = -[T_n^s r_s](x)$$

where the equality is pointwise over x. $\partial_s r_s(x)$ is a continuous function of x since K_s is continuous and is thus in L^2. Therefore we can consider

$$\langle \partial_s r_s, \phi_i\rangle_2 = \langle -T_n^s r_s, \phi_i\rangle_2.$$

By the continuity of $s \mapsto \theta_s$ we have the parameters are locally bounded in time and thus by Lemma B.5 we have that $\|K_s\|_\infty$ is also locally bounded therefore for any $s_0, \delta > 0$: $\sup_{|s-s_0|\leq\delta} \|K_s\|_\infty < \infty$. Note then that

$$|\partial_s r_s(x)| \leq \frac{1}{n}\sum_{i=1}^n |K_s(x, x_i)||r_s(x_i)| \leq \|K_s\|_\infty \|\hat{r}_s\|_{\mathbb{R}^n} \leq \|K_s\|_\infty \|\hat{r}_0\|_{\mathbb{R}^n}$$

It follows that $\|\partial_s r_s\|_\infty$ is bounded locally uniformly in s. Therefore the following differentiation under the integral sign is justified

$$\frac{d}{ds}\langle r_s, \phi_i\rangle_2 = \langle \partial_s r_s, \phi_i\rangle_2.$$

Thus combined with our previous equality we get

$$\frac{d}{ds}\langle r_s, \phi_i\rangle_2 = \langle -T_n^s r_s, \phi_i\rangle_2 = \langle -T_K r_s, \phi_i\rangle_2 + \langle (T_K - T_n^s)r_s, \phi_i\rangle_2$$
$$= \langle r_s, -T_K\phi_i\rangle_2 + \langle (T_K - T_n^s)r_s, \phi_i\rangle_2 = -\sigma_i\langle r_s, \phi_i\rangle_2 + \langle (T_K - T_n^s)r_s, \phi_i\rangle_2.$$

where we have used that T_K is self-adjoint. Therefore

$$\frac{d}{ds}\langle r_s, \phi_i\rangle_2 + \sigma_i\langle r_s, \phi_i\rangle_2 = \langle (T_K - T_n^s)r_s, \phi_i\rangle_2.$$

Multiplying by the integrating factor $\exp(\sigma_i s)$ we get

$$\frac{d}{ds}[\exp(\sigma_i s)\langle r_s, \phi_i\rangle_2] = \exp(\sigma_i s)\langle (T_K - T_n^s)r_s, \phi_i\rangle_2$$

Therefore applying the fundamental theorem of calculus after rearrangement we get

$$\langle r_t, \phi_i\rangle_2 = \exp(-\sigma_i t)\langle r_0, \phi_i\rangle_2 + \int_0^t \exp(-\sigma_i(t-s))\langle (T_K - T_n^s)r_s, \phi_i\rangle_2 ds$$

which is just the coordinatewise version of the desired result.

$$r_t = \exp(-T_K t)r_0 + \int_0^t \exp(-T_K(t-s))(T_K - T_n^s)r_s ds$$

□

C.4 COVERING NUMBER OF CLASS

We will now estimate the covering number of the class of shallow networks with bounds on their parameter norms. This lemma is slightly more general than what we will use but we will particularize it latter as it's general formulation presents no additional difficulty.

Lemma C.1. *Let*

$$\mathcal{C} = \{ \frac{a^T}{\sqrt{m}}\sigma(Wx+b) + b_0 : \|a-a'\|_2 \le \rho_1, \|W-W'\|_F \le \rho_2, \\ \|b-b'\|_2 \le \rho_3, |b_0 - b_0'| \le \rho_4 \\ \frac{1}{\sqrt{m}}\|a\|_2 \le \rho_1', \frac{1}{\sqrt{m}}\|W\|_{op} \le \rho_2', \frac{1}{\sqrt{m}}\|b\|_2 \le \rho_3' \}$$

and

$$\gamma' := |\sigma(0)| + \|\sigma'\|_\infty [\rho_2' M + \rho_3']$$

Then the (proper) covering number of $\mathcal{C}$ in the uniform norm satisfies

$$\mathcal{N}(\mathcal{C}, \epsilon, \|\|_\infty) \le \left(\frac{C'}{\epsilon}\right)^p$$

where $p = md + 2m + 1$ is the total number of parameters and C' equals

$$C' = C \max\{\rho_1\gamma', \rho_2 M \|\sigma'\|_\infty \rho_1', \rho_3 \|\sigma'\|_\infty \rho_1', \rho_4\}$$

where $C > 0$ is an absolute constant.

Proof. We will bound the pertubation of the function when changing the weights, specifically we will bound

$$\sup_{x\in B_M} \left| \frac{a^T}{\sqrt{m}}\sigma(Wx+b) - \frac{\tilde{a}^T}{\sqrt{m}}\sigma(\tilde{W}x+\tilde{b}) \right|.$$

Let $x^{(1)} = \frac{1}{\sqrt{m}}\sigma(Wx+b)$ and $\tilde{x}^{(1)} = \frac{1}{\sqrt{m}}\sigma(\tilde{W}x+\tilde{b})$. Then note that we have

$$\begin{aligned}
\left\|x^{(1)} - \tilde{x}^{(1)}\right\|_2 &\le \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left\|(W-\tilde{W})x + b - \tilde{b}\right\|_2 \\
&\le \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\left\|W-\tilde{W}\right\|_{op}\|x\|_2 + \left\|b-\tilde{b}\right\|_2\right] \\
&\le \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\left\|W-\tilde{W}\right\|_F M + \left\|b-\tilde{b}\right\|_2\right] =: \gamma
\end{aligned}$$

Well then

$$\begin{aligned}
|a^T x^{(1)} - \tilde{a}^T\tilde{x}^{(1)}| &\le |a^T(x^{(1)} - \tilde{x}^{(1)})| + |(a-\tilde{a})^T\tilde{x}^{(1)}| \\
&\le \|a\|_2 \gamma + \|a-\tilde{a}\|_2 \left\|\tilde{x}^{(1)}\right\|_2
\end{aligned}$$

Finally

$$\begin{aligned}
\left\|\tilde{x}^{(1)}\right\|_2 = \left\|\frac{1}{\sqrt{m}}\sigma(\tilde{W}x+\tilde{b})\right\|_2 &\le |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left\|\tilde{W}x+\tilde{b}\right\|_2 \\
&\le |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\left\|\tilde{W}\right\|_{op}\|x\|_2 + \left\|\tilde{b}\right\|_2\right] \\
&\le |\sigma(0)| + \frac{1}{\sqrt{m}}\|\sigma'\|_\infty \left[\left\|\tilde{W}\right\|_{op} M + \left\|\tilde{b}\right\|_2\right] \\
&\le |\sigma(0)| + \|\sigma'\|_\infty [\rho_2' M + \rho_3'] =: \gamma'
\end{aligned}$$

Therefore

$$|a^T x^{(1)} - \tilde{a}^T\tilde{x}^{(1)}| \le \|a\|_2 \gamma + \|a-\tilde{a}\|_2 \gamma'$$

Thus if we have

$$\|a-\tilde{a}\|_2 \leq \frac{\epsilon}{4\gamma'} =: \epsilon_1, \quad \left\|W-\tilde{W}\right\|_F \leq \frac{\epsilon}{8M\|\sigma'\|_\infty \rho_1'} =: \epsilon_2, \quad \left\|b-\tilde{b}\right\|_2 \leq \frac{\epsilon}{8\|\sigma'\|_\infty \rho_1'} =: \epsilon_3$$

then

$$\|a\|_2 \gamma \leq \frac{\epsilon \|a\|_2}{4\rho_1'\sqrt{m}} \leq \frac{\epsilon}{4}$$

therefore

$$|a^T x^{(1)} - \tilde{a}^T \tilde{x}^{(1)}| \leq \epsilon/2$$

and this bound holds for any $x \in B_M$. If add biases b_0 and $\tilde{b_0}$ such that $|b_0 - \tilde{b_0}| \leq \epsilon/2$ we simply get by the triangle inequality

$$|a^T x^{(1)} + b_0 - (\tilde{a}^T \tilde{x}^{(1)} + \tilde{b_0})| \leq \epsilon$$

Thus to get a cover we can simply cover the sets

$$\{a : \|a-a'\|_2 \leq \rho_1\} \quad \{W : \|W-W'\|_F \leq \rho_2\}$$
$$\{b : \|b-b'\|_2 \leq \rho_3\} \quad \{b_0 : |b_0 - b_0'| \leq \rho_4\}$$

in the Euclidean norm and multiply the covering numbers. Recall that the ϵ covering number for a Euclidean ball of radius R in s dimensional space, say $\mathcal{N}_\epsilon$, using the Euclidean norm satisfies

$$\left(\frac{cR}{\epsilon}\right)^s \leq \mathcal{N}_\epsilon \leq \left(\frac{CR}{\epsilon}\right)^s$$

for two absolute constants $c, C > 0$. Therefore we get that

$$\mathcal{N}(\mathcal{C}, \epsilon, \|\|_\infty) \leq \left(\frac{C\rho_1}{\epsilon_1}\right)^m \left(\frac{C\rho_2}{\epsilon_2}\right)^{md} \left(\frac{C\rho_3}{\epsilon_3}\right)^m \left(\frac{2C\rho_4}{\epsilon}\right)$$

The desired result follows from

$$\max\left\{\frac{\rho_1}{\epsilon_1}, \frac{\rho_2}{\epsilon_2}, \frac{\rho_3}{\epsilon_3}, \frac{2\rho_4}{\epsilon}\right\} \leq \frac{C}{\epsilon} \max\left\{\rho_1\gamma', \rho_2 M\|\sigma'\|_\infty \rho_1', \rho_3\|\sigma'\|_\infty \rho_1', \rho_4\right\}$$

□

We can now prove the following corollary which is the version of the previous lemma that we will actually use for our neural network.

Corollary C.2. *Let*

$$\mathcal{C} = \{\, \frac{a^T}{\sqrt{m}}\sigma(Wx+b) + b_0 : \frac{1}{\sqrt{m}}\|a\|_2, \frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2 \leq A, |b_0| \leq B \,\}$$

and

$$\gamma' := |\sigma(0)| + \|\sigma'\|_\infty [AM + A]$$

and assume $m \geq d$. Then the (proper) covering number of $\mathcal{C}$ in the uniform norm satisfies

$$\mathcal{N}(\mathcal{C}, \epsilon, \|\|_\infty) \leq \left(\frac{\Psi(m,d)}{\epsilon}\right)^p$$

where

$$\Psi(m,d) = C\max\{\sqrt{m}A\gamma', \sqrt{md}A^2\|\sigma'\|_\infty M, \sqrt{m}A^2\|\sigma'\|_\infty, B\}$$
$$= \sqrt{md}O\left(\max\left\{A^2, \frac{B}{\sqrt{md}}\right\}\right)$$

Proof. The idea is to apply Lemma C.1 with $a' = 0$, $W' = 0$, $b' = 0$, and $b_0' = 0$. Note that $\|W\|_F \leq \sqrt{d}\|W\|_{op} \leq \sqrt{md}A$. The result then follows by applying lemma with $\rho_1 = \sqrt{m}A$, $\rho_2 = \sqrt{md}A$, $\rho_3 = \sqrt{m}A$ and $\rho_4 = B$ and $\rho_1' = \rho_2' = \rho_3' = A$. □

C.5 UNIFORM CONVERGENCE OVER THE CLASS

We now show that $\|(T_n - T_K)g\|_2$ is uniformly small for all g in a suitable class of functions $\mathcal{C}'$. Ultimately we will show that $r_t \in \mathcal{C}'$ and thus this result is towards proving that $\|(T_n - T_K)r_t\|_2$ is small.

Lemma C.3. *Let $\mathcal{C}$ and $\Psi(m,d)$ be defined as in Corollary C.2. We let $\mathcal{C}' = \{g - f^* : g \in \mathcal{C}\}$ be the set where $\mathcal{C}$ is translated by the target function f^*. Let*

$$S = \sup_{g \in \mathcal{C}'} \|g\|_\infty$$

Then with probability at least $1-\delta$ over the sampling of $x_1, \dots, x_n$

$$\begin{aligned}\sup_{g \in \mathcal{C}'} \|(T_n - T_K)g\|_2 &\leq \frac{2S\sqrt{\sigma_1 \kappa}\sqrt{2\log(c/\delta) + 2p\log(\|K^\infty\|_\infty \Psi(m,d)\sqrt{n})}}{\sqrt{n}} + \frac{2}{\sqrt{n}} \\ &= \frac{2\left[1 + S\sqrt{\sigma_1\kappa}\sqrt{2\log(c/\delta) + \tilde{O}(p)}\right]}{\sqrt{n}}.\end{aligned}$$

Proof. Let $g \in \mathcal{C}'$. We introduce the random variables $Y_i := K^\infty_{x_i} g(x_i) - \mathbb{E}_{x\sim\rho}[K^\infty_x g(x)]$ taking values in the Hilbert space $\mathcal{H}$ for $i \in [n]$ where $\mathcal{H}$ is the RKHS associated with K^∞. Note that for any x

$$\|K^\infty_x g(x)\|_{\mathcal{H}} = |g(x)|\sqrt{\langle K^\infty_x, K^\infty_x\rangle_{\mathcal{H}}} \leq S\sqrt{K^\infty(x,x)} \leq S\kappa^{1/2}.$$

Thus $\|Y_i\|_{\mathcal{H}} \leq 2S\kappa^{1/2}$ a.s. Thus by Hoeffding's inequality for random variables taking values in a separable Hilbert space (see Rosasco et al. (2010, Section 2.4)) we have

$$\mathbb{P}\left(\left\|\frac{1}{n}\sum_{i=1}^n Y_i\right\|_{\mathcal{H}} > t\right) \leq 2\exp\left(-nt^2/2[2S\kappa^{1/2}]^2\right)$$

Since translation by a fixed function does not change the covering number, by Corollary C.2 the covering number of $\mathcal{C}'$ satisfies

$$\mathcal{N}(\mathcal{C}', \epsilon, \|\|_\infty) \leq \left(\frac{\Psi(m,d)}{\epsilon}\right)^p.$$

Let Δ be an ϵ net of $\mathcal{C}'$ in the uniform norm. Note that $\frac{1}{n}\sum_{i=1}^n Y_i = (T_n - T_K)g$. Thus by taking a union bound we have

$$\mathbb{P}\left(\max_{g\in\Delta} \|(T_n - T_K)g\|_{\mathcal{H}} \geq t\right) \leq \left(\frac{\Psi(m,d)}{\epsilon}\right)^p 2\exp\left(-nt^2/2[2S\kappa^{1/2}]^2\right)$$

Note that for any probability measure ν and $h \in L^\infty$

$$\left|\int_X K^\infty(x,s)h(s)d\nu(s)\right| \leq \int_X |K^\infty(x,s)||h(s)|d\nu(s) \leq \|K^\infty\|_\infty \|h\|_\infty$$

It follows that for any $h \in L^\infty$

$$\|(T_K - T_n)h\|_\infty \leq 2\|K^\infty\|_\infty \|h\|_\infty.$$

Note for any $g \in \mathcal{C}'$ we can pick $\hat{g}$ in Δ such that $\|g - \hat{g}\|_\infty \leq \epsilon$. Then

$$\begin{aligned}\|(T_n - T_K)g\|_2 &\leq \|(T_n - T_K)\hat{g}\|_2 + \|(T_n - T_K)(g - \hat{g})\|_2 \\ &\leq \sqrt{\sigma_1}\|(T_n - T_K)\hat{g}\|_{\mathcal{H}} + \|(T_n - T_K)(g - \hat{g})\|_\infty \\ &\leq \sqrt{\sigma_1}t + 2\|K^\infty\|_\infty \|g - \hat{g}\|_\infty \\ &\leq \sqrt{\sigma_1}t + 2\|K^\infty\|_\infty \epsilon\end{aligned}$$

where we have used the fact that $\|\bullet\|_2 \leq \sqrt{\sigma_1}\|\bullet\|_{\mathcal{H}}$ and $\|\bullet\|_2 \leq \|\bullet\|_\infty$ in the second inequality. Thus by setting

$$t = \frac{2S\kappa^{1/2}\sqrt{2\log(c/\delta) + 2p\log(\Psi(m,d)/\epsilon)}}{\sqrt{n}}$$

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

$$\sup_{g\in\mathcal{C}'} \|(T_n - T_K)g\|_2 \leq$$
$$\sqrt{\sigma_1}\frac{2S\kappa^{1/2}\sqrt{2\log(c/\delta)+2p\log(\Psi(m,d)/\epsilon)}}{\sqrt{n}} + 2\|K^\infty\|_\infty \epsilon.$$

This argument runs through for any $\epsilon > 0$. Thus by setting $\epsilon = \frac{1}{\|K^\infty\|_\infty \sqrt{n}}$ we get the desired result. □

C.6 Neural Network Is In The Class

In this section we demonstrate that the neural network in such a class as $\mathcal{C}$ as defined in Lemma C.1. Once we have this we can use Lemma C.3 to show that $\|(T_K - T_n)r_t\|_2$ is uniformly small. The first step is to bound the parameter norms, hence the following lemma.

Lemma C.4. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$, $T > 0$, $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$, and*

$$\xi(t) = \max\{\frac{1}{\sqrt{m}}\|W\|_{op}, \frac{1}{\sqrt{m}}\|b\|_2, \frac{1}{\sqrt{m}}\|a\|_2, 1\}.$$

Furthermore assume

$$m \geq \frac{4D^2\|y\|^2_{\mathbb{R}^n}T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta)+\tilde{O}(d))\right\}.$$

Then with probability at least $1-\delta$

$$\max_{t\in[0,T]}\xi(t) \leq \Gamma\left[1 + C\frac{\sqrt{d}+K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right].$$

If one instead does the doubling trick then the second condition on m can be removed from the hypothesis and the same conclusion holds.

Proof. First assume we are not doing the doubling trick. Note that the hypothesis on m is strong enough to satisfy the hypothesis of Lemma B.23, therefore we have with probability at least $1-\delta$

$$\max_{t\leq T}\xi(t) \leq \Gamma\xi(0).$$

Well then separately by Lemma B.17 with probability at least $1-\delta$

$$\xi(0) \leq 1 + C\frac{\sqrt{d}+K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}.$$

Thus by replacing δ with $\delta/2$ in the previous statements and taking a union bound we have with probability at least $1-\delta$

$$\max_{t\in[0,T]}\xi(t) \leq \Gamma\left[1 + C\frac{\sqrt{d}+K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right]$$

which is the desired result. Now suppose instead one does the doubling trick. We recall that the doubling trick does not change $\xi(0)$. Thus we can run through the exact same argument as before except when we apply Lemma B.23 we can remove the second condition on m from the hypothesis. □

The following lemma bounds the bias term.

Lemma C.5. *For any initial conditions we have*

$$|b_0(t)| \leq |b_0(0)| + t\|\hat{r}(0)\|_{\mathbb{R}^n}.$$

Proof. Note that

$$|\partial_t b_0(t)| = \left| \frac{1}{n} \sum_{i=1}^{n} \hat{r}(t)_i \right| \leq \|\hat{r}(t)\|_{\mathbb{R}^n} \leq \|\hat{r}(0)\|_{\mathbb{R}^n}$$

Thus by the fundamental theorem of calculus

$$|b_0(t)| \leq |b_0(0)| + t \|\hat{r}(0)\|_{\mathbb{R}^n} .$$

□

The following lemma demonstrates that the residual $r_t = f_t - f^*$ is bounded.

Lemma C.6. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$, $T > 0$, $D := 3\max\{|\sigma(0)|, M \|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$, and assume*

$$m \geq \frac{4D^2 \|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{ \frac{4D^2 O(\log(c/\delta) + \tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta) + \tilde{O}(d)) \right\}.$$

Then with probability at least $1 - \delta$ for $t \leq T$

$$\|f_t - f^*\|_\infty \leq \|f_0 - f^*\|_\infty + t \|\hat{r}(0)\|_{\mathbb{R}^n} CD^2\Gamma^2 \left[1 + C \frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}} \right]^2$$

If one instead does the doubling trick then the second condition on m can be removed from the hypothesis and the same conclusion holds.

Proof. Recall that

$$\partial_t(f_t(x) - f^*(x)) = -\frac{1}{n} \sum_{i=1}^{n} K_t(x, x_i)(f_t(x_i) - f^*(x_i)) = -\frac{1}{n} \sum_{i=1}^{n} K_t(x, x_i)\hat{r}(t)_i$$

Thus

$$|\partial_t(f_t(x) - f^*(x))| \leq \frac{1}{n} \sum_{i=1}^{n} |K_t(x, x_i)||\hat{r}(t)_i| \leq \|K_t\|_\infty \|\hat{r}(t)\|_{\mathbb{R}^n} \leq \|K_t\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n}$$

Well by Lemma B.5 we have that $\|K_t\|_\infty \leq CD^2\xi^2(t)$ where

$$\xi(t) = \max\{\frac{1}{\sqrt{m}} \|W\|_{op}, \frac{1}{\sqrt{m}} \|b\|_2, \frac{1}{\sqrt{m}} \|a\|_2, 1\}.$$

Well by Lemma C.4 we have that with probability at least $1 - \delta$

$$\max_{t \in [0,T]} \xi(t) \leq \Gamma \left[1 + C \frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}} \right].$$

Thus by the fundamental theorem of calculus

$$|f_t(x) - f^*(x)| \leq |f_0(x) - f^*(x)| + t \|\hat{r}(0)\|_{\mathbb{R}^n} CD^2\Gamma^2 \left[1 + C \frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}} \right]^2$$

Thus by taking the supremum over x we get

$$\|f_t - f^*\|_\infty \leq \|f_0 - f^*\|_\infty + t \|\hat{r}(0)\|_{\mathbb{R}^n} CD^2\Gamma^2 \left[1 + C \frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}} \right]^2$$

which is the desired conclusion. □

We can now finally prove that $\|(T_K - T_n)r_t\|_2$ is uniformly small.

Lemma C.7. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$, $T > 0$, $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$, and assume*

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta) + \tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta) + \tilde{O}(d))\right\}.$$

If we are doing the doubling trick set $S' = 0$ and otherwise set

$$S' = CDK^2\sqrt{d\log(CM\tilde{O}(\sqrt{m})) + \log(c/\delta)} = \tilde{O}(\sqrt{d}).$$

Then with probability at least $1 - \delta$

$$\sup_{t \leq T} \|(T_n - T_K)r_t\|_2 = \tilde{O}\left(\frac{(\|f^*\|_\infty + S')(1 + T\Gamma^2)\sqrt{\sigma_1 \kappa p}}{\sqrt{n}}\right)$$

and

$$\|r_0\|_\infty \leq \|f^*\|_\infty + S'.$$

If we are performing the doubling trick the second condition on m can be removed and the same conclusion holds.

Proof. By Lemma C.4 we have with probability at least $1 - \delta$

$$\max_{t \in [0,T]} \xi(t) \leq \Gamma\left[1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right] =: A. \tag{8}$$

Also by Lemma C.5

$$|b_0(t)| \leq |b_0(0)| + t\|\hat{r}(0)\|_{\mathbb{R}^n}.$$

If we are doing the doubling trick then $b_0(0) = 0$. Otherwise by Lemma B.15 we have with probability at least $1 - \delta$

$$|b_0(0)| \leq CK\sqrt{\log(c/\delta)}.$$

Furthermore by Lemma B.22 we have

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \leq \|y\|_{\mathbb{R}^n} + \|f(\bullet;\theta_0)\|_\infty.$$

Let L be defined as in Lemma B.21, i.e.

$$L(m, \sigma, d, K, \delta) := \sqrt{m}\|\sigma'\|_\infty\left\{1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right\}^2 = \tilde{O}(\sqrt{m}).$$

If we are not performing the doubling trick set

$$S' = CDK^2\sqrt{d\log(CML) + \log(c/\delta)}.$$

Otherwise if we are performing the doubling trick set $S' = 0$. In either case by Lemma B.21 we have with probability at least $1 - \delta$

$$\|f(\bullet;\theta_0)\|_\infty \leq S'. \tag{9}$$

In particular by Lemma B.22 we have

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \leq \|y\|_{\mathbb{R}^n} + \|f(\bullet;\theta_0)\|_\infty \leq \|y\|_{\mathbb{R}^n} + S'.$$

Thus we can say

$$|b_0(t)| \leq |b_0(0)| + t\|\hat{r}(0)\|_{\mathbb{R}^n} \leq CK\sqrt{\log(c/\delta)} + T(\|y\|_{\mathbb{R}^n} + S') =: B$$

and this holds whether or not we are performing the doubling trick. Thus up until time T the neural network is in class $\mathcal{C}$ as defined in Corollary C.2 with parameters A and B as defined above. Moreover by Lemma C.6 separate from the randomness before we have that with probability at least $1 - \delta$

$$\|r_t\|_\infty \leq \|r_0\|_\infty + t\|\hat{r}(0)\|_{\mathbb{R}^n} CD^2\Gamma^2\left[1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right]^2$$

Well note that when Equation 9 holds we have

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \leq \|r_0\|_\infty \leq \|f^*\|_\infty + \|f(\bullet;\theta_0)\|_\infty \leq \|f^*\|_\infty + S'.$$

Thus

$$\|r_t\|_\infty \leq (\|f^*\|_\infty + S')\left\{1 + TCD^2\Gamma^2\left[1 + C\frac{\sqrt{d} + K^2\sqrt{\log(c/\delta)}}{\sqrt{m}}\right]^2\right\} =: S$$

Thus by taking a union bound and redefining δ we have by an application of Lemma C.3 with S as defined in the hypothesis of the current theorem that with probability at least $1-\delta$

$$\begin{aligned}\sup_{t\leq T}\|(T_n - T_K)r_t\|_2 &\leq \frac{2\left[1 + S\sqrt{\sigma_1\kappa}\sqrt{2\log(c/\delta) + \tilde{O}(p)}\right]}{\sqrt{n}} \\ &= \tilde{O}\left(\frac{(\|f^*\|_\infty + S')(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right)\end{aligned}$$

where we have used that $S = \tilde{O}([\|f^*\|_\infty + S'][1 + T\Gamma^2])$. □

C.7 Proof Of Theorem 3.5

We are almost ready to prove Theorem 3.5. However first we must introduce a couple lemmas. The following bounds $\|(T_K - T_n^s)r_s\|_2$.

Lemma C.8.

$$\sup_{s\leq T}\|(T_K - T_n^s)r_s\|_2 \leq \sup_{s\leq T}\|(T_K - T_n)r_s\|_2 + \sup_{s\leq T}\|K^\infty - K_s\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n}.$$

Proof. We have that

$$\|(T_K - T_n^s)r_s\|_2 \leq \|(T_K - T_n)r_s\|_2 + \|(T_n - T_n^s)r_s\|_2.$$

Now observe that

$$\begin{aligned}|(T_n - T_n^s)r_s(x)| &= \left|\frac{1}{n}\sum_{i=1}^n [K^\infty(x,x_i) - K_s(x,x_i)]r_s(x_i)\right| \\ &\leq \frac{1}{n}\sum_{i=1}^n |K^\infty(x,x_i) - K_s(x,x_i)||r_s(x_i)| \\ &\leq \|K^\infty - K_s\|_\infty \|\hat{r}(s)\|_{\mathbb{R}^n} \leq \|K^\infty - K_s\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n}.\end{aligned}$$

Therefore

$$\|(T_n - T_n^s)r_s\|_2 \leq \|(T_n - T_n^s)r_s\|_\infty \leq \|K^\infty - K_s\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n}.$$

Thus

$$\sup_{s\leq T}\|(T_K - T_n^s)r_s\|_2 \leq \sup_{s\leq T}\|(T_K - T_n)r_s\|_2 + \sup_{s\leq T}\|K^\infty - K_s\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n}.$$

□

We are almost ready to finally prove Theorem 3.5. We must prove one final lemma that combines Lemma C.7 with the NTK deviation bounds in Theorem B.26 to show that $\|(T_K - T_n^s)r_s\|_2$ is uniformly small.

Lemma C.9. *Assume that $W_{i,j} \sim \mathcal{W}$, $b_\ell \sim \mathcal{B}$, $a_\ell \sim \mathcal{A}$ are all i.i.d zero-mean, subgaussian random variables with unit variance. Furthermore assume $\|1\|_{\psi_2}, \|w_\ell\|_{\psi_2}, \|a_\ell\|_{\psi_2}, \|b_\ell\|_{\psi_2} \leq K$ for each $\ell \in [m]$ where $K \geq 1$. Let $\Gamma > 1$, $T > 0$, $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$, and assume*

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta) + \tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta) + \tilde{O}(d))\right\}.$$

If we are doing the doubling trick set $S' = 0$ and otherwise set

$$S' = CDK^2\sqrt{d\log(CM\tilde{O}(\sqrt{m})) + \log(c/\delta)} = \tilde{O}(\sqrt{d}), S = S' + \|f^*\|_\infty .$$

Then with probability at least $1-\delta$

$$\sup_{s\le t}\|(T_K - T_n^s)r_s\|_2 = \tilde{O}\left(S\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 S\right] + \frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right).$$

If we are performing the doubling trick the condition $m \ge \frac{4D^2O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}$ can be removed and the same conclusion holds.

Proof. Note by Lemma C.8 we have

$$\sup_{s\le T}\|(T_K - T_n^s)r_s\|_2 \le \sup_{s\le T}\|(T_K - T_n)r_s\|_2 + \sup_{s\le T}\|K^\infty - K_s\|_\infty \|\hat{r}(0)\|_{\mathbb{R}^n} .$$

Well then by Theorem B.26 we have with probability at least $1-\delta$ that

$$\sup_{t\le T}\|K_t - K^\infty\|_\infty = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right).$$

Separately by Lemma C.7 we have with probability at least $1-\delta$

$$\sup_{s\le T}\|(T_K - T_n)r_s\|_2 = \tilde{O}\left(\frac{(\|f^*\|_\infty + S')(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right) = \tilde{O}\left(\frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right)$$

and

$$\|\hat{r}(0)\|_{\mathbb{R}^n} \le \|r_0\|_\infty \le S.$$

The result follows then from taking a union bound and replacing δ with $\delta/2$. □

We now proceed to prove the main theorem of this paper.

Theorem 3.5. *Let P_k be the orthogonal projection in L^2 onto span$\{\phi_1,\dots,\phi_k\}$ and let $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$. If we are doing the doubling trick set $S' = 0$ and otherwise set $S' = O(\sqrt{d\log(CM\tilde{O}(\sqrt{m})) + \log(c/\delta)}) = \tilde{O}(\sqrt{d})$, $\quad S = \|f^*\|_\infty + S'$. Also let $\Gamma > 1, T > 0$. Assume*

$$m \ge \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \ge \max\left\{\frac{4D^2O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta)+\tilde{O}(d))\right\}.$$

Then with probability at least $1-\delta$ we have that for all $t \le T$ and $k \in \mathbb{N}$

$$\|P_k(r_t - \exp(-T_K t)r_0)\|_2 \le \frac{1-\exp(-\sigma_k t)}{\sigma_k}\tilde{O}\left(S\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 S\right] + \frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right)$$

and

$$\|r_t - \exp(-T_K t)r_0\|_2 \le t\tilde{O}\left(S\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 S\right] + \frac{S(1+T\Gamma^2)\sqrt{\sigma_1\kappa p}}{\sqrt{n}}\right).$$

If we are performing the doubling trick the hypothesis $m \ge \frac{4D^2O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}$ can be removed and the same conclusion holds.

Proof. From Lemma 2.3 we have

$$r_t = \exp(-T_K t)r_0 + \int_0^t \exp(-T_K(t-s))(T_K - T_n^s)r_s ds.$$

Thus for any $k \in \mathbb{N}$

$$P_k(r_t - \exp(-T_K t) r_0) = P_k \int_0^t \exp(-T_K(t-s))(T_K - T_n^s) r_s ds$$
$$= \int_0^t P_k \exp(-T_K(t-s))(T_K - T_n^s) r_s ds.$$

Therefore

$$\|P_k(r_t - \exp(-T_K t) r_0)\|_2 = \left\| \int_0^t P_k \exp(-T_K(t-s))(T_K - T_n^s) r_s ds \right\|_2$$
$$\leq \int_0^t \|P_k \exp(-T_K(t-s))(T_K - T_n^s) r_s\|_2 \, ds$$
$$\leq \int_0^t \|P_k \exp(-T_K(t-s))\| \, \|(T_K - T_n^s) r_s\|_2 \, ds$$
$$\leq \int_0^t \exp(-\sigma_k(t-s)) \, \|(T_K - T_n^s) r_s\|_2 \, ds$$
$$\leq \frac{1 - \exp(-\sigma_k t)}{\sigma_k} \sup_{s \leq t} \|(T_K - T_n^s) r_s\|_2$$

and the above bound holds for any k. Well by Lemma C.9 the conditions on m in the hypothesis suffice to ensure that with probability at least $1 - \delta$

$$\sup_{s \leq t} \|(T_K - T_n^s) r_s\|_2 = \tilde{O}\left(S \frac{\sqrt{d}}{\sqrt{m}} \left[1 + t\Gamma^3 S\right] + \frac{S(1 + T\Gamma^2)\sqrt{\sigma_1 \kappa p}}{\sqrt{n}} \right).$$

and this is completely independent of k. The first result then follows from the above bound. To show the second result note that after applying the basic inequality $1 + x \leq e^x$ we have just shown

$$\|P_k(r_t - \exp(-T_K t) r_0)\|_2 = t\tilde{O}\left(S \frac{\sqrt{d}}{\sqrt{m}} \left[1 + t\Gamma^3 S\right] + \frac{S(1 + T\Gamma^2)\sqrt{\sigma_1 \kappa p}}{\sqrt{n}} \right)$$

uniformly over k. The second result then follows by sending $k \to \infty$ and Parseval's identity. □

Theorem 3.5 is strong enough to get a bound on the test error, which is demonstrated by the following corollary.

Corollary 3.6. *Suppose that $f^* = O(1)$ and assume we are performing the doubling trick where $f_0 \equiv 0$ so that $r_0 = -f^*$. Let $k \in \mathbb{N}$ and let P_k be the orthogonal projection onto span$\{\phi_1, \ldots, \phi_k\}$. Set $t = \frac{\log(\sqrt{2}\|P_k f^*\|_2/\epsilon^{1/2})}{\sigma_k}$ Then we have that $m = \tilde{\Omega}(\frac{d}{\epsilon \sigma_k^4})$ and $n = \tilde{\Omega}\left(\frac{\sigma_1 \kappa p}{\sigma_k^4 \epsilon}\right)$ suffices to ensure with probability at least $1 - \delta$*

$$\frac{1}{2}\|r_t\|_2^2 \leq 2\epsilon + 2\|(I - P_k) f^*\|_2^2.$$

Proof. Set $t = \frac{\log(\sqrt{2}\|P_k f^*\|_2/\epsilon^{1/2})}{\sigma_k}$. Note that

$$\frac{1}{2}\|r_t\|_2^2 \leq \frac{1}{2}\left[\|\exp(-T_K t) r_0\|_2 + \|r_t - \exp(-T_K t) r_0\|_2\right]^2$$
$$\leq 2\max\{\|\exp(-T_K t) r_0\|_2, \|r_t - \exp(-T_K t) r_0\|_2\}^2$$
$$\leq 2\left[\|\exp(-T_K t) r_0\|_2^2 + \|r_t - \exp(-T_K t) r_0\|_2^2\right].$$

Note that

$$\|\exp(-T_K t) r_0\|_2^2 = \|\exp(-T_K t) f^*\|_2^2 = \sum_{i=1}^{\infty} \exp(-2\sigma_i t) |\langle f^*, \phi_i \rangle_2|^2$$
$$\leq \exp(-2\sigma_k t) \sum_{i=1}^{k} |\langle f^*, \phi_i \rangle_2|^2 + \sum_{i=k+1}^{\infty} |\langle f^*, \phi_i \rangle_2|^2$$
$$= \frac{\epsilon}{2} + \|(I - P_k) f^*\|_2^2.$$

We want to apply Theorem 3.5 with $T = t$. We need

$$m \geq \frac{4D^2 \|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq O(\log(c/\delta) + \tilde{O}(d)).$$

We can simply set $\Gamma = 2$. Note that since $f^* = O(1)$ we have that $\|\hat{r}(0)\|_{\mathbb{R}^n} = \|y\|_{\mathbb{R}^n} = O(1)$. Then

$$\frac{D^2 \|y\|_{\mathbb{R}^n}^2 t^2}{[\log(\Gamma)]^2} = \tilde{O}\left(t^2\right) = \tilde{O}\left(\frac{1}{\sigma_k^2}\right).$$

thus our condition on m is strong enough to satisfy the first condition. Also $O(\log(c/\delta) + d\tilde{O}(1)) = \tilde{O}(d)$ which is satisfied by our condition on m. Thus by an application of Theorem 3.5 with $T = t$ and $\Gamma = 2$ we have with probability at least $1 - \delta$

$$\|r_t - \exp(-T_K t) r_0\|_2 \leq t\tilde{O}\left(\|f^*\|_\infty \frac{\sqrt{d}}{\sqrt{m}} \left[1 + t\Gamma^3 \|f^*\|_\infty\right] + \frac{\|f^*\|_\infty (1 + t\Gamma^2)\sqrt{\sigma_1 \kappa p}}{\sqrt{n}}\right).$$

Recall that $f^* = O(1)$. Also since $\Gamma = 2 = O(1)$ it can be ignored. Thus the first term above is

$$\tilde{O}\left(t^2 \frac{\sqrt{d}}{\sqrt{m}}\right) = \tilde{O}\left(\frac{\sqrt{d}}{\sigma_k^2 \sqrt{m}}\right).$$

Thus setting $m = \tilde{\Omega}(\frac{d}{\epsilon \sigma_k^4})$ suffices to ensure the first term is bounded by $\epsilon^{1/2}/(2\sqrt{2})$. Similarly the second term is

$$\tilde{O}\left(\frac{t^2 \sqrt{\sigma_1 \kappa p}}{\sqrt{n}}\right) = \tilde{O}\left(\frac{\sqrt{\sigma_1 \kappa p}}{\sigma_k^2 \sqrt{n}}\right).$$

Thus setting $n = \tilde{\Omega}\left(\frac{\sigma_1 \kappa p}{\sigma_k^4 \epsilon}\right)$ suffices to ensure that the second term bounded by $\epsilon^{1/2}/(2\sqrt{2})$. Thus in this case we have

$$\|r_t - \exp(-T_K t) r_0\|_2 \leq \frac{\epsilon^{1/2}}{\sqrt{2}}.$$

Thus we have

$$\frac{1}{2}\|r_t\|_2^2 \leq 2\left[\|\exp(-T_K t) r_0\|_2^2 + \|r_t - \exp(-T_K t) r_0\|_2^2\right] \leq 2\epsilon + 2\|(I - P_k) f^*\|_2^2$$

□

D Damped Deviations on Training Set

The damped deviations lemma for the training set is incredibly simple to prove and yet is incredibly powerful as we will see later. Here is the proof.

Lemma 2.1. *Let $G \in \mathbb{R}^{n \times n}$ be an arbitrary positive semidefinite matrix G_s the time dependent NTK matrix at time s. Then*

$$\hat{r}_t = \exp(-Gt)\hat{r}_0 + \int_0^t \exp(-G(t-s))(G - G_s)\hat{r}_s ds.$$

Proof. Note that we have the equation

$$\partial_t \hat{r}_t = -G_t \hat{r}_t = -G\hat{r}_t + (G - G_t)\hat{r}_t$$

Thus by multiplying by the integrating factor $\exp(Gt)$ and using the fact that $\exp(Gt)$ and G commute we have that

$$\partial_t \exp(Gt)\hat{r}_t = \exp(Gt)(G - G_t)\hat{r}_t.$$

Therefore by the fundamental theorem of calculus

$$\exp(Gt)\hat{r}_t - \hat{r}_0 = \int_0^t \exp(Gs)(G - G_s)\hat{r}_s ds$$

which after rearrangement gives

$$\hat{r}_t = \exp(-Gt)\hat{r}_0 + \int_0^t \exp(-G(t-s))(G - G_s)\hat{r}_s ds$$

□

Throughout we will let $u_1, \ldots, u_n$ denote the eigenvectors of G^∞ with corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$, normalized to have unit norm in $\|\bullet\|_{\mathbb{R}^n}$, i.e. $\|u_i\|_{\mathbb{R}^n} = 1$. The following corollary demonstrates that if one is only interested in approximating the top eigenvectors, then the deviations of the NTK only need to be small relative to the cutoff eigenvalue λ_i that you care about.

Corollary D.1. *Let P_k be the orthogonal projection onto span$\{u_1, \ldots, u_k\}$. Then for any $k \in [n]$*

$$\begin{aligned}\|P_k(\hat{r}_t - \exp(-G^\infty t)\hat{r}_0)\|_{\mathbb{R}^n} &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} \frac{1 - \exp(-\lambda_k t)}{\lambda_k} \\ &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} t.\end{aligned}$$

In particular

$$\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \sup_{s \leq t} \|G^\infty - G_s\|_{\mathbb{R}^n} \|\hat{r}_0\|_{\mathbb{R}^n} \frac{1 - \exp(-\lambda_n t)}{\lambda_n} \leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} t.$$

Proof. Note by Lemma 2.1 we have that

$$\hat{r}_t - \exp(-G^\infty t)\hat{r}_0 = \int_0^t \exp(-G^\infty(t-s))(G^\infty - G_s)\hat{r}_s ds$$

Therefore for any $k \in [n]$

$$\begin{aligned}P_k(\hat{r}_t - \exp(-G^\infty t)\hat{r}_0) &= P_k \int_0^t \exp(-G^\infty(t-s))(G^\infty - G_s)\hat{r}_s ds \\ &= \int_0^t P_k \exp(-G^\infty(t-s))(G^\infty - G_s)\hat{r}_s ds\end{aligned}$$

Thus

$$\begin{aligned}\|P_k(\hat{r}_t - \exp(-G^\infty t)\hat{r}_0)\|_{\mathbb{R}^n} &= \left\| \int_0^t P_k \exp(-G^\infty(t-s))(G^\infty - G_s)\hat{r}_s ds \right\|_{\mathbb{R}^n} \\ &\leq \int_0^t \|P_k \exp(-G^\infty(t-s))(G^\infty - G_s)\hat{r}_s\|_{\mathbb{R}^n} ds \\ &\leq \int_0^t \|P_k \exp(-G^\infty(t-s))\|_{op} \|G^\infty - G_s\|_{op} \|\hat{r}_s\|_{\mathbb{R}^n} ds \\ &\leq \int_0^t \exp(-\lambda_k(t-s)) \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} ds \\ &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} \int_0^t \exp(-\lambda_k(t-s)) ds \\ &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} \frac{1 - \exp(-\lambda_k t)}{\lambda_k} \\ &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} t\end{aligned}$$

where we have used the inequality $1 + x \leq \exp(x)$ in the last inequality. By specializing to the case $k = n$ since span$\{u_1, \ldots, u_n\} = \mathbb{R}^n$ we have

$$\begin{aligned}\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} \frac{1 - \exp(-\lambda_n t)}{\lambda_n} \\ &\leq \sup_{s \leq t} \|G^\infty - G_s\|_{op} \|\hat{r}_0\|_{\mathbb{R}^n} t.\end{aligned}$$

This completes the proof. □

Theorem 3.5 uses the concept of damped deviations to compare r_t with $\exp(-T_K t)r_0$. We can also prove the analogous statement on the training set that compares $\hat{r}_t$ to $\exp(-G^\infty t)\hat{r}_0$. The following is the analog of Theorem 3.5 on the training set.

Theorem D.2. *Let* $D := 3\max\{|\sigma(0)|, M\|\sigma'\|_\infty, \|\sigma'\|_\infty, 1\}$. *Also let* $\Gamma > 1, T > 0$. *Furthermore assume*

$$m \geq \frac{4D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(\Gamma)]^2} \text{ and } m \geq \max\left\{\frac{4D^2 O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}, O(\log(c/\delta)+\tilde{O}(d))\right\}$$

Let P_k *be the orthogonal projection onto span*$\{u_1, \ldots, u_k\}$. *Then with probability at least* $1-\delta$ *we have for any* $k \in [n]$ *and* $t \leq T$

$$\|P_k(\hat{r}_t - \exp(-G^\infty t)\hat{r}_0)\|_{\mathbb{R}^n} \leq \frac{1-\exp(-\lambda_k t)}{\lambda_k}\|\hat{r}_0\|_{\mathbb{R}^n}\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1+t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$
$$t\|\hat{r}_0\|_{\mathbb{R}^n}\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1+t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

in particular

$$\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \frac{1-\exp(-\lambda_n t)}{\lambda_n}\|\hat{r}_0\|_{\mathbb{R}^n}\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1+t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$
$$t\|\hat{r}_0\|_{\mathbb{R}^n}\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1+t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

If one instead does the doubling trick the condition $\frac{4D^2 O(\log(c/\delta)+\tilde{O}(d))T^2}{[\log(\Gamma)]^2}$ *can be removed from the hypothesis and the same conclusion holds.*

Proof. By Corollary D.1 we have

$$\|P_k(\hat{r}_t - \exp(-G^\infty t)\hat{r}_0)\|_{\mathbb{R}^n} \leq \sup_{s\leq t}\|G^\infty - G_s\|_{\mathbb{R}^n}\|\hat{r}_0\|_{\mathbb{R}^n}\frac{1-\exp(-\lambda_k t)}{\lambda_k}$$
$$\leq \sup_{s\leq t}\|G^\infty - G_s\|_{\mathbb{R}^n}\|\hat{r}_0\|_{\mathbb{R}^n} t$$

Well by Theorem B.27 we have with probability at least $1-\delta$

$$\sup_{s\leq t}\|G^\infty - G_t\|_{op} \leq \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1+t\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

The desired result follows from plugging this in to the previous bounds. □

E Proof of Theorem 3.7

We can now quickly prove our analog of Theorem 4.1 from Arora et al. (2019).

Theorem 3.7. *Assume* $m = \tilde{\Omega}(dn^5\epsilon^{-2}\lambda_n(H^\infty)^{-4})$ *and* $m \geq O(\log(c/\delta)+\tilde{O}(d))$ *and* $f^* = O(1)$. *Assume we are performing the doubling trick so that* $\hat{r}_0 = -y$. *Let* $v_1, \ldots, v_n$ *denote the eigenvectors of* G^∞ *normalized to have unit L2 norm* $\|v_i\|_2 = 1$. *Then with probability at least* $1-\delta$

$$\hat{r}_t = \exp(-G^\infty t)(-y) + \delta(t),$$

where $\sup_{t\geq 0}\|\delta(t)\|_2 \leq \epsilon$. *In particular*

$$\|\hat{r}_t\|_2 = \sqrt{\sum_{i=1}^n \exp(-2\lambda_i t)|\langle y, v_i\rangle_2|^2} \pm \epsilon.$$

Proof. Set $T = \log(\|\hat{r}(0)\|_{\mathbb{R}^n}\sqrt{n}/\epsilon)/\lambda_n$. Note that since $f^* = O(1)$ and we are performing the doubling trick we have that $\|\hat{r}_0\|_{\mathbb{R}^n} = \|y\|_{\mathbb{R}^n} = O(1)$. Recall that $\lambda_n := \frac{1}{n}\lambda_n(H^\infty)$ therefore $m = \tilde{\Omega}(dn^5\epsilon^{-2}\lambda_n(H^\infty)^{-4}) = \tilde{\Omega}(dn\epsilon^{-2}\lambda_n^{-4})$ is strong enough to ensure that

$$m \geq \frac{D^2\|y\|_{\mathbb{R}^n}^2 T^2}{[\log(2)]^2} = \tilde{O}(\lambda_n^{-2}) \quad m \geq O(\log(c/\delta)+\tilde{O}(d)) = \tilde{O}(d)$$

Then by an application of Theorem D.2 with $\Gamma = 2$ we have with probability at least $1-\delta$ that for all $t \leq T$

$$\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \frac{1-\exp(-\lambda_n t)}{\lambda_n} \|\hat{r}_0\|_{\mathbb{R}^n} \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + t\Gamma^3 \|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$
$$\leq \frac{\|\hat{r}_0\|_{\mathbb{R}^n}}{\lambda_n} \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + T\Gamma^3 \|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

Since $f^* = O(1)$ we have that $\|\hat{r}_0\|_{\mathbb{R}^n} = \|y\|_{\mathbb{R}^n} = O(1)$ therefore the above bound is

$$\tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\frac{T}{\lambda_n}\right) = \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\frac{1}{\lambda_n^2}\right)$$

Thus $m = \tilde{\Omega}(dn^5\epsilon^{-2}\lambda_n(H^\infty)^{-4}) = \tilde{\Omega}(dn\epsilon^{-2}\lambda_n^{-4})$ suffices to make the above term bounded by $\epsilon/\sqrt{n}$. Thus in this case

$$\sup_{t\leq T} \|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \epsilon/\sqrt{n}.$$

Let $\delta(t) = \hat{r}_t - \exp(-G^\infty t)\hat{r}_0$. We have just shown that $\sup_{t\leq T} \|\delta(t)\|_{\mathbb{R}^n} \leq \epsilon/\sqrt{n}$. We will now bound $\delta(t)$ for $t \geq T$. Note that for $t \geq T$

$$\|\exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \exp(-\lambda_n t)\|\hat{r}_0\|_{\mathbb{R}^n} \leq \exp(-\lambda_n T)\|\hat{r}_0\|_{\mathbb{R}^n} \leq \epsilon/\sqrt{n}$$

Also for $t \geq T$

$$\|\hat{r}_t\|_{\mathbb{R}^n} \leq \|\hat{r}_T\|_{\mathbb{R}^n} \leq \|\exp(-G^\infty T)\hat{r}_0\|_{\mathbb{R}^n} + \|\delta(T)\|_{\mathbb{R}^n} \leq 2\epsilon/\sqrt{n}$$

where we have used that $\|\hat{r}_t\|_{\mathbb{R}^n}$ is nonincreasing for gradient flow. Therefore for $t \geq T$

$$\|\delta(t)\|_{\mathbb{R}^n} \leq \|\hat{r}_t\|_{\mathbb{R}^n} + \|\exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq 3\epsilon/\sqrt{n}$$

Thus we have shown

$$\sup_{t\geq 0} \|\delta(t)\|_{\mathbb{R}^n} \leq 3\epsilon/\sqrt{n}.$$

The desired result follows from replacing ϵ with $\epsilon/3$ in the previous argument and using the fact that $\|\bullet\|_2 = \sqrt{n}\|\bullet\|_{\mathbb{R}^n}$ and $\hat{r}_0 = -y$. □

F Proof of Theorem 3.8

F.1 Main Theorem

Theorem 3.8. *Assume $m = \tilde{\Omega}\left(\epsilon^{-2}dT^2\|f^*\|_\infty^2(1+T\|f^*\|_\infty)^2\right)$ where $T > 0$ is a time parameter and $m \geq O(\log(c/\delta) + \tilde{O}(d))$ and $n \geq \frac{128\kappa^2\log(2/\delta)}{(\sigma_k-\sigma_{k+1})^2}$ Also assume $f^* \in L^\infty(X) \subset L^2(X)$ and let P^{T_K} be the orthogonal projection onto the eigenspaces of T_K corresponding to the eigenvalue $\alpha \in \sigma(T_K)$ and higher. Assume that $\left\|(I-P^{T_K})f^*\right\|_\infty \leq \epsilon'$ for some $\epsilon' > 0$. Pick k so that $\sigma_k = \alpha$ and $\sigma_{k+1} < \alpha$, i.e. k is the index of the last repeated eigenvalue corresponding to α in the ordered sequence $\{\sigma_i\}_i$. Also assume we are performing the doubling trick so that $\hat{r}(0) = -y$. Then we have with probability at least $1-3\delta$ over the sampling of $x_1,\ldots,x_n$ and θ_0 that for $t \leq T$*

$$\|\hat{r}_t\|_{\mathbb{R}^n} \leq \exp(-\lambda_k t)\|y\|_{\mathbb{R}^n} + \frac{4\kappa\|f^*\|_2\sqrt{10\log(2/\delta)}}{(\sigma_k-\sigma_{k+1})\sqrt{n}} + 2\epsilon' + \epsilon.$$

Proof. Recall that we have $\|\hat{r}(0)\|_{\mathbb{R}^n} = \|-y\|_{\mathbb{R}^n} \leq \|f^*\|_\infty$. Note that $m = \tilde{\Omega}\left(\epsilon^{-2}dT^2\|f^*\|_\infty^2(1+T\|f^*\|_\infty)^2\right)$ and $m \geq O(\log(c/\delta) + \tilde{O}(d))$ are strong enough to ensure the hypothesis of Theorem D.2 is satisfied with $\Gamma = 2$. From now on $\Gamma = 2 = O(1)$ and will be treated as a constant. Then by Theorem D.2 we have for $t \leq T$

$$\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq T\|\hat{r}_0\|_{\mathbb{R}^n} \tilde{O}\left(\frac{\sqrt{d}}{\sqrt{m}}\left[1 + T\Gamma^3\|\hat{r}(0)\|_{\mathbb{R}^n}\right]\right)$$

Thus using the fact from the doubling trick that $\|\hat{r}(0)\|_{\mathbb{R}^n} = \|y\|_{\mathbb{R}^n} \leq \|f^*\|_\infty$ setting $m = \tilde{\Omega}\left(\epsilon^{-2} dT^2 \|f^*\|_\infty^2 (1 + T\|f^*\|_\infty)^2\right)$ suffices to ensure that $\|\hat{r}_t - \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} \leq \epsilon$ for $t \leq T$. Let P_k be the orthogonal projection onto span$\{u_1, \ldots, u_k\}$. Well then for $t \leq T$

$$\begin{aligned}\|\hat{r}_t\|_{\mathbb{R}^n} &\leq \|\exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} + \epsilon \leq \|P_k \exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} + \|(I - P_k)\exp(-G^\infty t)\hat{r}_0\|_{\mathbb{R}^n} + \epsilon \\ &\leq \exp(-\lambda_k t)\|\hat{r}_0\|_{\mathbb{R}^n} + \|(I - P_k)\hat{r}_0\|_{\mathbb{R}^n} + \epsilon\end{aligned}$$

By Theorem F.6 we have with probability at least $1 - 2\delta$ over the sampling of $x_1, \ldots, x_n$ that

$$\|(I - P_k)y\|_{\mathbb{R}^n} \leq 2\epsilon' + \frac{4\kappa \|f^*\|_2 \sqrt{10\log(2/\delta)}}{(\sigma_k - \sigma_{k+1})\sqrt{n}}$$

Since we are using the doubling trick we have $\hat{r}_0 = -y$. Thus we have

$$\|(I - P_k)\hat{r}_0\|_{\mathbb{R}^n} \leq 2\epsilon' + \frac{4\kappa \|f^*\|_2 \sqrt{10\log(2/\delta)}}{(\sigma_k - \sigma_{k+1})\sqrt{n}}$$

Thus by taking a union bound we have with probability at least $1 - 3\delta$ for all $t \leq T$

$$\|\hat{r}_t\|_{\mathbb{R}^n} \leq \exp(-\lambda_k t)\|\hat{r}_0\|_{\mathbb{R}^n} + \frac{4\kappa \|f^*\|_2 \sqrt{10\log(2/\delta)}}{(\sigma_k - \sigma_{k+1})\sqrt{n}} + +2\epsilon' + \epsilon$$

The desired result follows from $\hat{r}_0 = -y$. □

F.2 Control of Initial Residual

We will use some of the notation and operator theory from Section C.1 and Section C.2 in this section, thus it is recommended to have read those sections first. Let $u_1, \ldots, u_n$ denote the eigenvectors of G^∞ normalized to have unit norm in $\|\bullet\|_{\mathbb{R}^n}$, i.e. $\|u_i\|_{\mathbb{R}^n} = 1$. Let P_k be the orthogonal projection onto span$\{u_1, \ldots, u_k\}$. The goal of this section is to upper bound the extent to which the labels y participate in the bottom eigendirections of G^∞, i.e. to show that $\|(I - P_k)y\|_{\mathbb{R}^n}$ is small. Let P^{T_K} be some projection onto the top eigenspaces of T_K. The idea is to show that if $\left\|(I - P^{T_K})f^*\right\|_2$ is small then by picking P_k so that rank$(P_k) =$ rank(P^{T_K}) then $\|(I - P_k)y\|_{\mathbb{R}^n}$ is also small with high probability. The results in this section essentially all appear in the proofs in Su & Yang (2019). We repeat the arguments here for completeness and due to differences in notation and constants.

We use some of the same machinery in (Rosasco et al., 2010). We define operators $L_{\mathcal{H}} : \mathcal{H} \to \mathcal{H}$ and $T_n : \mathcal{H} \to \mathcal{H}$ by

$$T_{\mathcal{H}} f := \int_X \langle f, K_s \rangle_{\mathcal{H}} K_s d\rho(s)$$

$$T_n f := \frac{1}{n}\sum_{i=1}^n \langle f, K_{x_i} \rangle_{\mathcal{H}} K_{x_i}$$

Note that $T_{\mathcal{H}}$ is equal to T_K on $\mathcal{H}$ and T_n is simply the operator you get if you replace ρ in the defintion of $T_{\mathcal{H}}$ with the empirical measure $\frac{1}{n}\sum_{i=1}^n \delta_{x_i}$. We define the "restriction" operator $R_n : \mathcal{H} \to \mathbb{R}^n$ by

$$R_n f = [f(x_1), f(x_2), \ldots, f(x_n)]^T$$

Note here the domain of R_n is $\mathcal{H}$ but in other parts of this paper we will allow R_n to take more general functions as input. Define $R_n^* : \mathbb{R}^n \to \mathcal{H}$ by

$$R_n^*(v_1, \ldots, v_n) = \frac{1}{n}\sum_{i=1}^n v_i K_{x_i}$$

It can be seen that

$$\langle R_n^* v, f \rangle_{\mathcal{H}} = \langle v, R_n f \rangle_{\mathbb{R}^n}$$

and thus R_n^* is the adjoint of R_n. Using these operators we may write $T_n = R_n^* R_n$ and $G^\infty = R_n R_n^*$. It will follow that T_n and G^∞ have the same eigenvalues (up to some zero eigenvalues) and their eigenvectors are related. We recall the following result from (Rosasco et al., 2010) (Proposition 9)

Theorem F.1. *(Rosasco et al., 2010) The following hold*

- *The operator T_n is finite rank, self-adjoint and positive, and the matrix G^∞ is symmetric and semi-positive definite. In particular the spectrum $\sigma(T_n)$ of T_n has finitely many non-zero elements and they are contained in $[0, \kappa]$.*
- *The spectrum of T_n and G^∞ are the same up to zero, specifically $\sigma(G^\infty) \setminus \{0\} = \sigma(T_n) \setminus \{0\}$. Moreover if λ_i is a nonzero eigenvalue and u_i and v_i are the corresponding eigenvector and eigenfunction for G^∞ and T_n respectively (normalized to norm 1 in $\|\bullet\|_{\mathbb{R}^n}$ and $\|\bullet\|_{\mathcal{H}}$ respectively), then*

$$u_i = \frac{1}{\lambda_i^{1/2}} R_n v_i$$

$$v_i = \frac{1}{\lambda_i^{1/2}} R_n^* u_i = \frac{1}{\lambda_i^{1/2}} \frac{1}{n} \sum_{j=1}^{n} K_{x_j} (u_i)_j$$

  where $(u_i)_j$ is the jth component of the vector u_i.
- *The following decompositions hold*

$$G^\infty w = \sum_{j=1}^{k} \lambda_j \langle w, u_j \rangle_{\mathbb{R}^n} u_j$$

$$T_n f = \sum_{j=1}^{k} \lambda_j \langle f, v_j \rangle_{\mathcal{H}} v_j$$

  where $k = rank(G^\infty) = rank(T_n)$ and both sums run over the positive eigenvalues. $\{u_i\}_{i=1}^k$ is an orthonormal basis for $ker(G^\infty)^\perp$ and $\{v_i\}_{i=1}^k$ is an orthonormal basis for $ker(T_n)^\perp$.

Note in our setting we will have that G^∞ is strictly positive definite a.s. Thus in our setting $\text{rank}(G^\infty) = \text{rank}(T_n) = n$. We will order the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$ (eigenvalues repeated according to multiplicity).

We will make use of the following lemma from Rosasco et al. (2010, Proposition 6):

Lemma F.2. *(Rosasco et al., 2010) Let $\alpha_1 > \alpha_2 > \ldots > \alpha_N > \alpha_{N+1}$ be the top $N+1$ distinct eigenvalues of $T_{\mathcal{H}}$. Let $P^{T_{\mathcal{H}}}$ be the orthogonal projection onto the eigenfunctions of $T_{\mathcal{H}}$ corresponding to eigenvalues α_N and above. Let P^{T_n} be the projection onto the top k eigenvectors of T_n so that $k = dim(range(T_n)) = dim(range(T_{\mathcal{H}}))$. Assume further that*

$$\|T_{\mathcal{H}} - T_n\|_{HS} \leq \frac{\alpha_N - \alpha_{N+1}}{4}.$$

Then

$$\left\|P^{T_{\mathcal{H}}} - P^{T_n}\right\|_{HS} \leq \frac{2}{\alpha_N - \alpha_{N+1}} \|T_{\mathcal{H}} - T_n\|_{HS}$$

The following lemma will be useful.

Lemma F.3. *Let $f^* \in L^2$ and let $P^{T_{\mathcal{H}}}$ and P^{T_n} be defined as in Lemma F.2. Then*

$$\sum_{i=k+1}^{n} |\langle R_n P^{T_K} f^*), u_i \rangle_{\mathbb{R}^n}|^2 \leq \frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\|P^{T_{\mathcal{H}}} - P^{T_n}\right\|_{HS}^2$$

Proof. We repeat the same proof as in (Su & Yang, 2019) for completeness and to remove confusion that may arise from differences in notation. The proof was originally given in (Rosasco et al., 2010) albeit with a minor error involving missing multiplicative factors. Note that

$$P^{T_K} f^* = \sum_{j=1}^{k} \langle f^*, \phi_j \rangle_2 \phi_j$$

Therefore

$$\langle R_n P^{T_K} f^*, u_i \rangle_{\mathbb{R}^n} = \sum_{j=1}^{k} \langle f^*, \phi_j \rangle_2 \langle R_n \phi_j, u_i \rangle_{\mathbb{R}^n}.$$

Applying Cauchy-Schwarz we get

$$\begin{aligned} |\langle R_n P^{T_K} f^*, u_i \rangle_{\mathbb{R}^n}|^2 &\leq \left[\sum_{j=1}^{k} |\langle f^*, \phi_j \rangle_2|^2 \right] \left[\sum_{j=1}^{k} |\langle R_n \phi_j, u_i \rangle_{\mathbb{R}^n}|^2 \right] \\ &\leq \|f^*\|_2^2 \sum_{j=1}^{k} |\langle R_n \phi_j, u_i \rangle_{\mathbb{R}^n}|^2 \end{aligned}$$

Well then note that

$$\sum_{j=1}^{k} |\langle R_n \phi_j, u_i \rangle_{\mathbb{R}^n}|^2 = \sum_{j=1}^{k} |\langle \phi_j, R_n^* u_i \rangle_{\mathcal{H}}|^2 = \sum_{j=1}^{k} \lambda_i |\langle \phi_j, v_i \rangle_{\mathcal{H}}|^2.$$

Therefore

$$\begin{aligned} \sum_{i=k+1}^{n} |\langle R_n P^{T_K} f^*), u_i \rangle_{\mathbb{R}^n}|^2 &\leq \|f^*\|_2^2 \sum_{i=k+1}^{n} \sum_{j=1}^{k} \lambda_i |\langle \phi_j, v_i \rangle_{\mathcal{H}}|^2 \\ &\leq \|f^*\|_2^2 \, \lambda_{k+1} \sum_{i=k+1}^{n} \sum_{j=1}^{k} |\langle \phi_j, v_i \rangle_{\mathcal{H}}|^2 \end{aligned} \tag{10}$$

On the other hand

$$\begin{aligned} \left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS}^2 &\geq \sum_{j=1}^{k} \left\| (P^{T_{\mathcal{H}}} - P^{T_n}) \sqrt{\sigma_j} \phi_j \right\|_{\mathcal{H}}^2 \\ &\geq \sum_{j=1}^{k} \sum_{i=k+1}^{n} |\langle (P^{T_{\mathcal{H}}} - P^{T_n}) \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}}|^2 \end{aligned}$$

Note that for $1 \leq j \leq k$ and $k+1 \leq i \leq n$ we have

$$\begin{aligned} \langle (P^{T_{\mathcal{H}}} - P^{T_n}) \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}} &= \langle P^{T_{\mathcal{H}}} \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}} - \langle P^{T_n} \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}} \\ &= \langle \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}} - \langle \sqrt{\sigma_j} \phi_j, P^{T_n} v_i \rangle_{\mathcal{H}} = \langle \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}}. \end{aligned}$$

So

$$\begin{aligned} \sum_{j=1}^{k} \sum_{i=k+1}^{n} |\langle (P^{T_{\mathcal{H}}} - P^{T_n}) \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}}|^2 &= \sum_{j=1}^{k} \sum_{i=k+1}^{n} |\langle \sqrt{\sigma_j} \phi_j, v_i \rangle_{\mathcal{H}}|^2 \\ &\geq \sigma_k \sum_{j=1}^{k} \sum_{i=k+1}^{n} |\langle \phi_j, v_i \rangle_{\mathcal{H}}|^2 \end{aligned}$$

To summarize we have shown

$$\frac{1}{\sigma_k} \left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS}^2 \geq \sum_{j=1}^{k} \sum_{i=k+1}^{n} |\langle \phi_j, v_i \rangle_{\mathcal{H}}|^2.$$

Combining this with equation 10 we get the final result

$$\sum_{i=k+1}^{n} |\langle R_n P^{T_K} f^*), u_i \rangle_{\mathbb{R}^n}|^2 \leq \frac{\|f^*\|_2^2 \, \lambda_{k+1}}{\sigma_k} \left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS}^2$$

□

We can use Lemma F.3 to produce the following bound.

Lemma F.4. *Let $f^* \in L^2$ and let $P^{T_{\mathcal{H}}}$ and P^{T_n} be defined as in Lemma F.2. Then*

$$\sum_{i=k+1}^{n} |\langle R_n f^*, u_i\rangle_{\mathbb{R}^n}|^2 \leq \frac{2}{n}\sum_{i=1}^{n} |(I - P^{T_K})f^*(x_i)|^2 + 2\frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\|P^{T_{\mathcal{H}}} - P^{T_n}\right\|_{HS}^2$$

Proof. We have that

$$\langle R_n f^*, u_i\rangle_{\mathbb{R}^n} = \langle R_n(I - P^{T_K})f^*, u_i\rangle_{\mathbb{R}^n} + \langle R_n P^{T_K} f^*, u_i\rangle_{\mathbb{R}^n}$$

Thus from the inequality $(a+b)^2 \leq 2(a^2+b^2)$ we get

$$\sum_{i=k+1}^{n} |\langle R_n f^*, u_i\rangle_{\mathbb{R}^n}|^2 \leq 2\sum_{i=k+1}^{n} |\langle R_n(I - P^{T_K})f^*, u_i\rangle_{\mathbb{R}^n}|^2 + 2\sum_{i=k+1}^{n} |\langle R_n P^{T_K} f^*, u_i\rangle_{\mathbb{R}^n}|^2$$

To control the first term we have

$$\sum_{i=k+1}^{n} |\langle R_n(I - P^{T_K})f^*, u_i\rangle_{\mathbb{R}^n}|^2 \leq \left\|(I - P^{T_K})f^*\right\|_{\mathbb{R}^n}^2 = \frac{1}{n}\sum_{i=1}^{n} |(I - P^{T_K})f^*(x_i)|^2$$

Then by applying Lemma F.3 to the second term we get the desired result. □

We recall the following lemma from Rosasco et al. (2010, Theorem 7)

Lemma F.5. *(Rosasco et al., 2010) With probability at least $1-\delta$ over the sampling of $x_1, \ldots, x_n$*

$$\|T_{\mathcal{H}} - T_n\|_{HS} \leq \frac{2\kappa\sqrt{2\log(2/\delta)}}{\sqrt{n}}$$

Now finally we can provide a bound on the labels participation in the bottom eigendirections.

Theorem F.6. *Assume $f^* \in L^2(X)$ and let P^{T_K} be the orthogonal projection onto the eigenspaces of T_K corresponding to the eigenvalue $\alpha \in \sigma(T_K)$ and higher. Assume that*

$$\left\|(I - P^{T_K})f^*\right\|_\infty \leq \epsilon'$$

for some $\epsilon' \geq 0$. Pick k so that $\sigma_k = \alpha$ and $\sigma_{k+1} < \alpha$, i.e. k is the index of the last repeated eigenvalue corresponding to α in the ordered sequence $\{\sigma_i\}_i$. Let P_k denote the orthogonal projection onto span$\{u_1, \ldots, u_k\}$. Finally assume

$$n \geq \frac{128\kappa^2\log(2/\delta)}{(\sigma_k - \sigma_{k+1})^2}.$$

Then we have with probability at least $1-2\delta$ over the sampling of $x_1, \ldots, x_n$ that

$$\|(I - P_k)R_n f^*\|_{\mathbb{R}^n} = \|(I - P_k)y\|_{\mathbb{R}^n} \leq 2\epsilon' + \frac{4\kappa\|f^*\|_2\sqrt{10\log(2/\delta)}}{(\sigma_k - \sigma_{k+1})\sqrt{n}}.$$

Proof. From Lemma F.4 we have

$$\sum_{i=k+1}^{n} |\langle R_n f^*, u_i\rangle_{\mathbb{R}^n}|^2 \leq \frac{2}{n}\sum_{i=1}^{n} |(I - P^{T_K})f^*(x_i)|^2 + 2\frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\|P^{T_{\mathcal{H}}} - P^{T_n}\right\|_{HS}^2$$

By assumption we have that the first term is bounded by $2(\epsilon')^2$. Now we must control the term

$$2\frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\|P^{T_{\mathcal{H}}} - P^{T_n}\right\|_{HS}^2$$

By Lemma F.5 we have with probability at least $1-\delta$

$$\|T_{\mathcal{H}} - T_n\|_{HS} \leq \frac{2\kappa\sqrt{2\log(2/\delta)}}{\sqrt{n}}.$$

Then

$$n \geq \frac{128\kappa^2 \log(2/\delta)}{(\sigma_k - \sigma_{k+1})^2}$$

suffices so that the right hand side above is less than or equal to $\frac{\sigma_k - \sigma_{k+1}}{4}$. Thus by Lemma F.2 we have that

$$\left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS} \leq \frac{2}{\sigma_k - \sigma_{k+1}} \left\| T_{\mathcal{H}} - T_n \right\|_{HS} \leq \frac{2}{\sigma_k - \sigma_{k+1}} \frac{2\kappa\sqrt{2\log(2/\delta)}}{\sqrt{n}}.$$

Thus from the above inequality we get that

$$2\frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS}^2 \leq \frac{64\kappa^2 \|f^*\|_2^2 \lambda_{k+1} \log(2/\delta)}{\sigma_k(\sigma_k - \sigma_{k+1})^2 \cdot n}$$

By Proposition 10 in Rosasco et al. (2010) we have separately with probability at least $1 - \delta$

$$\lambda_{k+1} \leq \sigma_{k+1} + \frac{2\kappa\sqrt{2\log(2/\delta)}}{\sqrt{n}}$$

Note that

$$n \geq \frac{128\kappa^2 \log(2/\delta)}{(\sigma_k - \sigma_{k+1})^2}$$

implies that

$$\frac{1}{\sqrt{n}} \leq \frac{\sigma_k - \sigma_{k+1}}{8\kappa\sqrt{2\log(2/\delta)}}$$

therefore

$$\lambda_{k+1} \leq \sigma_{k+1} + \frac{2\kappa\sqrt{2\log(2/\delta)}}{\sqrt{n}} \leq \sigma_k + \frac{1}{4}(\sigma_k - \sigma_{k+1}) \leq \frac{5}{4}\sigma_k$$

Thus

$$2\frac{\|f^*\|_2^2 \lambda_{k+1}}{\sigma_k} \left\| P^{T_{\mathcal{H}}} - P^{T_n} \right\|_{HS}^2 \leq \frac{64\kappa^2 \|f^*\|_2^2 \lambda_{k+1} \log(2/\delta)}{\sigma_k(\sigma_k - \sigma_{k+1})^2 n} \leq \frac{80\kappa^2 \|f^*\|_2^2 \log(2/\delta)}{(\sigma_k - \sigma_{k+1})^2 n}$$

Thus combined with our previous results we finally get that

$$\|(I - P_k)R_n f^*\|_{\mathbb{R}^n}^2 = \sum_{i=k+1}^{n} |\langle R_n f^*, u_i \rangle_{\mathbb{R}^n}|^2 \leq 2(\epsilon')^2 + \frac{80\kappa^2 \|f^*\|_2^2 \log(2/\delta)}{(\sigma_k - \sigma_{k+1})^2 n}$$

Thus from the inequality $\sqrt{a+b} \leq \sqrt{2}(\sqrt{a} + \sqrt{b})$ which holds for all $a, b \geq 0$ we have

$$\|(I - P_k)R_n f^*\|_{\mathbb{R}^n} \leq 2\epsilon' + \frac{4\kappa \|f^*\|_2 \sqrt{10\log(2/\delta)}}{(\sigma_k - \sigma_{k+1})\sqrt{n}}$$

Since $y = R_n f^*$ this provides the desired conclusion. □

G T_K IS STRICTLY POSITIVE

Note that

$$K^\infty(x, x') = \mathbb{E}[\sigma(\langle w, x \rangle_2 + b)\sigma(\langle w, x' \rangle_2 + b)] + \mathbb{E}[a^2 \sigma'(\langle w, x \rangle_2 + b)\sigma'(\langle w, x' \rangle_2 + b)][\langle x, x' \rangle_2 + 1] + 1$$

where the expectation is taken with respect to the parameter initialization. It suffices to show that the kernel corresponding to the first term above

$$K_a(x, x') := \mathbb{E}[\sigma(\langle w, x \rangle_2 + b)\sigma(\langle w, x' \rangle_2 + b)]$$

induces a strictly positive operator $T_{K_a} f(x) = \int_X K_a(x, s) f(s) d\rho(s)$. From the discussion in Section C.1 it suffices to show that the RKHS corresponding to K_a is dense in L^2. In Proposition 4.1 in Rahimi & Recht (2008) they showed that the RKHS associated with K_a has dense subset

$$\mathcal{F} := \left\{ x \mapsto \int_\Theta a(w, b)\sigma(\langle w, x \rangle_2 + b) d\mu(w, b) : \int_\Theta |a(w, b)|^2 d\mu(w, b) < \infty \right\}$$

where μ is the measure for the parameter initialization, i.e. $(w, b) \sim \mu$. Since $C(X)$ is dense in $L^2(X)$ it suffices to show that $\mathcal{F}$ is dense in $C(X)$ which is provided by the following theorem:

Theorem G.1. *Let σ be L-Lipschitz and not a polynomial. Assume that μ is a strictly positive measure supported on all of $\mathbb{R}^{d+1}$. Also assume that*

$$\int_{\mathbb{R}^{d+1}} [\|w\|_2^2 + \|b\|_2^2] d\mu(w,b) < \infty.$$

Then $\mathcal{F}$ is dense in $C(X)$ under the uniform norm.

Proof. We first show that $\mathcal{F} \subset C(X)$. Suppose we have $f \in \mathcal{F}$ and write $f(x) = \int_{\mathbb{R}^{d+1}} a(w,b)\sigma(\langle w,x\rangle_2 + b)d\mu(w,b)$. Well then

$$\begin{aligned}
|f(x) - f(x')| &= \left| \int_{\mathbb{R}^{d+1}} a(w,b)[\sigma(\langle w,x\rangle_2 + b) - \sigma(\langle w,x'\rangle_2 + b)]d\mu(w,b) \right| \\
&\leq \int_{\mathbb{R}^{d+1}} |a(w,b)||\sigma(\langle w,x\rangle_2 + b) - \sigma(\langle w,x'\rangle_2 + b)|d\mu(w,b) \\
\leq \int_{\mathbb{R}^{d+1}} |a(w,b)|L|\langle w, x - x'\rangle|d\mu(w,b) &\leq \int_{\mathbb{R}^{d+1}} |a(w,b)|L \|w\|_2 \|x - x'\|_2 \, d\mu(w,b) \\
&\leq L \|x - x'\|_2 \left[\int_{\mathbb{R}^{d+1}} |a(w,b)|^2 d\mu(w,b) \right]^{1/2} \left[\int_{\mathbb{R}^{d+1}} \|w\|_2^2 \, d\mu(w,b) \right]^{1/2}
\end{aligned}$$

Thus f is Lipschitz and thus continuous. Now suppose that $\mathcal{F}$ is not dense in $C(X)$. Then by the Riesz representation theorem there exists a nonzero signed measure $\nu(x)$ with finite total variation such that $\int_X f(x)d\nu(x) = 0$ for all $f \in \mathcal{F}$. Well then writing $f(x) = \int_{\mathbb{R}^{d+1}} a(w,b)\sigma(\langle w,x\rangle_2 + b)d\mu(w,b)$ as before we have

$$\int_X \int_{\mathbb{R}^{d+1}} a(w,b)\sigma(\langle w,x\rangle_2 + b)d\mu(w,b)d\nu(x) = 0 \tag{11}$$

Note that

$$\begin{aligned}
&\int_{\mathbb{R}^{d+1}} |a(w,b)||\sigma(\langle w,x\rangle_2 + b)|d\mu(w,b) \\
&\leq \int_{\mathbb{R}^{d+1}} |a(w,b)|[|\sigma(0)| + L|\langle w,x\rangle_2 + b|]d\mu(w,b) \\
&\leq \int_{\mathbb{R}^{d+1}} |a(w,b)|[|\sigma(0)| + L(\|w\|_2 M + \|b\|_2)]d\mu(w,b) < \infty
\end{aligned}$$

where we have used Cauchy-Schwarz and the hypothesis on the integrability of $\|w\|_2^2, \|b\|_2^2$ in the last step. Thus the integrand in Equation 11 is $\mu \times \nu$ integrable thus by Fubini's theorem we may interchange the order of integration. To get that

$$\int_{\mathbb{R}^{d+1}} a(w,b) \int_X \sigma(\langle w,x\rangle_2 + b)d\nu(x)d\mu(w,b)$$

and the above holds for any $a \in L^2(\mathbb{R}^{d+1}, \mu)$. Thus $\int_X \sigma(\langle w,x\rangle_2 + b)d\nu(x) = 0$ for μ-almost every w, b. However by essentially the same proof as when we showed $\mathcal{F} \subset C(X)$ we may show that $\int_X \sigma(\langle w,x\rangle_2 + b)d\nu(x) = 0$ is a continuous function of (w,b). Thus since μ is a strictly positive measure on $\mathbb{R}^{d+1}$ this implies that $\int_X \sigma(\langle w,x\rangle_2 + b)d\nu(x) = 0$ for every $(w,b) \in \mathbb{R}^{d+1}$. However by Theorem 1 in Leshno et al. (1993) we have that span$\{\sigma(\langle w,x\rangle_2 + b) : (w,b) \in \mathbb{R}^{d+1}\}$ is dense in $C(X)$. However by our previous conclusion and linearity we have that $\int g(x)d\nu(x) = 0$ for any g in span$\{\sigma(\langle w,x\rangle_2 + b) : (w,b) \in \mathbb{R}^{d+1}\}$, which implies then that ν must equal 0. Thus $\mathcal{F}$ is dense in $C(X)$. □

Since Gaussians are supported on all of $\mathbb{R}^{d+1}$ we have the following corollary:

Corollary G.2. *If $(w,b) \sim N(0, I_{d+1})$ then K^∞ is strictly positive.*