Tight Bounds on the Smallest Eigenvalue of the Neural Tanger Kernel for Deep ReLU Networks

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Abstract

A recent line of work has analyzed the theoretical properties of deep neural networks via the Neural Tanger Kernel (NTK). In particular, the smallest eigenvalue of the NTK has been related to memorization capacity, convergence of gradient descent algorithms and generalization of deep nets. However, existing results either provide bounds in the two-layer setting or assume that the spectrum of the NTK is bounded away from 0 for multi-layer networks. In this paper, we provide tight bounds on the smallest eigenvalue of NTK matrices for deep ReLU networks, both in the limiting case of infinite widths and for finite widths. In the finite-width setting, the network architectures we consider are quite general: we require the existence of a wide layer with roughly order of $N$ neurons, $N$ being the number of data samples; and the scaling of the remaining widths is arbitrary (up to logarithmic factors). To obtain our results, we analyze various quantities of independent interest: we give lower bounds on the smallest singular value of feature matrices, and upper bounds on the Lipschitz constant of input-output feature maps.

1 Introduction

Consider an $L$-layer ReLU network with feature maps $f_l : \mathbb{R}^d \to \mathbb{R}^{n_l}$ defined for every $x \in \mathbb{R}^d$ as

$$f_l(x) = \begin{cases} x & l = 0, \\ \sigma(W^T_l f_{l-1}) & l \in [L-1], \\ W^T_l f_{L-1} & l = L, \end{cases}$$

where $W_l \in \mathbb{R}^{n_{l-1} \times n_l}$, and $\sigma(x) = \max(0, x)$. We assume that the network has a single output, namely $n_L = 1$ and $W_L \in \mathbb{R}^{n_{L-1}}$. For consistency, let $n_0 = d$. Let $g_l : \mathbb{R}^d \to \mathbb{R}^{n_l}$ be the pre-activation feature map so that $f_l(x) = \sigma(g_l(x))$. Let $(x_1, \ldots, x_N)$ be $N$ samples in $\mathbb{R}^d$, $\theta = [\text{vec}(W_1), \ldots, \text{vec}(W_L)]$, and $F_L(\theta) = [f_L(x_1), \ldots, f_L(x_N)]^T$. Let $J$ be the Jacobian of $F_L$ with respect to all the weights:

$$J = \left[ \frac{\partial F_L}{\partial \text{vec}(W_1)}, \ldots, \frac{\partial F_L}{\partial \text{vec}(W_L)} \right] \in \mathbb{R}^{N \times \sum_{l=1}^L n_{l-1} n_l}.$$
If not mentioned otherwise, we will assume throughout the paper that all the partial derivatives are computed by the standard back-propagation with the convention that $\sigma'(0) = 0$. The empirical Neural Tangent Kernel (NTK) Gram matrix, denoted by $\tilde{K}^{(L)}$, is defined as:

$$\tilde{K}^{(L)} = J J^T = \sum_{l=1}^{L} \left[ \frac{\partial F_L}{\partial \text{vec}(W_l)} \right] \left[ \frac{\partial F_L}{\partial \text{vec}(W_l)} \right]^T \in \mathbb{R}^{N \times N}. \tag{3}$$

As shown in [21], when $(W_l)_{ij} \sim \mathcal{N}(0, 1)$ for all $l \in [L]$ and $\min \{n_1, \ldots, n_{L-1}\} \to \infty$, the normalized NTK matrix converges in probability to a non-random limit, called the limiting NTK matrix:

$$\left( \prod_{l=1}^{L-1} \frac{2}{n_l} \right) \tilde{K}^{(L)} \xrightarrow{p} K^{(L)}. \tag{4}$$

A quantitative bound for the convergence rate is provided in [4].

Several theoretical aspects of training neural networks have been related to the spectrum of the NTK matrices. For instance, considering the square loss $\Phi(\theta) = \frac{1}{2} \| F_L - Y \|_2^2$, one has

$$\| \nabla \Phi(\theta) \|_2^2 = (F_L - Y)^T \tilde{K}^{(L)} (F_L - Y) \geq \lambda_{\min} \left( \tilde{K}^{(L)} \right) 2\Phi(\theta). \tag{5}$$

The idea is that, if the spectrum of $\tilde{K}^{(L)}$ is bounded away from zero at initialization, then under suitable conditions, one can show that this property continues to hold during training. In that case, $\lambda_{\min} (\tilde{K}^{(L)})$ from (5) can be replaced by a positive constant, and thus minimizing the gradient on the LHS will drive the loss to zero. This property, together with other smoothness conditions of the loss, has been used for proving the global convergence of gradient descent in many prior works: [13, 32, 42, 46] consider two layer nets; [2, 12, 48, 49] consider deep nets with polynomially wide layers, and most recently [31] considers deep nets with one wide layer of linear width followed by a pyramidal shape. Beside optimization, the smallest eigenvalue of the NTK is also related to generalization [3, 27] and memorization capacity [27]. All these analyses show that understanding the scaling of the smallest eigenvalue of the NTK is a problem of fundamental importance.

The recent work [14] has characterized the full spectrum of the limiting NTK via an iterated Marchenko-Pastur map. Yet, this does not have implications on the scaling of any individual eigenvalue. In [27], the authors give a quantitative lower bound on $\lambda_{\min} (\tilde{K}^{(L)})$ in a regime in which the number of parameters scales linearly with $N$. This result is particularly interesting but currently restricted to a two-layer setup. To the best of our knowledge, for multi-layer architectures, the fact that the spectrum of the NTK is bounded away from zero is a typical working assumption [12, 20].

**Main contributions.** The aim of this paper is to provide tight lower bounds on the smallest eigenvalues of the empirical NTK matrices for deep ReLU networks.

First, we consider the asymptotic setting. For i.i.d. data from a class of distributions that satisfy a Lipschitz concentration property and for $(W_l)_{ij} \sim \mathcal{N}(0, 1)$, we show that the smallest eigenvalue of the limiting NTK matrix scales as

$$\text{LO}(d) \geq \lim_{\min \{n_1, \ldots, n_{L-1}\} \to \infty} \lambda_{\min} \left( \left( \prod_{l=1}^{L-1} \frac{2}{n_l} \right) \tilde{K}^{(L)} \right) = \lambda_{\min} \left( K^{(L)} \right) \geq \Omega(d), \tag{6}$$
where \( d \) captures the scaling of the average \( L^2 \) norm of the data. This is proved in Theorem 3.2.

Then, we consider a non-asymptotic setting where the network has large but finite widths, and the depth \( L \) is fixed. For the same data as before and for \((W_l)_{i,j} \sim \mathcal{N}(0, \beta_l^2)\), we show that

\[
O \left( \left( d \prod_{l=1}^{L-1} n_l \right) \left( \prod_{l=1}^{L} \beta_l^2 \right) \left( \sum_{l=1}^{L} \beta_l^{-2} \right) \right) \geq \lambda_{\min} \left( \tilde{K}^L \right) \geq \Omega \left( \left( d \prod_{l=1}^{L-1} n_l \right) \left( \prod_{l=1}^{L} \beta_l^2 \right) \left( L \sum_{l=1}^{L} \xi_l \beta_l^{-2} \right) \right),
\]

where \( \tilde{\Omega} \) neglects logarithmic factors and \( \xi_l = 1 \) if \( n_l = \tilde{\Omega}(N) \), and 0 otherwise. This is proved in Theorem 4.1. Our result immediately implies that the spectrum of the NTK matrix is bounded away from zero whenever the network contains one wide layer of order \( N \). This holds regardless of the position of the wide layer and the widths of the remaining ones (up to log factors). This last property allows for networks with bottleneck layers. When all the layers are wide, i.e. \( \min_{l \in [L-1]} n_l = \tilde{\Omega}(N) \), the scaling of the lower bound in (7) is optimal, as seen from the corresponding upper bound. Note also that our bound for finite widths is consistent with the asymptotic one in (6) (except that we do not track the dependence on \( L \) in (7)).

During the proofs of our main theorems, we obtain other intermediate results which could be of independent interest:

- We give a tight characterization of the smallest singular value of the hidden feature matrices. In the infinite width limit, the output features of the last hidden layer can be associated with the so-called conjugate kernel (CK) (or equivalently, the Gaussian process kernel), which has been the object of study for a popular line of research, see e.g. [10, 14, 22, 37, 38].

- We obtain a new bound on the Lipschitz constant of hidden feature maps under Gaussian initialization of the weights. This bound is tighter than the one typically appearing in the literature (i.e., given by the product of the operator norms of all the layers). The proof exploits a particular characterization of the Lipschitz constant of the feature maps and leverages existing bounds on the number of activation patterns of deep ReLU networks [41].

**Organization.** Section 2 introduces our setting. Section 3 provides bounds on \( \lambda_{\min} \left( K^{(L)} \right) \), and Section 4 provide bounds for \( \lambda_{\min} \left( \bar{K}^{(L)} \right) \). Section 5 gives bounds on the smallest singular values of the feature matrices, and Section 6 discusses bounds for the Lipschitz constant of the feature maps. Section 7 discusses further related works. All the missing proofs are deferred to the appendix.

## 2 Preliminaries

**Hermite expansion.** Our bounds depend on the \( r \)-th Hermite coefficient of the ReLU activation function \( \sigma \). Let us denote it by \( \mu_r(\sigma) \). By standard calculations, we have for any even integer \( r \geq 2 \),

\[
\mu_r(\sigma) = \frac{1}{\sqrt{2\pi}} (-1)^{r-2} \frac{(r-3)!!}{\sqrt{r!}}.
\]

(8)

**Weight and data distribution.** We consider the setting where both the weights of the network and the data are random. In particular, \((W_l)_{i,j} \sim \text{i.i.d.} \mathcal{N}(0, \beta_l^2)\) for all \( l \in [L], i \in [n_{l-1}], j \in [n_l] \), where the variable \( \beta_l \) may depend on layer widths. Throughout the paper, we let \((x_1, \ldots, x_N)\) be \( N \) i.i.d. samples from a data distribution, say \( P_X \), such that the following conditions are satisfied.

1. As introduced later, \( d \) is also the input dimension. However, only the scaling of the data matters for our bounds.
Assumption 2.1 (Data scaling) The data distribution $P_X$ satisfies the following properties:

1. $\int \|x\|^2 dP_X(x) = \Theta(\sqrt{d})$.
2. $\int \|x\|^2 dP_X(x) = \Theta(\|x\|)$.
3. $\int \|x - \int x' dP_X(x')\|^2 dP_X(x) = \Omega(d)$.

These are just scaling conditions on the data vector $x$ or its centered counterpart $x - \mathbb{E} x$. We remark that the data can have any scaling, but in this paper we fix it to be of order $d$ for convenience. We further assume the following condition on the data distribution.

Assumption 2.2 (Lipschitz concentration) The data distribution $P_X$ satisfies the Lipschitz concentration property. Namely, for every Lipschitz continuous function $f : \mathbb{R}^d \to \mathbb{R}$, there exists an absolute constant $c > 0$ such that, for all $t > 0$,

$$\mathbb{P} \left( \left| f(x) - \int f(x) dP_X(x) \right| > t \right) \leq 2 \exp \left( -ct^2/\|f\|_{\text{Lip}}^2 \right).$$

In general, Assumption 2.2 covers the whole family of distributions which satisfies the log-Sobolev inequality with a dimension-independent constant (or distributions with log-concave densities). This includes, for instance, the standard Gaussian distribution, the uniform distribution on the sphere, or uniform distributions on the unit (binary or continuous) hypercube [44]. Let us remark that the coordinates of a random sample need not be independent under the above assumptions. Note also that, by applying a Lipschitz map to the data, Assumption 2.2 still holds. Thus, data produced via a Generative Adversarial Network (GAN) fulfills our assumption, see [40].

Notations. We use the following notations throughout the paper: $X = [x_1, \ldots, x_N]^T \in \mathbb{R}^{N \times d}$; the feature matrices at layer $l$ are defined as $F_l = [f_l(x_1), \ldots, f_l(x_N)]^T \in \mathbb{R}^{N \times n_l}$; the centered feature matrices are $\bar{F}_l = F_l - \mathbb{E}_X[F_l]$ for $l \in [L-1]$, where the expectation is taken over all the samples; $\Sigma_l(x) = \text{diag}(\sigma'(g_{l,j}(x)))_{j=1}^{n_l}$ for $l \in [L-1]$, where $g_{l,j}(x)$ is the pre-activation neuron. Given two matrices $A, B \in \mathbb{R}^{m \times n}$, we denote by $A \circ B$ their Hadamard product, and by $A \ast B = [(A_1 \otimes B_1), \ldots, (A_m \otimes B_m)]^T \in \mathbb{R}^{m \times n^2}$ their row-wise Khatri-Rao product. Given a p.s.d. matrix $A$, we denote by $\sqrt{A}$ its square root (i.e. $\sqrt{A} = \sqrt{A}^T$ and $\sqrt{A} \sqrt{A} = A$), and by $\|A\|_\text{op}$ the operator norm (or the largest singular value) of $A$. We denote by $\|f\|_{\text{Lip}}$ the Lipschitz constant of the function $f$. All the complexity notations $\Omega(\cdot)$ and $\mathcal{O}(\cdot)$ are understood for sufficiently large $N, d, n_1, n_2, \ldots, n_{L-1}$. The depth of the network $L$ is considered to be a constant.

3 Limiting NTK Matrix with All Wide Layers

This section provides tight bounds on the smallest eigenvalue of the limiting NTK matrix $K^{(L)} \in \mathbb{R}^{N \times N}$ from [11]. As shown in [21], one can compute this matrix recursively as follows:

$$K_{ij}^{(1)} = G_{ij}^{(1)}, \quad K_{ij}^{(l)} = K_{ij}^{(l-1)} G_{ij}^{(l)} + G_{ij}^{(l)}, \quad G_{ij}^{(l)} = 2 \mathbb{E}_{(u,v) \sim \mathcal{N}(0,A_{ij}^{(l)})} [\sigma'(u)\sigma'(v)], \quad \forall l \in [2, L], \quad (9)$$

4
where the matrices $G^{(l)} \in \mathbb{R}^{N \times N}$ and $A^{(l)}_{ij} \in \mathbb{R}^{2 \times 2}$ are given by

$$G_{ij}^{(1)} = \langle x_i, x_j \rangle, \quad A_{ij}^{(l)} = \begin{bmatrix} G_{jj}^{(l-1)} & G_{ij}^{(l-1)} \\ G_{ji}^{(l-1)} & G_{ii}^{(l-1)} \end{bmatrix}, \quad G_{ij}^{(l)} = 2 \mathbb{E}_{(u,v) \sim \mathcal{N}(0,A_{ij}^{(l)})}[\sigma(u)\sigma(v)], \quad \forall l \in [2, L].$$

(10)

In order to prove our main result of this section, we first need to rewrite the entry-wise formula of the NTK as given in (9) in a more compact form. In particular, the following lemma provides a helpful characterization of the limiting NTK matrix.

**Lemma 3.1** The following holds for the matrices (9)-(10):

$$G^{(1)} = XX^T,$$

(11)

$$G^{(2)} = 2 \mathbb{E}_{w \sim \mathcal{N}(0, I_d)} \left[ \sigma(Xw)\sigma(Xw)^T \right],$$

(12)

$$G^{(l)} = 2 \mathbb{E}_{w \sim \mathcal{N}(0, I_N)} \left[ \sigma(\sqrt{G^{(l-1)} w}) \sigma(\sqrt{G^{(l-1)} w})^T \right], \quad \forall l \in [3, L],$$

(13)

$$K^{(1)} = G^{(1)},$$

(14)

$$K^{(l)} = K^{(l-1)} \circ G^{(l)} + G^{(l)}, \quad \forall l \in [2, L],$$

(15)

$$\dot{G}^{(l)} = 2 \mathbb{E}_{w \sim \mathcal{N}(0, I_N)} \left[ \sigma'(\sqrt{G^{(l-1)} w}) \sigma'(\sqrt{G^{(l-1)} w})^T \right], \quad \forall l \in [2, L].$$

(16)

Moreover, we have

$$K^{(L)} = G^{(L)} + \sum_{l=1}^{L-1} G^{(l)} \circ G^{(l+1)} \circ \dot{G}^{(l+2)} \circ \ldots \circ \dot{G}^{(L)}.$$

(17)

**Proof:** Fix $l \in [2, L]$, and let $B = \sqrt{G^{(l-1)}}$. Then, one has $B = B^T$ and $B^2 = G^{(l-1)}$. Furthermore, (13) can be rewritten as

$$G^{(l)}_{ij} = 2 \mathbb{E}_{w \sim \mathcal{N}(0, I_N)} \left[ \sigma(\langle B_{i} ; w \rangle) \sigma(\langle B_{j} ; w \rangle) \right].$$

Let $u = \langle B_{i} ; w \rangle$ and $v = \langle B_{j} ; w \rangle$. Then, $(u, v) \sim \mathcal{N} \left( 0, \begin{bmatrix} G_{ii}^{(l-1)} & G_{ij}^{(l-1)} \\ G_{ji}^{(l-1)} & G_{jj}^{(l-1)} \end{bmatrix} \right)$, which suffices to prove the expressions for $G^{(l)}$. A similar argument applies to $\dot{G}^{(l)}$. The last equation of $K^{(L)}$ is obtained by unrolling the equation (15). \qed

We are now ready to state the main result of this section. A proof sketch is given below, and the full proof is deferred to Appendix B.

**Theorem 3.2 (Smallest eigenvalue of limiting NTK)** Let $\{x_i\}_{i=1}^N$ be a set of i.i.d. data points from $P_X$, where $P_X$ has zero mean and satisfies the Assumptions 2.7 and 2.3. Let $K^{(L)}$ be the limiting NTK recursively defined in (9). Then, for any even integer constant $r \geq 2$, we have w.p. at least $1 - Ne^{-\Omega(d)} - N^2e^{-\Omega(dN^{-2/(r-0.5)})}$ that

$$LO(d) \geq \lambda_{\min} \left( K^{(L)} \right) \geq \mu_r(\sigma)^2 \Omega(d),$$

(18)

where $\mu_r(\sigma)$ is the $r$-th Hermite coefficient of the ReLU function given by (8).
**Proof:** Recall that for two p.s.d. matrices $P$ and $Q$, it holds $\lambda_{\min}(P \circ Q) \geq \lambda_{\min}(P) \min_{i \in [n]} Q_{ii}$ [39]. By applying this inequality to the formula for the matrix $K_L$ in Lemma 3.1 and exploiting the fact that $G^{(p)}_{ii} = 1$ for all $p \in [2, L]$, $i \in [N]$, we obtain that $\lambda_{\min}(K^{(L)}) \geq \sum_{l=1}^{L} \lambda_{\min}(G^{(l)})$. By using the Hermite expansion and homogeneity of ReLU, we can bound $\lambda_{\min}(G^{(l)})$ in terms of $\lambda_{\min}(\left( (G^{(l-1)})^{sr} \right) G^{(l-1)})$, for any integer $r > 0$, where $(G^{(l-1)})^{sr}$ denotes the $r$-th Khatri Rao power of $G^{(l-1)}$. Iterating this argument, it suffices to bound $\lambda_{\min}(\left( X^{sr} \right) (X^{sr})^T)$. This last step can be done via the Gershgorin circle theorem, and by using Assumptions 2.1 [2.2]

Let us make a few remarks about the result of Theorem 3.2. First, the probability can be made arbitrarily close to 1 as long as $N$ does not grow super-polynomially in $d$. Second, the $\Omega$ and $O$ notations in (18) do not hide any other dependencies on the depth $L$. Finally, the proof of the theorem can be extended to other types of architectures, such as ResNet.

As mentioned in the introduction, non-trivial lower bounds on the smallest eigenvalue of the NTK have been used as a key assumption for proving optimization and generalization results in many previous works, see e.g. [3, 8, 13] for shallow models and [12, 20] for deep models. While quantitative lower bounds have been developed for shallow networks [16], this is the first time, to the best of our knowledge, that these bounds are proved for deep ReLU models.

For finite-width networks, when all the layer widths are sufficiently large, one would expect that, at initialization, the smallest eigenvalue of the NTK matrix [3] has a scaling similar to that given by Theorem 3.2. A quantitative result can be obtained whenever the convergence rates of $\tilde{K}^{(L)}$ to $K^{(L)}$ is available. For instance, by using Theorem 3.1 of [4], one has that, for $(W_l)_{ij} \sim \mathcal{N}(0, 1)$,

$$\left\| \left( \prod_{l=1}^{L} \frac{2}{n_l} \right) \tilde{K}^{(L)}_{ij} - K^{(L)}_{ij} \right\| \leq (L + 1) \epsilon,$$

provided that $\min_{l \in [L-1]} n_l = \Omega \left( \epsilon^{-4} \text{poly}(L) \right)$. By taking $\epsilon = (2(L + 1)N)^{-1} \lambda_{\min}(K^{(L)})$, it follows that $\left\| \left( \prod_{l=1}^{L} \frac{2}{n_l} \right) \tilde{K}^{(L)} - K^{(L)} \right\|_F \leq \frac{3}{2} \lambda_{\min}(K^{(L)}) / 2$, and thus

$$\frac{1}{2} \lambda_{\min}(K^{(L)}) \leq \lambda_{\min}\left( \left( \prod_{l=1}^{L} \frac{2}{n_l} \right) \tilde{K}^{(L)} \right) \leq \frac{3}{2} \lambda_{\min}(K^{(L)}),$$

(20)

By applying Theorem 3.2, one concludes that

$$\lambda_{\min}(\tilde{K}^{(L)}) = \Theta \left( d \prod_{l=1}^{L-1} n_l \right)$$

(21)

provided that $\min_{l \in [L-1]} n_l = \Omega \left( N^4 \right)$. However, this raises two questions: (i) can one further relax the current condition on layer widths? And (ii) is it necessary to require all the layers to be wide to get a similar lower bound on the smallest eigenvalue? We address these questions in the next section.

## 4 NTK Matrix with a Single Wide Layer

In this section, we provide bounds on the smallest eigenvalue of the empirical NTK matrix for networks of finite widths and fixed depth. The network we consider may have any given subset of
layers with widths linear in $N$ (up to logarithmic factors), while all the remaining layers may have poly-logarithmic scaling. Our main result of this section is stated below and proved in Section 4.1.

**Theorem 4.1 (Finite-width scaling of smallest eigenvalue of NTK matrix)** Consider an $L$-layer ReLU network (1). Let $\{x_i\}_{i=1}^N$ be a set of i.i.d. data points from $P_X$, where $P_X$ satisfies the Assumptions 2.1-2.2, and let $K(L)$ be the NTK Gram matrix, as defined in (3). Let the weights of the network be initialized as $[W_l]_{i,j} \sim \mathcal{N}(0, \beta_l^2)$, for all $l \in [L]$. Fix any $\delta > 0$ and any even integer $r \geq 2$. For $k \in [L-1]$, let $\xi_k$ be 1 if the following condition holds:

$$n_k = \Omega \left( N \log(N) \log \left( \frac{N}{\delta} \right) \right), \quad \prod_{l=1}^{k-2} \log(n_l) = o \left( \min_{l \in [0,k-1]} n_l \right),$$

and let $\xi_k$ be 0 otherwise. Let $\mu_r(\sigma)$ be given by (8). Then, we have

$$\lambda_{\min} \left( K(L) \right) \geq \sum_{k=2}^{L} \xi_{k-1} \mu_r(\sigma)^2 \Omega \left( d \prod_{l=1}^{L-1} n_l \prod_{l=1}^{L} \beta_l^2 \right) + \lambda_{\min} \left( XX^T \right) \Omega \left( \prod_{l=1}^{L-1} n_l \prod_{l=2}^{L} \beta_l^2 \right)$$

w.p. at least

$$1 - \delta - \sum_{k=1}^{L-1} \xi_k N^2 \exp \left( -\Omega \left( \frac{\min_{l \in [0,k-1]} n_l}{N^{2/(r-0.1)} \prod_{l=1}^{k-2} \log(n_l)} \right) \right) - N \sum_{l=1}^{L-1} \exp (-\Omega (n_l)) - N \exp(-\Omega (d)).$$

Moreover, we have that, w.p. at least $1 - \sum_{l=1}^{L-1} \exp (-\Omega (n_l)) - \exp(-\Omega (d))$,

$$\lambda_{\min} \left( K(L) \right) \leq \sum_{k=1}^{L} \Omega \left( d \prod_{l=1}^{L-1} n_l \prod_{l=1}^{L} \beta_l^2 \right).$$

The lower bound (22) and the upper bound (24) have the same scaling if one of the following two sufficient conditions hold: (i) the leading term in the sum over $k$ occurs for $k \neq 1$, or (ii) $\lambda_{\min} \left( XX^T \right) = \Omega(d)$. In this case, Theorem 4.1 shows that the smallest eigenvalue of the NTK matrix scales as the product of all the layer widths, all the variances and the sum of their reciprocals. Note also that the probability in (23) can be made arbitrarily close to 1 provided that all the layers before the wide layer $k$ do not exhibit exponential bottlenecks in their widths.

In a nutshell, Theorem 4.1 shows (in a quantitative way) that the spectrum of the NTK matrix is bounded away from zero. The requirements on the network architecture are mild: (i) existence of a wide layer with $\Omega(N)$ neurons, and (ii) absence of exponential bottlenecks before the wide layer. This last condition means that after the wide layer(s), the widths of the network need not have any relation with each other, thus can scale differently. This is a more general setting than the one considered in [29, 30, 31] where the network contains a single wide layer, and then it is followed by a pyramidal shape (i.e. the widths are non-increasing towards the output layer).

Our result immediately implies that such a class of networks (as considered in Theorem 4.1) can approximate $N$ distinct data points within arbitrary precision, for any real labels. The fact that
the positive definiteness of the NTK implies a property on memorization capacity of neural nets has been observed in [27] (albeit for a two-layer model). For other results on memorization capacity which do not require the existence of a wide layer, we refer the reader to [5, 7, 15, 43, 47]. The following corollary should be seen as a proof of concept, and it is proved in Appendix D.1.

**Corollary 4.2 (Memorization capacity)** Consider an L-layer ReLU network (1). Let \{x_i\}_{i=1}^N be a set of i.i.d. data points from \(P_X\), where \(P_X\) satisfies the Assumptions 2.1-2.2. Fix any \(\delta, \delta' > 0\). Assume that there exists a layer \(k \in [L-1]\) such that \(n_k = \Omega \left( N \log(N) \log \left( \frac{N}{\delta} \right) \right)\) and \(\prod_{l=1}^{k-1} \log(n_l) = o \left( \min_{l \in [0,k-1]} n_l \right)\). Then, the following holds

\[
\forall Y, \forall \epsilon > 0, \exists \theta : \|F_L(\theta) - Y\|_2 \leq \epsilon
\]

w.p. at least \(1 - \delta - N^2 e^{-\Omega \left( \frac{\min_{l \in [0,k-1]} n_l}{N^2 \prod_{l=1}^{k-1} \log(n_l)} \right)} - N \sum_{l=1}^{L-1} e^{-\Omega(n_l)} - N e^{-\Omega(d)}\) over the data.

Our Theorem 4.1 gives hope that gradient descent methods will be successful in optimizing deep ReLU nets with a single wide layer, regardless of its position, as long as the wide layer has roughly order of \(N\) neurons. We note that it is not possible to directly apply existing results in the literature such as [9] since the Jacobian matrix is not Lipschitz with respect to the weights. Also, to get optimization guarantees, one often has to track the movement of the NTK-related quantities during the course of training, which is not done in this paper. Providing rigorous convergence guarantees for deep ReLU nets with a single wide layer of linear width is an interesting avenue for future research.

### 4.1 Proof of Theorem 4.1

By chain rules and some standard manipulations (see Lemma 4.1 of [31] for a closed-formed expression of the Jacobian of a network with multiple outputs), one obtains for every \(i, j \in [N]\) that

\[
(JJ^T)_{ij} = \sum_{k=0}^{L-3} \langle f_k(x_i), f_k(x_j) \rangle \left( \sum_{l=k+2}^{L-1} W_l \Sigma_l(x_i) \right) \left( \sum_{l=k+2}^{L-1} W_l \Sigma_l(x_j) \right) W_L + \langle f_{L-2}(x_i), f_{L-2}(x_j) \rangle \langle \Sigma_{L-1}(x_i)W_L, \Sigma_{L-1}(x_j)W_L \rangle + \langle f_{L-1}(x_i), f_{L-1}(x_j) \rangle.
\]

Let \(B_k \in \mathbb{R}^{N \times N}\) be a matrix whose \(i\)-th row is defined as

\[
(B_k)_{i} = \begin{cases} 
\Sigma_k(x_i) \left( \prod_{l=k+1}^{L-1} W_l \Sigma_l(x_i) \right) W_L, & k \in [0, L-2] \\
\sqrt{N} 1_N, & k = L-1 \\
\sqrt{N} 1_N, & k = L
\end{cases}
\]

Then, one can rewrite \(JJ^T = \sum_{k=0}^{L-1} F_k F_k^T \circ B_{k+1} B_{k+1}^T\). For two p.s.d. matrices \(P, Q \in \mathbb{R}^{n \times n}\), it holds \(\lambda_{\min}(P \circ Q) \geq \lambda_{\min}(P) \cdot \min_{i \in [n]} Q_{ii}\) [39]. Thus,

\[
\lambda_{\min} \left( JJ^T \right) \geq \sum_{k=0}^{L-1} \lambda_{\min}(F_k F_k^T) \min_{i \in [N]} \| (B_{k+1})_{i} \|_2^2.
\] (25)
We now bound every term on the RHS of (25). Doing so requires a careful analysis of various quantities involving the hidden layers. This includes the smallest singular value of the feature matrices $F_k \in \mathbb{R}^{N \times n_k}$, and the Lipschitz constant of the feature maps $f_k, g_k : \mathbb{R}^d \to \mathbb{R}^{n_k}$. As these results could be of independent interest, we put them separately in the following sections. In particular, our Theorem 5.1 from the next section proves bounds for these results could be of independent interest, we put them separately in the following sections. In particular, our Theorem 5.1 from the next section proves bounds for $\lambda_{\text{min}}(F_k F_k^T)$. To bound the norm of the rows of $B_{k+1}$, one can use the following lemma (for the proof, see Appendix D).

**Lemma 4.3** Fix any layer $k \in [L - 2]$, and $x \sim P_X$. Then,

$$
\left\| \Sigma_{k+1}(x) \left( \prod_{l=k+2}^{L-1} W_l \Sigma_l(x) \right) W_L \right\|_2^2 = \Theta \left( \beta_k^2 n_{k+1} \prod_{l=k+2}^{L-1} n_l \beta_l^2 \right),
$$

w.p. at least $1 - \sum_{l=1}^{L-1} \exp(-\Omega(n_l)) - \exp(-\Omega(d))$. Here, we assume by convention that the product term $\prod_{l=k+2}^{L-1}(\cdot)$ is inactive for $k = L - 2$.

By plugging the bounds of Lemma 4.3 and Theorem 5.1 into (25), the lower bound in (22) immediately follows. For the upper bound, note that

$$
\lambda_{\text{min}}(JJ^T) \leq (JJ^T)_{11} = \sum_{k=0}^{L-1} \|F_k \|_2^2 \|B_{k+1} \|_2^2. \tag{26}
$$

The second term in the RHS of (26) can be bounded by using Lemma 4.3 above. To bound the first term, we note that $(F_k)_{1:} = f_k(x_1)$ and that, for every $0 \leq k \leq L - 1$,

$$
\|f_k(x_1)\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right), \tag{27}
$$

w.p. at least $1 - \sum_{l=1}^{k} \exp(-\Omega(n_l)) - \exp(-\Omega(d))$. This last statement follows from Lemma C.1 in Appendix C. By plugging (27) and the bound of Lemma 4.3 into (26), the upper bound in (24) immediately follows.

## 5 Smallest Singular Values of Feature Matrices

Throughout this section, we assume that $(W_l)_{ij} \sim \text{i.i.d.} \mathcal{N}(0, \beta^2_l)$ for $l \in [L]$, and that the data points are i.i.d. from a distribution $P_X$ satisfying Assumption 2.1 and 2.2. Recall the definition of the feature matrices at various hidden layers: $F_k = [f_k(x_1), \ldots, f_k(x_N)]^T \in \mathbb{R}^{N \times n_k}$. Our main result of this section is the following tight bound on the smallest singular values of these matrices.

**Theorem 5.1 (Smallest singular value of feature matrices)** Fix any $k \in [L - 1]$ and any integer constant $r > 0$. Let $\delta > 0$ be given. Assume that

$$
n_k = \Omega \left( N \log(N) \log \left( \frac{N}{\delta} \right) \right), \quad \prod_{l=1}^{k-2} \log(n_l) = o(\min_{i\in[0,k-1]} n_i),
$$

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Let $\mu_r(\sigma)$ be given by $\mathbb{E}_w \sum_{i=1}^k n_i \beta_i^2 I_{n_i,k-1}$, then the smallest singular value of the feature matrix $F_k$ satisfies

$$O \left( d \prod_{l=1}^k n_l \beta_l^2 \right) \geq \sigma_{\min}(F_k)^2 \geq \mu_r(\sigma)^2 \Omega \left( d \prod_{l=1}^k n_l \beta_l^2 \right)$$

w.p. at least

$$1 - \delta - N^2 \exp \left( -\Omega \left( \min_{i \in [0,k-1]} n_i \prod_{l=1}^{k-1} \log(n_l) \right) \right) - N \sum_{l=1}^{k-1} \exp \left( -\Omega \left( n_l \right) \right) - N \exp(-\Omega(d)).$$

**Proof of Theorem 5.1.** First of all, the conditions of Theorem 5.1 imply that $n_k \geq N$, which further implies $\sigma_{\min}(F_k)^2 = \lambda_{\min}(F_k F_k^T)$. To bound this quantity, we first relate it to the smallest eigenvalue of the expected Gram matrix, namely $\mathbb{E}[F_k F_k^T]$, where the expectation is taken over $W_k$. Note that $\mathbb{E}[F_k F_k^T] = n_k \mathbb{E}[\sigma(F_{k-1} w) \sigma(F_{k-1} w)^T]$, where $w$ has the same distribution as any column of $W_k$. This is formalized in the following lemma, which is proved in Appendix [E.1].

**Lemma 5.2** Let $\lambda = \lambda_{\min} \left( \mathbb{E}_{w \sim N(0, \beta_k^2 1_{n_k-1})} [\sigma(F_{k-1} w) \sigma(F_{k-1} w)^T] \right)$. Fix any $\delta > 0$. Assume that

$$n_k \geq \max \left( N, c \frac{\beta_k^2 \|F_{k-1}\|_F^2}{\lambda} \max \left( 1, \log \frac{4 \beta_k^2 \|F_{k-1}\|_F^2}{\lambda} \right) \log \frac{N}{\delta} \right),$$

where $c$ is an absolute constant. Then, we have w.p. at least $1 - \delta$ over $W_k$ that

$$\sigma_{\min}(F_k)^2 \geq \frac{n_k \lambda}{4}.$$  

From here, it suffices to bound $\|F_{k-1}\|_F^2$ and $\lambda$. The first quantity can be bounded by using a standard induction argument over $k$. In particular, from Lemma [C.1] in Appendix [C] it follows that $\|F_{k-1}\|_F^2 = \Theta \left( N d \prod_{l=1}^{k-1} n_l \beta_l^2 \right)$ w.p. at least $1 - \sum_{l=1}^{k-1} \exp \left( -\Omega \left( n_l \right) \right) - \exp(-\Omega(d))$.

A more challenging task is to bound $\lambda$, which is done in the remainder of this section. First, we relate $\lambda$ to the smallest eigenvalue of (row-wise) Khatri-Rao powers of $F_{k-1}$. This is obtained via the following lemma, which is proved in Appendix [E.2].

**Lemma 5.3** Fix any $k \in [L - 1]$ and any integer $r > 0$. Then, we have

$$\lambda_{\min} \left( \mathbb{E}_{w \sim N(0, \beta_k^2 1_{n_k})} [\sigma(F_k w) \sigma(F_k w)^T] \right) \geq \beta_{k+1}^2 \mu_r(\sigma)^2 \max_{i \in [N]} \| (F_k)_i : \|_2^{2(r-1)},$$

Next, we show that the smallest singular value of the Khatri-Rao powers of $F_k$ does not decrease if one considers the centered features $\tilde{F}_k = F_k - \mathbb{E}_X[F_k]$. This is formalized in the following lemma, which is proved in Appendix [E.3].

**Lemma 5.4 (Centering features)** Fix any $k \in [L - 1]$, and any integer $r > 0$. Then, we have

$$(F_k^{sr})(F_k^{sr})^T \geq (\tilde{F}_k^{sr})(\tilde{F}_k^{sr})^T$$  \hspace{1cm} (28)

w.p. at least

$$1 - N \exp \left( -\Omega \left( \min_{i \in [0,k]} n_i \prod_{l=1}^{k-1} \log(n_l) \right) \right) - \sum_{l=1}^{k-1} \exp \left( -\Omega \left( n_l \right) \right).$$  \hspace{1cm} (29)

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The last step is to bound the smallest eigenvalue of \((\tilde{F}_k^{tr})(\tilde{F}_k^{sr})^T\), as done in the following lemma which is proved in Appendix E.4.

**Lemma 5.5 (Khatri-Rao powers of centered feature matrices)** Fix any \(k \in [L-1]\) and any integer \(r > 0\). Assume \(\prod_{l=1}^{k-1} \log(n_l) = o\left(\min_{l \in [0,k]} n_l\right)\). Then, we have

\[
\lambda_{\min} \left((\tilde{F}_k^{tr})(\tilde{F}_k^{sr})^T\right) = \Theta \left(\left(d \prod_{l=1}^{k} n_l \beta_l^2\right)^r\right)
\]

w.p. at least

\[
1 - N^2 \exp \left(-\Omega \left(\frac{\min_{l \in [0,k]} n_l}{N^{2/(r-0.1)} \prod_{l=1}^{k-1} \log(n_l)}\right)\right) = N \sum_{l=1}^{k} \exp \left(-\Omega (n_l)\right).
\]

Combining all these lemmas, one obtains the desired lower bound of \(\sigma_{\min}(F_k)^2\) as stated in Theorem 4.1. For the upper bound, one has \(\lambda_{\min}(F_k F_k^T) \leq \min_{i \in [N]} \|F_ki\|_2^2 = O \left(d \prod_{l=1}^{k} n_l \beta_l^2\right)\), where the last estimate follows from Lemma C.1 in Appendix C.

### 6 Lipschitz Constant of Feature Maps

The Lipschitz constants of the feature maps \(g_k : \mathbb{R}^d \to \mathbb{R}^{nk}\) appear in several results of this paper, including Lemma 5.4 and Lemma 5.5. A simple upper bound is given by \(\|g_k\|_{\text{Lip}} \leq \prod_{l=1}^{k} \|W_l\|_{\text{op}}\). From standard bounds on the operator norm of Gaussian random matrices (see Theorem 2.12 of [14]), one obtains that \(\prod_{l=1}^{k} \|W_l\|_{\text{op}}\) scales as \(\prod_{l=1}^{k} \beta_l \max(\sqrt{n_l}, 1)\). However, this simple estimate would lead to restrictions on the neural network architectures for which our main Theorem 4.1 holds.

In this section, we provide a sharp bound for such Lipschitz constants. As usual, \((W_l)_{ij} \sim \mathcal{N}(0, \beta_l^2)\) for \(l \in [L]\). For every \(z \in \mathbb{R}^d\), the activation pattern of \(z\) up to layer \(k\) is denoted by

\[
A_{1\rightarrow k}(z) = (\text{sign}(g_{lj}(z)))_{l \in [k], j \in [n_l]} = (-1, 0, 1)^{\sum_{l=1}^{k} n_l}.
\]

where \(\text{sign}(g_{lj}(z)) = 1\) if \(g_{lj}(z) > 0\), \(-1\) if \(g_{lj}(z) < 0\) and 0 otherwise. For every differentiable point of \(g_k\), we denote by \(J(g_k)(z) \in \mathbb{R}^{nk \times d}\) the corresponding Jacobian matrix.

Our starting point is to relate the Lipschitz constant of \(g_k\) with the operator norm of the Jacobian. First, we have via the Rademacher theorem that \(\|g_k\|_{\text{Lip}} = \sup_{x \in \mathbb{R}^d \setminus \Omega_{g_k}} \|J(g_k)(z)\|_{\text{op}}\), where \(\Omega_{g_k}\) is the set of non-differentiable points of \(g_k\) which has measure zero. The issue here is that even if we restrict ourself to the “good” set \(\mathbb{R}^d \setminus \Omega_{g_k}\), the Jacobian matrix as computed by the standard back-propagation algorithm 2 (which is also the object that we can analytically handle) may not represent the true Jacobian of \(g_k\). This happens, for example, when the input to any of the ReLU activations is 0. The following lemma circumvents this problem by restricting the supremum to the set of inputs where the two Jacobian matrices agree. Its proof is deferred to Appendix F.2.

**Lemma 6.1** Fix any \(k \in [L]\). Then w.p. 1 over \((W_l)_{l=1}^{k-1}\), the following holds for all \(W_k\):

\[
\|g_k\|_{\text{Lip}} = \max_{z \in \mathbb{R}^d, A_{1\rightarrow k-1}(z) \in \{-1, 1\}^{\sum_{l=1}^{k-1} n_l}} \|J(g_k)(z)\|_{\text{op}}.
\]

2 with a convention that \(\sigma'(0) = 0\)

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In words, Lemma 6.1 shows that the Lipschitz constant of $g_k$ is given by the maximum operator norm of its Jacobian over all the inputs $z$'s which fulfill $g_{lj}(z) \neq 0$ for all $l \in [k-1], j \in [n_l]$. This has two implications. First, $g_k$ is differentiable at every such input, and chain rules can be applied through all the layers to compute the true Jacobian. In particular, we have for all such $z$'s that:

$$J(g_k)(z) = W^T_k \prod_{l=1}^{k-1} \Sigma_{k-l}(z)W^T_{k-l}. \quad (32)$$

Second, one observes that $J(g_k)(z) = J(g_k)(z')$ for all $z, z'$ with $A_{1\rightarrow k-1}(z) = A_{1\rightarrow k-1}(z')$. Thus, the number of Jacobian matrices that one needs to bound in (31) is at most the number of activation patterns, which has been studied in [18, 28, 41]. By exploiting these facts via a careful induction argument, we obtain the following result.

**Theorem 6.2 (Lipschitz constant of feature maps)** Fix any $k \in [L]$. Then, we have w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ that

$$\|g_k\|_{Lip}^2 = O\left(\frac{\prod_{l=0}^{k} n_l}{\min_{l \in [0, k]} n_l} \prod_{l=1}^{k-1} \log(n_l) \prod_{l=1}^{k} \beta_l^2\right). \quad (33)$$

The idea of the proof is to bound the operator norm of the Jacobian matrix from (32) for all inputs with the same given activation pattern (via an $\epsilon$-net argument and concentration inequalities), and then to do a union bound over all the possible patterns. The details are deferred to Appendix F.1.

### 7 Further Related Work

The spectrum of various random matrices arising from deep learning models has been the subject of recent investigations. Most of the existing results focus on the linear-width asymptotic regime, where the widths of the various layers are linearly proportional. In particular, the spectrum of the conjugate kernel (CK) is studied in the single-layer case for Gaussian i.i.d. data [35], for Gaussian mixtures [23], for general training data [25], and for a model with an additive bias [1]. The multi-layer case is tackled in [6]. The Hessian matrix of a two-layer network can be decomposed into two pieces, one coming from the second derivatives and the other of the form $J^T J$ (a.k.a. the Fisher information matrix). This second term is studied in [33, 36]. Note that this is different from the NTK matrix, given by $JJ^T$, as analyzed in this paper. Typically, for an over-parameterized model, the Fisher information matrix is rank-deficient, whereas the NTK one is full-rank. The work [34] uses tools from free probability to study the spectrum of the input-output Jacobian of the network. Again, this is different from the parameter-output Jacobian considered in the current paper. The generalization error has been also studied via the spectrum of suitable random matrices, and this kind of analysis has been carried out for linear regression [19], for a random feature model [26], for random Fourier features [24], and most recently for a two-layer network [27].

Generally speaking, the line of literature reviewed above has studied the spectrum of various random matrices related to neural networks. Our work is complementary in the sense that it concerns the smallest eigenvalue of the NTK and the feature maps. We remark that obtaining an almost-sure convergence of the empirical spectral distribution of a random matrix in general does not have any implications on the limit of its individual eigenvalues. The closest existing work is [27], which focuses on a two-layer model and gives a lower bound on the smallest eigenvalue of the NTK matrix when the number of parameters of the network exceeds the number of training samples.
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\[d \Theta(\cdot) \] with the same probability as stated in the theorem.

Thus, it follows from Assumption 2.2 that \(p.s.d. \) matrices \(P, Q \) and doing a union bound over all data pairs, we get

\[
\max_{i,j} \left| \langle x_i, x_j \rangle \right| \leq dN^{-1/(r-0.5)} \text{ w.p. at least } 1 - N^2 e^{-\Omega(dN^{-2/(r-0.5)})}.
\]

Combining these two events, we obtain that the following hold

\[
\|x_i\|_2^2 = \Theta(d), \quad \forall i \in [N], \\
|\langle x_i, x_j \rangle| \leq dN^{-1/(r-0.5)}, \quad \forall i \neq j
\]

with the same probability as stated in the theorem.

We have from Lemma 3.1 that

\[
K^{(L)} = \sum_{l=1}^{L} G^{(l)} \circ \hat{G}^{(l+1)} \circ \hat{G}^{(l+2)} \circ \ldots \circ \hat{G}^{(L)}.
\]

One also observes that all the matrices \(G^{(l)}, \hat{G}^{(l)}, G^{(l)}\) are positive semidefinite. Recall that, for two p.s.d. matrices \(P, Q \in \mathbb{R}^{n \times n}\), one has \(\lambda_{\min}(P \circ Q) \geq \lambda_{\min}(P) \min_{i \in [n]} Q_{ii} \) [39]. Thus, it holds

\[
\lambda_{\min}(K^{(L)}) \geq \sum_{l=1}^{L} \lambda_{\min}(G^{(l)}) \min_{i \in [N]} \prod_{p=l+1}^{L} (G^p)_{ii} = \sum_{l=1}^{L} \lambda_{\min}(G^{(l)}),
\]

where

\[
\lambda_{\min}(G^{(l)})) = \frac{\min_{i \in [N]} \sum_{j=1}^{N} |G^{(l)}(i,j)|^2}{\max_{i \in [N]} \sum_{j=1}^{N} |G^{(l)}(i,j)|^2}
\]

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where the last equality follows from the fact that \( (\tilde{G}^{(p)})_{ii} = 1 \) for all \( p \in [2, L], i \in [N] \). From here, it suffices to bound \( \lambda_{\min}(G^{(2)}) \). Let \( D = \text{diag}([\|x_i\|_2]_{i=1}^N) \) and \( \tilde{X} = D^{-1}X \). Then, by the homogeneity of \( \sigma \), we have \( \sigma(Xw) = \sigma(D\tilde{X}w) = D\sigma(\tilde{X}w) \), and thus

\[
\lambda_{\min}(G^{(2)}) = \lambda_{\min}\left(D\mathbb{E}\left[\sigma(\tilde{X}w)\sigma(\tilde{X}w)^T\right]D\right)
= \lambda_{\min}\left(D\left[\mu_0(\sigma)^21_N1_N^T + \sum_{s=1}^{\infty} \mu_s(\sigma)^2(\tilde{X}^{*s})^T(\tilde{X}^{*s})\right]D\right)
\geq \mu_r(\sigma)^2 \lambda_{\min}\left(D(\tilde{X}^{*r})^T \tilde{X}^{*r} D\right)
= \mu_r(\sigma)^2 \lambda_{\min}\left(D^{-r-1}(\tilde{X}^{*r})^T \tilde{X}^{*r} D^{-r-1}\right)
\geq \mu_r(\sigma)^2 \lambda_{\min}\left((\tilde{X}^{*r})^T \tilde{X}^{*r}\right),
\]

where the second step uses the Hermite expansion of \( \sigma \) (for the proof see Lemma D.3 of [31]). By Gersgorin circle theorem, one has

\[
\lambda_{\min}\left((\tilde{X}^{*r})^T \tilde{X}^{*r}\right) \geq \min_{i \in [N]} \|x_i\|_2^{2r} - (N - 1) \max_{i \neq j} |\langle x_i, x_j \rangle|^r \geq \mathcal{O}(d),
\]

where the last estimate follows from (34). For the upper bound, note that

\[
\lambda_{\min}\left(K^{(L)}\right) \leq \frac{\text{tr}(K^{(L)})}{N} = \frac{1}{N} \sum_{i=1}^N \sum_{l=1}^L (G^{(l)})_{ii} \prod_{p=l+1}^L (\tilde{G}^{p})_{ii}.
\]

One observes that \((G^{(l)})_{ii} = 2\mathbb{E}_{g \sim N(0, (G_{i-1})_{ii})}[\sigma(g)^2] = (G^{(l-1)})_{ii}\). Iterating this argument gives \((G^{(l)})_{ii} = (G^{(1)})_{ii} = \|x_i\|_2^2\). Thus, it follows that

\[
\lambda_{\min}\left(K^{(L)}\right) \leq \frac{L}{N} \text{tr}(G^{(1)}) = \frac{L}{N} \sum_{i=1}^N \|x_i\|_2^2 = L \mathcal{O}(d),
\]

where we used again (34) in the last estimate.

### C Some Useful Estimates

**Lemma C.1** Fix any \( 0 \leq k \leq L - 1 \) and \( x \sim P_X \). Then, we have

\[
\|f_k(x)\|_2^2 = \Theta\left(d^{\frac{k}{2}} \prod_{l=1}^k n_l \beta_l^2\right)
\]

w.p. at least \( 1 - \sum_{i=1}^k \exp(-\Omega(n_i)) - \exp(-\Omega(d)) \) over \((W_i)_{i=1}^k\) and \( x \). Moreover,

\[
\mathbb{E}_x \|f_k(x)\|_2^2 = \Theta\left(d^{\frac{k}{2}} \prod_{l=1}^k n_l \beta_l^2\right)
\]

w.p. \( 1 - \sum_{i=1}^k \exp(-\Omega(n_i)) \) over \((W_i)_{i=1}^k\).
Lemma C.2 Fix any \( k \in [L-1] \). Then, we have
\[
\|\mathbb{E}_x[f_k(x)]\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right)
\]
w.p. at least \( 1 - \sum_{l=1}^{k} \exp(-\Omega(n_l)) \) over \((W_i)_{l=1}^{k}\).

Lemma C.3 Fix any \( k \in [L-1] \). Assume \( \prod_{l=1}^{k-1} \log(n_l) = o \left( \min_{l \in [0,k]} n_l \right) \). Then, we have
\[
\|f_k(x_i) - \mathbb{E}_x[f_k(x)]\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right), \quad \forall i \in [N]
\]
w.p. at least
\[
1 - N \exp \left( -\Omega \left( \frac{\min_{l \in [0,k]} n_l}{\prod_{l=1}^{k-1} \log(n_l)} \right) \right) - \sum_{l=1}^{k} \exp(-\Omega(n_l)).
\]

Lemma C.4 Fix any \( k \in [L-1] \). Then, we have
\[
\mathbb{E}_x \|f_k(x) - \mathbb{E}_x[f_k(x)]\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right)
\]
w.p. at least \( 1 - \sum_{l=1}^{k} \exp(-\Omega(n_l)) \) over \((W_i)_{l=1}^{k}\).

Lemma C.5 Fix any \( k \in [L-1] \), and \( x \sim P_X \). Then, we have that \( \|\Sigma_k(x)\|_F^2 = \Theta(n_k) \) w.p. at least \( 1 - \sum_{l=1}^{k} \exp(-\Omega(n_l)) - \exp(-\Omega(d)) \) over \((W_i)_{l=1}^{k}\) and \( x \).

Lemma C.6 Fix any \( k \in [L-1], k \leq p \leq L - 1 \), and \( x \sim P_X \). Then, we have that
\[
\left\| \Sigma_k(x) \prod_{l=k+1}^{p} W_l \Sigma_l(x) \right\|_F^2 = \Theta \left( n_k \prod_{l=k+1}^{p} n_l \beta_l^2 \right)
\]
w.p. at least \( 1 - \sum_{l=1}^{p} \exp(-\Omega(n_l)) - \exp(-\Omega(d)) \) over \((W_i)_{l=1}^{p}\) and \( x \).

C.1 Proof of Lemma [C.1]

The proof works by induction over \( k \). Note that the statement holds for \( k = 0 \) due to Assumptions 2.1 and 2.2. Assume that the lemma holds for some \( k - 1 \), i.e. \( \|f_{k-1}(x)\|_2^2 = \Theta \left( d \prod_{l=1}^{k-1} n_l \beta_l^2 \right) \) w.p. at least \( 1 - \sum_{l=1}^{k-1} N \exp(-\Omega(n_l)) - N \exp(-\Omega(d)) \). Let us condition on this event of \((W_i)_{l=1}^{k-1}\) and study probability bounds over \( W_k \). Let \( W_k = [w_1, \ldots, w_{n_k}]^T \) where \( w_j \sim \mathcal{N}(0, \beta_k^2 [I_{n_k - 1}]) \). Note that
\[
\|f_k(x)\|_2^2 = \sum_{j=1}^{n_k} f_{k,j}(x)^2,
\]
(36)
and that
\[ E_{W_k} \|f_k(x)\|_2^2 = \sum_{j=1}^{n_k} E_{w_j} [f_{k,j}(x)^2] = \frac{n_k \beta_k^2}{2} \|f_{k-1}(x)\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right), \]
where the last equality follows from the induction assumption. Furthermore,
\[ \|f_{k,j}(x)^2\|_{\psi_1} = \|f_{k,j}(x)\|_{\psi_2}^2 \leq c \beta_k^2 \|f_{k-1}(x)\|_2^2 = O \left( \beta_k^2 d \prod_{l=1}^{k-1} n_l \beta_l^2 \right), \]
where \( c \) is an absolute constant. Thus, by applying Bernstein’s inequality (see Theorem 2.8.1 of [44]) to the sum of i.i.d. random variables in \([30]\), we have
\[ \frac{1}{2} E_{W_k} \|f_k(x)\|_2^2 \leq \|f_k(x)\|_2^2 \leq \frac{3}{2} E_{W_k} \|f_k(x)\|_2^2 \]
w.p. at least \( 1 - \exp(-\Omega(n_k)) \). Taking the intersection of the two events finishes the proof for \( \|f_k(x)\|_2^2 \). The proof for \( E_x \|f_k(x)\|_2^2 \) can be done by following similar passages and using that \( \|E_x[f_{k,j}(x)^2]\|_{\psi_1} \leq E_x \|f_{k,j}(x)^2\|_{\psi_1} \).

C.2 Proof of Lemma [C.2]

The upper bound follows from Lemma [C.1] via Jensen’s inequality. The proof for the lower bound works by induction on \( k \). Assume it holds for \( k-1 \) that \( \|E_x[f_{k-1}(x)]\|_2^2 = \Omega \left( d \prod_{l=1}^{k-1} n_l \beta_l^2 \right) \) w.p. at least \( 1 - \sum_{l=1}^{k-1} \exp(-\Omega(n_l)) \) over \( (W_l)_{l=1}^{k-1} \). Let us condition on the intersection of this event and that of Lemma [C.1] for \( (W_l)_{l=1}^{k-1} \). Let \( W_k = [w_1, \ldots, w_{n_k}] \) where \( w_j \sim \mathcal{N}(0, \beta_k^2 I_{n_{k-1}}) \). For every \( j \in [n_k] \),
\[ \|(E_x[f_{k,j}(x)])^2\|_{\psi_1} = \|E_x[f_{k,j}(x)]\|_{\psi_2}^2 \leq E_x \|f_{k,j}(x)\|_{\psi_2}^2 \leq c \beta_k^2 E_x \|f_{k-1}(x)\|_2^2 = O \left( d \beta_k^2 \prod_{l=1}^{k-1} n_l \beta_l^2 \right), \]
where \( c \) is an absolute constant and the last equality follows from the above conditional event from Lemma [C.1]. Moreover,
\[ E_{W_k} \|E_x[f_k(x)]\|_2^2 = \sum_{j=1}^{n_k} E_{w_j} \|E_x[f_{k,j}(x)]\|_2^2 \geq \sum_{j=1}^{n_k} (E_x E_{w_j} [f_{k,j}(x)])^2 = \frac{n_k \beta_k^2}{2\pi} \|E_x[f_{k-1}(x)]\|_2^2 = \Omega \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right), \]
where the last estimate follows from our induction assumption. By Bernstein’s inequality (see Theorem 2.8.1 of [44]), we have
\[ \|E_x[f_k(x)]\|_2^2 \geq \frac{1}{2} E_{W_k} \|E_x[f_k(x)]\|_2^2 = \Omega \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right) \]
w.p. at least \( 1 - \exp(-n_k) \) over \( W_k \). Taking the intersection of all these events finishes the proof.
C.3 Proof of Lemma C.3

Let $Z : \mathbb{R}^d \rightarrow \mathbb{R}$ be a random function over $x_i$ defined as $Z(x_i) = \|f_k(x_i) - \mathbb{E}_x[f_k(x)]\|_2$. It follows from Theorem 6.2 that w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^k$,

$$\|Z\|_{\text{Lip}}^2 = \mathcal{O} \left( \prod_{l=0}^k n_l \log n_l \prod_{l=1}^{k-1} \beta^2_l \right) = o \left( d \prod_{l=1}^k n_l \beta^2_l \right). \quad (37)$$

Below, let us denote the shorthand

$$\mathbb{E}[Z] = \mathbb{E}_{x_i}[Z(x_i)] = \int_{\mathbb{R}^d} Z(x_i) dP_X(x_i).$$

It holds

$$\mathbb{E}[Z]^2 = \mathbb{E}[Z^2] - \mathbb{E}[Z - \mathbb{E}Z]^2$$

$$\geq \mathbb{E}[Z^2] - \int_0^\infty \mathbb{P}(|Z - \mathbb{E}Z| > \sqrt{t}) dt$$

$$\geq \mathbb{E}[Z^2] - \int_0^\infty 2 \exp \left( -\frac{ct}{\|Z\|_{\text{Lip}}^2} \right) dt$$

$$= \mathbb{E}[Z^2] - \frac{2}{c} \|Z\|^2_{\text{Lip}}, \quad (38)$$

where the 2nd inequality follows from Assumption 2.2. By Lemma C.4 we have w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^k$ that

$$\mathbb{E}[Z^2] = \Theta \left( d \prod_{l=1}^k n_l \beta^2_l \right). \quad (39)$$

By combining (37), (38) and (39), we obtain that $\mathbb{E}[Z] = \Omega \left( \sqrt{d \prod_{l=1}^k n_l \beta^2_l} \right)$. Moreover, $\mathbb{E}[Z] \leq \sqrt{\mathbb{E}[Z^2]} = \mathcal{O} \left( \sqrt{d \prod_{l=1}^k n_l \beta^2_l} \right)$. As a result, we have that $\mathbb{E}[Z] = \Theta \left( \sqrt{d \prod_{l=1}^k n_l \beta^2_l} \right)$ w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^k$. Let us condition on this event and study probability bounds over the samples. Using Assumption 2.2 we have $\frac{1}{2} \mathbb{E}[Z] \leq Z \leq \frac{3}{2} \mathbb{E}[Z]$, hence $Z = \Theta \left( \sqrt{d \prod_{l=1}^k n_l \beta^2_l} \right)$, w.p. at least

$$1 - \exp \left( -\Omega \left( \frac{\min_{l \in [0,k]} n_l}{\prod_{l=1}^{k-1} \log(n_l)} \right) \right).$$

Taking the union bound over $N$ samples, followed by an intersection with the above event over the weights, finishes the proof.

C.4 Proof of Lemma C.4

The proof works by induction on $k$. Note that the statement holds for $k = 0$ due to Assumption 2.1. Let us assume for now that the result holds for the first $k$ layers. To prove it for layer $k$, we condition
on the intersection of this event and the event of Lemma C.1 for \((W_l)_l^{k-1}\), and study probability bounds over \(W_k\). Define \(W_k = \{w_1, \ldots, w_n\} \in \mathbb{R}^{n_k \times n_k}\) where \(w_j \sim \mathcal{N}(0, \beta_k^2 I_{n_k})\). Recall that by definition, \(f_{k,j}(x) = \sigma(\langle w_j, f_{k-1}(x) \rangle)\) for \(j \in [n_k]\). We have that

\[
\mathbb{E}_x \|f_k(x) - \mathbb{E}_x[f_k(x)]\|^2 = \sum_{j=1}^{n_k} \mathbb{E}_x \left( f_{k,j}(x) - \mathbb{E}_x[f_{k,j}(x)] \right)^2.
\]

Taking the expectation over \(W_k\), we have

\[
\mathbb{E}_{W_k} \mathbb{E}_x \|f_k(x) - \mathbb{E}_x[f_k(x)]\|^2
= \mathbb{E}_{W_k} \mathbb{E}_x \|f_k(x)\|^2 - \mathbb{E}_{W_k} \mathbb{E}_x[f_k(x)]^2
= \frac{n_k \beta_k^2}{2} \mathbb{E}_x \|f_{k-1}(x)\|^2 - \mathbb{E}_x \mathbb{E}_y \sum_{j=1}^{n_k} \mathbb{E}_{w_j} \sigma(\langle w_j, f_{k-1}(x) \rangle) \sigma(\langle w_j, f_{k-1}(y) \rangle)
\]

\[
= \frac{n_k \beta_k^2}{2} \mathbb{E}_x \|f_{k-1}(x)\|^2 - n_k \beta_k^2 \mathbb{E}_x \|f_{k-1}(x)\| \|f_{k-1}(y)\|_{\mathbb{R}}^2 \sum_{r=0}^{\infty} \mu_r(\sigma)^2 \left\langle \frac{f_{k-1}(x)}{\|f_{k-1}(x)\|}, \frac{f_{k-1}(y)}{\|f_{k-1}(y)\|} \right\rangle^r
\]

\[
\geq \frac{n_k \beta_k^2}{2} \mathbb{E}_x \|f_{k-1}(x)\|^2 - \mu_1(\sigma)^2 n_k \beta_k^2 \mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2 - n_k \beta_k^2 \sum_{r=0}^{\infty} \mu_r(\sigma)^2 (\mathbb{E}_x \|f_{k-1}(x)\|^2)^2
\]

\[
= \frac{n_k \beta_k^2}{2} \mathbb{E}_x \|f_{k-1}(x)\|^2 - \frac{n_k \beta_k^2}{4} (\mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2 - \mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2)^2 - \frac{n_k \beta_k^2}{4} \mathbb{E}_x \|f_{k-1}(x)\|^2,
\]

where in the last step we use that \(\mu_1(\sigma)^2 = 1/4\) and that \(\sum_{r=0}^{\infty} \mu_r(\sigma)^2 = 1/4\). Furthermore, the RHS of the last expression can be lower bounded by

\[
\frac{n_k \beta_k^2}{4} \left( \mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2 - \mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2 \right) = \frac{n_k \beta_k^2}{4} \mathbb{E}_x \|f_{k-1}(x) - \mathbb{E}_x[f_{k-1}(x)]\|_{\mathbb{R}}^2 = \Omega \left( \prod_{l=1}^{k} \mu_l^2 \right),
\]

where the last step follows by induction assumption. Moreover, it follows from above that

\[
\mathbb{E}_{W_k} \mathbb{E}_x \|f_k(x) - \mathbb{E}_x[f_k(x)]\|^2 \leq \frac{n_k \beta_k^2}{2} \mathbb{E}_x \|f_{k-1}(x)\|_{\mathbb{R}}^2 = \mathcal{O} \left( \prod_{l=1}^{k} \mu_l^2 \right),
\]
where the last estimate follows from Lemma C.1. For every $j \in [n_k]$, 
\[
\left\| E_x \left( f_{k,j}(x) - E_x[f_{k,j}(x)] \right) \right\|_{\psi_1}^2 \leq E_x \left\| \left( f_{k,j}(x) - E_x[f_{k,j}(x)] \right) \right\|_{\psi_1}^2 - c E_x \left\| f_{k,j}(x) - E_x[f_{k,j}(x)] \right\|_{\psi_2}^2 \\
\leq c E_x \left\| f_{k,j}(x) \right\|_{\psi_2}^2 \\
\leq c E_x \left( \left\| f_{k,j}(x) - E_{w_j}[f_{k,j}(x)] \right\|_{\psi_2}^2 + \left\| E_{w_j}[f_{k,j}(x)] \right\|_{\psi_2}^2 \right) \\
\leq c E_x \left( \beta_k^2 \left\| f_{k,j}(x) \right\|_{\text{Lip}}^2 + \frac{\beta_k^2}{2\pi} \left\| f_{k-1}(x) \right\|_2^2 \right) \\
\leq c \beta_k^2 E_x \left\| f_{k-1}(x) \right\|_2^2 \\
= \mathcal{O} \left( \beta_k^2 d \prod_{l=1}^{k-1} \beta_l l_l \right),
\]
where $c$ is an absolute constant (which is allowed to change from line to line) and the last step uses Lemma C.1. By Bernstein’s inequality (see Theorem 2.8.1 of [44]),
\[
\frac{1}{2} E_{W_k} E_x \left\| f_k(x) - E_x[f_k(x)] \right\|_F^2 \leq E_x \left\| f_k(x) - E_x[f_k(x)] \right\|_2^2 \leq \frac{3}{2} E_{W_k} E_x \left\| f_k(x) - E_x[f_k(x)] \right\|_2^2,
\]
w.p. at least $1 - \exp (-\Omega(n_k))$ over $W_k$. Thus, with that probability, we have that
\[
E_x \left\| f_k(x) - E_x[f_k(x)] \right\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right).
\]
Taking the intersection of all the events finishes the proof.

C.5 Proof of Lemma C.5

**Proof:** By Lemma C.1 we have $f_{k-1}(x) \neq 0$ w.p. at least $1 - \sum_{i=1}^{k-1} \exp (-\Omega(n_i)) - \exp(-\Omega(d))$ over $(W_i)_{i=1}^{k-1}$ and $x$. Let us condition on this event and derive probability bounds over $W_k$. Let $W_k = \{w_1, \ldots, w_{n_k}\}$. Then, $\left\| \Sigma_k(x) \right\|_F^2 = \sum_{j=1}^{n_k} \sigma'((f_{k-1}(x), w_j))$. Thus,
\[
E_{W_k} \left\| \Sigma_k(x) \right\|_F^2 = n_k E_{w_1} \left[ \sigma'(-\langle f_{k-1}(x), w_1 \rangle) \right] = n_k E_{w_1} [(1 - \sigma'(\langle f_{k-1}(x), w_1 \rangle))] = n_k - E_{W_k} \left\| \Sigma_k(x) \right\|_F^2,
\]
where we used the fact that $w_j$ has a symmetric distribution, $\sigma'(t) = 1 - \sigma'(-t)$ for $t \neq 0$, and the set of $w_1 \in \mathbb{R}^{n_k}$ for which $\langle f_{k-1}(x), w_j \rangle = 0$ has measure zero. This implies that $E_{W_k} \left\| \Sigma_k(x) \right\|_F^2 = n_k/2$. By Hoeffding’s inequality on bounded random variables (see Theorem 2.2.6 of [44]), we have
\[
P \left( \left\| \Sigma_k(x) \right\|_F^2 - E_{W_k} \left\| \Sigma_k(x) \right\|_F^2 > t \right) \leq 2 \exp \left( -\frac{2t^2}{n_k} \right).
\]
Picking $t = n_k/4$ finishes the proof. \qed
C.6 Proof of Lemma C.6

The proof works by induction on \( p \). First, Lemma C.5 implies that the statement holds for \( p = k \). Suppose it holds for some \( p - 1 \). Note that this implies \( f_{p-1}(x) \neq 0 \) because otherwise \( \Sigma_{p-1}(x) = 0 \), which contradicts the induction assumption. Let \( S_p = \Sigma_k(x) \prod_{l=k+1}^p W_l \Sigma_l(x) \). Then, \( S_p = S_{p-1}W_p \Sigma_p(x) \). Let \( W_p = [w_1, \ldots, w_{n_p}] \). Then,

\[
\|S_p\|_F^2 = \sum_{j=1}^{n_p} \|S_{p-1}w_j\|_2^2 \sigma'(g_{p,j}(x)) = \sum_{j=1}^{n_p} \|S_{p-1}w_j\|_2^2 \sigma'((f_{p-1}(x), w_j))
\]

We have

\[
E_{W_p}\|S_p\|_F^2 = n_p E_{w_1} \|S_{p-1}w_1\|_2^2 \sigma'((f_{p-1}(x), w_1)) = n_p E_{w_1} \|S_{p-1}(-w_1)\|_2^2 \sigma'((f_{p-1}(x), (-w_1)))
\]

\[
= n_p E_{w_1} \|S_{p-1}w_1\|_2^2 (1 - \sigma'((f_{p-1}(x), w_1))) = n_p E_{w_1} \|S_{p-1}w_1\|_2^2 - E_{W_p}\|S_p\|_F^2 = n_p \beta_p^2 \|S_{p-1}\|^2_F - E_{W_p}\|S_p\|_F^2,
\]

where the second step uses that \( w_1 \) has a symmetric distribution, the third step uses the fact that \( \sigma'(t) = 1 - \sigma'(-t) \) for \( t \neq 0 \) and the set of \( w_1 \) for which \( (f_{p-1}(x), w_1)) = 0 \) has measure zero. Thus,

\[
E_{W_p}\|S_p\|_F^2 = \frac{n_p}{2} \beta_p^2 \|S_{p-1}\|^2_F = \Theta \left( n_k \prod_{l=k+1}^p n_l \beta_l^2 \right),
\]

where the last equality holds by induction assumption. Moreover,

\[
\left\|\|S_{p-1}w_j\|_2^2 \sigma'((f_{p-1}(x), w_j))\right\|_{\psi_1} \leq c \left\|\|S_{p-1}w_j\|_2\right\|_{\psi_2} \leq c \beta_p^2 \|S_{p-1}\|^2_F,
\]

where \( c \) is an absolute constant (which is allowed to change from passage to passage). By Bernstein’s inequality (see Theorem 2.8.1 of [44]), we have

\[
\frac{1}{2} E_{W_p}\|S_p\|_F^2 \leq \|S_p\|_F^2 \leq \frac{3}{2} E_{W_p}\|S_p\|_F^2
\]

w.p. at least \( 1 - e^{-\Omega(n_p)} \). Taking the intersection of all the events finishes the proof.

D Missing Proofs from Section 4

D.1 Proof of Corollary 4.2

Let \( p = \sum_{l=1}^L n_l m_{l-1} \). Let \( \frac{\partial F_L}{\partial \theta} \in \mathbb{R}^{N \times p} \) denote the true Jacobian of \( F_L \) (without the convention that \( \sigma'(0) = 0 \)) at a differentiable point \( \theta \). Note that, by Lemma B.2 of [31], \( F_L(\theta) \) is locally Lipschitz, thus a.e. differentiable. Let \( J(\theta) \in \mathbb{R}^{N \times p} \) be the Jacobian matrix defined in (2) (with the convention that \( \sigma'(0) = 0 \)). Let

\[
\Omega_1 = \{ \theta \in \mathbb{R}^p | \text{rank}(J(\theta)) = N \}
\]
and \( \Omega_0 = \{ \theta \in \mathbb{R}^p \mid \exists l \in [L-1], j \in [n_l], i \in [N] : g_{ij}(x_i) = 0 \} \).

Let \( \lambda_p \) denote the Lebesgue measure in \( \mathbb{R}^p \). Pick an even integer \( r \) s.t. \( r \geq 0.1 + 2/\delta' \). Then, Theorem 4.1 implies that, with high probability (as stated in the corollary) over the training data, we have \( \lambda_p(\Omega_1) > 0 \). For every \( \theta \in \Omega_1 \), it holds that \( f_l(\theta, x_i) \neq 0 \) for all \( 0 \leq l \leq L-2, i \in [N] \), because otherwise \( J(\theta)_i = 0 \) (which leads to a contradiction). Thus, every \( \theta \in \Omega_1 \cap \Omega_0 \) must satisfy \( 0 = g_{ij}(\theta, x_i) = \langle f_{l-1}(\theta, x_i), (W_l)_j \rangle \) for some \( l \in [L-1], j \in [n_l], i \in [N] \). The set of \( W_l \) which satisfies this equation has measure zero, and thus it holds \( \lambda_p(\Omega_1 \cap \Omega_0) = 0 \). Combining these facts, we get \( \lambda_p(\Omega_1 \setminus \Omega_0) > 0 \). Pick some \( \theta_0 \in \Omega_1 \setminus \Omega_0 \). Then clearly, we have the following: (i) \( J(\theta_0) = \frac{\partial F_0}{\partial \theta} |_{\theta=\theta_0} \) and (ii) \( \text{rank}(J(\theta_0)) = N \). This implies that there exists \( \theta' \in \mathbb{R}^p \) such that \( \left( \frac{\partial F_0}{\partial \theta} |_{\theta=\theta_0} \right) \theta' = Y \) and thus,

\[
y_i = \left( \left( \frac{\partial F_L}{\partial \theta} |_{\theta=\theta_0} \right) \theta' \right)_i = \left( \frac{\partial f_L(\theta, x_i)}{\partial \theta} |_{\theta=\theta_0} \right), \quad \forall i \in [N].
\]

The result follows by noting that \( h_\epsilon(x_i) \) can be implemented by a network of the same depth with twice more neurons at every hidden layer.

**D.2 Proof of Lemma 4.3**

By a change of index \( k+1 \rightarrow k \), it is equivalent to prove the following:

\[
\left\| \Sigma_k(x) \left( \prod_{l=k+1}^{L-1} W_l \Sigma_l(x) \right) W_L \right\|_2^2 = \Theta \left( \beta^2_L n_k \prod_{l=k+1}^{L-1} n_l \beta^2_l \right).
\]

Let \( B = \Sigma_k(x) \left( \prod_{l=k+1}^{L-1} W_l \Sigma_l(x) \right) \). By Lemma D.4, \( \|B\|_F^2 = \Theta \left( n_k \prod_{l=k+1}^{L-1} n_l \beta^2_l \right) \) w.p. at least \( 1 - \sum_{l=1}^{L-1} \exp(-\Omega(n_l)) \). Moreover, one can also show that with a similar probability,

\[
\|B\|_{op}^2 = O \left( \frac{n_k}{\min_{l \in [k,L-1]} n_l} \prod_{l=k+1}^{L-1} n_l \beta^2_l \right).
\]

The proof of this is postponed below. Let us condition on the intersection of these two events of \( (W_l)_{l=1}^{L-1} \). Then, by Hanson-Wright inequality (see Theorem 6.2.1 of [4]), we have

\[
\frac{1}{2} \|BW_L\|_2^2 \leq \|BW_L\|_2^2 \leq \frac{3}{2} \|BW_L\|_2^2.
\]

w.p. at least \( 1 - e^{-\Omega(\|B\|_F^2/\|B\|_{op}^2)} \) over \( W_L \). Plugging the above bounds leads to the desired result.

In the remainder of this proof, we verify the above bound of \( \|B\|_{op}^2 \). Concretely, we want to show that for every \( p, q \in [L-1] \), the following holds w.p. at least \( 1 - \sum_{l=p+1}^{q} \exp(-\Omega(n_l)) \)

\[
\left\| \prod_{l=p}^{q} W_l \Sigma_l(x) \right\|_{op}^2 = O \left( \frac{\prod_{l=p+1}^{q} n_l}{\min_{l \in [p-1,q]} n_l} \prod_{l=p}^{q} \beta^2_l \right).
\]
Given that, the bound of \( \|B\|_{op}^2 \) follows immediately by letting \( p = k + 1, q = L - 1 \), and noting \( \|\Sigma_k(x)\|_{op} \leq 1 \). The proof of (40) is by induction over the length \( s = q - p \). First, (40) holds for \( s = 0 \) since \( \|W_p\Sigma_p(x)\|_{op}^2 \leq \|W_p\|_{op}^2 = O(\beta_p^2 \max(n_p, n_{p-1})) \) where the last estimate follows from the standard bounds on the operator norm of Gaussian matrices (see Theorem 2.12 of [11]). Suppose that (40) holds for \( p, q \) such that \( q - p \leq s - 1 \), and we want to prove it for all pairs \( p, q \) with \( q - p = s \). It suffices to provide bound for one pair of \((p, q)\) and then do a union bound over all possible pairs. In the following, let

\[
 j = \arg \min_{l \in [p-1, q]} n_l, \quad t = \arg \min_{l \in [p-1, q] \setminus \{j\}} n_l.
\]

We analyze three cases below. In the first case, namely \( j \in [p, q - 1] \), then

\[
 \left\| \prod_{l=p}^q W_l \Sigma_l(x) \right\|_{op}^2 \leq \left\| \prod_{l=p}^j W_l \Sigma_l(x) \right\|_{op}^2 \left\| \prod_{l=j+1}^q W_l \Sigma_l(x) \right\|_{op}^2 = O \left( \prod_{l=p}^j n_l \prod_{l=j+1}^q n_l \prod_{l=p}^q \beta_l^2 \right)
\]

\[
 = O \left( \prod_{l=p}^{q-1} n_l \prod_{l=p}^q \beta_l^2 \right) = O \left( \prod_{l=p}^{q-1} n_l \prod_{l=p}^q \beta_l^2 \right)
\]

where the first equality follows from our induction assumption, the second equality follows from the current choice of \( j \). In the second case, if \( j = q \) and \( t \in [p, q - 1] \), then similarly one has

\[
 \left\| \prod_{l=p}^q W_l \Sigma_l(x) \right\|_{op}^2 \leq \left\| \prod_{l=p}^t W_l \Sigma_l(x) \right\|_{op}^2 \left\| \prod_{l=t+1}^q W_l \Sigma_l(x) \right\|_{op}^2 = O \left( \prod_{l=p}^t n_l \prod_{l=p}^q n_l \prod_{l=p}^q \beta_l^2 \right)
\]

\[
 = O \left( \prod_{l=p}^{q-1} n_l \prod_{l=p}^q n_l \prod_{l=p}^q \beta_l^2 \right) = O \left( \prod_{l=p}^{q-1} n_l \prod_{l=p}^q \beta_l^2 \right)
\]

It remains to handle the case in which either \((j = p - 1)\) or \((j = q \text{ and } t = p - 1)\). To do so, we use an \( \epsilon \)-net argument. Since \( \|\Sigma_q(x)\|_{op} \leq 1 \), it holds that

\[
 \left\| \prod_{l=p}^q W_l \Sigma_l(x) \right\|_{op}^2 \leq \left( \prod_{l=p}^{q-1} W_l \Sigma_l(x) \right) W_q \left\| W_q \right\|_{op}^2.
\]  

(41)

Furthermore, by using Lemma 4.4.1 of [11],

\[
 \left\| \left( \prod_{l=p}^{q-1} W_l \Sigma_l(x) \right) W_q \right\|_{op}^2 \leq 2 \sup_{y \in \mathbb{N}^{p-1}_{1/2}} \left\| y^T \left( \prod_{l=p}^{q-1} W_l \Sigma_l(x) \right) W_q \right\|_2^2,
\]  

(42)

where \( \mathbb{N}^{p-1}_{1/2} \) is a \( \frac{1}{2} \)-net of the unit sphere in \( \mathbb{R}^{p-1} \). Fix \( y \in \mathbb{N}^{p-1}_{1/2} \), and let \( z \) be defined as above, then clearly \( z \) is independent of \( W_q \), and it holds by induction assumption

\[
 \|z\|_2^2 = O \left( \prod_{l=p}^{q-1} n_l \prod_{l=p}^{q-1} \beta_l^2 \right)
\]  

(43)
w.p. at least $1 - \sum_{l=p}^{q-1} \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^{q-1}$. Conditioned on this event of the first $q - 1$ layers, let us study concentration bound for $\|z^TW_q\|_2^2$ where the only randomness is over $W_q$. Note that $\|z^TW_q\|_2^2 = \sum_{j=1}^{n_q} \langle z, (W_q)_j \rangle^2$ and $\|z, (W_q)_j \|_{\psi_1} \leq c_1 \beta_q^2 \|z\|_2^2$. Thus by Bernstein’s inequality (see Theorem 2.8.1 of [44]),

$$\mathbb{P}\left( \|z^TW_q\|_2^2 - \mathbb{E}[z^TW_q] \|z^TW_q\|_2^2 > t \right) \leq \exp\left( -c_2 \min\left( \frac{t}{c_1 \beta_q^2 \|z\|_2^2}, \frac{t^2}{n_q c_1 \beta_q^4 \|z\|_2^4} \right) \right),$$

for some constant $c_2$. By plugging $t = Cc_1 \max(n_q, n_{p-1}) \beta_q^2 \|z\|_2^2 / c_2$ for some $C > \max(c_2, \log 5)$, and $\mathbb{E}[z^TW_q] \|z^TW_q\|_2^2 = n_q \beta_q^2 \|z\|_2^2$, one obtains $\|z^TW_q\|_2^2 = \mathcal{O}\left( \max(n_q, n_{p-1}) \beta_q^2 \|z\|_2^2 \right)$ w.p. at least $1 - e^{-C \max(n_q, n_{p-1})}$. Taking the union bound over $y \in \mathbb{N}_{1/2}^{p-1}$, we get

$$\sup_{y \in \mathbb{N}^{p-1}_{1/2}} \|z^TW_q\|_2^2 = \sup_{y \in \mathbb{N}^{p-1}_{1/2}} \left\| y^T \left( \prod_{l=p}^{q-1} W_l \Sigma_l(x) \right) W_q \right\|_2^2 = \mathcal{O}\left( \max(n_q, n_{p-1}) \beta_q^2 \|z\|_2^2 \right),$$

w.p. at least $1 - \mathbb{N}^{p-1}_{1/2} e^{-C \max(n_q, n_{p-1})} = 1 - e^{-\Omega(\max(n_q, n_{p-1}))}$, where we used the fact that $\mathbb{N}^{p-1}_{1/2} \leq 5^{p-1}$ and $C > \log 5$. This combined with (11), (12) and (13) implies

$$\left\| \prod_{l=p}^{q} W_l \Sigma_l(x) \right\|_{\text{op}}^2 = \mathcal{O}\left( \max_{(j, t)} \prod_{l=p}^{q-1} \frac{\beta_l^2}{\min_{i \in [p-1, q-1]} n_l} \prod_{l=p}^{q-1} \frac{n_l}{\min_{i \in [p-1, q-1]} n_l} \prod_{l=p}^{q-1} \frac{\beta_l^2}{\min_{i \in [p-1, q-1]} n_l} \right),$$

where the last estimate follows from the current conditions on $(j, t)$. To summarize, we have shown that (40) holds for every given pair $(p, q)$ such that $q - p = s$. Taking the union bound over all these pairs finishes the proof. Finally, note that doing the union bound above does not affect the probability of the final result since the number of all possible pairs is only a constant.

E Missing Proofs from Section 5

E.1 Proof of Lemma 5.2

For a subgaussian random variable $Z$, recall that $\mathbb{P}(Z > t) \leq \exp(-c t^2 / \|Z\|_{\psi_2}^2)$, where $c$ is an absolute constant. In the following, let $t = \frac{4 \beta_k \|F_{k-1}\|_F}{\|z\|_{\psi_2}} \sqrt{\max\left( 1, \log \frac{8 \beta_k^2 \|F_{k-1}\|_F^2}{c \lambda} \right)}$. Let us denote the shorthand $W_k = [w_1, \ldots, w_{n_k}] \in \mathbb{R}^{n_{k-1} \times n_k}$, and denote by $A \in \mathbb{R}^{n \times n_k}$ a matrix such that $A_{j \cdot} = \sigma(F_{k-1} w_j) \mathbb{I}_{\|\sigma(F_{k-1} w_j)\|_2 \leq t}$ for all $j \in [n_k]$. Let

$$G = \mathbb{E}_{w \sim \mathbb{N}(0, \beta_k^2 1_{n_{k-1}})} \left[ \sigma(F_{k-1} w) \sigma(F_{k-1} w)^T \right],$$

$$\hat{G} = \mathbb{E}_{w \sim \mathbb{N}(0, \beta_k^2 1_{n_{k-1}})} \left[ \sigma(F_{k-1} w) \sigma(F_{k-1} w)^T \mathbb{I}_{\|\sigma(F_{k-1} w)\|_2 \leq t} \right].$$

Note $\lambda = \lambda_{\min}(G)$, $\lambda_{\min}(F_k T_k^T) \geq \lambda_{\min}(A A^T)$ and $\lambda_{\max}(A_j A_j^T) \leq t^2$. By Matrix Chernoff inequality (see Theorem 1.1 of [13]), it holds for every $\epsilon \in [0, 1)$

$$\mathbb{P}\left( \lambda_{\min}(A A^T) \leq (1 - \epsilon) \lambda_{\min}(E A A^T) \right) \leq N \left[ \frac{e^{-\epsilon}}{(1 - \epsilon)^{1-\epsilon}} \right]^{\lambda_{min}(E A A^T) / t^2}.$$
Pick $\epsilon = 1/2$. Then,
\[
\Pr \left( \lambda_{\min} \left( AA^T \right) \leq n_k \lambda_{\min} \left( \hat{G} \right) / 2 \right) \leq \exp \left( -c_1 n_k \lambda_{\min} \left( \hat{G} \right) / t^2 + \log N \right).
\]
Thus, for $n_k \geq \frac{t^2}{c_1 \lambda_{\min}(\hat{G})} \log \frac{N}{\delta}$ we have $\lambda_{\min} \left( AA^T \right) \geq \frac{n_k \lambda_{\min}(\hat{G})}{2}$ w.p. $\geq 1 - \delta$. Moreover,
\[
\left\| \hat{G} - G \right\|_2 \leq \mathbb{E} \left\| \sigma(F_{k-1}w)\sigma(F_{k-1}w)^T \mathbb{1}_{\|\sigma(F_{k-1}w)\|_2 \leq t} - \sigma(F_{k-1}w)\sigma(F_{k-1}w)^T \right\|_2
\]
\[
= \mathbb{E} \left[ \|\sigma(F_{k-1}w)\|_2^2 \mathbb{1}_{\|\sigma(F_{k-1}w)\|_2 > t} \right]
\]
\[
= \int_{s=0}^{\infty} \mathbb{P} \left( \|\sigma(F_{k-1}w)\|_2 > t \right) \mathbb{P} \left( \|\sigma(F_{k-1}w)\|_2 > \sqrt{s} \right) ds
\]
\[
= \int_{s=0}^{\infty} \mathbb{P} \left( \|\sigma(F_{k-1}w)\|_2 > t \right) \mathbb{P} \left( \|\sigma(F_{k-1}w)\|_2 > \sqrt{s} \right) ds
\]
\[
\leq \int_{s=0}^{\infty} \exp \left( -c_1 \frac{t^2 + s}{4 \beta_k^2 \|F_{k-1}\|_F^2} \right) ds
\]
\[
\leq \lambda/2,
\]
where the second inequality uses the fact that $\|\sigma(F_{k-1}w)\|_2 \leq 2 \beta_k \|F_{k-1}\|_F$. It follows that $\lambda_{\min} \left( \hat{G} \right) \geq \lambda/2$. In total, for $n_k \geq \frac{2 \beta_k^2}{c_1 \lambda} \log \frac{N}{\delta}$, it holds w.p. at least $1 - \delta$ that
\[
\sigma_{\min}(F_k)^2 = \lambda_{\min}(F_k F_k^T) \geq \lambda_{\min}(AA^T) \geq n_k \lambda_{\min} \left( \hat{G} \right) / 2 \geq n_k \lambda/4,
\]
where we used the condition $n_k \geq N$ in the above equality.

### E.2 Proof of Lemma 5.3
Let $D = \text{diag}(\|F_1\|_2, \ldots, \|F_N\|_2)$ and $\hat{F}_k = D^{-1}F_k$. Then, by the homogeneity of $\sigma$, we have
\[
\lambda_{\min} \left( \mathbb{E}[\sigma(F_k w)\sigma(F_k w)^T] \right) = \lambda_{\min} \left( D \mathbb{E} \left[ \sigma(\hat{F}_k w)\sigma(\hat{F}_k w)^T \right] D \right)
\]
\[
= \beta_{k+1}^2 \lambda_{\min} \left( D \left[ \mu_0(\sigma)^2 1_N 1_N^T + \sum_{s=1}^{\infty} \mu_s(\sigma)^2 (\hat{F}_k^{ss})(\hat{F}_k^{ss})^T \right] D \right)
\]
\[
\geq \beta_{k+1}^2 \mu_r(\sigma)^2 \lambda_{\min} \left( D (\hat{F}_k^{sr})(\hat{F}_k^{sr})^T D \right)
\]
\[
= \beta_{k+1}^2 \mu_r(\sigma)^2 \lambda_{\min} \left( D^{-r-1}(F_k^{sr})(F_k^{sr})^T D^{-(r-1)} \right)
\]
\[
\geq \beta_{k+1}^2 \mu_r(\sigma)^2 \lambda_{\min} \left( (F_k^{sr})(F_k^{sr})^T \right) \frac{\lambda_{\max}(F_i)}{\max_{i \in [N]} \|F_i\|_2^{2(r-1)}}
\]
where the second equality uses the Hermite expansion of $\sigma$ (for the proof see Lemma D.3 of [31]).
E.3 Proof of Lemma 5.4

Let $\mu = \mathbb{E}_x[f_k(x)] \in \mathbb{R}^n$. Denote $A = F_k$ and $\tilde{A} = \tilde{F}_k = A - 1_N \mu^T$ where $1_N \in \mathbb{R}^N$ is the all-one vector. By Lemma C.2 it holds w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^k$ that

$$\|\mu\|_2^2 = \Theta \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right). \quad (44)$$

Also, Theorem 6.2 shows that w.p. at least $1 - \sum_{l=1}^k \exp(-\Omega(n_l))$ over $(W_l)_{l=1}^k$,

$$\|f_k\|_{\text{Lip}}^2 = O \left( \prod_{l=0}^{k-1} \frac{n_l}{\min_{i \in [0,k]} n_l} \prod_{l=1}^{k} \log(n_l) \prod_{l=1}^{k} \beta_l^2 \right). \quad (45)$$

Let us condition on the intersection of these two events of the weights and study probability bounds over the data. We have

$$ (F^r_k) (F^r_k)^T = (A A^T) \circ \ldots \circ (A A^T), \quad (46) $$

where the Hadamard product is repeated $r$ times. By definition, it holds

$$ AA^T = \tilde{A} \tilde{A}^T + \|\mu\|_2^2 1_N 1_N^T + (1_N \mu^T) \tilde{A}^T + \tilde{A} (1_N \mu^T)^T $$

$$ = \tilde{A} \tilde{A}^T + \|\mu\|_2^2 1_N 1_N^T + 1_N \left( A \mu - \|\mu\|_2^2 1_N \right)^T + \left( A \mu - \|\mu\|_2^2 1_N \right) 1_N^T $$

$$ = \tilde{A} \tilde{A}^T + 1_N 1_N^T \left( \Lambda + \frac{\|\mu\|_2^2}{2} \right) + \left( \Lambda + \frac{\|\mu\|_2^2}{2} \right) 1_N^T, $$

where $\Lambda = \text{diag}(A \mu - \|\mu\|_2^2 1_N)$. Let $h : \mathbb{R}^d \to \mathbb{R}$ be a function over a random sample $x$, defined as $h(x) = (f_k(x), \mu)$. Then, $\Lambda_{ii} = h(x_i) - \mathbb{E}_x[h(x)]$. Since $\|h\|_{\text{Lip}}^2 \leq \|\mu\|_2^2 \|f_k\|_{\text{Lip}}^2$, it holds

$$ \mathbb{P}(|\Lambda_{ii}| \geq t) \leq \exp \left( -\frac{t^2}{2 \|\mu\|_2^2 \|f_k\|_{\text{Lip}}^2} \right). \quad (47) $$

Pick $t = \|\mu\|_2^2 / 2$. Then, taking the union bound over all the samples, we have

$$ \min_{i \in [N]} \Lambda_{ii} \geq -\frac{\|\mu\|_2^2}{2} \implies AA^T \succeq \tilde{A} \tilde{A}^T $$

w.p. at least

$$ 1 - N \exp \left( -\frac{\|\mu\|_2^2}{8 \|f_k\|_{\text{Lip}}^2} \right). $$

Taking the intersection with $(44)$, $(45)$ and plugging the bounds leads to the desired result.
E.4 Proof of Lemma 5.5

From Gershgorin circle theorem, one obtains

\[
\lambda_{\min}\left(\left(F^r_k\right)^T(F^r_k)\right) \geq \min_{i \in [N]} \left\|\left(F^r_k\right)_i\right\|_2^2 - \frac{N}{\max_{i \neq j} \left|\left(F^r_k\right)_i, (F^r_k)_j\right|}, \tag{48}
\]

\[
\lambda_{\min}\left(\left(F^r_k\right)^T(F^r_k)\right) \leq \max_{i \in [N]} \left\|\left(F^r_k\right)_i\right\|_2^2 + \frac{N}{\max_{i \neq j} \left|\left(F^r_k\right)_i, (F^r_k)_j\right|}. \tag{49}
\]

By Lemma C.3, it holds w.p. at least 1 \(- N \exp\left( - \Omega \left( \frac{\min_{i \in [0,k]} n_i}{\prod_{l=1}^k \log(n_l)} \right) \right) \) that

\[
\left\|\left(F^r_k\right)_i\right\|_2 = \Theta \left( \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right)^r \right), \quad \forall i \in [N]. \tag{50}
\]

In the following, we bound the second term on the RHS of (49). For a fixed \( j \in [N] \), Lemma C.3 implies that w.p. at least 1 \(- \exp\left( - \Omega \left( \frac{\min_{i \in [0,k]} n_i}{\prod_{l=1}^k \log(n_l)} \right) \right) \)\(- \sum_{l=1}^k \exp(-\Omega(n_l)) \) over \( (W^l_i)_{l=1}^k \) and \( x_j \), we have

\[
\left\|\left(F^r_k\right)_j\right\|_2^2 = \Theta \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right). \tag{51}
\]

Moreover, Theorem 6.2 implies that w.p. at least 1 \(- \sum_{l=1}^k \exp(-\Omega(n_l)) \) over \( (W^l_i)_{l=1}^k \),

\[
\left\|f_k(x) - \mathbb{E}_x f_k(x)\right\|_{\text{Lip}}^2 = \mathcal{O} \left( \prod_{l=0}^{k-1} n_l \prod_{l=1}^{k} \log(n_l) \prod_{l=1}^{k} \beta_l^2 \right). \tag{52}
\]

Let us condition on the intersection of these two events of \( (W^l_i)_{l=1}^k \) and \( x_j \), and derive probability bounds over \( x_i \), for every \( i \neq j \). Let \( h(x_i) = \left( (F^r_k)_i, (F^r_k)_j \right) \) be a function of \( x_i \), then

\[
\left\|h\right\|_{\text{Lip}}^2 \leq \left\|\left(F^r_k\right)_j\right\|_2^2 \left\|f_k(x_i) - \mathbb{E}_x f_k(x_i)\right\|_{\text{Lip}}^2 = \mathcal{O} \left( \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right)^2 \prod_{l=1}^{k-1} \log(n_l) \prod_{l=1}^k \min_{i \in [0,k]} n_i \right),
\]

where the last estimate follows from (51) and (52). Using Assumption 2.2 followed by a union bound over \( \{x_i\}_{i \neq j} \), we have for every \( t > 0 \) that

\[
\mathbb{P} \left( \max_{i \in [N], i \neq j} \left|\left(F^r_k\right)_i, (F^r_k)_j\right| \geq t \right) \leq (N - 1) \exp \left( - \frac{t^2}{\mathcal{O} \left( \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right)^2 \prod_{l=1}^{k-1} \log(n_l) \prod_{l=1}^k \min_{i \in [0,k]} n_i \right)} \right). \tag{53}
\]

Pick \( t = N^{-1/(r-0.1)} \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right) \). Then, taking the intersection bound with (51) and (52) yields

\[
N \max_{i \in [N], i \neq j} \left|\left(F^r_k\right)_i, (F^r_k)_j\right|^r \leq N \left( \frac{d \prod_{l=1}^k n_l^{\beta_l^2}}{N^{r/(r-0.1)}} \right)^r = o \left( \left( d \prod_{l=1}^k n_l^{\beta_l^2} \right)^r \right) \tag{54}
\]
w.p. at least
\[ 1 - (N - 1) \exp \left( -\Omega \left( \frac{\min_{l \in [0,k]} n_l}{N^{2/(r-0.1)} \prod_{l=1}^{k-1} \log(n_l)} \right) \right) - \sum_{l=1}^{k} \exp(-\Omega(n_l)). \]

Since this holds for every given \( x_j \), taking the union bound over \( j \in [N] \) yields that
\[ N \max_{i \neq j} |\langle (\tilde{F}_k)_i, (\tilde{F}_k)_j \rangle| = o \left( \left( d \prod_{l=1}^{k} n_l \beta_l^2 \right)^{r} \right) \]
w.p. at least
\[ 1 - N^2 \exp \left( -\Omega \left( \frac{\min_{l \in [0,k]} n_l}{N^{2/(r-0.1)} \prod_{l=1}^{k-1} \log(n_l)} \right) \right) - N \sum_{l=1}^{k} \exp(-\Omega(n_l)). \]

Combining (48), (49), (50), (55) finishes the proof.

### F Missing Proofs from Section 6

**Definition F.1** A subset \( A \subseteq \mathbb{R}^n \) is called a polyhedron if it is the intersection of a finite family of (closed) half-spaces. A function \( f : \mathbb{R}^n \to \mathbb{R}^m \) is called piecewise linear if there exist a finite family of polyhedra \( \{P_i\}_{i=1}^{T} \) such that \( \mathbb{R}^n = \bigcup_{i=1}^{T} P_i \) and \( f \) coincides with a linear function on each \( P_i \).

The following lemma establishes a formal connection between ReLU networks and PWL functions. Its proof is contained in Appendix F.3.

**Lemma F.2** For every \( k \in [L] \), \( f_k, g_k : \mathbb{R}^d \to \mathbb{R}^{n_k} \) as defined in (1) are piecewise linear functions.

An equivalent way of defining piecewise linear maps is the following, see e.g. [17].

**Lemma F.3** A function \( f : \mathbb{R}^n \to \mathbb{R}^m \) is piecewise linear if and only if there exist a finite family of polyhedra \( \{P_i\}_{i=1}^{T} \) and matrices \( \{A_i\}_{i=1}^{T} \in \mathbb{R}^{m \times n} \) such that:

1. \( \mathbb{R}^n = \bigcup_{i=1}^{T} P_i \),
2. \( \text{int}(P_i) \neq \emptyset \) \( \forall i \in [T] \),
3. \( \text{int}(P_i) \cap \text{int}(P_j) = \emptyset \) \( \forall i \neq j \),
4. \( f(x) = A_i x \) for every \( x \in P_i \).

### F.1 Proof of Theorem 6.2

Let \( h_{p \to q} : \mathbb{R}^{n_p} \to \mathbb{R}^{n_q} \) be defined as
\[ h_{p \to q} = \hat{A}_q \circ \hat{\sigma}_{q-1} \circ \hat{A}_{q-1} \circ \ldots \circ \hat{\sigma}_{p+1} \circ \hat{A}_{p+1}, \]
where the mapping $A_t : \mathbb{R}^{n_{i-1}} \rightarrow \mathbb{R}^{n_i}$ is given by $A_t(x) = W_t^T x$, and the mapping $\hat{\sigma}_t : \mathbb{R}^{n_i} \rightarrow \mathbb{R}^{n_i}$ is given by $\hat{\sigma}(x) = [\sigma(x_1), \ldots, \sigma(x_{n_i})]^T$ for every $x \in \mathbb{R}^{n_i}$. By definition, it holds $g_{k}(x) = h_{0\rightarrow k}(x)$. In the following, we prove that for every $0 \leq p < q \leq L$, it holds w.p. $1 - \sum_{l=p+1}^q \exp (-\Omega(n_l))$ that

\[
\|h_{p\rightarrow q}\|_{\text{Lip}} = O \left( \frac{\prod_{l=p}^q n_l}{\min_{[p,q]} n_l} \prod_{l=p+1}^{q-1} \log(n_l) \prod_{l=p+1}^q \beta_l^2 \right). 
\] (56)

The desired result follows by letting $p = 0, q = k$. The proof of (56) is by induction over the length $s = q - p$. First, (56) holds for $s = 1$. Suppose that (56) holds for all $(p, q)$ such that $q - p \leq s - 1$, and we want to prove it for all $(p, q)$ with $q - p = s$. It suffices to show the result for one pair and then do a union bound over all the possible pairs. Let us define

\[
j = \arg \min_{l \in [p,q]} n_l, \quad t = \arg \min_{l \in [p,q]\setminus\{j\}} n_l.
\]

Consider three cases below. In the first case, $j \in [p + 1, q - 1]$. By noting that

\[h_{p\rightarrow q} = h_{j\rightarrow q} \circ \hat{\sigma}_j \circ h_{p\rightarrow j}\]

and using the Lipschitz property of a composition of Lipschitz continuous functions, one obtains

\[
\|h_{p\rightarrow q}\|_{\text{Lip}} \leq \|h_{p\rightarrow j}\|_{\text{Lip}} \|\hat{\sigma}_j\|_{\text{Lip}} \|h_{j\rightarrow q}\|_{\text{Lip}}
\]

\[= O \left( \frac{\prod_{l=p}^q n_l}{\min_{[p,q]} n_l} \prod_{l=p+1}^{j-1} \log(n_l) \frac{\prod_{l=j}^q n_l}{\min_{[j,q]} n_l} \prod_{l=j+1}^{q-1} \log(n_l) \prod_{l=p+1}^q \beta_l^2 \right).
\]

where the first equality follows from induction assumption and $\|\hat{\sigma}\|_{\text{Lip}} \leq 1$, the second equality follows from definition of $j$. In the second case, $j = q$ and $t \in [p + 1, q - 1]$, then similarly,

\[
\|h_{p\rightarrow q}\|_{\text{Lip}} \leq \|h_{p\rightarrow t}\|_{\text{Lip}} \|\hat{\sigma}_t\|_{\text{Lip}} \|h_{t\rightarrow q}\|_{\text{Lip}}
\]

\[= O \left( \frac{\prod_{l=p}^q n_l}{\min_{[p,q]} n_l} \prod_{l=p+1}^{t-1} \log(n_l) \frac{\prod_{l=t}^q n_l}{\min_{[t,q]} n_l} \prod_{l=t+1}^{q-1} \log(n_l) \prod_{l=p+1}^q \beta_l^2 \right).
\]

It remains to handle the case where either $(j = p)$ or $(j = q$ and $t = p)$. By Lemma 6.1, it holds w.p. 1 over $(W_t)_{t=p+1}^{q-1}$ that there exists a set of $R$ tuples of diagonal matrices, say $\mathcal{D}$ =
\{(\Sigma_{p+1}^1, \ldots, \Sigma_{q-1}^1), \ldots, (\Sigma_{p+1}^R, \ldots, \Sigma_{q-1}^R)\}$, with 0-1 entries on the diagonals such that

$$\|h_{p\rightarrow q}\|_{\text{Lip}} \leq \max_{(\Sigma_{p+1}^1, \ldots, \Sigma_{q-1}^1) \in \mathcal{D}} \left\| \left( \prod_{t=p+1}^{q-1} W_t \Sigma_t \right) W_q \right\|_{\text{op}}.$$  

(57)

According to Lemma 6.1, $R$ can be interpreted as the maximum number of activation patterns of a $q - p$ layer network with layer widths $(n_p, n_{p+1}, \ldots, n_q)$, where every hidden neuron has a definite sign pattern $\{-1, +1\}$. Let $n_{\text{max}} = \max_{t \in [p+1,q-1]} n_t$, then $R = \mathcal{O}((n_{\text{max}})^{n_p})$ (see e.g. [18, 41]). Using the definition of operator norm and an $\epsilon$-net argument, the inequality (57) becomes

$$\|h_{p\rightarrow q}\|_{\text{Lip}} \leq \max_{(\Sigma_{p+1}^1, \ldots, \Sigma_{q-1}^1) \in \mathcal{D}} \sup_{\|y\|_2 = 1} \left\| y^T \left( \prod_{t=p+1}^{q-1} W_t \Sigma_t \right) W_q \right\|_2 \leq \max_{(\Sigma_{p+1}^1, \ldots, \Sigma_{q-1}^1) \in \mathcal{D}} \sup_{y \in N_{1/2}^p} \left\| y^T \left( \prod_{t=p+1}^{q-1} W_t \Sigma_t \right) W_q \right\|_2,$$  

(58)

where $N_{1/2}^p$ is a $\frac{1}{2}$-net of the unit sphere in $\mathbb{R}^{n_p}$ and the last inequality follows from Lemma 4.4.1 in [44]. Fix $y \in N_{1/2}^p$, and let $z$ be defined as above. Note that $z$ is independent of $W_q$. From the proof of Lemma 4.3 we have

$$\|z\|_2 \leq \left\| \prod_{t=p+1}^{q-1} W_t \Sigma_t \right\|_{\text{op}}^2 \leq \mathcal{O} \left( \frac{\prod_{l=p+1}^{q-1} n_l}{\min_{t \in [p,q-1]} n_t} \prod_{t=p+1}^{q-1} \beta_t^2 \right)$$  

(59)

w.p. at least $1 - \sum_{l=p}^{q-1} \exp(-\Omega(n_l))$ over $(W_l)_{l=p+1}^{q-1}$. Conditioned on the intersection of this event with the event (57), let us now study a concentration bound for $\|z^T W_q\|_2^2$ where the only randomness is $W_q$. We have $\|z^T W_q\|_2^2 = \sum_{j=1}^{n_q} \langle z, W_q, j \rangle^2$ and $\|z, (W_Q, j)\|_1^2 \leq c_1 \beta_q^2 \|z\|_2^2$. Thus by Bernstein’s inequality (see Theorem 2.8.1 of [44]),

$$\mathbb{P} \left( \|z^T W_q\|_2^2 - \mathbb{E}_{W_q} \|z^T W_q\|_2^2 > t \right) \leq \exp \left( -c_2 \min \left( \frac{t}{c_1 \beta_q^2 \|z\|_2^2}, \frac{t^2}{n_q c_1^2 \beta_q^4 \|z\|_2^4} \right) \right),$$

for some constant $c_2$. Let $C = \max(c_2, 2)$. Then by substituting to the above inequality the values

$$t = \frac{C_1}{C_2} \max(n_q, n_p) \log(R) n_p \beta_q^2 \|z\|_2^2, \quad \mathbb{E}_{W_q} \|z^T W_q\|_2^2 = n_q \beta_q^2 \|z\|_2^2,$$

we have w.p. at least $1 - e^{-C \max(n_q, n_p) \log(R)/n_p}$ that

$$\|z^T W_q\|_2^2 = \mathcal{O} \left( \max(n_q, n_p) \frac{\log(R)}{n_p} \beta_q^2 \|z\|_2^2 \right).$$
Now taking the union bound over \( y \in N^p_{1/2} \) and all tuples from \( D \), the RHS of (53) is bounded as
\[
\max_{(\Sigma_{p+1}, \ldots, \Sigma_{q-1}) \in D} 2 \sup_{y \in N^p_{1/2}} \| T W_t \|_2^2 = O \left( \max(n_q, n_p) \frac{\log(R)}{n_p} \beta_q^2 \| z \|_2^2 \right)
= O \left( \max(n_q, n_p) \log(n_{\max}) \beta_q^2 \| z \|_2^2 \right)
\]
w.p. at least
\[
1 - R \left| N^p_{1/2} \right| e^{-C \max(n_q, n_p) \log(R) / n_p} \geq 1 - e^{-\Omega(\max(n_q, n_p))},
\]
where we used \( \left| N^p_{1/2} \right| \leq 5^n, R = O \left( (n_{\max})^n \right) \) and \( C > 1 \). This combined with (58), (59) implies
\[
\| h_{p \rightarrow q} \|_{\text{Lip}} = O \left( \max(n_q, n_p) \log(n_{\max}) \beta_q^2 \frac{\prod_{l=p}^{q-1} n_l}{\min_{l \in [p,q-1]} n_l} \prod_{l=p+1}^{q} \beta_l^2 \right)
= O \left( \frac{\prod_{l=p}^{q} n_l}{\min_{l \in [p,q]} n_l} \log(n_{\max}) \prod_{l=p+1}^{q} \beta_l^2 \right)
= O \left( \frac{\prod_{l=p}^{q} n_l}{\min_{l \in [p,q]} n_l} \prod_{l=p+1}^{q} \log(n_l) \prod_{l=p+1}^{q} \beta_l^2 \right),
\]
where the second estimate follows from the current value of \( (j, t) \). So, we have shown that (53) holds for every pair \( (p, q) \) with \( q - p = s \). Taking the union bound over all these pairs finishes the proof. Note that this last step does not affect the final probability as the number of pairs is only a constant.

### F.2 Proof of Lemma 6.1

Let \( \gamma_d \) be the Lebesgue measure in \( \mathbb{R}^d \). Let us associate to \( g_k : \mathbb{R}^d \rightarrow \mathbb{R}^{n_k} \) a set of polyhedra \( \{P_i\}_{i=1}^T \) and matrices \( \{A_i\}_{i=1}^T \in \mathbb{R}^{n_k \times n_d} \) as in Lemma F.3. First, let us show that
\[
\| g_k \|_{\text{Lip}} = \max_{i \in [T]} \| A_i \|_{\text{op}}.
\]

Pick any \( x, y \in \mathbb{R}^d \). By intersecting the line segment \([x, y]\) with the polyhedra, there exists a finite set of points \( \{u_i\}_{i=1}^r \) on \([x, y]\) such that: (i) \( u_0 = x, u_r = y \), (ii) \( \| x - y \|_2 = \sum_{i=0}^{r-1} \| u_i - u_{i+1} \|_2 \), and (iii) \( [u_i, u_{i+1}] \) is contained in \( P_{j_i} \) for some \( j_i \in [T] \). This implies
\[
\| g_k(x) - g_k(y) \|_2 \leq \sum_{i=0}^{r-1} \| g_k(u_i) - g_k(u_{i+1}) \|_2 = \sum_{i=0}^{r-1} \| A_{j_i}(u_i - u_{i+1}) \|_2 \leq \sum_{i=0}^{r-1} \| A_{j_i} \|_{\text{op}} \| u_i - u_{i+1} \|_2 \leq \max_{i \in [T]} \| A_i \|_{\text{op}} \| x - y \|_2,
\]
which means
\[
\| g_k \|_{\text{Lip}} = \sup_{x, y} \frac{\| g_k(x) - g_k(y) \|_2}{\| x - y \|_2} \leq \max_{i \in [T]} \| A_i \|_{\text{op}}.
\]
To show that the above inequality can be attained, let \( i_\ast = \arg \max_{i \in [T]} \| A_i \|_{\text{op}} \). Since \( \text{int}(P_\ast) \neq \emptyset \), it holds
\[
\left\{ \frac{x - y}{\| x - y \|_2} \bigg| x, y \in P_\ast \right\} = S^{n-1},
\]
where \( S^{n-1} \) denotes the unit sphere in \( \mathbb{R}^n \), and thus
\[
\sup_{x,y} \frac{\| g_k(x) - g_k(y) \|_2}{\| x - y \|_2} \geq \sup_{x,y \in P_\ast} \frac{\| g_k(x) - g_k(y) \|_2}{\| x - y \|_2} = \sup_{x,y \in P_\ast} \frac{\| A_{i_\ast}(x - y) \|_2}{\| x - y \|_2} = \| A_{i_\ast} \|_{\text{op}}.
\]
This proves the equation (60). Next, let us define the following sets:
\[
S = \left\{ x \in \mathbb{R}^d \bigg| f_{k-1}(x) = 0 \right\},
\]
\[
B = \left\{ x \in \mathbb{R}^d \setminus S \bigg| \exists l \in [k-1], i_l \in [n_l] : g_{i_l,i_l}(x) = 0 \right\},
\]
\[
G = \mathbb{R}^d \setminus (B \cup S).
\]

Let \( \partial S = S \setminus \text{int}(S) \). Then clearly, \( \mathbb{R}^d = G \cup B \cup \partial S \cup \text{int}(S) \). Let us show that \( \gamma_d(B) = \gamma_d(\partial S) = 0 \). By Lemma [2], \( f_{k-1} \) is a PWL function, thus every level set of \( f_{k-1} \) can be written as a union of finitely many polyhedra in \( \mathbb{R}^d \). This means that \( \partial S \) is a union of finitely many polyhedra with dimension at most \( d - 1 \), thus \( \gamma_d(\partial S) = 0 \). Concerning the set \( B \), note that for every \( l \in [k-1], i_l \in [n_l] \),
\[
g_{i_l,i_l}(x) = \sum_{i_0=1}^{d} \sum_{i_1=1}^{n_1} \cdots \sum_{i_{l-1}=1}^{n_{l-1}} \prod_{p=1}^{l} x_{i_0}(W_p)_{i_{p-1},i_p} \prod_{q=1}^{l-1} \mathbb{I}_{g_{q,i_q}(x)>0}.
\]

By definition, any \( x \in B \) satisfies \( f_l(x) \neq 0 \) for all \( l \in [k-1] \). This implies that at each layer \( q \in [k-1] \), there exists at least one active neuron, i.e. some \( i_q \in [n_q] \) such that \( g_{q,i_q}(x) > 0 \). Let \( \mathbb{I}_l \) denote the set of active neurons that an input \( x \in B \) may have at layer \( l \in [k-1] \). Then it holds
\[
B \subseteq \bigcup_{l \in [k-1]} \bigcup_{i_l \in [n_l]} \bigcup_{x_l \in [n_l]} \bigcup_{i_{l-1} \in [n_{l-1}]} \cdots \bigcup_{i_2 \in [n_2]} \left\{ x \in \mathbb{R}^d \bigg| \sum_{i_0=1}^{d} \sum_{i_1=1}^{n_1} \cdots \sum_{i_{l-1} \in \mathbb{I}_{l-1}}^{n_{l-1}} \prod_{p=1}^{l} x_{i_0}(W_p)_{i_{p-1},i_p} = 0 \right\}.
\]

With probability 1 over \( (W_l)_{l=1}^{k-1} \), the set of zeros of each polynomial inside the bracket above has measure zero. Since there are only finitely many such polynomials, one obtains \( \gamma_d(B) = 0 \).

We are now ready to prove the lemma. From \( \text{int}(P_\ast) \neq \emptyset \) and \( \gamma_d(B \cup \partial S) = 0 \), it follows that
\[
\text{int}(P_\ast) \cap (G \cup \text{int}(S)) = \text{int}(P_\ast) \cap (\mathbb{R}^d \setminus (B \cup \partial S)) \neq \emptyset.
\]

For every \( i \in [T] \), let \( z_i \in \text{int}(P_\ast) \cap (G \cup \text{int}(S)) \). Since \( z_i \in \text{int}(P_\ast) \), it follows from (60) that
\[
\| g_k \|_{\text{Lip}} = \max_{i \in [T]} \| A_i \|_{\text{op}} = \max_{i \in [T]} \| J(g_k)(z_i) \|_{\text{op}}.
\]

Now if \( z_i \in \text{int}(S) \), then \( J(g_k)(z_i) = 0 \), as \( g_k \) is constant zero in a neighborhood of \( z_i \). Otherwise, we must have \( z_i \in G \), which implies \( A_{1 \rightarrow k-1}(z_i) \in \{-1,+1\}^{\sum_{l=1}^{k-1} n_l} \). Combining all these facts, we get
\[
\| g_k \|_{\text{Lip}} = \max_{z : A_{1 \rightarrow k-1}(z) \in \{-1,+1\}^{\sum_{l=1}^{k-1} n_l}} \| J(g_k)(z) \|_{\text{op}}.
\]

Finally, the inequality \( \| f_k \|_{\text{Lip}} \leq \| g_k \|_{\text{Lip}} \) follows from the 1-Lipschitz property of ReLU.
F.3 Proof of Lemma [F.1]

Let $T = 2 \sum_{i=1}^{n_l} n_i$, and $\{A_1, \ldots, A_T\} \in \{-1, +1\}^{\sum_{i=1}^{n_l}}$ denote the set of all possible binary strings of dimension $\sum_{i=1}^{n_l}$, where each entry takes value $-1$ or $+1$. Let us index the entries of each string by $A_j = \{A_{j,l,i} \}_{l \in [k], i \in [n_i]}$. Let $P_j \subseteq \mathbb{R}^d$ be the set of inputs where the activation pattern of all neurons up to layer $k$ matches perfectly with $A_j$, namely

$$P_j = \bigcap_{l \in [k]} \bigcap_{i \in [n_i]} \left\{ x \in \mathbb{R}^d \mid g_{l,i_l}(x)A_{j,l,i_l} \geq 0 \right\}$$

$$= \bigcap_{l \in [k]} \bigcap_{i \in [n_i]} \left\{ x \in \mathbb{R}^d \mid \sum_{i_0=1}^{d} \sum_{i_1=1}^{n_1} \ldots \sum_{i_{l-1}=1}^{n_{l-1}} \prod_{p=1}^{l-1} x_{i_0}(W_p)_{i_{p-1},i_p} \prod_{p=1}^{l-1} \mathbb{1}_{A_{j,p,i_p} > 0} A_{j,l,i_l} \geq 0 \right\}.$$ 

It is clear that $P_j$ is a polyhedron. Also, every coordinate function $f_{k,i_k}$ admits the following linear representation on $P_j$

$$f_{k,i_k}(x) = \sum_{i_0=1}^{d} \sum_{i_1=1}^{n_1} \ldots \sum_{i_{k-1}=1}^{n_{k-1}} \prod_{p=1}^{k} x_{i_0}(W_p)_{i_{p-1},i_p} \mathbb{1}_{A_{j,p,i_p} > 0}, \quad \forall x \in P_j.$$ 

This implies that $f_k$ coincides with a linear function on $P_j$. As every input must take one of the $T$ strings as an activation pattern, we also have $\mathbb{R}^d = \bigcup_{j=1}^{T} P_j$. Thus according to Definition [F.1], $f_k$ is a PWL function. Similarly, $g_k$ is also piecewise linear.