Spectra of the Conjugate Kernel and Neural Tangent Kernel for Linear-Width Neural Networks

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Abstract

We study the eigenvalue distributions of the Conjugate Kernel and Neural Tangent Kernel associated to multi-layer feedforward neural networks. In an asymptotic regime where network width is increasing linearly in sample size, under random initialization of the weights, and for input samples satisfying a notion of approximate pairwise orthogonality, we show that the eigenvalue distributions of the CK and NTK converge to deterministic limits. The limit for the CK is described by iterating the Marcenko-Pastur map across the hidden layers. The limit for the NTK is equivalent to that of a linear combination of the CK matrices across layers, and may be described by recursive fixed-point equations that extend this Marcenko-Pastur map. We demonstrate the agreement of these asymptotic predictions with the observed spectra for both synthetic and CIFAR-10 training data, and we perform a small simulation to investigate the evolutions of these spectra over training.

1 Introduction

Recent progress in our theoretical understanding of neural networks has connected their training and generalization to two associated kernel matrices. The first is the Conjugate Kernel (CK) or the equivalent Gaussian process kernel [Nea95, Wil97, CS09, DFS16, PLR16, SGGSD17, LBN18]. This is the gram matrix of the derived features produced by the final hidden layer of the network. The network predictions are linear in these derived features, and the CK governs training and generalization in this linear model.

The second is the Neural Tangent Kernel (NTK) [JGH18, DZPS19, AZLS19]. This is the gram matrix of the Jacobian of in-sample predictions with respect to the network weights, and was introduced to study full network training. Under gradient-flow training dynamics, the in-sample predictions follow a differential equation governed by the NTK. We provide a brief review of these matrices in Section 2.1.

The spectral decompositions of these kernel matrices are related to training and generalization properties of the underlying network. Training occurs most rapidly along the eigenvectors of the largest eigenvalues [AS17], and the eigenvalue distribution may determine the trainability of the model and the extent of implicit bias towards simpler functions [XPS19, YS19a]. It is thus of interest to understand the spectral properties of these matrices, both at random initialization and over the course of training.
1.1 Summary of contributions

In this work, we apply techniques of random matrix theory to derive an exact asymptotic characterization of the eigenvalue distributions of the CK and NTK at random initialization, in a multi-layer feedforward network architecture. We study a “linear-width” asymptotic regime, where each hidden layer has width proportional to the training sample size. We impose an assumption of approximate pairwise orthogonality for the training samples, which encompasses general settings of independent samples that need not have independent entries.

We show that the eigenvalue distributions for both the CK and the NTK converge to deterministic limits, depending on the eigenvalue distribution of the training data. The limit distribution for the CK at each intermediate hidden layer is a Marcenko-Pastur map of a linear transformation of that of the previous layer. The limit for the NTK may be described by a recursively defined sequence of fixed-point equations that extend this Marcenko-Pastur map.

We demonstrate the agreement of these asymptotic limits with the observed spectra on both synthetic and CIFAR-10 training data of moderate size. We conclude by examining empirically the evolutions of these spectra during training, on a simple example of learning a single neuron. In this example, the bulk eigenvalue distributions of the CK and NTK undergo small elongations, and isolated principal components emerge that are highly predictive of the training labels.

1.2 Related literature

Under linear-width asymptotics, the limit CK spectrum for one hidden layer was characterized in [PW17] for training data with i.i.d. Gaussian entries. For activations satisfying $E_{\xi \sim \mathcal{N}(0,1)} [\sigma'(\xi)] = 0$, [PW17] conjectured that this limit is a Marcenko-Pastur law also in multi-layer networks, and this was proven under a more general subgaussian assumption in [BP19]. [LLC18] studied the one-hidden-layer CK with general training data, and [LC18] specialized this to Gaussian mixture models. These works [LLC18, LC18] showed that the limit spectrum is a Marcenko-Pastur map of the inter-neuron covariance. We build on this insight by analyzing this covariance across multiple layers, under approximate orthogonality of the training samples. This orthogonality condition is similar to that of [ALP19], which recently studied the one-hidden-layer CK with a bias term. This condition is also more general than the assumption of i.i.d. entries, and we describe in Appendix I the reduction to the one-hidden-layer result of [PW17], as this reduction is not immediately clear.

We believe that our characterization of the limit NTK spectrum is new in the linear-width regime even for one hidden layer. The equivalent spectrum of the covariance matrix $JJ^\top$, which is one of two components of the Hessian of the training loss, was studied for one hidden layer in [PB17, PW18] in a slightly different setting. [PB17, PW18] considered an output dimension that is also proportional to $n$, and [PW18] further studied the expectation of $JJ^\top$ over the input samples $X$, rather than $JJ^\top$ itself.

The spectrum of a gram matrix $X^\top X$ is equivalent (up to the addition/removal of 0’s) to $XX^\top$, which is the sample covariance matrix for linear regression using the features $X$. As recognized in [Dic16, PW17, LLC18], its Stieltjes transform is directly related to the in-sample training error of ridge regression using $X$. Thus our results have direct bearing on the training error for random features regression using the derived features of the final layer or of the Jacobian $J = \nabla_{\theta} f_{\theta}(X)$. Analysis of generalization error uses similar techniques but is more involved, as this requires understanding the joint spectral limit of $XX^\top$ with its expectation [DW18]. This was carried out for the one-hidden-layer CK in [HMRT19, MM19], for inputs with i.i.d. Gaussian entries or with uniform distribution on the sphere.

Many properties of the CK and NTK have been established in the limit of infinite width and fixed
sample size $n$. In this limit, both the CK [Nea95, Wil97, DFS16, LBN+18] and the NTK [JGH18, LXS+19, Yan19] at random initialization converge to fixed $n \times n$ kernel matrices. The associated random features regression models converge to kernel linear regression in the RKHS of these limit kernels. Furthermore, network training occurs in a “lazy” regime [COB19], where the NTK remains constant throughout training [JGH18, DZPS19, DLL+19, AZLS19, LXS+19, ADH+19]. Spectral properties of the CK, NTK, and Hessian of the training loss have been previously studied in this infinite-width limit in [PLR+16, SEG+17, XPS19, KAA19, Gsd+19, JGH19]. Limitations of lazy training and these equivalent kernel regression models have been studied theoretically and empirically in [COB19, ADH+19, YS19b, GMMM19a, GMMM19b, LRZ19], suggesting that trained neural networks of practical width are not fully described by this type of infinite-width kernel equivalence. The asymptotic behavior is different in the linear-width regime that we study in our work: For example, for the simple linear activation $\sigma(x) = x$, the infinite-width limit of the CK at random initialization is the input Gram matrix $X^\top X$, whereas its limit spectrum under linear-width asymptotics has an additional noise component from iterating the Marcenko-Pastur map.

In the linear-width regime, the CK and NTK are expected to evolve over training, as feature learning is expected to occur. Our results characterize these spectra only at random initialization of the weights. Recent work has studied the evolution of the NTK in an entrywise sense [HY19, DGA19], and we believe it is an interesting open question to translate this understanding to a more spectral perspective.

2 Background

2.1 Neural network model and kernel matrices

We consider a fully-connected, feedforward neural network with input dimension $d_0$, hidden layers of dimensions $d_1, \ldots, d_L$, and a scalar output. For an input $x \in \mathbb{R}^{d_0}$, we parametrize the network as

$$f_\theta(x) = w^\top \frac{1}{\sqrt{d_L}} \sigma(W_L \frac{1}{\sqrt{d_{L-1}}} \sigma(\ldots \frac{1}{\sqrt{d_2}} \sigma(W_2 \frac{1}{\sqrt{d_1}} \sigma(W_1 x)))) \in \mathbb{R}. \quad (1)$$

Here, $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function (applied entrywise) and

$$W_\ell \in \mathbb{R}^{d_{\ell} \times d_{\ell-1}} \quad \text{for } 1 \leq \ell \leq L, \quad w \in \mathbb{R}^{d_L}$$

are the network weights. We denote by $\theta = (W_1, \ldots, W_L, w)$ the weights across all layers. The scalings by $1/\sqrt{d_\ell}$ reflect the “NTK-parametrization” of the network [JGH18]. We discuss alternative scalings and an extension to multi-dimensional outputs in Section 3.4.

Given $n$ training samples $x_1, \ldots, x_n \in \mathbb{R}^{d_0}$, we denote the matrices of inputs and post-activations by

$$X \equiv X_0 = (x_1 \ldots x_n) \in \mathbb{R}^{d_0 \times n}, \quad X_\ell = \frac{1}{\sqrt{d_\ell}} \sigma(W_\ell X_{\ell-1}) \in \mathbb{R}^{d_\ell \times n} \quad \text{for } 1 \leq \ell \leq L.$$ 

Then the in-sample predictions of the network are given by $f_\theta(X) = (f_\theta(x_1), \ldots, f_\theta(x_n)) = w^\top X_L \in \mathbb{R}^{1 \times n}$. The Conjugate Kernel (CK) is the matrix

$$K^{\text{CK}} = X_L^\top X_L \in \mathbb{R}^{n \times n}.$$ 

More generally, we will call $X_\ell^\top X_\ell$ the conjugate kernel at the intermediate layer $\ell$. Fixing the matrix $X_L$, the CK governs training and generalization in the linear regression model $y = w^\top X_L$. 


For very wide networks, $K^{\text{CK}}$ may be viewed as an approximation of its infinite-width limit and regression using $X_L$ is an approximation of regression in the RKHS defined by this limit kernel $K^{\text{RR08}}$.

We denote the Jacobian matrix of the network predictions with respect to the weights $\theta$ as

$$J = \nabla_{\theta} f_{\theta}(X) = (\nabla_{\theta} f(x_1) \cdots \nabla_{\theta} f(x_n)) \in \mathbb{R}^{\dim(\theta) \times n}.$$  

The **Neural Tangent Kernel (NTK)** is the matrix

$$K^{\text{NTK}} = J^\top J = (\nabla_{\theta} f_{\theta}(X))^\top (\nabla_{\theta} f_{\theta}(X)) \in \mathbb{R}^{n \times n}. \quad (2)$$

Under gradient-flow training of the network weights $\theta$ with training loss $\|y - f_{\theta}(X)\|^2/2$, the time evolutions of residual errors and in-sample predictions are given by

$$\frac{d}{dt} (y - f_{\theta(t)}(X)) = -K^{\text{NTK}}(t) \cdot (y - f_{\theta(t)}(X)), \quad \frac{d}{dt} f_{\theta(t)}(X) = K^{\text{NTK}}(t) \cdot (y - f_{\theta(t)}(X)) \quad (3)$$

where $\theta(t)$ and $K^{\text{NTK}}(t)$ are the parameters and NTK at training time $t$. Denoting the eigenvalues and eigenvectors of $K^{\text{NTK}}(t)$ by $(\lambda_\alpha(t), v_\alpha(t))_{\alpha=1}^n$, and the spectral components of the residual error by $r_\alpha(t) = v_\alpha(t)^\top (y - f_{\theta(t)}(X))$, these training dynamics are expressed spectrally as

$$\frac{d}{dt} r_\alpha(t) = -\lambda_\alpha(t) r_\alpha(t), \quad \frac{d}{dt} f_{\theta(t)}(X) = \sum_{\alpha=1}^n \lambda_\alpha(t) r_\alpha(t) \cdot v_\alpha(t).$$

Hence, $\lambda_\alpha(t)$ controls the instantaneous rate of decay of the residual error in the direction of $v_\alpha(t)$. For very wide networks, $K^{\text{NTK}}$, $\lambda_\alpha$, and $v_\alpha$ are all approximately constant over the entirety of training $[\text{JGH18}, \text{DZPS19}]$. Denoting the eigenvalues and eigenvectors of $K^{\text{NTK}}$ by $(\lambda_\alpha(t), v_\alpha(t))_{\alpha=1}^n$, and the spectral components of the residual error by $r_\alpha(t) = v_\alpha(t)^\top (y - f_{\theta(t)}(X))$, these training dynamics are expressed spectrally as

$$\frac{d}{dt} r_\alpha(t) = -\lambda_\alpha(t) r_\alpha(t), \quad \frac{d}{dt} f_{\theta(t)}(X) = \sum_{\alpha=1}^n \lambda_\alpha(t) r_\alpha(t) \cdot v_\alpha(t).$$

Hence, $\lambda_\alpha(t)$ controls the instantaneous rate of decay of the residual error in the direction of $v_\alpha(t)$. For very wide networks, $K^{\text{NTK}}$, $\lambda_\alpha$, and $v_\alpha$ are all approximately constant over the entirety of training $[\text{JGH18}, \text{DZPS19}, \text{DLL}^{\dag}19, \text{AZLS19}, \text{COB19}]$. This yields the closed-form solution $r_\alpha(t) \approx r_\alpha(0) e^{-t\lambda_\alpha}$, so that the in-sample predictions $f_{\theta(t)}(X)$ converge exponentially fast to the observed training labels $y$, with a different exponential rate $\lambda_\alpha$ along each eigenvector $v_\alpha$ of $K^{\text{NTK}}$.

### 2.2 Eigenvalue distributions, Stieltjes transforms, and the Marcenko-Pastur map

We will derive almost-sure weak limits for the empirical eigenvalue distributions of random symmetric kernel matrices $K \in \mathbb{R}^{n \times n}$ as $n \to \infty$. Throughout this paper, we will denote this as

$$\lim \text{spec } K = \mu$$

where $\mu$ is the limit probability distribution on $\mathbb{R}$. Letting $\{\lambda_\alpha\}_{\alpha=1}^n$ be the eigenvalues of $K$, this means

$$\frac{1}{n} \sum_{\alpha=1}^n f(\lambda_\alpha) \to \mathbb{E}_{x \sim \mu}[f(x)] \quad (4)$$

a.s. as $n \to \infty$, for any continuous bounded function $f : \mathbb{R} \to \mathbb{R}$. Intuitively, this may be understood as the convergence of the “bulk” of the eigenvalue distribution of $K[\text{F}]$. We will also show that $\|K\| \leq C$ a.s., for a constant $C > 0$ and all large $n$. Then $[\text{F}]$ in fact holds for any continuous function $f : \mathbb{R} \to \mathbb{R}$, as such a function must be bounded on $[-C, C]$.

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1In this paper, we use “conjugate kernel” and “neural tangent kernel” to refer to these matrices for a finite-width network, rather than their infinite-width limits.

2We caution that this does not imply convergence of the largest and smallest eigenvalues of $K$ to the support of $\mu$, which is a stronger notion of convergence than what we study in this work.
We will characterize the probability distribution \( \mu \) and the empirical eigenvalue distribution of \( K \) by their Stieltjes transforms. These are defined, respectively, for a spectral argument \( z \in \mathbb{C}^+ \) as
\[
m_\mu(z) = \int \frac{1}{x-z} \, d\mu(x), \quad m_K(z) = \frac{1}{n} \sum_{\alpha=1}^{n} \frac{1}{\lambda_\alpha - z} = \frac{1}{n} \text{Tr}(K - z \text{Id})^{-1}.
\]
The pointwise convergence \( m_K(z) \to m_\mu(z) \) a.s. over \( z \in \mathbb{C}^+ \) implies \( \lim \text{spec} K = \mu \). For \( z = x + i\eta \in \mathbb{C}^+ \), the value \( \pi^{-1} \text{Im} m_\mu(z) \) is the density function of the convolution of \( \mu \) with the distribution Cauchy\((0, \eta)\) at \( x \in \mathbb{R} \). Hence, the function \( m_\mu(z) \) uniquely defines \( \mu \), and evaluating \( \pi^{-1} \text{Im} m_\mu(x + i\eta) \) for small \( \eta > 0 \) yields an approximation for the density of \( \mu \).

An example of this type of characterization is given by the Marcenko-Pastur map, which describes the spectra of sample covariance matrices [MP67]: Let \( X \in \mathbb{R}^{d \times n} \) have i.i.d. \( \mathcal{N}(0, 1/d) \) entries, let \( \Phi \in \mathbb{R}^{n \times n} \) be positive semi-definite, and let \( n \to \infty \) such that \( \lim \text{spec} \Phi = \mu \) and \( n/d \to \gamma \in (0, \infty) \). Then the sample covariance matrix \( \Phi^{1/2}X^\top X \Phi^{1/2} \) has an almost sure spectral limit,
\[
\lim \text{spec} \Phi^{1/2}X^\top X \Phi^{1/2} = \rho^\text{MP}_\gamma \boxtimes \mu.
\]
We will call this limit \( \rho^\text{MP}_\gamma \boxtimes \mu \) the Marcenko-Pastur map of \( \mu \) with aspect ratio \( \gamma \). This distribution \( \rho^\text{MP}_\gamma \boxtimes \mu \) may be defined by its Stieltjes transform \( m(z) \), which solves the Marcenko-Pastur fixed point equation
\[
m(z) = \int \frac{1}{x(1 - \gamma - \gamma zm(z)) - z} \, d\mu(x).
\]

3 Main results

3.1 Assumptions

We use Greek indices \( \alpha, \beta \), etc. for samples in \( \{1, \ldots, n\} \), and Roman indices \( i, j \), etc. for neurons in \( \{1, \ldots, d\} \). For a matrix \( X \in \mathbb{R}^{d \times n} \), we denote by \( x_\alpha \) its \( \alpha \text{th} \) column and by \( x_i^\top \) its \( i \text{th} \) row. \( \| \cdot \| \) is the \( \ell_2 \)-norm for vectors and \( \ell_2 \to \ell_2 \) operator norm for matrices. \( \text{Id} \) is the identity matrix.

\textbf{Definition 3.1.} Let \( \varepsilon, B > 0 \). A matrix \( X \in \mathbb{R}^{d \times n} \) is \((\varepsilon, B)\)-orthonormal if its columns satisfy, for every \( \alpha \neq \beta \in \{1, \ldots, n\} \),
\[
\|x_\alpha^2 - 1\| \leq \varepsilon, \quad |x_\alpha^\top x_\beta| \leq \varepsilon, \quad \|X\| \leq B, \quad \sum_{\alpha=1}^{n} (\|x_\alpha\|^2 - 1)^2 \leq B^2.
\]

\textbf{Assumption 3.2.} The number of layers \( L \geq 1 \) is fixed, and \( n, d_0, d_1, \ldots, d_L \to \infty \), such that
(a) The weights \( \theta = (W_1, \ldots, W_L, w) \) are i.i.d. and distributed as \( \mathcal{N}(0, 1) \).
(b) The activation \( \sigma(x) \) is twice differentiable, with \( \sup_{x \in \mathbb{R}} |\sigma'(x)|, |\sigma''(x)| \leq \lambda_{\sigma} \) for some \( \lambda_{\sigma} < \infty \). For \( \xi \sim \mathcal{N}(0, 1) \), we have \( \mathbb{E}[\sigma(\xi)] = 0 \) and \( \mathbb{E}[\sigma^2(\xi)] = 1 \).
(c) The input \( X \in \mathbb{R}^{d_0 \times n} \) is \((\varepsilon_n, B)\)-orthonormal in the sense of Definition 3.1 where \( B \) is a constant, and \( \varepsilon_n n^{1/4} \to 0 \) as \( n \to \infty \).
(d) As \( n \to \infty \), \( \lim \text{spec} X^\top X = \mu_0 \) for a probability distribution \( \mu_0 \) on \([0, \infty)\), and \( \lim n/d_\ell = \gamma_\ell \) for constants \( \gamma_\ell \in (0, \infty) \) and each \( \ell = 1, 2, \ldots, L \).

\footnote{Note that some authors use a negative sign convention and define \( m_\mu(z) \) as \( \int 1/(z-x) \, d\mu(x) \).}
achieved in practice by batch normalization [IS15]. For 1, ensure that all pre-activations have approximate mean 0 and variance 1. This scaling may be for every 1-Lipschitz convex function \( \varphi : \mathbb{R}^{d_0} \to \mathbb{R} \). Then for any k > 0, with probability \( 1 - n^{-k} \), X is \( (\sqrt{\frac{K \log n}{d_0}}, B) \)-orthonormal for some \( K, B > 0 \) depending only on \( c_0, k \).

The scaling of \( \theta \), together with the scalings in (1) and the conditions \( E[\sigma(\xi)] = 0 \) and \( E[\sigma^2(\xi)] = 1 \), ensure that all pre-activations have approximate mean 0 and variance 1. This scaling may be achieved in practice by batch normalization [IS15]. For \( \xi \sim \mathcal{N}(0, 1) \), we define the following constants associated to \( \sigma(x) \). We verify in Proposition C.1 that under Assumption 3.2(b), we have \( b_\sigma^2 \leq 1 \leq a_\sigma \).

\[
 b_\sigma = E[\sigma'(\xi)], \quad a_\sigma = E[\sigma'(\xi)^2], \quad q_\ell = (b_\sigma^2)^{L-\ell}, \quad r_\ell = a_\sigma^{L-\ell}, \quad r_+ = \sum_{\ell=0}^{L-1} r_\ell - q_\ell. \tag{7}
\]

### 3.2 Spectrum of the Conjugate Kernel

Recall the Marcenko-Pastur map (5). Let \( \mu_1, \mu_2, \mu_3, \ldots \) be the sequence of probability distributions on \([0, \infty)\) defined recursively by

\[
 \mu_\ell = \rho_{\gamma_\ell}^{\text{MP}} \otimes \left( (1 - b_\sigma^2) + b_\sigma^2 \cdot \mu_{\ell-1} \right). \tag{8}
\]

Here, \( \mu_0 \) is the input limit spectrum in Assumption 3.2(d), \( b_\sigma \) is defined in (7), and \( (1 - b_\sigma^2) + b_\sigma^2 \cdot \mu \) denotes the translation and rescaling of \( \mu \) that is the distribution of \( (1 - b_\sigma^2) + b_\sigma^2 x \) when \( x \sim \mu \).

**Theorem 3.4.** Suppose Assumption 3.2 holds, and define \( \mu_1, \ldots, \mu_L \) by (8). Then

\[
 \lim \text{spec} X_\ell^T X_\ell = \mu_\ell \quad \text{for each } \ell = 1, \ldots, L, \quad \lim \text{spec} K^{\text{CK}} = \mu_L.
\]

Furthermore, \( \|K^{\text{CK}}\| \leq C \) a.s. for a constant \( C > 0 \) and all large n.

If \( \sigma(x) \) is such that \( b_\sigma = 0 \), then each distribution \( \mu_\ell \) is simply the Marcenko-Pastur law \( \rho_{2\ell}^{\text{MP}} \). This special case was previously conjectured in [PW17] and proven in [BP19], for input data \( X \) with i.i.d. entries.

To connect Theorem 3.4 to our next result on the NTK, let us describe the iteration (8) more explicitly using a recursive sequence of fixed-point equations derived from the Marcenko-Pastur equation (6): Let \( m_\ell(z) \) be the Stieltjes transform of \( \mu_\ell \), and define

\[
 \tilde{\ell}(z_{-1}, z_\ell) = \lim_{n \to \infty} \frac{1}{n} \text{Tr}(z_{-1} \text{Id} + z_\ell X_\ell^T X_\ell)^{-1} = \frac{1}{z_\ell} m_\ell \left( \frac{z_{-1}}{z_\ell} \right).
\]
Applying the Marcenko-Pastur equation \([6]\) to \(m_\ell(-z_1/z_\ell)\), and introducing \(\tilde{s}_\ell(z_1,z_\ell) = [z_\ell(1 - \gamma_\ell + \gamma_\ell z_1 \tilde{t}_\ell(z_1,z_\ell))]^{-1}\), one may check that \([8]\) may be written as the pair of equations
\[
\begin{align*}
\tilde{t}_\ell(z_1,z_\ell) &= \tilde{t}_{\ell-1}(z_1 + \frac{1 - b_\sigma^2}{\tilde{s}_\ell(z_1,z_\ell)}, \frac{b_\sigma^2}{\tilde{s}_\ell(z_1,z_\ell)}), \\
\tilde{s}_\ell(z_1,z_\ell) &= (1/z_\ell) + \gamma_\ell(\tilde{s}_\ell(z_1,z_\ell) - z_1 \tilde{s}_\ell(z_1,z_\ell) \tilde{t}_\ell(z_1,z_\ell)).
\end{align*}
\]
where \([10]\) is a rearrangement of the definition of \(\tilde{s}_\ell\). Applying \([9]\) to substitute \(\tilde{t}_\ell(z_1,z_\ell)\) in \([10]\), the equation \([10]\) is a fixed-point equation that defines \(\tilde{s}_\ell\) in terms of \(\tilde{t}_{\ell-1}\). Then \([9]\) defines \(t_\ell\) in terms of \(\tilde{s}_\ell\) and \(t_{\ell-1}\). The limit Stieltjes transform for \(K^{\text{CK}}\) is the specialization \(m^{\text{CK}}(z) = \tilde{t}_L(-z,1)\).

### 3.3 Spectrum of the Neural Tangent Kernel

In the neural network model \([1]\), an application of the chain rule yields an explicit form
\[
K^{\text{NTK}} = X_L^\top X_L + \sum_{\ell=1}^L (S_\ell^\top S_\ell) \odot (X_{\ell-1}^\top X_{\ell-1}),
\]
where \(\odot\) is the Hadamard (entrywise) product. We refer to Appendix \[G.1\] for the exact expression; see also \[HY19\] Eq. (1.7)]. Our spectral analysis of \(K^{\text{NTK}}\) relies on the following approximation, which shows that the limit spectrum of \(K^{\text{NTK}}\) is equivalent to a linear combination of the conjugate kernel matrices \(X_0^\top X_0, \ldots, X_L^\top X_L\) and \(\text{Id}\). We prove this result in Appendix \[G.1\].

**Lemma 3.5.** Under Assumption \[3.2\] letting \(r_+\) and \(q_\ell\) be as defined in \(7\),
\[
\lim \text{spec } K^{\text{NTK}} = \lim \text{spec } \left( r_+ \text{Id} + X_L^\top X_L + \sum_{\ell=0}^{L-1} q_\ell X_\ell^\top X_\ell \right).
\]

To provide an analytic description of this spectrum, we extend \([9,10]\) to characterize the trace of rational functions of \(X_0^\top X_0, \ldots, X_L^\top X_L\) and \(\text{Id}\). Denote the closed lower-half complex plane with 0 removed as \(\mathbb{C}^* = \overline{\mathbb{C}}^{-}\ \{0\}\). For \(\ell = 0, 1, 2, \ldots\), we define recursively two sequences of functions
\[
\begin{align*}
t_\ell &: (\mathbb{C}^- \times \mathbb{R}^\ell \times \mathbb{C}^*) \times \mathbb{C}^{\ell+2} \to \mathbb{C}, \\
s_\ell &: \mathbb{C}^- \times \mathbb{R}^\ell \times \mathbb{C}^* \to \mathbb{C}^+,
\end{align*}
\]
where \(z = (z_1, z_0, \ldots, z_\ell) \in \mathbb{C}^- \times \mathbb{R}^\ell \times \mathbb{C}^*\) and \(w = (w_{-1}, w_0, \ldots, w_\ell) \in \mathbb{C}^{\ell+2}\). We will define these functions such that \(t_\ell(z, w)\) will be the value of
\[
\lim_{n \to \infty} n^{-1} \text{Tr}(z_{-1} \text{Id} + z_0 X_0^\top X_0 + \ldots + z_\ell X_\ell^\top X_\ell)^{-1}(w_{-1} \text{Id} + w_0 X_0^\top X_0 + \ldots + w_\ell X_\ell^\top X_\ell).
\]
For \(\ell = 0\), we define the first function \(t_0\) by
\[
t_0\left((z_1, z_0), (w_{-1}, w_0)\right) = \int \frac{w_{-1} + w_0 x}{z_{-1} + z_0 x} d\mu_0(x)
\]
(11)
For \(\ell \geq 1\), we then define the functions \(s_\ell\) and \(t_\ell\) recursively by
\[
\begin{align*}
s_\ell(z) &= (1/z_\ell) + \gamma_{\ell-1}(s_{\ell-1}(z_{\text{prev}}(z)), (1 - b_\sigma^2, 0, \ldots, 0, b_\sigma^2)), \\
t_\ell(z, w) &= (w_\ell/z_\ell) + t_{\ell-1}(s_{\ell-1}(z_{\text{prev}}(z)), w_{\text{prev}})
\end{align*}
\]
(13)
where we write as shorthand
\[
\begin{align*}
    z_{\text{prev}}(s_l(z)) & \equiv \left( z_{-1} + \frac{1 - b_{\sigma}^2}{s_l(z)}, z_0, \ldots, z_{l-2}, z_{l-1} + \frac{b_{\sigma}^2}{s_l(z)} \right) \in \mathbb{C}^- \times \mathbb{R}^{\ell-1} \times \mathbb{C}^*, \\
    w_{\text{prev}}(w_{l-1}, w_{\ell-1}) &= (w_{\ell-1} - (w_{\ell}/z_{\ell}) \cdot (z_{-1}, \ldots, z_{l-1})) \in \mathbb{C}^{\ell+1}.
\end{align*}
\]

**Proposition 3.6.** For each \( \ell \geq 1 \) and any \( z \in \mathbb{C}^- \times \mathbb{R}^{\ell} \times \mathbb{C}^* \), there is a unique solution \( s_l(z) \in \mathbb{C}^+ \) to the fixed-point equation (12).

Hence, (12) defines \( s_l(z) \) in terms of \( t_{\ell-1}(z, w) \), and this is then used in (13) to define \( t_\ell(z, w) \). This is illustrated diagrammatically as
\[
\begin{align*}
    t_0(z, w) \rightarrow t_1(z, w) \rightarrow t_2(z, w) \rightarrow \cdots \\
    \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \\
    s_1(z) \quad s_2(z) \quad s_3(z)
\end{align*}
\]

**Theorem 3.7.** Under Assumption 3.2, for any fixed values \( z_{-1}, z_0, \ldots, z_L \in \mathbb{R} \) where \( z_L \neq 0 \), \lim \text{spec}(z_{-1} \text{Id} + z_0X_L^*X_0 + \ldots + z_LX_L^*X_L) = \nu \) where \( \nu \) is the probability distribution with Stieltjes transform \( m_\nu(z) = t_L((-z + z_{-1}, z_0, \ldots, z_L), (1, 0, \ldots, 0)) \).

In particular, \( \lim \text{spec} K_{\text{NTK}} \) is the probability distribution with Stieltjes transform
\[
m_{\text{NTK}}(z) = t_L\left((-z + r_+, q_0, \ldots, q_{L-1}, 1, (1, 0, \ldots, 0)\right).
\]
Furthermore, \( \|K_{\text{NTK}}\| \leq C \) a.s. for a constant \( C > 0 \) and all large \( n \).

This also describes the limit for \( K_{\text{CK}} = X_L^*X_L \), by specializing to \((z_{-1}, \ldots, z_L) = (0, \ldots, 0, 1)\). One may check that \( s_{\ell}(z_{-1}, 0, \ldots, 0, z_{\ell}) = \tilde{s}_{\ell}(z_{-1}, z_{\ell}) \) and \( t_{\ell}(z_{-1}, 0, \ldots, 0, z_{\ell}), (1, 0, \ldots, 0)) = \tilde{t}_{\ell}(z_{-1}, z_{\ell}) \), where \( \tilde{s}_{\ell}, \tilde{t}_{\ell} \) are defined by (9, 10), and (12, 13) reduce to (9, 10) under this specialization.

### 3.4 Extension to multi-dimensional outputs and rescaled parametrizations

Theorem 3.7 pertains to \( K_{\text{NTK}} \) for a network with scalar outputs, under the “NTK-parametrization” of network weights in [1]. We consider here a network with \( k \)-dimensional output, defined as
\[
f_\theta(x) = W_{L+1}^\top \frac{1}{\sqrt{d_L}} \sigma\left(W_L \frac{1}{\sqrt{d_{L-1}}} \sigma\left( \ldots \frac{1}{\sqrt{d_2}} \sigma\left(W_2 \frac{1}{\sqrt{d_1}} \sigma(W_1 x)\right)\right)\right) \in \mathbb{R}^k
\]
where \( W_{L+1}^\top \in \mathbb{R}^{k \times d_L} \). We write the coordinates of \( f_\theta \) as \((f_{\theta}^1, \ldots, f_{\theta}^k)\), and the vectorized output for all training samples \( X \in \mathbb{R}^{d_0 \times n} \) as \( f_\theta(X) = (f_{\theta}^1(X), \ldots, f_{\theta}^k(X)) \in \mathbb{R}^{nk} \). We consider the NTK
\[
K_{\text{NTK}} = \sum_{\ell=1}^{L+1} \tau_{\ell} \left( \nabla W_{\ell} f_\theta(X) \right)^\top \left( \nabla W_{\ell} f_\theta(X) \right) \in \mathbb{R}^{nk \times nk}.
\]
For \( \tau_1 = \cdots = \tau_{L+1} = 1 \), this is a flattening of the NTK defined in [JGH18], and we recall briefly its derivation from gradient-flow training in Appendix H.1. We consider general constants \( \tau_1, \ldots, \tau_{L+1} > 0 \) to allow for a different learning rate for each weight matrix \( W_\ell \), which may arise from backpropagation in the model (16) using a parametrization with different scalings of the weights.

**Theorem 3.8.** Fix any \( k \geq 1 \). Suppose Assumption 3.2 holds. Then \( \|K_{\text{NTK}}\| \leq C \) a.s. for a constant \( C > 0 \) and all large \( n \), and \( \lim \text{spec} K_{\text{NTK}} \) is the probability distribution with Stieltjes transform
\[
m_{\text{NTK}}(z) = t_L\left((-z + \tau \cdot r_+, \tau_1 q_0, \ldots, \tau_L q_{L-1}, \tau_{L+1}), (1, 0, \ldots, 0)\right), \quad \tau \cdot r_+ = \sum_{\ell=0}^{L-1} \tau_{\ell+1} (r_\ell - q_\ell).
\]
4 Experiments

We describe in Appendix A an algorithm to numerically compute the limit spectral densities of Theorem 3.7. The computational cost is independent of the dimensions \((n, d_0, \ldots, d_L)\), and each limit density below was computed within a few seconds on our laptop computer. Using this procedure, we investigate the accuracy of the theoretical predictions of Theorems 3.4 and 3.7. Finally, we conclude by examining the spectra of \(K_{\text{CK}}\) and \(K_{\text{NTK}}\) after network training, on a simple example.

4.1 Simulated Gaussian training data

We consider \(n = 3000\) training samples with i.i.d. \(\mathcal{N}(0, 1/d_0)\) entries, input dimension \(d_0 = 1000\), and \(L = 5\) hidden layers of dimensions \(d_1 = \ldots = d_5 = 6000\). We take \(\sigma(x) \propto \tan^{-1}(x)\), normalized so that \(E[\sigma(\xi)^2] = 1\). A close agreement between the observed and limit spectra is displayed in Figure 1 for both \(K_{\text{CK}}\) and \(K_{\text{NTK}}\). Intermediate layers are depicted in Appendix J.3.

We highlight two qualitative phenomena: The spectral distribution of the NTK (at initialization) is separated from 0, as explained by the Id component in Lemma 3.5. Across layers \(\ell = 1, \ldots, L\), there is a merging of the spectral bulk components of the CK, and an extension of its spectral support.
4.2 CIFAR-10 training data

We consider $n = 5000$ samples randomly selected from the CIFAR-10 training set [Kri09], with input dimension $d_0 = 3072$, and $L = 5$ hidden layers of dimensions $d_1 = \ldots = d_5 = 10000$. Strong principal component structure may cause the training samples to have large pairwise inner-products. Thus, we pre-process the training samples by removing the leading 10 PCs. A close agreement between the observed and limit spectra is displayed in Figure 2, for both $K^{CK}$ and $K^{NTK}$. Results without removing these leading 10 PCs are presented in Appendix J.2, where there is close agreement for $K^{CK}$ but a deviation from the theoretical prediction for $K^{NTK}$. This suggests that the approximation in Lemma 3.5 is sensitive to large but low-rank perturbations of $X$.

4.3 CK and NTK spectra after training

We consider $n = 1000$ training samples $(x_\alpha, y_\alpha)$, with $x_\alpha$ uniformly distributed on the unit sphere of dimension $d_0 = 800$, and $y_\alpha = \sigma(x_\alpha^\top v)$ for $v \in \mathbb{R}^{d_0}$ on the sphere of radius $\sqrt{d_0}$. We train a 3-layer network with widths $d_1 = d_2 = d_3 = 800$, without biases, using the Adam optimizer in Keras with learning rate 0.01, batch size 32, and 300 training epochs. The final mean-squared training error is $10^{-4}$, and the test-sample prediction-$R^2$ is 0.81.

Figure 3 depicts the spectra of $K^{CK}$ and $K^{NTK}$ for the trained weights $\theta$. Intermediate layers are shown in Appendix J.3. We observe that the bulk spectra of $K^{CK}$ and $K^{NTK}$ are slightly elongated from their random initializations. Furthermore, large outlier eigenvalues emerge in both $K^{CK}$ and $K^{NTK}$ over training. The corresponding eigenvectors are highly predictive of the training labels $y$, suggesting the emergence of these eigenvectors as the primary mechanism of training in this example.

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A Numerical solution of the fixed-point equations

Theorem 3.7 characterizes the limit Stieltjes transform $m(z)$ of matrices such as $K^{CK}$ and $K^{NTK}$. By the discussion in Section 2.2, a numerical approximation to the density functions of the corresponding spectral distributions may be obtained by computing $m(z)$ for $z = x + i\eta$, across a fine grid of values $x \in \mathbb{R}$ and for a fixed small imaginary part $\eta > 0$. We describe here one possible approach for this computation.

To compute the limit spectrum for $z_{-1}$ $\text{Id} + z_{0}X_{0}^{\top}X_{0} + \ldots + z_{L}X_{L}^{\top}X_{L}$ and general values $z_{-1}, \ldots, z_{L} \in \mathbb{R}$, fix the spectral argument $z = x + i\eta$ and denote

$$z_{L} = (-z + z_{-1}, z_{0}, \ldots, z_{L}),$$

$z_{L-1} = z_{\text{prev}}(s_{L}(z_{L}), z_{L}),$  $z_{L-2} = z_{\text{prev}}(s_{L-1}(z_{L-1}), z_{L-1}),$ etc.

Here, for $s \in \mathbb{C}^{+}$ and $z \in \mathbb{C}^{-} \times \mathbb{R}^{\ell} \times \mathbb{C}^{*}$, the quantity

$$z_{\text{prev}}(s, z) = \left(z_{-1} + \frac{1 - b_{s}^{2}}{s}, z_{0}, \ldots, z_{\ell-2}, z_{\ell-1} + \frac{b_{s}^{2}}{s}\right) \in \mathbb{C}^{-} \times \mathbb{R}^{\ell-1} \times \mathbb{C}^{*}$$

is as defined in [14], and we are making its dependence on $z$ explicit. Denote $s_{\ell} \equiv s_{\ell}(z_{\ell})$ for each $\ell = 1, \ldots, L$. Observe that, if we are given $s_{1}, \ldots, s_{L}$, then the value $t_{\ell}(z_{\ell}, w)$ may be directly computed from [13], for any $\ell \in \{0, \ldots, L\}$ and any vector $w \in \mathbb{C}^{L+2}$. This is because the fixed points needed to compute the arguments $z_{\text{prev}}(s_{\ell}(z_{\ell}), z_{\ell}), z_{\text{prev}}(s_{\ell-1}(z_{\ell-1}), z_{\ell-1}),$ etc. for the successive evaluations of $t_{\ell}, t_{\ell-1},$ etc. are provided by this given sequence $s_{1}, \ldots, s_{L}$.

Thus, we apply an iterative procedure of initializing $s_{1}^{(0)}, \ldots, s_{L}^{(0)} \in \mathbb{C}^{+}$, and computing the simultaneous updates $s_{1}^{(l+1)}, \ldots, s_{L}^{(l+1)}$ using the previous values $s_{1}^{(l)}, \ldots, s_{L}^{(l)}$. That is, we compute the right side of (12) for each $\ell = 1, \ldots, L$, using $z_{\text{prev}}(s_{\ell}^{(l)}, z)$ in place of $z_{\text{prev}}(s_{\ell}(z), z)$. After this iteration converges to fixed points $s_{1}^{*}, \ldots, s_{L}^{*}$, we then compute $m(z) = t_{L}(z_{L}, (1, 0, \ldots, 0))$ using (13) and these fixed points. For each successive value $z = x + i\eta$ along the grid of values $x \in \mathbb{R}$, we initialize $s_{1}^{(0)}, \ldots, s_{L}^{(0)}$ by linear interpolation from the computed fixed points at the preceding two values of $x$ along this grid, for faster computation.

Note that for each value $z = x + i\eta$, if the above iteration converges to fixed points $s_{1}^{*}, \ldots, s_{L}^{*} \in \mathbb{C}^{+}$, then this procedure computes the correct value for $m(z)$: This is because, denoting

$$z_{L-1}^{*} = z_{\text{prev}}(s_{L}^{*}, z_{L}),$$  $$z_{L-2}^{*} = z_{\text{prev}}(s_{L-1}^{*}, z_{L-1}^{*}),$$  $$\ldots,$$  $$z_{1}^{*} = z_{\text{prev}}(s_{2}^{*}, z_{2}^{*}),$$

it may be checked iteratively from [12, 13] and the uniqueness guarantee of Proposition 3.6 that $s_{1}^{*} = s_{1}(z_{1}^{*})$, then $s_{2}^{*} = s_{2}(z_{2}^{*})$, etc., and finally that $s_{L}^{*} = s_{L}(z_{L})$. This then means that $z_{L-1}^{*} = z_{\text{prev}}(s_{L}(z_{L}), z_{L}) = z_{L-1}$, then $z_{L-2}^{*} = z_{\text{prev}}(s_{L-1}(z_{L-1}), z_{L-1}) = z_{L-2}$, etc., and so $s_{\ell}^{*} = s_{\ell}(z_{\ell})$ for each $\ell$. Then this method computes the correct value for $m(z) = t_{L}(z_{L}, (1, 0, \ldots, 0))$.

We have found in practice that the above iteration occasionally converges to fixed points $s_{1}, \ldots, s_{L}$ not belonging to $\mathbb{C}^{+}$ (i.e. this is not a mapping from $(\mathbb{C}^{+})^{L}$ to $(\mathbb{C}^{+})^{L}$). If this occurs, we randomly re-initialize $s_{1}^{(0)}, \ldots, s_{L}^{(0)} \in \mathbb{C}^{+}$, and we have found that the method reaches the correct fixed point within a small number of random initializations.

B Proof of $(\varepsilon, B)$-orthonormality for independent input training samples

We prove Proposition 3.3. For convenience, in this section, we denote the input dimension $d_{0}$ simply as $d$, and we denote the rescaled input by $\tilde{X} = \sqrt{d}X$, with columns $\tilde{x}_{a} = \sqrt{d} \cdot x_{a}$.
Bound for \( \| \bar{x}_\alpha \|^2 \): Note that \( \mathbb{E}[\| \bar{x}_\alpha \|^2] = d \). Applying the convex concentration property and [Ada15, Theorem 2.5] with \( A = \text{Id} \), we have for any \( t > 0 \) that
\[
P \left[ \| \bar{x}_\alpha \|^2 - d > t \right] \leq 2 \exp \left( -c \min \left( \frac{t^2}{d}, t \right) \right) \tag{18}
\]
for a constant \( c \) depending only on \( c_0 \). Applying this for \( t = \sqrt{Kd \log n} \) and a union bound, with probability \( 1 - 2ne^{-cK \log n} \),
\[
\| \bar{x}_\alpha \|^2 - d \leq \sqrt{Kd \log n} \quad \text{for all } \alpha \in [n]. \tag{19}
\]
Rescaling, this shows \( \| x_\alpha \|^2 - 1 \leq \sqrt{(K \log n)/d} \).

Bound for \( \bar{x}_\alpha^\top \bar{x}_\beta \): Since \( \bar{x}_\alpha \) and \( \bar{x}_\beta \) are independent, conditional on \( \bar{x}_\beta \), we have \( \mathbb{E}[\bar{x}_\alpha^\top \bar{x}_\beta | \bar{x}_\beta] = 0 \), and the map \( \bar{x}_\alpha \mapsto \bar{x}_\alpha^\top \bar{x}_\beta \) is convex and \( \| \bar{x}_\beta \| \)-Lipschitz. Then the convex concentration property implies, for any \( t > 0 \),
\[
P \left[ \| \bar{x}_\alpha^\top \bar{x}_\beta \| > t \| \bar{x}_\beta \| \right] \leq 2e^{-c_0 t^2/\| \bar{x}_\beta \|^2}.
\]
On the event (19), applying this for \( t = \sqrt{Kd \log n} \), this probability is at most \( 2e^{-cK \log n} \). Taking a union bound, with probability \( 1 - 2n^2e^{-cK \log n} \),
\[
\| \bar{x}_\alpha^\top \bar{x}_\beta \| \leq \sqrt{Kd \log n} \quad \text{for all } \alpha \neq \beta \in [n].
\]
Rescaling, this shows \( |x_\alpha^\top x_\beta| \leq \sqrt{(K \log n)/d} \).

Bound for \( \| \tilde{X} \| \): Fix any unit vector \( v = (v_1, \ldots, v_n) \in \mathbb{R}^n \). By [KR19, Lemma C.11], the random vector \( \tilde{X} v \) also satisfies the convex concentration property, with a modified constant \( c'_0 \). Note that \( \mathbb{E}[\| \tilde{X} v \|^2] = d \| v \|^2 = d \). Then, as in (18), we have
\[
P \left[ \| \tilde{X} v \|^2 - d > t \right] \leq 2 \exp \left( -c \min \left( \frac{t^2}{d}, t \right) \right).
\]
Applying this with \( t = (B^2/4 - 1)d \), and taking a union bound over a \( 1/2 \)-net \( \mathcal{N} \) of the unit ball \( \{ v \in \mathbb{R}^n : \| v \| = 1 \} \) with cardinality \( 5^n \), we have with probability at least \( 1 - 5^n \cdot 2e^{-cB^2d} \) that
\[
\| \tilde{X} v \| \leq (B/2) \sqrt{d} \quad \text{for all } v \in \mathcal{N}.
\]
Since
\[
\| \tilde{X} \| = \sup_{v : \| v \| = 1} \| \tilde{X} v \| \leq \sup_{v \in \mathcal{N}} \| \tilde{X} v \| + \| \tilde{X} \| / 2,
\]
we have \( \| \tilde{X} \| \leq B \sqrt{d} \) on this event. Rescaling, this shows \( \| X \| \leq B \).

Bound for \( \sum_{\alpha=1}^n (\| \bar{x}_\alpha \|^2 - d)^2 \): Define \( z = (z_1, \ldots, z_n) \) where \( z_\alpha = \| \bar{x}_\alpha \|^2 - d \). Fixing any unit vector \( v = (v_1, \ldots, v_n) \in \mathbb{R}^n \), let us first bound \( v^\top z \): We have
\[
v^\top z = \sum_{\alpha=1}^n v_\alpha (\| \bar{x}_\alpha \|^2 - d),
\]
which has mean 0. Note that integrating the tail bound (18) yields the sub-exponential condition
\[
\mathbb{E} \left[ \exp \left( \lambda (\| \bar{x}_\alpha \|^2 - d) \right) \right] \leq \exp(Cd\lambda^2) \quad \text{for all } |\lambda| \leq c'
\]
and some constants $C, c' > 0$. (See e.g. [BLM13, Theorem 2.3], applied with $(v, c) = (C d', C')$ and a large enough constant $C' > 0$.) Then, as $\bar{x}_1, \ldots, \bar{x}_n$ are independent and $\|v\|^2 = 1$, also

$$
E[e^{\lambda v^\top z}] = E \left[ \exp \left( \lambda \sum_{\alpha=1}^n v_{\alpha} (\|\bar{x}_\alpha\|^2 - d) \right) \right] \leq \exp(C d \lambda^2) \quad \text{for all } |\lambda| \leq c'.
$$

For any $t > 0$, applying this with $\lambda = \min(t/(2C d), c')$ yields the sub-exponential tail bound

$$
P[v^\top z \geq t] \leq e^{-\lambda t} E[e^{\lambda v^\top z}] \leq \exp\left( -c \min\left( \frac{t^2}{d}, t \right) \right).
$$

Now applying this for $t = (B/2)d$, and again taking a union bound over a 1/2-net $\mathcal{N}$ of the unit ball, we have with probability $1 - 5^n \cdot e^{-c B d}$ that

$$
v^\top z \leq (B/2)d \quad \text{for all } v \in \mathcal{N}.
$$

On this event, we have as above that $\|z\| \leq B d$, so $\|z\|^2 \leq B^2 d^2$. Rescaling, this shows $\sum_{\alpha=1}^n (\|\bar{x}_\alpha\|^2 - 1)^2 \leq B^2$.

Applying all of the above bounds for sufficiently large constants $K, B > 0$, we obtain that these hold with probability at least $n^{-k}$, which yields Proposition 3.3.

### C Overview of proofs for the main results

The proofs of Theorems 3.4, 3.7, and 3.8 are contained in the subsequent Appendices D–H. We provide here an outline of the argument.

We will apply induction across the layers $\ell = 1, \ldots, L$, analyzing the post-activation matrix $X_\ell$ of each layer conditional on the previous post-activations $X_0, \ldots, X_{\ell-1}$ (i.e. with respect to only the randomness of $W_\ell$). For the Conjugate Kernel, this will entail analyzing the Stieltjes transform

$$
\frac{1}{n} \text{Tr}(X_L^\top X_L - z \text{Id})^{-1}
$$

conditional on the previous layers. For the Neural Tangent Kernel, given the approximation in Lemma 3.5, this will entail analyzing the Stieltjes transform

$$
\frac{1}{n} \text{Tr}(A + X_L^\top X_L - z \text{Id})^{-1}
$$

conditional on the previous layers, where $A$ is a linear combination of $X_0^\top X_0, \ldots, X_{L-1}^\top X_{L-1}$, and Id. Note that this matrix $A$ is deterministic conditional on the previous layers.

In Appendix D, we carry out a non-asymptotic analysis of $(\varepsilon, B)$-orthonormality. In particular, we show that if the deterministic input $X \equiv X_0$ is $(\varepsilon, B)$-orthonormal, then $X_1$ is $(C\varepsilon, C B)$-orthonormal with high probability, for a constant $C > 0$ depending only on $\lambda_\sigma$. Note that we require the fourth technical condition

$$
\sum_{\alpha=1}^n (\|x_\alpha\|^2 - 1)^2 \leq B^2
$$

in Definition 3.1 to ensure that the operator norm $\|X_1\|$ remains of constant order, as otherwise $X_1$ may have a rank-one component whose norm grows slowly with $n$. Applying this result conditionally for every layer, Assumption 3.2 then implies that $X_0, \ldots, X_L$ are all $(\tilde{\varepsilon}_n, \tilde{B})$-orthonormal for modified parameters $(\tilde{\varepsilon}_n, \tilde{B})$. 

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In Appendix E we carry out the analysis of the trace
\[ \frac{1}{n} \text{Tr}(A + \alpha X_1^T X_1 - z \text{Id})^{-1} \]
in a single layer, for a deterministic \((\epsilon_n, B)\)-orthonormal input \(X_0\), symmetric matrix \(A \in \mathbb{R}^{n \times n}\), and spectral parameters \(\alpha \in \mathbb{C}^\ast \equiv \mathbb{C}^\ast \setminus \{0\}\) and \(z \in \mathbb{C}\). We allow \(\alpha \in \mathbb{C}^\ast\) (rather than fixing \(\alpha = 1\)), as the subsequent induction argument for the NTK will require this extension. When \(A = 0\) and \(\alpha = 1\), this reduces to the analysis in [LLC18], and also mirrors the proof of the Marcenko-Pastur equation (6). For \(A \neq 0\), this trace will depend jointly on \(A\) and the second-moment matrix \(\Phi_1 \in \mathbb{R}^{n \times n}\) for the rows of \(X_1\). We derive a fixed-point equation in terms of \(A\) and \(\Phi_1\), which approximates this trace in the \(n \to \infty\) limit.

In Appendix F we prove Theorem 3.4 on the CK, by specializing this analysis to the setting \(A = 0\) and \(\alpha = 1\). The inductive loop is closed via an entrywise approximation of the second-moment matrix \(\Phi_\ell\) in each layer by a linear combination of \(X_\ell^T X_{\ell-1}\) and \(\text{Id}\) in the previous layer. The main argument for this approximation has been carried out in Appendix [I].

In Appendix G we prove Theorem 3.7 on the NTK. Our analysis reduces the trace of any linear combination of \(X_0^T X_0, \ldots, X_L^T X_L, \text{Id}\) to the trace of a more general rational function of \(X_0^T X_0, \ldots, X_{\ell-1}^T X_{\ell-1}, \text{Id}\) in the previous layer. In order to close the inductive loop, we analyze the trace of such a rational function across layers, and show that it may be characterized by the recursive fixed-point equations (12) and (13). In Appendix G, we also establish the approximation in Lemma 3.5 and the existence and uniqueness of the fixed point to (12).

Finally, in Appendix H, we prove Theorem 3.8, which is a minor extension of Theorem 3.7.

**Notation.** In the proof, \(v^*\) and \(M^*\) denote the conjugate transpose. For a complex matrix \(M \in \mathbb{C}^{n \times n}\), we denote by
\[ \text{tr} M = n^{-1} \text{Tr} M \]
the normalized matrix trace, by \(\|M\| = \sup_{v \in \mathbb{C}^n, \|v\| = 1} \|Mv\|\) the operator norm, and by \(\|M\|_F = (\text{tr} M^* M)^{1/2} = (\sum_{\alpha, \beta} |M_{\alpha \beta}|^2)^{1/2}\) the Frobenius norm. Note that we have
\[ |\text{tr} M| \leq \|M\| \leq \|M\|_F, \quad \|M\|_F \leq \sqrt{n}\|M\|, \quad |\text{tr} AB| \leq n^{-1}\|A\|_F\|B\|_F. \]

Let us collect here a few basic results, which we will use in the subsequent sections.

**Proposition C.1.** Under Assumption 3.2(b), the constants \(a_\sigma\) and \(b_\sigma\) in (7) satisfy
\[ |b_\sigma| \leq 1 \leq \sqrt{a_\sigma} \leq \lambda_\sigma. \]
For a universal constant \(C > 0\), the activation function \(\sigma\) satisfies
\[ |\sigma(x)| \leq C \lambda_\sigma(|x| + 1) \quad \text{for all } x \in \mathbb{R}. \]  

**Proof.** It is clear from definition that \(a_\sigma \leq \lambda_\sigma^2\). By the Gaussian Poincaré inequality,
\[ 1 = \mathbb{E}[\sigma(\xi)^2] = \text{Var}[\sigma(\xi)] \leq \mathbb{E}[\sigma'(\xi)^2] = a_\sigma. \]

By Gaussian integration-by-parts and Cauchy-Schwarz,
\[ |b_\sigma| = \mathbb{E}[\sigma'(\xi)] = |\mathbb{E}[\xi \cdot \sigma(\xi)]| \leq \mathbb{E}[\xi^2]^{1/2}\mathbb{E}[\sigma(\xi)^2]^{1/2} = 1. \]

We have
\[ |\sigma(0)| \leq \mathbb{E}[|\sigma(0) - \sigma(\xi)| + \mathbb{E}[|\sigma(\xi)|] \leq \lambda_\sigma \mathbb{E}[|\xi|] + \mathbb{E}[\sigma(\xi)^2]^{1/2} \leq C \lambda_\sigma \]
(the last inequality applying \(\lambda_\sigma \geq 1\)). Then \(|\sigma(x)| \leq |\sigma(0)| + \lambda_\sigma |x| \leq C \lambda_\sigma (|x| + 1). \]

\[ \square \]
Proposition C.2. Suppose \( M = U + iV \in \mathbb{C}^{n \times n} \), where the real and imaginary parts \( U, V \in \mathbb{R}^{n \times n} \) are symmetric, and \( V \) is invertible with either \( V \succeq c_0 \text{Id} \) or \( V \preceq -c_0 \text{Id} \) for a value \( c_0 > 0 \). Then \( M \) is invertible, and \( \| M^{-1} \| \leq 1/c_0 \).

Proof. For any unit vector \( v \in \mathbb{C}^n \),
\[
\| M v \| = \| M v \cdot |v| \| \geq |v^* M v| = |v^* U v + i \cdot v^* V v| \geq |v^* V v|,
\]
the last step holding because \( U, V \) are real-symmetric so that \( v^* U v \) and \( v^* V v \) are both real. By the given assumption on \( V \), we have \(|v^* V v| \geq c_0 \), so \( \| M v \| \geq c_0 \) for every unit vector \( v \in \mathbb{C}^n \). Then \( M \) is invertible, and \( \| M^{-1} \| \leq 1/c_0 \).

Proposition C.3. Let \( M, \tilde{M} \in \mathbb{R}^{n \times n} \) be any two symmetric matrices satisfying
\[
\frac{1}{n} \| M - \tilde{M} \|_F^2 \to 0
\]
a.s. as \( n \to \infty \). If \( \lim \text{spec} \ M = \nu \) for a probability distribution \( \nu \) on \( \mathbb{R} \), then also \( \lim \text{spec} \ \tilde{M} = \nu \).

Proof. For fixed \( z \in \mathbb{C}^+ \), let \( m(z) = \text{tr}(M - z \text{Id})^{-1} \) and \( \tilde{m}(z) = \text{tr}(\tilde{M} - z \text{Id})^{-1} \) be the Stieltjes transforms. Then applying \( A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1} \), we may bound their difference by
\[
|m(z) - \tilde{m}(z)|^2 = \frac{1}{n^2} \left| \text{Tr}[(M - z \text{Id})^{-1} - (\tilde{M} - z \text{Id})^{-1}] \right|
= \frac{1}{n^2} \left| \text{Tr}(M - z \text{Id})^{-1}(\tilde{M} - M)(\tilde{M} - z \text{Id})^{-1} \right|
\leq \frac{1}{n^2} \| \tilde{M} - M \|_F^2 \|(M - z \text{Id})^{-1}\|_F \|\tilde{M} - M \|_F \|(M - z \text{Id})^{-1}\|_F
\leq \frac{1}{n^2} \| \tilde{M} - M \|_F^2 \|(M - z \text{Id})^{-1}\|_F \|\tilde{M} - M \|_F \|(M - z \text{Id})^{-1}\|_F
\]
Applying \( \|(M - z \text{Id})^{-1}\|_F \leq 1/\text{Im} \, z \) by Proposition C.2 and similarly for \( \tilde{M} \), the given condition shows that \( m(z) - \tilde{m}(z) \to 0 \) a.s., pointwise over \( z \in \mathbb{C}^+ \). If \( \lim \text{spec} \ M = \nu \), then \( m(z) \to m_\nu(z) = \int (x - z)^{-1} d\nu(x) \) a.s., and hence also \( \tilde{m}(z) \to m_\nu(z) \) a.s. and \( \lim \text{spec} \ \tilde{M} = \nu \).

D Propagation of approximate pairwise orthogonality

In this section, we work in the following (non-asymptotic) setting of a single layer: Consider any deterministic matrix \( X \in \mathbb{R}^{d \times n} \), let \( W \in \mathbb{R}^{d \times d} \) have i.i.d. \( \mathcal{N}(0, 1) \) entries, and set
\[
\tilde{X} = \frac{1}{\sqrt{d}} \sigma(WX) \in \mathbb{R}^{d \times n}.
\]
(22)

Note that \( \tilde{X} \) has i.i.d. rows with distribution \( \sigma(w^\top X) / \sqrt{d} \), where \( w \sim \mathcal{N}(0, \text{Id}) \). Define the second-moment matrix of \( \tilde{X} \) by
\[
\Phi = \mathbb{E}[(\tilde{X}^\top \tilde{X})] = \mathbb{E}[\sigma(w^\top X)^\top \sigma(w^\top X)] \in \mathbb{R}^{n \times n}
\]
(23)
where the expectations are over the standard Gaussian matrix \( W \) and standard Gaussian vector \( w \). We show in this section the following result.
Lemma D.1. Suppose $X$ is $(\varepsilon, B)$-orthonormal where $\varepsilon < 1/\lambda_\sigma$. Then for universal constants $C, c > 0$, with probability at least $1 - 2n^2e^{-cd}\varepsilon^2 - 3e^{-cn}$, the matrix $\tilde{X}$ remains $(\tilde{\varepsilon}, \tilde{B})$-orthonormal with

$$\tilde{\varepsilon} = C\lambda^2_\sigma \varepsilon, \quad \tilde{B} = C\left(1 + n/d\right)\lambda^2_\sigma B.$$ 

Proof. For part (a), observe that $(\varepsilon, B)$ in our later arguments which approximate $\Phi$ in Frobenius norm.

(b) With probability at least $1/n$ such that a.s. for all large $n$, every matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal.

Proof. Note that increasing $\varepsilon_n$ represents a weaker assumption, so we may assume without loss of generality that $\varepsilon_n \geq n^{-0.49}$. Then by Lemma D.1, there is a constant $C_0 \geq 1$ depending on $\lambda_\sigma, \gamma_1, \ldots, \gamma_L$, such that if $X_{\ell-1}$ is $(C^\ell_0 \varepsilon_n, C^\ell_0 B)$-orthonormal, then conditional on this event, $X_\ell$ is $(C^\ell_0 \varepsilon_n, C^\ell_0 B)$-orthonormal with probability at least $1 - e^{-n^{0.001}}$ for all large $n$. Thus, setting $\varepsilon_n = C^0_0 \varepsilon_n$ and $B = C^0_0 B$, with probability at least $1 - L e^{-n^{0.01}}$, every matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal. The almost sure statement then follows from Borel-Cantelli.

In the remainder of this section, we prove Lemma D.1. We divide the proof into Lemmas D.3, D.4, and D.5 below, which check the individual requirements for $(\varepsilon, B)$-orthonormality of $\tilde{X}$. We denote by $C, C', c, c' > 0$ universal constants that may change from instance to instance.

Lemma D.3. If $X$ is $(\varepsilon, B)$-orthonormal where $\varepsilon < 1/\lambda_\sigma$, then for universal constants $C, c > 0$:

(a) For all $\alpha \neq \beta \in [n],$

$$|\Phi_{\alpha\beta} - b^2_{\alpha\beta} x^\top_{\alpha} x_{\beta}| \leq C\lambda^2_\sigma \varepsilon^2$$

$$\left|\mathbb{E}_{w \sim N(0,1)}[\sigma(w^\top x_{\alpha})]\right| \leq C\lambda_\sigma \|x_{\alpha}\|^2 - 1 \leq C\lambda_\sigma \varepsilon$$

$$|\Phi_{\alpha\alpha} - 1| \leq C\lambda_\sigma \|x_{\alpha}\|^2 - 1 \leq C\lambda_\sigma \varepsilon$$

(b) With probability at least $1 - 2n^2e^{-cd}$, simultaneously for all $\alpha \neq \beta \in [n]$, the columns of $\tilde{X}$ satisfy

$$\|\tilde{x}_{\alpha}\|^2 - 1 \leq C\lambda^2_\sigma \varepsilon, \quad \|\tilde{x}_{\alpha}^\top \tilde{x}_{\beta}\| \leq C\lambda^2_\sigma \varepsilon.$$

Note that (24) establishes an approximation which is second-order in $\varepsilon$—this will be important in our later arguments which approximate $\Phi$ in Frobenius norm.

Proof. For part (a), observe that $(\zeta_\alpha, \zeta_\beta) \equiv (w^\top x_{\alpha}, w^\top x_{\beta})$ is bivariate Gaussian, with mean 0 and covariance

$$\Sigma = \begin{pmatrix} \|x_{\alpha}\|^2 & x^\top_{\alpha} x_{\beta} \\ x^\top_{\alpha} x_{\beta} & \|x_{\beta}\|^2 \end{pmatrix} = \text{Id} + \Delta$$

where $\Delta$ is entrywise bounded by $\varepsilon$. Then performing a Gram-Schmidt orthogonalization procedure, for some standard Gaussian variables $\xi_\alpha, \xi_\beta \sim N(0, 1)$, we have

$$\zeta_\alpha = u_\alpha \xi_\alpha, \quad \zeta_\beta = u_\beta \xi_\beta + v_\beta \xi_\alpha$$

where $u_\alpha, u_\beta > 0$ and $v_\beta \in \mathbb{R}$ satisfy $|u_\alpha - 1|, |u_\beta - 1|, |v_\beta| \leq C\varepsilon$ for a universal constant $C > 0$.

By a Taylor expansion of $\sigma(\zeta)$ around $\zeta = \xi$, there exists a random variable $\eta$ between $\zeta$ and $\xi$ such that

$$\sigma(\zeta) = \sigma(\xi) + \sigma'(\xi)(\zeta - \xi) + \frac{1}{2}\sigma''(\eta)(\zeta - \xi)^2.$$ (28)
For \( \alpha \neq \beta \), applying this for both \( \zeta_\alpha \) and \( \zeta_\beta \), noting that the product of leading terms satisfies \( \mathbb{E}[\sigma(\zeta_\alpha)\sigma(\zeta_\beta)] = 0 \), and applying also the bounds \(|\sigma'(x)|, |\sigma''(x)| \leq \lambda_\sigma\) where \( \lambda_\sigma \geq 1 \), it is easy to check that

\[
\Phi_{\alpha\beta} = \mathbb{E}[\sigma(\zeta_\alpha)\sigma(\zeta_\beta)] = \mathbb{E}\left[ \sigma(\zeta_\alpha) \cdot \sigma'(\zeta_\beta)(\zeta_\beta - \xi_\beta) + \sigma(\zeta_\beta) \cdot \sigma'(\zeta_\alpha)(\zeta_\alpha - \xi_\alpha) \right] + \text{remainder}
\]

where this remainder has magnitude at most \( C\lambda_\sigma^2 \varepsilon^2 \). For the first term, substituting (27) and applying independence of \( \zeta_\alpha \) and \( \zeta_\beta \), we have

\[
\mathbb{E}\left[ \sigma(\zeta_\alpha) \cdot \sigma'(\zeta_\beta)(\zeta_\beta - \xi_\beta) + \sigma(\zeta_\beta) \cdot \sigma'(\zeta_\alpha)(\zeta_\alpha - \xi_\alpha) \right]
\]

\[
= (u_\beta - 1)\mathbb{E}[\sigma(\zeta_\alpha)] \cdot \mathbb{E}[\sigma'(\zeta_\beta)\xi_\beta] + v_\beta \mathbb{E}[\sigma(\zeta_\alpha)\xi_\alpha] \cdot \mathbb{E}[\sigma'(\zeta_\beta)] + (u_\alpha - 1)\mathbb{E}[\sigma(\zeta_\beta)] \cdot \mathbb{E}[\sigma'(\zeta_\alpha)\xi_\alpha].
\]

Applying \( \mathbb{E}[\sigma(\xi)] = 0 \) and the integration-by-parts identity \( \mathbb{E}[\sigma(\xi)\xi] = \mathbb{E}[\sigma'(\xi)] = b_\sigma \), this term equals \( v_\beta b_\sigma \). From (27), we have \( u_\alpha v_\beta = \mathbb{E}[\zeta_\alpha \zeta_\beta] = x_\alpha^\top x_\beta \). Since \( |u_\alpha - 1| \leq C\varepsilon \), this implies \( |v_\beta b_\sigma^2 - b_\sigma^2 x_\alpha^\top x_\beta| \leq Cb_\sigma^2 \varepsilon^2 \leq C\lambda_\sigma^2 \varepsilon^2 \). Combining these yields (24). Similarly, from a first-order Taylor expansion analogous to (28),

\[
\left| \mathbb{E}[\sigma(w^\top x_\alpha)] - \mathbb{E}[\sigma(\xi_\alpha)] \right| = \left| \mathbb{E}[\sigma(\zeta_\alpha)] \right| = \mathbb{E}[\sigma(\xi_\alpha)] \leq C\lambda_\sigma \cdot |u_\alpha - 1|,
\]

\[
|\Phi_{\alpha\alpha} - 1| = |\mathbb{E}[\sigma(\zeta_\alpha)^2] - \mathbb{E}[\sigma(\xi_\alpha)^2]| \leq C \max(\lambda_\sigma \cdot |u_\alpha - 1|, \lambda_\sigma^2 \cdot |u_\alpha - 1|^2). \]

The bounds (25) and (26) follow from the observations \( u_\alpha^2 = \mathbb{E}[\zeta_\alpha^2] = \|x_\alpha\|^2 \) and \( |u_\alpha - 1| \leq |u_\alpha^2 - 1| \leq \varepsilon \).

For part (b), let \( w_k \) be the \( k \)th row of \( W \). Then by definition of \( \bar{X} \), for any \( \alpha, \beta \in [n] \) (including \( \alpha = \beta \)),

\[
\bar{X}_\alpha^\top \bar{X}_\beta = \frac{1}{d} \sum_{k=1}^d \sigma(w_k^\top x_\alpha) \sigma(w_k^\top x_\beta).
\]

We apply Bernstein’s inequality: Denote by \( \| \cdot \|_{\psi_2} \) and \( \| \cdot \|_{\psi_1} \) the sub-Gaussian and sub-exponential norms of a random variable. For any deterministic vector \( x \in \mathbb{R}^d \), the function \( w \mapsto \sigma(w^\top x) \) is \( \lambda_\sigma \|x\|\)-Lipschitz. Then for \( w \sim \mathcal{N}(0, \text{Id}) \) and a universal constant \( C > 0 \), we have by Gaussian concentration-of-measure

\[
\|\sigma(w^\top x_\alpha) - \mathbb{E}[\sigma(w^\top x_\alpha)]\|_{\psi_2} \leq C\lambda_\sigma \|x_\alpha\|.
\]

From (25), \( \|\mathbb{E}[\sigma(w^\top x_\alpha)]\| \leq C\lambda_\sigma \varepsilon \). Thus (recalling that \( \|x_\alpha\| - 1 \leq \varepsilon \)), we have \( \|\sigma(w^\top x_\alpha)\|_{\psi_2} \leq C\lambda_\sigma \) for a constant \( C > 0 \), and similarly for \( x_\beta \). So

\[
\|\sigma(w^\top x_\alpha)\|_{\psi_1} \leq \|\sigma(w^\top x_\alpha)\|_{\psi_2} \leq C\lambda_\sigma^2.
\]

Applying Bernstein’s inequality (see [Ver18 Theorem 2.8.1]), for a universal constant \( c > 0 \) and any \( t > 0 \),

\[
\mathbb{P}\left[|\bar{X}_\alpha^\top \bar{X}_\beta - \mathbb{E}[\bar{X}_\alpha^\top \bar{X}_\beta]| > t \right] \leq 2 \exp\left(-cd \min\left(\frac{t^2}{\lambda_\sigma^4}, \frac{t}{\lambda_\sigma^2}\right)\right).
\]

Applying this for \( t = \lambda_\sigma^2 \varepsilon \) and taking a union bound over all \( \alpha, \beta \in [n] \), we get

\[
\mathbb{P}\left[|\bar{X}_\alpha^\top \bar{X}_\beta - \mathbb{E}[\bar{X}_\alpha^\top \bar{X}_\beta]| \leq \lambda_\sigma^2 \varepsilon \text{ for all } \alpha, \beta \in [n]\right] \geq 1 - 2n^2 \exp(-cd \cdot \varepsilon^2).
\]

Since \( \mathbb{E}[\bar{X}_\alpha^\top \bar{X}_\beta] = \Phi_{\alpha\beta} \), part (b) now follows from part (a). \( \square \)
Lemma D.4. If $X$ is $(\varepsilon,B)$-orthonormal, then for universal constants $C,c > 0$:

(a) $\|\Phi\| \leq C\lambda_d^2B^2$.

(b) With probability at least $1 - 2e^{-cn}$, $\|\tilde{X}\| \leq C\left(1 + \sqrt{n/d}\right)\lambda_\sigma B$.

Proof. For part (a), define

$$\Sigma = \mathbb{E}[\sigma(w^T X)^\top \sigma(w^T X)] - \mathbb{E}[\sigma(w^T X)]^\top \mathbb{E}[\sigma(w^T X)]$$

where the first term on the right is $\Phi$. Then

$$\|\Sigma\| = \sup_{v:||v||=1} v^\top \Sigma v = \sup_{v:||v||=1} \mathbb{E}[\left(\sigma(w^T X)v\right)^2] - \mathbb{E}[\sigma(w^T X)v]^2 = \sup_{v:||v||=1} \text{Var}[\sigma(w^T X)v].$$

We bound this variance using the Gaussian Poincaré inequality: Let us fix $v \in \mathbb{R}^n$ with $||v|| = 1$ and define

$$F(w) = \sigma(w^T X)v = \sum_{\alpha=1}^n v_\alpha \sigma(w^T x_\alpha).$$

Then, letting $u \in \mathbb{R}^n$ be the vector with entries $u_\alpha = v_\alpha \sigma'(w^T x_\alpha)$,

$$\nabla F(w) = \sum_{\alpha=1}^n v_\alpha \sigma'(w^T x_\alpha) \cdot x_\alpha = Xu, \quad ||\nabla F(w)|| \leq ||X|| \cdot ||u|| \leq \lambda_\sigma B.$$

Then by the Gaussian Poincaré inequality, $\text{Var}[F(w)] \leq \mathbb{E}[||\nabla F(w)||^2] \leq \lambda_\sigma^2 B^2$, so $||\Sigma|| \leq \lambda_\sigma^2 B^2$. In addition, by (25), the difference between $\Phi$ and $\Sigma$ is a rank-one perturbation controlled by

$$||\Phi - \Sigma|| = ||\mathbb{E}[\sigma(w^T X)]||^2 = \sum_{\alpha=1}^n \mathbb{E}[\sigma(w^T x_\alpha)]^2 \leq C\lambda_\sigma^2 \sum_{\alpha=1}^n (||x_\alpha||^2 - 1)^2 \leq C\lambda_\sigma^2 B^2,$$

the last inequality using the final condition of $(\varepsilon,B)$-orthonormality in Definition 3.1. This establishes part (a).

For part (b), we apply the concentration result of [Ver10, Eq. (5.26)] for matrices with independent sub-Gaussian rows. For any fixed unit vector $v \in \mathbb{R}^n$, recall from (32) that $F(w) = \sigma(w^T X)v$ is $\lambda_\sigma B$-Lipschitz. Then by Gaussian concentration-of-measure,

$$||F(w) - \mathbb{E}[F(w)||_{\psi_2} \leq C\lambda_\sigma B.$$

We have $||\mathbb{E}[F(w)]|| \leq ||\mathbb{E}[\sigma(w^T X)]|| \leq C\lambda_\sigma B$ by (33), so also $||F(w)||_{\psi_2} \leq C\lambda_\sigma B$. This holds for any unit vector $v \in \mathbb{R}^n$, hence $||\sigma(w^T X)||_{\psi_2} \leq C\lambda_\sigma B$ for the vector sub-Gaussian norm. Thus, $\sqrt{\lambda_\sigma B} \tilde{X}$ has i.i.d. rows whose sub-Gaussian norm is at most a universal constant. Recalling $\Phi = \tilde{X}^\top \tilde{X}$ and applying [Ver10, Eq. (5.26)] with $A = \sqrt{\lambda_\sigma B}$, we obtain for some universal constants $C,c > 0$ that

$$\mathbb{P}\left[||\tilde{X}^\top \tilde{X} - \Phi|| > \max(\delta,\delta^2)||\Phi||\right] \leq 2e^{-ct^2}, \quad \delta = C\sqrt{n/d}t + t/\sqrt{d}.$$

Note that the complementary event $||\tilde{X}^\top \tilde{X} - \Phi|| \leq \max(\delta,\delta^2)||\Phi||$ implies

$$||\tilde{X}|| \leq \sqrt{(1 + \max(\delta,\delta^2)||\Phi||} \leq (1 + C')\sqrt{||\Phi||}$$

for a constant $C' > 0$. Then choosing $t = \sqrt{n}$ and applying part (a) yields part (b). \qed
Lemma D.5. If \( X \) is \((\varepsilon, B)\)-orthonormal, then for universal constants \( C, c > 0 \), with probability at least \( 1 - \exp(-cn) \), the columns of \( \bar{X} \) satisfy

\[
\sum_{\alpha=1}^{n} (\|\bar{x}_\alpha\|^2 - 1)^2 \leq C \left( 1 + n^2/d^2 \right) \lambda_\alpha^4 B^2.
\]

Let us remark that in settings where \( \varepsilon \gg 1/\sqrt{n} \), applying Lemma D.3(b) to bound each term \((\|\bar{x}_\alpha\|^2 - 1)^2\) separately would not yield a constant-order bound for this sum. The proof below performs a more careful analysis of the combined fluctuations of \((\|\bar{x}_\alpha\|^2 - 1)^2\).

Proof. Let \( z = (z_1, \ldots, z_n) \in \mathbb{R}^n \) and \( r = (r_1, \ldots, r_n) \in \mathbb{R}^n \) be defined as

\[
z_\alpha = \|\bar{x}_\alpha\|^2 - \mathbb{E}[\|\bar{x}_\alpha\|^2], \quad r_\alpha = \mathbb{E}[\|\bar{x}_\alpha\|^2] - 1.
\]

The quantity to be bounded is \( \|z + r\|^2 \). Note that \( \|z + r\|^2 \leq 2\|z\|^2 + 2\|r\|^2 \). We have

\[
\mathbb{E}[\|\bar{x}_\alpha\|^2] = \mathbb{E} \left[ \frac{1}{d} \sum_{i=1}^{d} \sigma(w_i^\top x_\alpha)^2 \right] = \Phi_{\alpha\alpha},
\]

so applying (26) from Lemma D.3

\[
\|r\|^2 = \sum_{\alpha=1}^{n} (\Phi_{\alpha\alpha} - 1)^2 \leq C\lambda_\alpha^4 \sum_{\alpha=1}^{n} (\|x_\alpha\|^2 - 1)^2 \leq C\lambda_\alpha^4 B^2.
\]

Thus it remains to bound \( \|z\|^2 \).

Let \( \mathcal{N} \) be a 1/2-net of the unit ball \( \{w \in \mathbb{R}^n : \|w\| = 1\} \), of cardinality \( |\mathcal{N}| \leq 5^n \). Then

\[
\|z\| = \sup_{w : \|w\| \leq 1} w^\top z \leq \sup_{v \in \mathcal{N}} v^\top z + \|z\|/2,
\]

so \( \|z\| \leq 2 \sup_{v \in \mathcal{N}} v^\top z \). For each fixed vector \( v = (v_1, \ldots, v_n) \in \mathcal{N} \), we have

\[
v^\top z = \sum_{\alpha=1}^{n} v_\alpha \cdot \frac{1}{d} \sum_{i=1}^{d} \left( \sigma(w_i^\top x_\alpha)^2 - \mathbb{E}[\sigma(w_i^\top x_\alpha)^2] \right) = \frac{1}{d} \sum_{i=1}^{d} \left( \sum_{\alpha=1}^{n} \left( \sigma(w_i^\top x_\alpha)^2 - \mathbb{E}[\sigma(w_i^\top x_\alpha)^2] \right) v_\alpha \right).
\]

We will bound the sub-exponential norm of each summand \( i = 1, \ldots, d \) and apply Bernstein’s inequality.

For \( w \sim \mathcal{N}(0, \text{Id}) \), denote

\[
q = (q_1, \ldots, q_n) = (w^\top x_1, \ldots, w^\top x_n), \quad F(q) = \sum_{\alpha=1}^{n} (\sigma(q_\alpha)^2 - \mathbb{E}[\sigma(q_\alpha)^2]) v_\alpha.
\]

Observe that \( q = X^\top w \). Thus we wish to bound the sub-exponential norm of \( F(q(w)) \) when \( w \sim \mathcal{N}(0, \text{Id}) \). By the Gaussian Sobolev inequality (see [AW15, Eq. (3)]), for any \( p \geq 2 \),

\[
\|F(q(w))\|_{L^p} \leq \sqrt{p} \cdot \left\| \nabla_w F(q(w)) \right\|_{L^p} \quad (36)
\]
where $\|Y\|_{L^p} = \mathbb{E}[|Y|^p]^{1/p}$ denotes the $L^p$-norm of a random variable (and $\|\nabla_w F(q(w))\|$ is the usual $\ell_2$ vector norm of the gradient of $F(q(w))$ in $w$). By the chain rule,
\[
\nabla_w F(q(w)) = X \cdot \nabla_q F(q),
\]
so
\[
\|\nabla_w F(q(w))\|^2 \leq \|X\|^2 \|\nabla_q F(q)\|^2 \leq B^2 \|\nabla_q F(q)\|^2.
\]
We have $\frac{\partial}{\partial q_{\alpha}} F(q) = 2\sigma(q_{\alpha})\sigma'(q_{\alpha})v_{\alpha}$, so
\[
\|\nabla_q F(q)\|^2 = \sum_{\alpha=1}^{n} 4\sigma(q_{\alpha})^2\sigma'(q_{\alpha})^2 v_{\alpha}^2 \leq 4\lambda_\sigma^2 \sum_{\alpha=1}^{n} \sigma(q_{\alpha})^2 v_{\alpha}^2.
\]
Recalling (29), we have
\[
\|\sigma(q_{\alpha})^2\|_{\psi_1} = \|\sigma(w^T x_{\alpha})^2\|_{\psi_1} \leq C\lambda_\sigma^2. Then
\[
\left\| \sum_{\alpha=1}^{n} \sigma(q_{\alpha})^2 v_{\alpha}^2 \right\|_{\psi_1} \leq C\lambda_\sigma^2 \sum_{\alpha=1}^{n} v_{\alpha}^2 = C\lambda_\sigma^2,
\]
so
\[
\left\| \|\nabla_w F(q(w))\|_{\psi_1}^2 \right\|_{\psi_1} \leq C\lambda_\sigma^2 B^2.
\]
This implies the bound (see [Ver18, Proposition 2.7.1]), for any $p \geq 1$,
\[
\left\| \|\nabla_w F(q(w))\|_{L^{2p}} \right\|_{L^p} ^{2p} = \mathbb{E}[\|\nabla_w F(q(w))\|^{2p}] = \|\|\nabla_w F(q(w))\|_{L^p}^{2p} \leq (C'\lambda_\sigma^4 B^2 \cdot p)^p
\]
for a universal constant $C' > 0$. Thus, applying this to (36), we obtain for any $p \geq 2$
\[
\|F(q(w))\|_{L^p} \leq \sqrt{p} \cdot C\lambda_\sigma^2 B \sqrt{p} = C\lambda_\sigma^2 B \cdot p.
\]
Finally, this implies (see again [Ver18, Proposition 2.7.1]) $\|F(q(w))\|_{\psi_1} \leq C'\lambda_\sigma^2 B$ for a universal constant $C' > 0$, which is our desired bound on the sub-exponential norm of $F(q(w))$.

Applying this and Bernstein’s inequality to (35), for any $t > 0$,
\[
\mathbb{P}[v^T z > t] \leq \exp \left(-cd \min \left(\frac{t^2}{\lambda_\sigma^2 B^2}, \frac{t}{\lambda_\sigma^2 B} \right) \right).
\]
Setting
\[
t = C_0\lambda_\sigma^2 B \cdot \max(\delta, \delta^2), \quad \delta = \sqrt{n/d}
\]
for a large enough constant $C_0 > 0$, and taking the union bound over all $5^n$ vectors $v \in \mathcal{N}$, we get
\[
\mathbb{P}[\|z\| > 2t] \leq \mathbb{P} \left[ \sup_{v \in \mathcal{N}} v^T z > t \right] \leq e^{-ct}
\]
for a constant $c > 0$. Combining with the bound on $\|r\|^2$ in (34), we obtain the lemma. \(\square\)
E Resolvent analysis for a single layer

We consider the same setting of a single layer as in the preceding section. Let $\tilde{X}$ and $\Phi$ be defined by the deterministic input $X \in \mathbb{R}^{d \times n}$ and Gaussian matrix $W \in \mathbb{R}^{\tilde{d} \times d}$ as in (22) and (23), and define the $(n$-dependent) aspect ratio

$$\gamma = n/\tilde{d}.$$ Consider a deterministic real-symmetric matrix $A \in \mathbb{R}^{n \times n}$, and two (possibly $n$-dependent) spectral arguments $\alpha \in \mathbb{C}^*$ and $z \in \mathbb{C}^+$, where $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$. We study the matrix

$$A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id}.$$ We collect here the set of assumptions that we will use in this section.

**Assumption E.1.** There are constants $B, C_0, c_0 > 0$ such that

(a) $\alpha \in \mathbb{C}^*$ and $z \in \mathbb{C}^+$, and $\gamma, |\alpha|, |z|, \text{Im} z \in [c_0, C_0]$.

(b) $X$ is $(\varepsilon_n, B)$-orthonormal, where $\varepsilon_n < n^{-0.01}$.

(c) $A \in \mathbb{R}^{n \times n}$ is deterministic and symmetric, satisfying $\|A\| \leq C_0$.

(d) $W$ has i.i.d. $\mathcal{N}(0, 1)$ entries, and $\sigma(x)$ satisfies Assumption 3.2(b).

Throughout this section, $C, C', c, c', n_0 > 0$ denote constants changing from instance to instance that may depend on $\lambda_\sigma$ and the above values $B, C_0, c_0$.

Proposition 3.2 ensures that $A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id}$ is invertible. Define the resolvent

$$R = (A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id})^{-1} \in \mathbb{C}^{n \times n}$$

and the deterministic $(n$-dependent) parameter

$$\bar{s} = \alpha^{-1} + \gamma \cdot \mathbb{E}[\text{tr} R\Phi].$$

The goal of this section is to prove the following result, which approximates this resolvent $R$ by replacing the random matrix $\alpha \tilde{X}^\top \tilde{X}$ with a deterministic matrix $\bar{s}^{-1}\Phi$, and provides an approximate fixed-point equation that defines this parameter $\bar{s}$.

For $A = 0$ and $\alpha = 1$, we will verify in Appendix F that this result reduces to the Marcenko-Pastur equation (6).

**Lemma E.2.** Under Assumption E.1, there are constants $C, c, c_0, n_0 > 0$ such that for all $n \geq n_0$, any deterministic matrix $M \in \mathbb{C}^{n \times n}$, and any $t \in (n^{-1}, c_0)$,

(a) $\mathbb{P}\left[|\text{tr} RM - \text{tr} (A + \bar{s}^{-1}\Phi - z \text{Id})^{-1} M| > \|M\|t\right] \leq Cne^{-cnt^2}$

(b) $\mathbb{P}\left[|\bar{s} - (\alpha^{-1} + \gamma \text{tr} (A + \bar{s}^{-1}\Phi - z \text{Id})^{-1} \Phi)| > t\right] \leq Cne^{-cnt^2}$
E.1 Basic bounds

**Proposition E.3.** Under Assumption E.1, deterministically for some constants $C, c, n_0 > 0$ and all $n \geq n_0$,

$$\|R\| \leq C, \quad \|\Phi\| \leq C, \quad \|\bar{s}\| \leq C, \quad \text{Im} \bar{s} \geq c.$$

Furthermore, with probability at least $1 - 2e^{-c'n}$ for a constant $c' > 0$,

$$\text{Im tr } R\Phi \geq c.$$

*Proof.* We may write $A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id} = U + iV$ where $U = A + (\text{Re }\alpha)\tilde{X}^\top \tilde{X} - (\text{Re }z) \text{Id}$ and $V = (\text{Im }\alpha)\tilde{X}^\top \tilde{X}^\top - (\text{Im }z) \text{Id}$. Both $U$ and $V$ are symmetric, and $V \leq (\text{Im }z) \text{Id}$ because $\text{Im }\alpha \leq 0$ and Im $z > 0$. Then $\|R\| \leq 1/\text{Im }z \leq C$ by Proposition C.2.

The bound $\|\Phi\| \leq C$ comes from Lemma D.4(a) and the $(\epsilon_n, B)$-orthonormality assumption for $X$. Then from the definition of $\bar{s}$ in (38) and the bounds $\|R\|, \|\Phi\| \leq C$, we have also $\|\bar{s}\| \leq C$. For the lower bound for $\text{Im }\bar{s}$ and $\text{Im tr } R\Phi$, let us write

$$\text{tr } R\Phi = \text{tr } \left( \frac{R + R^*}{2} \right) \Phi + \text{tr } \left( \frac{R - R^*}{2} \right) \Phi.$$ 

The first trace is real because $R + R^*$ is Hermitian, so

$$\text{Im tr } R\Phi = \text{Im } \text{tr } \left( \frac{R - R^*}{2} \right) \Phi.$$

Denoting $Y = A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id}$ and applying the identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$, we have

$$R - R^* = Y^{-1} - (Y^*)^{-1} = Y^{-1}(Y^* - Y)(Y^*)^{-1} = R(Y^* - Y)R^*.$$

Then, writing $Y = U + iV$ as above and applying $Y^* - Y = -2iV$, we get

$$\text{Im tr } R\Phi = \text{Im}( -i \cdot \text{tr } RV R^* \Phi ) = \text{Re}( -i (\text{Im }\alpha) \cdot \text{tr } R\tilde{X}^\top \tilde{X} R^* \Phi + (\text{Im }z) \cdot \text{tr } RR^* \Phi ).$$

Since $\text{tr } R\tilde{X}^\top \tilde{X} R^* \Phi = \Phi \Phi^1/2 R\tilde{X}^\top \tilde{X} R^* \Phi^{1/2}$, where this matrix is positive semi-definite, this trace is real and non-negative. Similarly, $\text{tr } RR^* \Phi$ is real and non-negative. Then the above yields the lower bound

$$\text{Im tr } R\Phi \geq \text{Im }z \cdot \text{tr } RR^* \Phi \geq \text{Im }z \cdot \lambda_{\min}(RR^*) \cdot \text{tr } \Phi,$$

where $\lambda_{\min}(RR^*)$ is the smallest eigenvalue of $RR^*$. By [26] and the condition $\epsilon_n < n^{-0.01}$, we have $\text{tr } \Phi \geq c$ for a constant $c > 0$ and large enough $n_0$. Observe that $\lambda_{\min}(RR^*) = 1/\|Y\|^2$, and $\|Y\| \leq \|A\| + |\alpha| \cdot \|\tilde{X}\|^2 + |z|$. By Lemma D.4(b), with probability $1 - 2e^{-c'n}$, we have $\|\tilde{X}\| \leq C$, so putting this together yields $\text{Im tr } R\Phi \geq c$ with this probability. Finally, for the deterministic bound $\text{Im }\bar{s} \geq c$, we may apply $\text{Im tr } R\Phi \geq c$ on the event where $\|\tilde{X}\| \leq C$ holds, and $\text{Im tr } R\Phi \geq 0$ on the complementary event. Taking an expectation and applying the definition (38) yields $\text{Im }\bar{s} \geq c$.

E.2 Resolvent approximation

We recall the result of [LLC18, Lemma 1], which establishes concentration of quadratic forms in the rows of $\tilde{X}$. The following is its specialization to standard Gaussian matrices $W$, and stated in our notation.
Lemma E.4 ([LLC18]). Suppose \( \sigma(x) \) is \( \lambda_\sigma \)-Lipschitz, and let \( \bar{x}_i^\top \) be a row of \( \bar{X} \). Then for any deterministic matrix \( Y \in \mathbb{R}^{n \times n} \) with \( \|Y\| \leq 1 \), for some constants \( C, c > 0 \) (depending on \( \lambda_\sigma \)), and for any \( t > 0 \),

\[
\mathbb{P} \left( \frac{1}{n} \bar{x}_i^\top Y \bar{x}_i - \operatorname{tr} Y \Phi > t \right) \leq C \exp \left( -\frac{cn}{\|X\|^2} \min \left( \frac{t^2}{t_0^2}; t \right) \right)
\]

where \( t_0 = |\sigma(0)| + \lambda_\sigma \|X\| \sqrt{1/\gamma} \).

Using this result, we establish the following approximation for the resolvent \( R \) in (37).

Lemma E.5. Consider any deterministic matrix \( M \in \mathbb{C}^{n \times n} \), and set

\[
\delta_n = \operatorname{tr} M - \operatorname{tr} R \left( A + \frac{1}{\alpha^{-1} + \gamma \operatorname{tr} \Phi} \Phi - z \operatorname{Id} \right) M.
\]

Under Assumption [E,1] there exist constants \( c, c_0, n_0 > 0 \) such that for all \( n \geq n_0 \) and \( t \in (n^{-1}, c_0) \),

\[
\mathbb{P} [ |\delta_n| > \|M\| t ] \leq C n e^{-cnt^2}.
\]

Proof. By rescaling \( M \), we may assume that \( \|M\| \leq 1 \). We have \( \operatorname{Id} = R(A + \alpha \bar{X}^\top \bar{X} - z \operatorname{Id}) = RA + \alpha R \bar{X}^\top \bar{X} - z R \). Writing \( \bar{X}^\top \bar{X} = \sum_i x_i x_i^\top \) (where \( x_i^\top \) is the \( i \)-th row of \( \bar{X} \)), multiplying by \( M \), and taking the normalized trace \( \operatorname{tr} = n^{-1} \operatorname{Tr} \),

\[
\operatorname{tr} M = \operatorname{tr} RAM + \alpha \operatorname{tr} R \bar{X}^\top \bar{X} M - z \operatorname{tr} RM
\]

\[
= \operatorname{tr} RAM + \frac{\alpha}{n} \sum_{i=1}^{d} \bar{x}_i^\top M R \bar{x}_i - z \operatorname{tr} RM.
\]

Hence

\[
\delta_n = \frac{\alpha}{n} \sum_{i=1}^{d} \bar{x}_i^\top M R \bar{x}_i - \frac{\operatorname{tr} R \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} \Phi}.
\]

Let us define the leave-one-out resolvent

\[
R^{(i)} = \left( A + \alpha \sum_{j: j \neq i} \bar{x}_j \bar{x}_j^\top - z \operatorname{Id} \right)^{-1}.
\]

We may then decompose \( \delta_n \) as \( \delta_n = J_1 + \gamma J_2 \) where (recalling \( \gamma = n/d \))

\[
J_1 = \frac{1}{n} \sum_{i=1}^{d} \left( \alpha \bar{x}_i^\top M R \bar{x}_i - \frac{\gamma \operatorname{tr} R^{(i)} \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} R^{(i)} \Phi} \right),
\]

\[
J_2 = \frac{1}{n} \sum_{i=1}^{d} \left( \frac{\operatorname{tr} R^{(i)} \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} R^{(i)} \Phi} - \frac{\operatorname{tr} R \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} \Phi} \right).
\]

Let us denote these summands as

\[
J_1^{(i)} = \alpha \bar{x}_i^\top M R \bar{x}_i - \frac{\gamma \operatorname{tr} R^{(i)} \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} R^{(i)} \Phi} \quad \text{and} \quad J_2^{(i)} = \frac{\operatorname{tr} R^{(i)} \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} R^{(i)} \Phi} - \frac{\operatorname{tr} R \Phi M}{\alpha^{-1} + \gamma \operatorname{tr} \Phi}.
\]
Bound for $J_1$. Momentarily fix the index $i \in \{1, \ldots, \tilde{d}\}$. Applying the Sherman-Morrison identity, we have
\[ R = R^{(i)} - \frac{\alpha R^{(i)} \tilde{x}_i \tilde{x}_i^\top R^{(i)}}{1 + \alpha \tilde{x}_i R^{(i)} \tilde{x}_i}. \] (40)
Then, introducing $A_1 = \tilde{x}_i^\top MR^{(i)} \tilde{x}_i$ and $A_2 = \tilde{x}_i^\top R^{(i)} \tilde{x}_i$,
\[ \alpha \tilde{x}_i^\top MR \tilde{x}_i = \alpha A_1 - \frac{\alpha^2 A_1 A_2}{1 + \alpha A_2} = \frac{A_1}{\alpha^{-1} + A_2}. \]
Recall that the rows of $\tilde{X}$ are i.i.d. Let $\tilde{X}^{(i)}$ be the matrix $\tilde{X}$ with the $t^{th}$ row $\tilde{x}_i$ removed, and let $E_{\tilde{x}_i}[\cdot]$ be the expectation over only $\tilde{x}_i$ (i.e. conditional on $\tilde{X}^{(i)}$). Observe that $R^{(i)}$ is a function of $\tilde{X}^{(i)}$. Applying Proposition E.3 with $\tilde{X}^{(i)}$ in place of $\tilde{X}$, we see that $\|R^{(i)}\|$ and $\|MR^{(i)}\|$ are both bounded by a constant. Then applying Lemma E.4 conditional on $\tilde{X}^{(i)}$, and recalling the bound (20) for $\sigma(0)$, there are constants $C, c > 0$ for which
\[ \mathbb{P}[|A_k - E_{\tilde{x}_i}[A_k]| > t] \leq Ce^{-cn\min(t^2, t)} \quad \text{for } k = 1, 2. \]

Note that
\[ E_{\tilde{x}_i}[A_1] = \text{Tr} MR^{(i)}E[\tilde{x}_i \tilde{x}_i^\top] = \frac{1}{d} \text{Tr} M R^{(i)} \Phi = \gamma \text{tr} R^{(i)} \Phi M. \]
Similarly, $E_{\tilde{x}_i}[A_2] = \gamma \text{tr} R^{(i)} \Phi$, so
\[ J_1^{(i)} = \frac{A_1}{\alpha^{-1} + A_2} - \frac{E_{\tilde{x}_i}[A_1]}{\alpha^{-1} + E_{\tilde{x}_i}[A_2]}. \]
Applying Proposition E.3, we have for some constants $C, c, c' > 0$, on an event $\mathcal{E}(X^{(i)})$ of probability $1 - 2e^{-cn}$, that
\[ |E_{\tilde{x}_i}[A_1]| \leq C, \quad |\alpha^{-1} + E_{\tilde{x}_i}[A_2]| \geq \text{Im}(\alpha^{-1} + E_{\tilde{x}_i}[A_2]) \geq c. \]
Then, for any $t$ such that $t < c/2$, on the event where $|A_1 - E_{\tilde{x}_i}[A_1]| \leq t$, $|A_2 - E_{\tilde{x}_i}[A_2]| \leq t$, and $\mathcal{E}(X^{(i)})$ all hold,
\[ |J_1^{(i)}| \leq \frac{|A_1 - E_{\tilde{x}_i}[A_1]|}{|\alpha^{-1} + A_2|} + |E_{\tilde{x}_i}[A_1]| \cdot \frac{|A_2 - E_{\tilde{x}_i}[A_2]|}{|\alpha^{-1} + E_{\tilde{x}_i}[A_2]|} \leq Ct. \] (41)
Thus, for $t < c_0$ and a sufficiently small constant $c_0 > 0$, we have $\mathbb{P}[|J_1^{(i)}| \geq t] \leq C e^{-cn t^2}$. Applying a union bound over $i \in \{1, \ldots, \tilde{d}\}$, this yields $\mathbb{P}[|J_1| \geq t] \leq Cne^{-cn t^2}$.

Bound for $J_2$. Applying the identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$,
\[ R^{(i)} - R = R^{(i)}(R^{-1} - (R^{(i)})^{-1})R = \alpha R^{(i)} \tilde{x}_i \tilde{x}_i^\top R. \]
Then, applying also the bounds $\|R\|, \|R^{(i)}\| \leq C$ from Proposition E.3,
\[ |\text{tr}(R^{(i)} - R) \Phi M| = \frac{1}{n} |\alpha \tilde{x}_i \tilde{x}_i^\top R \Phi M R^{(i)} \tilde{x}_i| \leq \frac{C\|\tilde{X}\|^2}{n}. \]
Applying Lemma D.4(b), with probability $1 - 2e^{-cn}$, this is at most $C/n$ for every $i \in \{1, \ldots, \tilde{d}\}$. Similarly, $|\text{tr}(R^{(i)} - R) \Phi| \leq C/n$ with this probability. Applying again $|\text{tr} R \Phi M| \leq C$, $|\alpha^{-1} + \gamma \text{tr} R \Phi| \geq c$, and an argument similar to (41), we obtain $|J_2^{(i)}| \leq C'/n$ for a constant $C' > 0$. Taking a union bound over $i \in \{1, \ldots, \tilde{d}\}$, this yields $\mathbb{P}[|J_2| > C/n] \leq C'ne^{-cn}$. Combining these bounds for $J_1$ and $J_2$, choosing $t > cn^{-1}$, and re-adjusting the constants yields the lemma. \qed
E.3 Proof of Lemma E.2

We now prove Lemma E.2 using Lemma E.5. Define the random $n$-dependent parameter

$$s = \alpha^{-1} + \gamma \text{tr} \Phi,$$

so that $\bar{s} = \mathbb{E}[s]$. The following establishes concentration of $s$ around $\bar{s}$.

**Lemma E.6.** Under Assumption E.1, for some constants $c, n_0 > 0$, all $n \geq n_0$, and any $t > 0$,

$$\mathbb{P}[|s - \bar{s}| > t] \leq 2e^{-cnt^2}.$$

**Proof.** Define $F(W) = \gamma \text{tr} \Phi$, where $R$ and $\tilde{X}$ are considered as a function of $W$. Fix any matrices $W, \Delta \in \mathbb{R}^{d \times n}$ where $\|\Delta\|_F = 1$, and define $W_t = W + t\Delta$. Then, applying $\partial R = -R(\partial(R^{-1}))R$ and $R = R^\top$,

$$\vec(\Delta)^\top(\nabla F(W)) = \left| \frac{d}{dt} \right|_{t=0} F(W_t) = -\gamma \text{tr} R \left( \left| \frac{d}{dt} \right|_{t=0} R^{-1} \right) R\Phi$$

$$= -2\gamma \alpha \text{tr} R^{\top} \left( \frac{d}{dt} \right|_{t=0} R \tilde{X}^{\top} \right) R\Phi$$

$$= -2\gamma \alpha \sqrt{\frac{d}{\beta}} \text{tr} \left( R^{\top} \cdot (\sigma'(WX) \odot (\Delta X)) \right) R\Phi,$$

where $\odot$ is the Hadamard product, and $\sigma'$ is applied entrywise. Applying Proposition E.3,

$$\left| \vec(\Delta)^\top(\nabla F(W)) \right| \leq \frac{C}{\sqrt{d}} \cdot \|R\tilde{X}^{\top} \cdot (\sigma'(WX) \odot (\Delta X)) \cdot R\| \leq \frac{C'}{\sqrt{d}} \cdot \|R\tilde{X}^{\top}\| \cdot \|\sigma'(WX) \odot (\Delta X)\|.$$

For the first term,

$$\|R\tilde{X}^{\top}\|^2 = \frac{1}{|\alpha|} \|R(\alpha \tilde{X}^{\top} \tilde{X})R^*\| \leq \frac{1}{|\alpha|} \left( \|R(A + \alpha \tilde{X}^{\top} \tilde{X} - z \text{Id})R^*\| + \|R(A - z \text{Id})R^*\| \right)$$

$$\leq \frac{1}{|\alpha|}(\|R\| + \|R\|^2(\|A\| + |z|)) \leq C.$$

For the second term,

$$\|\sigma'(WX) \odot (\Delta X)\| \leq \|\sigma'(WX) \odot (\Delta X)\|_F \leq \lambda_{\sigma}\|\Delta X\|_F \leq \lambda_{\sigma}\|\Delta\|_F \cdot \|X\| \leq C.$$

Thus $|\vec(\Delta)^\top(\nabla F(W))| \leq C/\sqrt{n}$. This holds for every $\Delta$ such that $\|\Delta\|_F = 1$, so $F(W)$ is $C/\sqrt{n}$-Lipschitz in $W$ with respect to the Frobenius norm. Then the result follows from Gaussian concentration of measure. \hfill \Box

To conclude the proof of Lemma E.2, we may again assume $\|M\| \leq 1$ by rescaling $M$. Set

$$\tilde{M} = (A + \bar{s}^{-1} \Phi - z \text{Id})^{-1} M.$$

Note that $\bar{s}^{-1} \in \mathbb{C}^-$, so $\|\tilde{M}\| \leq \|(A + \bar{s}^{-1} \Phi - z \text{Id})^{-1}\| \leq C$ by Proposition C.2. Applying Lemma E.5 with $\tilde{M}$,

$$\mathbb{P} \left[ \text{tr} \tilde{M} - \text{tr} R \left( A + s^{-1} \Phi - z \text{Id} \right) \tilde{M} > t \right] \leq Cne^{-cnt^2} \quad (42)$$

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for all $t \in (n^{-1}, c_0)$. Furthermore, applying the definition of $\tilde{M}$,
\[
|\text{tr} R (A + s^{-1}\Phi - z \text{Id}) \tilde{M} - \text{tr} RM| = |\text{tr} R ((A + s^{-1}\Phi - z \text{Id}) - (A + \bar{s}^{-1}\Phi - z \text{Id})) \tilde{M}| = |s^{-1} - \bar{s}^{-1}| \cdot |\text{tr} R\Phi \tilde{M}| \leq C|s^{-1} - \bar{s}^{-1}|.
\]
Recall that $|\bar{s}| \geq \text{Im} \bar{s} \geq c$. Then, on the event where $|s - \bar{s}| \leq t$ and $t < c/2$, we have $|s^{-1} - \bar{s}^{-1}| \leq Ct$. Then applying Lemma E.6 for some constants $c, c_0 > 0$ and all $t \in (0, c_0)$,
\[
\mathbb{P}\left[|\text{tr} R (A + s^{-1}\Phi - z \text{Id}) \tilde{M} - \text{tr} RM| > t\right] \leq 2e^{-cnt^2}.
\]
Combining this with (42) yields Lemma E.2(a). Specializing Lemma E.2(a) to $M = \Phi$, we obtain
\[
\mathbb{P}\left[|s - (\alpha^{-1} + \gamma \text{tr}(A + \bar{s}^{-1}\Phi - z \text{Id})^{-1}\Phi)| > t\right] \leq Cn e^{-cnt^2}.
\]
Applying again Lemma E.6 to bound $|s - \bar{s}|$, we obtain Lemma E.2(b).

\section{Analysis for the Conjugate Kernel}

Theorem 3.4 is a special case of Theorem 3.7, but let us provide here a simpler argument. Define, for each layer, the $n \times n$ matrices
\[
\Phi_\ell = \mathbb{E}_w\left[\sigma(w^T X_{\ell-1})^\top \sigma(w^T X_{\ell-1})\right] \\
\tilde{\Phi}_\ell = b_\sigma^2 X_{\ell-1}^\top X_{\ell-1} + (1 - b_\sigma^2) \text{Id}
\]
where $\mathbb{E}_w$ denotes the expectation over only the random vector $w \sim \mathcal{N}(0, \text{Id})$. Here, $\Phi_\ell, \tilde{\Phi}_\ell$ are deterministic conditional on $X_{\ell-1}$, but are random unconditionally for $\ell \geq 2$. For each fixed $\ell = 1, \ldots, L$, we will show
\[
\lim \text{spec} \Phi_\ell = \lim \text{spec} \tilde{\Phi}_\ell. 
\]
Conditioned on $X_{\ell-1}$, the spectral limit of $X_{\ell}^\top X_{\ell}$ was shown in [LLC18] to be a Marčenko-Pastur map of the spectral limit of $\Phi_\ell$—we reproduce a short proof below under our assumptions, by specializing Lemma E.2 to $\alpha = 1$ and $A = 0$. Combining with (45) and iterating from $\ell = 1, \ldots, L$ yields Theorem 3.4.

\textbf{Lemma F.1.} \textit{Under Assumption 3.2, for each $\ell = 1, \ldots, L$, almost surely as $n \to \infty$,}
\[
\frac{1}{n}\|\Phi_\ell - \tilde{\Phi}_\ell\|_F^2 \to 0.
\]
\textbf{Proof.} By Corollary D.2, increasing $(\varepsilon_n, B)$ as needed, we may assume that each matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal. Denote by $\Phi_\ell[\alpha, \beta]$ and $\tilde{\Phi}_\ell[\alpha, \beta]$ the $(\alpha, \beta)$ entries of these matrices. Then Lemma D.3(a) shows for $\alpha \neq \beta$ that
\[
|\Phi_\ell[\alpha, \beta] - \tilde{\Phi}_\ell[\alpha, \beta]| \leq C\varepsilon_n^2.
\]
For $\alpha = \beta$, applying $\tilde{\Phi}_\ell[\alpha, \alpha] = 1 - b_\sigma^2 + b_\sigma^2\|x_{\alpha-1}\|^2$, we have
\[
|\Phi_\ell[\alpha, \alpha] - \tilde{\Phi}_\ell[\alpha, \alpha]| \leq |\Phi_\ell[\alpha, \alpha] - 1| + b_\sigma^2\|x_{\alpha-1}\|^2 - 1| \leq C\varepsilon_n.
\]
Then
\[
\|\Phi_\ell - \tilde{\Phi}_\ell\|_F^2 \leq Cn(n-1)\varepsilon_n^4 + Cn\varepsilon_n^2,
\]
and the result follows from the condition $\varepsilon_n n^{1/4} \to 0$. \hfill $\square$
Proof of Theorem 3.4. By Corollary D.2, we may assume that each matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal. This implies the bounds $\|X_\ell\| \leq C$ and $\|K^{CK}\| \leq C$ for all large $n$.

For the spectral convergence, suppose by induction that $\lim \text{spec } X_{\ell-1}^\top X_{\ell-1} = \mu_{\ell-1}$, where the base case $\lim \text{spec } X_0^\top X_0 = \mu_0$ holds by assumption. Defining

$$\nu_\ell = (1 - b_\sigma^2) + b_\sigma^2 \cdot \mu_{\ell-1},$$

Proposition C.3 and Lemma F.1 together show that

$$\lim \text{spec } \Phi_\ell = \lim \text{spec } \tilde{\Phi}_\ell = \nu_\ell.$$ Specializing Lemma E.2(b) to the setting $A = 0, \alpha = 1, X = X_{\ell-1}$, and $\tilde{X} = X_\ell$, and choosing $t \equiv t_n$ such that $t_n \to 0$ and $nt_n^2 \gg \log n$, we obtain

$$|\bar{s} - 1 - (n/d_\ell) \operatorname{tr}(\bar{s}^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell| \to 0$$

a.s. as $n \to \infty$, where

$$\bar{s} = 1 + \frac{n}{d_\ell} \mathbb{E}_{W_\ell}[\operatorname{tr}(X_\ell^\top X_\ell - z \operatorname{Id})^{-1}\Phi_\ell].$$

Here, this expectation is taken over only $W_\ell$ (i.e., conditional on $X_0, \ldots, X_{\ell-1}$).

Proposition E.3 verifies that $\bar{s}$ is bounded as $n \to \infty$, so for any subsequence in $n$, there is a further sub-subsequence along which $\bar{s} \to s_0$ for a limit $s_0 \equiv s_0(z) \in \mathbb{C}^\sigma$. Applying $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$ and Propositions C.2 and E.3

$$|\operatorname{tr}(\bar{s}^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell - \operatorname{tr}(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell|$$

$$= |s_0^{-1} - s^{-1}| \cdot |(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell(\bar{s}^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell|$$

$$\leq |s_0^{-1} - s^{-1}| \cdot \|(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\| \cdot \|(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell\|^2$$

$$\leq C|s_0^{-1} - s^{-1}|.$$

Thus, along the sub-subsequence where $\bar{s} \to s_0$, we get

$$\operatorname{tr}(\bar{s}^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell - \operatorname{tr}(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell \to 0.$$ (46)

We have also

$$\operatorname{tr}(s_0^{-1}\Phi_\ell - z \operatorname{Id})^{-1}\Phi_\ell \to \int \frac{x}{s_0^{-1}x - z} d\nu_\ell(x),$$ (48)

since the function $x \mapsto x/(s_0^{-1}x - z)$ is continuous and bounded over $\mathbb{R}$, and $\lim \text{spec } \Phi_\ell = \nu_\ell$. Thus, taking the limit of (46) along this sub-subsequence, the value $s_0$ must satisfy

$$s_0 - 1 - \gamma_\ell \int \frac{x}{s_0^{-1}x - z} d\nu_\ell(x) = 0.$$ (49)

Now applying Lemma E.2(a) with $M = \operatorname{Id}$, and taking the limit along this sub-subsequence, by a similar argument we obtain that

$$\operatorname{tr}(X_\ell^\top X_\ell - z \operatorname{Id})^{-1} \to \int \frac{1}{s_0^{-1}x - z} d\nu_\ell(x).$$ (50)
Denoting this limit by \( m_\ell(z) \), and rewriting \([49]\) by applying
\[
\int \frac{x}{s_0^{-1}x - z} d\nu_\ell(x) = s_0 \int \left( 1 + \frac{z}{s_0^{-1}x - z} \right) d\nu_\ell(x) = s_0 (1 + zm_\ell(z)),
\]
we get \( s_0^{-1} = 1 - \gamma_\ell - \gamma_\ell zm_\ell(z) \). Applying this back to the definition of \( m_\ell(z) \) in \([50]\), this shows that \( m_\ell(z) \) satisfies the Marcenko-Pastur equation
\[
m(z) = \int \frac{1}{x(1 - \gamma_\ell - \gamma_\ell zm(z)) - z} d\nu_\ell(x),
\]
so \( m_\ell(z) \) is the Stieltjes transform of \( \mu_\ell = \rho_{\gamma_\ell}^{\text{MP}} \otimes \nu_\ell = \rho_{\gamma_\ell}^{\text{MP}} \otimes ((1 - b^2_\sigma) + b^2_\sigma \cdot \mu_{\ell-1}) \).

We have shown that \( \text{tr}(X_\ell^\top X_\ell - z \text{Id})^{-1} \to m_\ell(z) \) almost surely along this sub-subsequence in \( n \). Since, for every subsequence in \( n \), there exists such a sub-subsequence, this implies \( \lim_{n \to \infty} \text{tr}(X_\ell^\top X_\ell - z \text{Id})^{-1} = m_\ell(z) \) almost surely. Thus \( \lim \text{spec} X_\ell^\top X_\ell = \mu_\ell \), which completes the induction. \( \square \)

G Analysis for the Neural Tangent Kernel

G.1 Spectral approximation and operator norm bound

We first prove the spectral approximation stated in Lemma 3.5, as well as the operator norm bound \( \| K^{\text{NTK}} \| \leq C \). The following form of \( K^{\text{NTK}} \) is derived also in [HY19, Eq. (1.7)]: Denote by \( x_\alpha^\ell \) the \( \alpha \)th column of \( X_\ell \). For each \( \ell = 1, \ldots, L \), define the matrix \( S_\ell \in \mathbb{R}^{d_\ell \times n} \) whose \( \alpha \)th column is given by
\[
s_\alpha^\ell = D_\alpha^\ell W_\ell^\top \frac{W_{\ell+1}^\top}{\sqrt{d_\ell}} D_\alpha^{\ell+1} \frac{W_{\ell+2}^\top}{\sqrt{d_{\ell+1}}} \cdots \frac{W_L^\top}{\sqrt{d_L}} D_\alpha^L \frac{w}{\sqrt{d_L}},
\]
where we define diagonal matrices indexed by \( \alpha \in [n] \) and \( k \in [L] \) as
\[
D_k^\alpha \equiv \text{diag} \left( \sigma'(W_k x_\alpha^{k-1}) \right) \in \mathbb{R}^{d_\alpha \times d_k}.
\]
Applying the chain rule, we may verify for each input sample \( x_\alpha \) that
\[
\nabla_w f_\theta(x_\alpha) = x_\alpha^L \in \mathbb{R}^{d_L}, \quad \nabla_{W_\ell} f_\theta(x_\alpha) = s_\alpha^\ell \otimes x_\alpha^{\ell-1} \in \mathbb{R}^{d_\ell d_{\ell-1}}.
\]
Then
\[
\nabla_w f_\theta(X) = X_L^\top X_L, \quad \nabla_{W_\ell} f_\theta(X) = (S_\ell^\top S_\ell) \odot (X_{\ell-1}^\top X_{\ell-1}),
\]
where \( \odot \) is the Hadamard product. Thus, the NTK is given by
\[
K^{\text{NTK}} = \left( \nabla_\theta f_\theta(X) \right)^\top \left( \nabla_\theta f_\theta(X) \right) = X_L^\top X_L + \sum_{\ell=1}^L (S_\ell^\top S_\ell) \odot (X_{\ell-1}^\top X_{\ell-1}).
\]

Lemma G.1. Let \( X \in \mathbb{R}^{d \times n} \) be \((\varepsilon, B)\)-orthonormal, let \( W \in \mathbb{R}^{d \times d} \) have i.i.d. \( \mathcal{N}(0,1) \) entries, and let \( x_\alpha, x_\beta \) be two columns of \( X \) where \( \alpha \neq \beta \). Then for universal constants \( C, c > 0 \) and any \( t > 0 \):

(a) With probability at least \( 1 - 2e^{-cd^2} \),
\[
\left| \frac{1}{d} \text{Tr} \left( \text{diag} \left( \sigma'(W x_\alpha) \right) \text{diag} \left( \sigma'(W x_\beta) \right) \right) - b_\sigma^2 \right| \leq C\lambda_\sigma^2(\varepsilon + t).
\]
(b) Let $M \in \mathbb{R}^{d \times d}$ be any deterministic symmetric matrix, and denote

$$T(x_\alpha, x_\beta) = \frac{1}{d} \text{Tr} \left( \text{diag} \left( \sigma'(Wx_\alpha) \right) W MW^\top \text{diag} \left( \sigma'(Wx_\beta) \right) \right).$$

With probability at least $1 - (2d + 2)e^{-c \min(t^2 d, t \sqrt{d})}$,

$$|T(x_\alpha, x_\beta) - b_\sigma^2 \text{Tr} M| \leq C \lambda_\sigma^2 \left( \varepsilon \sqrt{d} + t \sqrt{d} + t \sqrt{d} \right) \|M\|_F.$$

Furthermore, both (a) and (b) hold with $(x_\alpha, x_\alpha)$ in place of $(x_\alpha, x_\beta)$, upon replacing $b_\sigma^2$ by $a_\sigma$.

Proof. Write $w_k^\top \in \mathbb{R}^d$ for the $k$th row of $W$. Then

$$\frac{1}{d} \text{Tr} \left( \text{diag} \left( \sigma'(Wx_\alpha) \right) \text{diag} \left( \sigma'(Wx_\beta) \right) \right) = \frac{1}{d} \sum_{k=1}^d \sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta).$$

Applying $\sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta) \in [-\lambda_\sigma^2, \lambda_\sigma^2]$ and Hoeffding’s inequality,

$$\mathbb{P} \left[ \frac{1}{d} \sum_{k=1}^d \left( \sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta) - \mathbb{E} \left[ \sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta) \right] \right) > \lambda_\sigma^2 t \right] \leq 2e^{-ct^2}.$$

To bound the mean, recall that $(\zeta_\alpha, \zeta_\beta) \equiv (w_k^\top x_\alpha, w_k^\top x_\beta)$ is bivariate Gaussian, which we may write as

$$\zeta_\alpha = u_\alpha \xi_\alpha, \quad \zeta_\beta = u_\beta \xi_\beta + v_\beta \xi_\alpha$$

as in (27). Here, $\xi_\alpha, \xi_\beta \sim \mathcal{N}(0, 1)$ are independent, $u_\alpha, u_\beta > 0$ and $v_\beta \in \mathbb{R}$, and these satisfy $|u_\alpha - 1|, |u_\beta - 1|, |v_\beta| \leq C \varepsilon$. Applying the Taylor expansion

$$\sigma'(\zeta) = \sigma'(\xi) + \sigma''(\eta)(\zeta - \xi)$$

for some $\eta$ between $\zeta$ and $\xi$, and the conditions $\mathbb{E}[\sigma'(\xi)] = b_\sigma$ and $|\sigma''(x)| \leq \lambda_\sigma$, it is easy to check that $|\mathbb{E}[\sigma'(\zeta_\alpha) \sigma'(\zeta_\beta)] - b_\sigma^2| \leq C \lambda_\sigma^2 \varepsilon$. Then part (a) follows. The statement with $(x_\alpha, x_\alpha)$ and $a_\sigma$ follows similarly from this Taylor expansion and the bound $|\mathbb{E}[\sigma'(\zeta_\alpha)^2] - a_\sigma| \leq C \lambda_\sigma^2 \varepsilon$.

For part (b), we write

$$T(x_\alpha, x_\beta) = \frac{1}{d} \sum_{k=1}^d \sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta) \cdot w_k^\top M w_k.$$

By the Hanson-Wright inequality (see [RV13 Theorem 1.1]),

$$\mathbb{P} \left[ \|w_k^\top M w_k - \text{Tr} M\|_F > \|M\|_F \cdot t \sqrt{d} \right] \leq 2e^{-c \min(t^2 d, t \sqrt{d})}$$

for a constant $c > 0$. Then, applying $|\sigma'(x)| \leq \lambda_\sigma$ and a union bound over $k = 1, \ldots, d$, with probability at least $1 - 2de^{-c \min(t^2 d, t \sqrt{d})}$,

$$|T(x_\alpha, x_\beta) - \text{Tr} M \cdot \frac{1}{d} \sum_{k=1}^d \sigma'(w_k^\top x_\alpha) \sigma'(w_k^\top x_\beta)| \leq \|M\|_F \cdot \lambda_\sigma^2 t \sqrt{d}.$$

Then part (b) follows from combining with part (a), and applying $\text{Tr} M \leq \sqrt{d} \|M\|_F$. \qed
Corollary G.2. Let $s_\ell^\ell$ be as defined in (51), and let $q_\ell, r_\ell$ be the constants in (7). Under Assumption 3.2 for a constant $C > 0$, almost surely for all large $n$ and for all $\ell \in [L]$ and $\alpha \neq \beta \in [n],$

$$\left| s_\alpha^\ell s_\beta^\ell - q_{\ell-1} \right| \leq C \max(\varepsilon_n, n^{-0.48}), \quad \|s_\alpha^\ell\|^2 - r_{\ell-1} \leq C \max(\varepsilon_n, n^{-0.48}).$$

(53)

Proof. By Corollary D.2 we may assume that each matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal. Since a larger value of $\varepsilon_n$ corresponds to a weaker assumption, we may assume without loss of generality that $\varepsilon_n \geq n^{-0.48}$.

Fix $\ell \in [L]$ and $\alpha, \beta \in [n]$, and define

$$M_\ell = D_\alpha^\ell D_\beta^\ell$$

$$M_k = D_\alpha^k \frac{W_k}{\sqrt{d_{k-1}}} \cdots D_\alpha^{\ell+1} \frac{W_{\ell+1}}{\sqrt{d_\ell}} D_\beta^{\ell} \frac{W_{\ell+1}}{\sqrt{d_\ell}} D_\beta^{\ell+1} \cdots \frac{W_{k}}{\sqrt{d_{k-1}}} D_\beta^k \quad \text{for} \quad \ell + 1 \leq k \leq L. \quad (54)$$

Recalling the definition (51) and applying the Hanson-Wright inequality conditional on $W_1, \ldots, W_L,$

$$\left| s_\alpha^\ell s_\beta^\ell - \frac{1}{d_L} \Tr M_\ell \right| \leq C \varepsilon_n \sqrt{n} \cdot \frac{1}{d_L} \|M_\ell\|_F \quad (55)$$

with probability $1 - e^{-c \min(\varepsilon_n^n, \varepsilon_n \sqrt{n})} \geq 1 - e^{-n^{0.01}}$. Next, for each $k = L, L-1, \ldots, \ell + 1$, we apply Lemma G.1(b) conditional on $W_1, \ldots, W_{k-1},$ with $t = \varepsilon_n, M = M_{k-1}/d_{k-1}, d = d_{k-1},$ and $\bar{d} = d_k + 1.$ Note that $k - 1 \geq \ell \geq 1$, so that both $d_{k-1}$ and $d_k$ are proportional to $n$. Then

$$\left| \frac{1}{d_k} \Tr M_k - b_\alpha^2 \cdot \frac{1}{d_{k-1}} \Tr M_{k-1} \right| \leq C \varepsilon_n \sqrt{n} \cdot \frac{1}{d_{k-1}} \|M_{k-1}\|_F$$

with probability $1 - e^{-n^{0.01}}$. Finally, for $k = \ell$, applying Lemma G.1(a) conditional on $W_1, \ldots, W_{\ell-1}$ and with $t = \varepsilon_n,$

$$\left| \frac{1}{d_\ell} \Tr M_\ell - b_\alpha^2 \right| \leq C \varepsilon_n$$

with probability $1 - e^{-n^{0.01}}$. Combining these bounds, with probability $1 - C'e^{-n^{0.01}},$

$$\left| s_\alpha^\ell s_\beta^\ell - (b_\alpha^2)^{L-\ell+1} \right| \leq C \varepsilon_n \sqrt{n} \left( \|M_\ell\|_F + \ldots + \|M_k\|_F + \sqrt{n} \right).$$

We also have $\|W_k/\sqrt{d_k}\| \leq C$ for each $k = 2, \ldots, L$ with probability $1 - C'e^{-cn}$, see e.g. Ver18 Theorem 4.4.5). Then, applying $\|D_k\| \leq \lambda_\sigma$, we have $\|M_k\| \leq C' \sqrt{n} \|M_k\| \leq C' \sqrt{n}$ for every $k = 1, \ldots, L$. Then the first bound of (53) follows. The second bound of (53) is the same, applying Lemma G.1 for $(x_\alpha, x_\beta)$ instead of $(x_\alpha, x_\beta)$. The almost sure statement follows from Borel-Cantelli. 

Lemma G.3. Under Assumption 3.2, almost surely as $n \to \infty,$

$$\frac{1}{n} \left\| K^{NTK} - \left( r_+ \Id + X_L^\ell X_L + \sum_{\ell=0}^{L-1} q_{\ell} X_{\ell}^\ell X_{\ell} \right) \right\|_F^2 \to 0.$$

Furthermore, for a constant $C > 0$, almost surely for all large $n, \|K^{NTK}\| \leq C.$
Proof. By Corollary [D.2] we may assume that each matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal. Then

$$\left| x^{\ell-1}_i x^{\ell-1}_j \right| \leq \varepsilon_n, \quad \|x^{\ell-1}_i\|^2 - 1 \leq \varepsilon_n.$$ 

Increasing $\varepsilon_n$ if necessary, we may assume $\varepsilon_n \geq n^{-0.48}$. Combining with (53), we have for the off-diagonal entries of the Hadamard product that

$$\left| (S^{T}_\ell S_{\ell}) \odot (X^{T}_{\ell-1}X_{\ell-1}) \right| \leq C\varepsilon_n^2,$$

and for the diagonal entries that

$$\left| (S^{T}_\ell S_{\ell}) \odot (X^{T}_{\ell-1}X_{\ell-1}) \right| \leq C\varepsilon_n.$$

Then applying this to (52),

$$\left\| K^{NTK} - \left( r_+ \text{Id} + X_L^T X_L + \sum_{\ell=0}^{L-1} q_{\ell} X_{\ell}^T X_{\ell} \right) \right\|_F^2 \leq Cn(n-1)\varepsilon_n^4 + Cn\varepsilon_n^2.$$

The first statement of the lemma then follows from the assumption $\varepsilon_n n^{1/4} \to 0$.

For the second statement on the operator norm, we have

$$\| (S^{T}_\ell S_{\ell}) \odot (X^{T}_{\ell-1}X_{\ell-1}) \| \leq \max_{\ell=1}^{n} \left| s^{T}_\alpha s^{\ell}_\alpha \right| \cdot \| X^{T}_{\ell-1}X_{\ell-1} \|.$$

See [Joh90, Eq. (3.7.9)], applied with $X = Y = S_{\ell}$. Then $\|K^{NTK}\| \leq C$ follows from (52), the $(\varepsilon_n, B)$-orthonormality of each matrix $X_{\ell-1}$, and the bound for the diagonal entries of $S_{\ell}$ in (53).

Combining Lemma [G.3] and Proposition [C.3] this proves Lemma [3.5].

G.2 Unique solution of the fixed-point equation

Let $A, \Phi \in \mathbb{R}^{n \times n}$ be symmetric matrices, where $\Phi$ is positive semi-definite. Let $z \in \mathbb{C}^+$, $\alpha \in \mathbb{C}^*$, and $\gamma > 0$. For $s \in \mathbb{C}^+$, define

$$S(s) = (A + s^{-1} \Phi - z \text{Id})^{-1}, \quad f_n(s) = \alpha^{-1} + \gamma \text{tr} S(s) \Phi.$$ 

Lemma G.4. (a) For any $s \in \mathbb{C}^+$, setting $S \equiv S(s)$,

$$\text{Im } f_n(s) \geq \text{Im } z \cdot \gamma \text{tr } S \Phi S^* \geq 0.$$ 

(b) For any $s_1, s_2 \in \mathbb{C}^+$, setting $S_1 \equiv S(s_1)$ and $S_2 \equiv S(s_2)$,

$$\left| f_n(s_1) - f_n(s_2) \right| \leq |s_1 - s_2| \cdot \left( \frac{\text{Im } f_n(s_1) - \text{Im } z \cdot \gamma \text{tr } S_1 \Phi S_1^*}{\text{Im } s_1} \right)^{1/2} \left( \frac{\text{Im } f_n(s_2) - \text{Im } z \cdot \gamma \text{tr } S_2 \Phi S_2^*}{\text{Im } s_2} \right)^{1/2}$$

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Dropping Im $\alpha$

Let us first show that for each $\Phi$

Proof. For part (a), let us write

\[ S\Phi = S\Phi S^*(A + s^{-1}\Phi - z\text{Id})^* = S\Phi S^*A + (1/s^*)S\Phi S^*\Phi - z^*S\Phi S^*. \]

Since $S\Phi S^*$ is Hermitian and positive semi-definite, the quantities $\text{tr} S\Phi S^* A$, $\text{tr} S\Phi S^* \Phi$, and $\text{tr} S\Phi S^*$ are all real, and the latter two are nonnegative. Then

\[ \text{Im} f_n(s) = \text{Im} \alpha^{-1} + \gamma \text{Im} \text{tr} S\Phi = \text{Im} \alpha^{-1} + \frac{\text{Im}s}{|s|^2} \cdot \gamma \text{tr} S\Phi S^* \Phi + \text{Im} z \cdot \gamma \text{tr} S\Phi S^*. \] (56)

Each term on the right side of (56) is nonnegative, and dropping the first two of these terms yields (a).

For part (b), applying the identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$, we have

\[ S_1 - S_2 = S_1(s_2^{-1}\Phi - s_1^{-1}\Phi)S_2 = \frac{s_1 - s_2}{s_1 s_2} S_1 \Phi S_2, \]

so

\[ f_n(s_1) - f_n(s_2) = \gamma \text{tr} S_1 \Phi - \gamma \text{tr} S_2 \Phi = \frac{\gamma (s_1 - s_2)}{s_1 s_2} \text{tr} S_1 \Phi S_2 \Phi. \]

Applying Cauchy-Schwarz to the inner-product $\langle S_1, S_2 \rangle_{\Phi} = \text{tr} S_1 \Phi S_2^* \Phi$,

\[ |\text{tr} S_1 \Phi S_2 \Phi|^2 = |\langle S_1, S_2 \rangle_{\Phi}|^2 \leq \langle S_1, S_1 \rangle_{\Phi} \cdot \langle S_2, S_2 \rangle_{\Phi} = \text{tr} S_1 \Phi S_1^* \Phi \cdot \text{tr} S_2 \Phi S_2^* \Phi. \]

Then

\[ |f_n(s_1) - f_n(s_2)| \leq |s_1 - s_2| \cdot \left( \frac{\gamma \text{tr} S_1 \Phi S_1^* \Phi}{|s_1|^2} \right)^{1/2} \left( \frac{\gamma \text{tr} S_2 \Phi S_2^* \Phi}{|s_2|^2} \right)^{1/2}. \]

Dropping Im $\alpha^{-1}$ in (56) and applying this to upper-bound $\gamma \text{tr} S\Phi S^* \Phi/|s|^2$, part (b) follows. \(\square\)

**Corollary G.5.** As $n \to \infty$, suppose that $f_n(s) \to f(s)$ pointwise for each $s \in \mathbb{C}^+$, the empirical spectral distributions of $\Phi$ and $A$ converge weakly to deterministic limits, and the limit for $\Phi$ is not the point distribution at 0. Then the fixed-point equation $s = f(s)$ has at most one solution $s \in \mathbb{C}^+$.

Proof. Let us first show that for each $s \in \mathbb{C}^+$ and a value $c_0(s) > 0$ independent of $n$,

\[ \liminf_{n \to \infty} \text{tr} S(s) \Phi S^*(s) \geq c_0(s) > 0. \] (57)

Denoting $S \equiv S(s)$ and applying the von Neumann trace inequality,

\[ \text{tr} S\Phi S^* = \frac{1}{n} \text{Tr} S^* S \geq \frac{1}{n} \sum_{\alpha=1}^n \lambda_{\alpha}(\Phi) \lambda_{n+1-\alpha}(S^* S), \]

where $\lambda_1(\cdot) \geq \ldots \geq \lambda_n(\cdot)$ denote the sorted eigenvalues. Since $\Phi$ has a non-degenerate limit spectrum, there is a constant $\varepsilon > 0$ for which $\lambda_{\varepsilon n}(\Phi) > \varepsilon$ for all large $n$. (Throughout the proof, $\varepsilon n$, $\varepsilon n/2$, etc. should be understood as their roundings to the nearest integer.) Then

\[ \text{tr} S\Phi S^* \geq \varepsilon \cdot \frac{1}{n} \sum_{\alpha=1}^{\varepsilon n} \lambda_{n+1-\alpha}(S^* S). \]

Denoting by $\sigma_{\alpha}(\cdot)$ the $\alpha^{\text{th}}$ largest singular value, observe that

\[ \lambda_{n+1-\alpha}(S^* S) = \sigma_{n+1-\alpha}(S) = \sigma_{\alpha}(A + s^{-1}\Phi - z \text{Id})^{-2}. \]
Applying $\sigma_{\alpha+\beta}(A + B) \leq \sigma_{\alpha}(A) + \sigma_{\beta}(B)$, we have
\[
\sigma_{\alpha}(A + s^{-1}\Phi - z \text{Id}) \leq \sigma_{\alpha/2}(A) + |s|^{-1}\sigma_{\alpha/2+1}(\Phi) + |z|.
\]
Since the spectra of $A$ and $\Phi$ converge to deterministic limits, this implies that there is a constant $C(s) > 0$ (also depending on $z$ and $\varepsilon$) such that $\sigma_{\alpha}(A + s^{-1}\Phi - z \text{Id}) \leq C(s)$ for every $\alpha \in [\varepsilon n/2, \varepsilon n]$ and all large $n$. Thus
\[
\text{tr } S \Phi S^* \geq \varepsilon \cdot \frac{\varepsilon n - \varepsilon n/2}{n} \cdot C(s)^{-2}
\]
for all large $n$, and this shows the claim \([57]\).

Then, taking the limit $n \to \infty$ in Lemma \([G.4]\)(b), we get
\[
|f(s_1) - f(s_2)| \leq |s_1 - s_2| \cdot \left( \frac{\text{Im } f(s_1) - \text{Im } z \cdot \gamma c_0(s_1)}{\text{Im } s_1} \right)^{1/2} \left( \frac{\text{Im } f(s_2) - \text{Im } z \cdot \gamma c_0(s_2)}{\text{Im } s_2} \right)^{1/2}.
\]
If $s_1 = f(s_1)$ and $s_2 = f(s_2)$, then this yields $|s_1 - s_2| \leq |s_1 - s_2| \cdot h(s_1, s_2)$ for some quantity $h(s_1, s_2) \in [0, 1)$, where $h(s_1, s_2) < 1$ strictly because $c_0(s_1), c_0(s_2) > 0$. This implies $s_1 = s_2$, so the equation $s = f(s)$ has at most one solution $s \in \mathbb{C}^+$.

**G.3 Proof of Proposition 3.6 and Theorem 3.7**

The operator norm bound in Theorem 3.7 was shown in Lemma G.3. For the spectral convergence, note that by Lemma 3.5, the limit Stieltjes transform of $K_{\text{NTK}}$ at any $z \in \mathbb{C}^+$ is given by
\[
m_{\text{NTK}}(z) = \lim_{n \to \infty} \text{tr } \left( (-z + r_+) \text{Id} + X_L^\top X_L + \sum_{\ell=0}^{L-1} q_{\ell} X_\ell^\top X_\ell \right)^{-1},
\]
provided that this limit exists and defines the Stieltjes transform of a probability measure. For $z = (z_{-1}, \ldots, z_L) \in \mathbb{C}^- \times \mathbb{R}^L \times \mathbb{C}^*$, $w = (w_{-1}, \ldots, w_L) \in \mathbb{C}^{L+2}$, recall the functions
\[
z \mapsto s_\ell(z), \quad (z, w) \mapsto t_\ell(z, w)
\]
defined recursively by \([12]\) and \([13]\). Proposition 3.6 and Theorem 3.7 are immediate consequences of the following extended result.

**Lemma G.6.** Under Assumption 3.2, for each $\ell = 1, \ldots, L$:

(a) For every $z \in \mathbb{C}^- \times \mathbb{R}^L \times \mathbb{C}^*$, the equation \([12]\) has a unique fixed point $s_\ell(z) \in \mathbb{C}^+$.

(b) For every $(z, w) \in (\mathbb{C}^- \times \mathbb{R}^L \times \mathbb{C}^*) \times \mathbb{C}^{L+2}$, almost surely
\[
t_\ell(z, w)
= \lim_{n \to \infty} \text{tr } \left( z_{-1} \text{Id} + z_0 X_0^\top X_0 + \ldots + z_L X_L^\top X_L \right)^{-1} \left( w_{-1} \text{Id} + w_0 X_0^\top X_0 + \ldots + w_L X_L^\top X_L \right).
\]

In particular, for any $z_{-1}, \ldots, z_L \in \mathbb{R}$ where $z_\ell \neq 0$,
\[
\lim \text{spec } z_{-1} \text{Id} + z_0 X_0^\top X_0 + \ldots + z_L X_L^\top X_L = \nu
\]
where $\nu$ is a probability measure on $\mathbb{R}$ with Stieltjes transform
\[
m(z) = t_\ell((z_{-1} + z_0, \ldots, z_\ell), (1, 0, \ldots, 0)).
\]

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Proof. By Corollary \text{D.2}, we may assume that each matrix $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal.

Define $\Phi_\ell, \tilde{\Phi}_\ell$ by \eqref{eq:E.37} and \eqref{eq:E.38}. For $z = (z_1, \ldots, z_L)$, let us write as shorthand
\[ z \cdot X^\top X(\ell) = z_{-1} \text{Id} + z_0 X_0^\top X_0 + \ldots + z_L X_L^\top X_L, \]
where the parenthetical ($\ell$) signifies the index of the last term in this sum. Let us define similarly $w \cdot X^\top X(\ell)$.

Note that part (b) holds for $\ell = 0$, by the assumption $\lim \text{spec} X_0^\top X_0 = \mu_0$, the definition of $t_0((z_1, z_0), (w_1, w_0))$ in \eqref{eq:E.32}, and the fact that the function $x \mapsto (w_{-1} + w_0 x)/(z_{-1} + z_0 x)$ is continuous and bounded when $z_{-1} \in \mathbb{C}^-$ and $z_0 \in \mathbb{C}^*$.

We induct on $\ell$. Suppose that part (b) holds for $\ell - 1$. To show part (a) for $\ell$, fix any $z = (z_1, \ldots, z_L) \in \mathbb{C}^- \times \mathbb{R}^L \times \mathbb{C}^*$ (not depending on $n$) and consider the matrix
\[ R = \left( z \cdot X^\top X(\ell) \right)^{-1}. \] (59)

We apply the analysis of Appendix \text{E} conditional on $X_0, \ldots, X_{\ell-1}$, and with the identifications
\[ \tilde{X} = X_\ell, \quad X = X_{\ell-1}, \quad d = d_\ell, \quad d = d_{\ell-1}, \]
\[ A = z_0 X_0^\top X_0 + \ldots + z_{\ell-1} X_{\ell-1}^\top X_{\ell-1}, \quad \alpha = z_\ell, \quad z = -z_{-1}. \]
Observe that $\alpha \in \mathbb{C}^*$ and $z \in \mathbb{C}^-$. The matrix $R$ in (59) is exactly
\[ R = (A + \alpha \tilde{X}^\top \tilde{X} - z \text{Id})^{-1}. \]

Since each $X_0, \ldots, X_{\ell-1}$ is $(\varepsilon_n, B)$-orthonormal, we have $|A| \leq C$ for some constant $C > 0$ (depending on $z_1, \ldots, z_L, \lambda_\sigma$). Thus Assumption \text{E.1} holds, conditional on $X_0, \ldots, X_{\ell-1}$. Let us define the $n$-dependent parameter
\[ \bar{s} = \frac{1}{\alpha} + \frac{n}{d_\ell} \text{tr} E_{W_\ell} [R \Phi_\ell], \]
where this expectation is over only the weights $W_\ell$. Then, applying Lemma \text{E.2}(b) with a value $t \equiv t_n$ such that $t \to 0$ and $nt^2 \gg \log n$, we obtain
\[ \left| \bar{s} - \frac{1}{\alpha} - \frac{n}{d_\ell} \text{tr}(A + \bar{s}^{-1} \Phi_\ell - z \text{Id})^{-1} \Phi_\ell \right| \to 0 \] (60)
almost surely as $n \to \infty$.

Proposition \text{E.3} shows that $|\bar{s}|$ is bounded, so for any subsequence in $n$, there is a further subsequence where $\bar{s} \to s_0$ for a limit $s_0 \equiv s_0(z) \in \mathbb{C}^+$. Let us now replace $\bar{s}$ and $\Phi_\ell$ above by $s_0$ and $\tilde{\Phi}_\ell$: First we have
\[ \text{tr} \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} \tilde{\Phi}_\ell - \text{tr} \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} \tilde{\Phi}_\ell \to 0 \]
by the same argument as \eqref{eq:47}. Then, we have
\[ \left| \text{tr} \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} \tilde{\Phi}_\ell - \text{tr} \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} \tilde{\Phi}_\ell \right| \]
\[ = \left| s_0^{-1} \text{tr} \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} (\tilde{\Phi}_\ell - \Phi_\ell) \left( A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} \right)^{-1} \tilde{\Phi}_\ell \right| \]
\[ \leq \frac{C}{n} \| \tilde{\Phi}_\ell - \Phi_\ell \|_F \cdot \| (A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id})^{-1} \Phi (A + s_0^{-1} \Phi - z \text{Id})^{-1} \|_F \]
\[ \leq \frac{C}{\sqrt{n}} \| \tilde{\Phi}_\ell - \Phi_\ell \|_F \cdot \| (A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id})^{-1} \| \cdot \| \Phi \| \cdot \| (A + s_0^{-1} \Phi - z \text{Id})^{-1} \| \to 0, \]
where the convergence to 0 follows from Lemma G.3. Finally, we have

\[
\left| \text{tr} \left( A + s_0^{-1} \Phi_\ell - z \right) \right| - \text{tr} \left( A + s_0^{-1} \Phi_\ell - z \right)^{-1} \Phi_\ell \leq \frac{1}{n} \|(A + s_0^{-1} \Phi_\ell - z)^{-1} \Phi_\ell \|_F \leq \frac{1}{\sqrt{n}} \|(A + s_0^{-1} \Phi_\ell - z)^{-1} \| \cdot \| \Phi_\ell - \Phi_\ell \|_F \to 0.
\]

Applying these approximations to 60, we have almost surely along this sub-subsequence that

\[
\left| s_0 - \frac{1}{\alpha} - \gamma_\ell \text{tr} (A + s_0^{-1} \Phi_\ell - z \text{Id})^{-1} \Phi_\ell \right| \to 0.
\]

Now observe from the definitions of \( A, \tilde{\Phi}_\ell, \) and \( z \) that

\[
A + s_0^{-1} \tilde{\Phi}_\ell - z \text{Id} = \left( z_{-1} + \frac{1 - b^2_0}{s_0} \right) \text{Id} + \sum_{k=0}^{\ell-2} z_k X_k^T X_k + \left( z_{\ell-1} + \frac{b^2_0}{s_0} \right) X_{\ell-1}^T X_{\ell-1},
\]

\[
\tilde{\Phi}_\ell = (1 - b^2_0) \text{Id} + b^2_0 X_{\ell-1}^T X_{\ell-1}.
\]

Then, applying (61) and the induction hypothesis that part (b) holds for \( \ell - 1 \), we obtain that the value \( s_0 \) must satisfy

\[
s_0 = \frac{1}{\alpha} + \gamma_{\ell+1} \left( z_{\text{prev}}(s_0), (1 - b^2_0, 0, \ldots, 0, b^2_0) \right),
\]

where \( z_{\text{prev}} \) is defined in (14). This shows the existence of a solution (in \( \mathbb{C}^+ \)) to the fixed-point equation (12).

To show uniqueness, we apply Corollary G.5. For any fixed \( s \in \mathbb{C}^+ \), defining

\[
f_\ell(s) = \frac{1}{\alpha} + (n/d_\ell) \text{tr} (A + s^{-1} \Phi_\ell - z \text{Id})^{-1} \Phi,
\]

the same arguments as above establish that

\[
\lim_{n \to \infty} f_\ell(s) = f(s) \equiv \frac{1}{\alpha} + \gamma_{\ell+1} \left( z_{\text{prev}}(s), (1 - b^2_0, 0, \ldots, 0, b^2_0) \right).
\]

Part (b) holding for \( \ell - 1 \) implies that both \( A \) and \( \Phi_\ell \) have deterministic spectral limits, where

\[
\lim \text{spec} \Phi_\ell = \lim \text{spec} \tilde{\Phi}_\ell
\]

by (45). This cannot be the point distribution at 0, because (26) implies that \( \text{tr} \Phi \geq 1/2 \) for all large \( n \), and \( \| \Phi \| \leq C \) so at least \( n/(2C) \) eigenvalues of \( \Phi \) exceed 1/2 for every \( n \). Thus, Corollary G.5 implies that the fixed point \( s = f(s) \) is unique. So the fixed point \( s_\ell(z) \in \mathbb{C}^+ \) is uniquely defined by (12), and this shows part (a) for \( \ell \).

By the uniqueness of this fixed point, we have also shown that \( s_0 = s_\ell(z) \), where \( s_0 \) is the limit of \( \bar{s} \) along the above sub-subsequence. Since for any subsequence in \( n \), there exists a sub-subsequence for this which holds, this shows that \( \lim_{n \to \infty} \bar{s} = s_\ell(z) \) almost surely.

Now, to show that part (b) holds for \( \ell \), let us also fix any \( w = (w_{-1}, \ldots, w_\ell) \in \mathbb{C}^{\ell+2} \). Using that \( z_\ell \neq 0 \), we may write

\[
w \cdot X^T X(\ell) = \frac{w_\ell}{z_\ell} \cdot z \cdot X^T X(\ell) + w_{\text{prev}} \cdot X^T X(\ell - 1),
\]

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where $w_{\text{prev}}$ is as defined in [15]. Then
\[
(z \cdot X^\top X(\ell))^{-1} (w \cdot X^\top X(\ell)) = \frac{w_\ell}{z_\ell} \text{Id} + (z \cdot X^\top X(\ell))^{-1} (w_{\text{prev}} \cdot X^\top X(\ell - 1)).
\]

We now apply Lemma E.2(a) conditional on $X_0, \ldots, X_{\ell - 1}$, with the same identifications as above and with
\[
M = w_{\text{prev}} \cdot X^\top X(\ell - 1).
\]

Note that $M$ is indeed deterministic conditional on $X_0, \ldots, X_{\ell - 1}$, and $\|M\| \leq C$ for a constant $C > 0$ (depending on $z$ and $w$) since $X_0, \ldots, X_{\ell - 1}$ are $(\varepsilon_n, B)$-orthonormal. Then, applying Lemma E.2(a),
\[
\text{tr} \left[ (z \cdot X^\top X(\ell))^{-1} (w_{\text{prev}} \cdot X^\top X(\ell - 1)) \right] - \text{tr} \left[ (A + s^{-1} \Phi_\ell - z \text{Id})^{-1} (w_{\text{prev}} \cdot X^\top X(\ell - 1)) \right] \to 0.
\]

By the same arguments as above, we may replace $\bar{s}$ by $s_0 = s_\ell(z)$ and $\Phi_\ell$ by $\tilde{\Phi}_\ell$. Then, applying this to (62),
\[
\text{tr} \left[ (z \cdot X^\top X(\ell))^{-1} (w \cdot X^\top X(\ell)) \right] - \frac{w_\ell}{z_\ell} - \text{tr} \left[ (A + s_\ell(z) - 1\tilde{\Phi}_\ell - z \text{Id})^{-1} (w_{\text{prev}} \cdot X^\top X(\ell - 1)) \right] \to 0.
\]

Finally, applying that part (b) holds for $\ell - 1$, this yields
\[
\lim_{n \to \infty} \text{tr} \left[ (z \cdot X^\top X(\ell))^{-1} (w \cdot X^\top X(\ell)) \right] = \frac{w_\ell}{z_\ell} + t_{\ell - 1}(z_{\text{prev}}(s_\ell(z)), w_{\text{prev}}),
\]
which is the definition of $t_\ell(z, w)$. This establishes (58).

For any fixed $z_{-1}, \ldots, z_\ell \in \mathbb{R}$ where $z_\ell \neq 0$, and any fixed $z \in \mathbb{C}^+$, this implies that the Stieltjes transform of $z \cdot X^\top X(\ell)$ has the almost sure limit
\[
m(z) = t_\ell((-z + z_{-1}, 0, \ldots, z_\ell), (1, 0, \ldots, 0)).
\]

So $m(z)$ defines the Stieltjes transform of a sub-probability distribution $\nu$, and the empirical eigenvalue distribution of $z \cdot X^\top X(\ell)$ converges vaguely a.s. to $\nu$. Since $\|z \cdot X^\top X(\ell)\|$ is bounded because $X_0, \ldots, X_L$ are $(\varepsilon_n, B)$-orthonormal, this limit $\nu$ must in fact be a probability distribution, and the eigenvalue distribution converges weakly to $\nu$. This concludes the induction and the proof. \hfill \Box

**H** Multi-dimensional outputs and rescaled parametrizations

In this section, we provide some motivation for the form of the NTK in (17) for networks with a $k$-dimensional output, and we prove Theorem 3.8 regarding its spectrum.

**H.1 Derivation of (17) from gradient flow training**

Consider gradient flow training of the network [16], with training samples $(x_\alpha, y_\alpha)_{\alpha=1}^n$ where $x_\alpha \in \mathbb{R}^{d_0}$ and $y_\alpha \in \mathbb{R}^k$, under the general training loss
\[
F(\theta) = \sum_{\alpha=1}^n \mathcal{L}(f_\theta(x_\alpha), y_\alpha).
\]
Here, $\mathcal{L} : \mathbb{R}^k \times \mathbb{R}^k \rightarrow \mathbb{R}$ is the loss function. We denote by $\nabla \mathcal{L}(f_\theta(x_\alpha), y_\alpha) \in \mathbb{R}^k$ the gradient of $\mathcal{L}$ with respect to its first argument, and by $\nabla_{W_\ell} f_\theta(x_\alpha) \in \mathbb{R}^{\dim(W_\ell) \times k}$ the Jacobian of $f_\theta(x_\alpha)$ with respect to the weights $W_\ell$.

Consider a possibly reweighted gradient-flow training of $\theta$, where the evolution of weights $W_\ell$ is given by

$$\frac{d}{dt} W_\ell(t) = -\tau_\ell \cdot \nabla_{W_\ell} F(\theta(t)) = -\tau_\ell \sum_{\alpha=1}^{n} \nabla_{W_\ell} f_\theta(x_\alpha) \cdot \nabla \mathcal{L}(f_\theta(x_\alpha), y_\alpha).$$

The learning rate for each weight matrix $W_\ell$ is scaled by a constant $\tau_\ell$—this may arise, for example, from reparametrizing the network (16) using $\tilde{W}_\ell = \tau_\ell^{-1} \cdot W_\ell$ and considering gradient flow training for $\tilde{W}_\ell$. Denoting the vectorization of all training predictions and its Jacobian by

$$f_\theta(X) = (f_\theta^1(X), \ldots, f_\theta^k(X)) \in \mathbb{R}^{nk}, \quad \nabla_{W_\ell} f_\theta(X) \in \mathbb{R}^{\dim(W_\ell) \times nk},$$

and the corresponding vectorization of $(\nabla \mathcal{L}(f_\theta(x_\alpha), y_\alpha))_{\alpha=1}^{n}$ by $\nabla \mathcal{L}(f_\theta(X), y) \in \mathbb{R}^{nk}$, this may be written succinctly as

$$\frac{d}{dt} W_\ell(t) = -\tau_\ell \cdot \nabla_{W_\ell} f_\theta(X) \cdot \nabla \mathcal{L}(f_\theta(X), y).$$

Then the time evolution of in-sample predictions is given by

$$\frac{d}{dt} f_\theta(t)(X) = (\nabla_{\theta} f_\theta(t)(X))^\top \cdot \frac{d}{dt} \theta(t)$$

$$= -\sum_{\ell=1}^{L+1} \tau_\ell \left( \nabla_{W_\ell} f_\theta(X) \right)^\top \left( \nabla_{W_\ell} f_\theta(X) \right) \cdot \nabla \mathcal{L}(f_\theta(X), y) = -K_{\text{NTK}} \cdot \nabla \mathcal{L}(f_\theta(X), y),$$

where $K_{\text{NTK}}$ is the matrix defined in (17). For $\tau_1 = \ldots = \tau_{L+1} = 1$, this matrix is simply

$$K_{\text{NTK}} = (\nabla_{\theta} f_\theta(X))^\top (\nabla_{\theta} f_\theta(X)) \in \mathbb{R}^{nk \times nk},$$

which is a flattening of the neural tangent kernel $K \in \mathbb{R}^{n \times n \times k \times k}$ (identified as a map $K : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{k \times k}$) that is defined in [JGH18].

### H.2 Proof of Theorem 3.8

The matrix $K_{\text{NTK}}$ in (17) admits a $k \times k$ block decomposition

$$K_{\text{NTK}} = \begin{pmatrix} K_{11} & \cdots & K_{1k} \\ \vdots & \ddots & \vdots \\ K_{k1} & \cdots & K_{kk} \end{pmatrix}, \quad K_{ij} = \sum_{\ell=1}^{L+1} \tau_\ell \left( \nabla_{W_\ell} f_\theta^i(X) \right)^\top \left( \nabla_{W_\ell} f_\theta^j(X) \right) \in \mathbb{R}^{nk}.$$

Writing

$$W_{L+1} = \begin{pmatrix} w_1^\top \\ \vdots \\ w_k^\top \end{pmatrix},$$

a computation using the chain rule similar to (52) verifies that

$$K_{ij} = 1 \{i = j\} \tau_{L+1} X_L^\top X_L + \sum_{\ell=1}^{L} \tau_\ell (S_{\ell}^i S_{\ell}^j) \odot (X_{\ell-1}^\top X_{\ell-1})$$

where $S_{\ell}^i \in \mathbb{R}^{d_{\ell} \times n}$ is the matrix with the same column-wise definition as in (51), replacing $w$ by $w_i$. 

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Lemma H.1. Under the assumptions of Theorem 3.8 for each $\ell \in [L]$ and any indices $i \neq j \in [k]$, almost surely as $n \to \infty$,
\[
\frac{1}{n} \|K_{ij}^{\text{NTK}}\|_F^2 \to 0.
\]
Furthermore, for a constant $C > 0$, almost surely for all large $n$, $\|K_{ij}^{\text{NTK}}\| \leq C$.

Proof. By Corollary D.2, we may assume that each $X_0, \ldots, X_L$ is $(\varepsilon_n, B)$-orthonormal.

Let us fix $i, j, \ell$ and denote the columns of $S_i^{\ell}$ and $S_j^{\ell}$ by $s_{\alpha}^{i, \ell}$ and $s_{\beta}^{j, \ell}$ for $\alpha, \beta \in [n]$. We apply the Hanson-Wright inequality conditional on $W_1, \ldots, W_L$, which is similar to (55). However, since $w_i$ and $w_j$ are independent, there is no trace term, and we obtain instead
\[
|s_{\alpha}^{\ell, i} s_{\beta}^{\ell, j}| \leq C \varepsilon_n \sqrt{n} \frac{1}{d_L} \|M_L\|_F
\]
for both $\alpha = \beta$ and $\alpha \neq \beta$ with probability $1 - e^{-n^{0.01}}$, where $M_L$ is the same matrix as defined in (54). Applying the bound $\|M_L\|_F \leq C \sqrt{n}$ as in the proof of Corollary G.2 this yields
\[
|s_{\alpha}^{\ell, i} s_{\beta}^{\ell, j}| \leq C \varepsilon_n
\]
almost surely for all $\alpha, \beta \in [n]$ and all large $n$. Combining with the $(\varepsilon_n, B)$-orthonormality of $X_{\ell-1}$, we get for $\alpha \neq \beta$ that
\[
|(S_{\ell}^{\ell, i} S_{\ell}^{\ell, j}) \circ (X_{\ell-1}^\top X_{\ell-1})[\alpha, \beta]| \leq C \varepsilon_n^2, \quad |(S_{\ell}^{\ell, i} S_{\ell}^{\ell, j}) \circ (X_{\ell-1}^\top X_{\ell-1})[\alpha, \alpha]| \leq C \varepsilon_n.
\]

Then
\[
\| (S_{\ell}^{\ell, i} S_{\ell}^{\ell, j}) \circ (X_{\ell-1}^\top X_{\ell-1}) \|_F^2 \leq C n(n - 1) \varepsilon_n^4 + C n \varepsilon_n^2,
\]
and the first statement follows from the assumption $\varepsilon_n n^{1/4} \to 0$. The second statement on the operator norm follows from the bound
\[
\| (S_{\ell}^{\ell, i} S_{\ell}^{\ell, j}) \circ (X_{\ell-1}^\top X_{\ell-1}) \| \leq \left( \max_{\alpha = 1} \left| s_{\alpha}^{\ell, i} s_{\alpha}^{\ell, i} \right| \right)^{1/2} \left( \max_{\alpha = 1} \left| s_{\alpha}^{\ell, j} s_{\alpha}^{\ell, j} \right| \right)^{1/2} \cdot \|X_{\ell-1}^\top X_{\ell-1}\|.
\]
See [Joh90, Eq. (3.7.9)] applied with $X = S_\ell^i$ and $Y = S_\ell^j$. The bound $\|K_{ij}^{\text{NTK}}\| \leq C$ then follows from the $(\varepsilon_n, B)$-orthonormality of $X_{\ell-1}$ and Corollary G.2 applied to $S_\ell^i$ and $S_\ell^j$.

Applying this lemma together with Proposition C.3 we obtain
\[
\lim \text{spec } K^{\text{NTK}} = \lim \text{spec } \begin{pmatrix} K^{\text{NTK}}_{11} & \cdots & \cdots \\ \cdot & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ K^{\text{NTK}}_{kk} \end{pmatrix}
\]
where the off-diagonal blocks $K_{ij}^{\text{NTK}}$ may be replaced by 0. Then the limit spectrum of $K^{\text{NTK}}$ is an equally weighted mixture of those of $K_{11}^{\text{NTK}}, \ldots, K_{kk}^{\text{NTK}}$. For each diagonal block $K_{ii}^{\text{NTK}}$, the argument of Lemma G.3 shows that
\[
\lim \text{spec } K_{ii}^{\text{NTK}} = \lim \text{spec } \left( \tau \cdot r_+ \text{Id} + \tau L+1 X_{\ell}^\top X_{\ell} + \sum_{\ell = 0}^{L-1} \tau_{\ell+1} q_{\ell} X_{\ell+1}^\top X_{\ell} \right).
\]

Then by Theorem 3.7 each diagonal block $K_{ii}^{\text{NTK}}$ has the same limit spectrum, whose Stieltjes transform is given by the function $m_{\text{NTK}}(z)$ in Theorem 3.8. Furthermore, since $\|K_{ij}^{\text{NTK}}\| \leq C$ by Lemma G.3 and $\|K_{ij}^{\text{NTK}}\| \leq C$ for $i \neq j$ by Lemma H.1 this shows $\|K^{\text{NTK}}\| \leq C$. This establishes Theorem 3.8.
I Reduction to result of Pennington and Worah [PW17] for one hidden layer

Consider the one-hidden-layer conjugate kernel

\[ K_{\text{CK}} = X_1^\top X_1 = \frac{1}{d_1} \sigma(W_1 X)^\top \sigma(W_1 X) \in \mathbb{R}^{n \times n}. \]

Define an associated covariance matrix

\[ M = \frac{1}{n} \sigma(W_1 X) \sigma(W_1 X)^\top \in \mathbb{R}^{d_1 \times d_1}, \]

and observe that the eigenvalues of \( K_{\text{CK}} \) are those of \( M \) multiplied by \( n/d_1 \) and padded by \( n - d_1 \) additional zeros (or with \( d_1 - n \) zeros removed, if \( n - d_1 < 0 \)). [PW17, Theorem 1] characterizes the limit spectrum of \( M \) in terms of a quartic equation in its Stieltjes transform, under the additional assumptions that \( X \) has i.i.d. \( \mathcal{N}(0,1/d_0) \) entries and \( n/d_0 \to \gamma_0 \in (0,\infty) \). By Theorem 3.4, this should be equivalent to the description

\[ \lim \text{spec} K_{\text{CK}} = \rho_{\text{MP}}^{\text{MP}} \bigotimes \left( (1 - b_2^2) + b_2^2 \mu_0 \right) \]

for the limit spectrum of \( K_{\text{CK}} \), if we specialize to \( \mu_0 = \rho_{\gamma_0}^{\text{MP}} \) being the Marcenko-Pastur limit spectrum of the input gram matrix \( X^\top X \). We derive this equivalence in this section.

Let \( m_K(z) \) and \( m_M(z) \) be the limit Stieltjes transforms for \( K_{\text{CK}} \) and \( M \). For any \( z \in \mathbb{C}^+ \), by the relation between the eigenvalues of \( K_{\text{CK}} \) and \( M \),

\[ \frac{1}{n} \text{Tr} \left( K_{\text{CK}} - \frac{n}{d_1} z I_d \right)^{-1} = - \frac{1}{1 - \frac{d_1}{n}} \frac{n}{d_1} \left( - \frac{n}{d_1} z \right)^{-1} \quad \text{and} \quad \frac{1}{n} \text{Tr} \left( M - \frac{n}{d_1} z I_d \right)^{-1} \]

\[ = - \left( 1 - \frac{d_1}{n} \right) \frac{d_1}{n} \cdot \frac{1}{z} + \frac{1}{d_1} \cdot \frac{1}{d_1} \text{Tr}(M - z I_d)^{-1}. \]

Taking the limit on both sides, we obtain the relation between \( m_K(z) \) and \( m_M(z) \), which is

\[ m_K(\gamma_1 z) = - \left( 1 - \frac{1}{\gamma_1} \right) \frac{1}{\gamma_1 z} + \frac{1}{\gamma_1^2} m_M(z) = \frac{1}{\gamma_1^2} \left( m_M(z) + \frac{1 - \gamma_1}{z} \right). \]

Following the notation of [PW17], let us set

\[ \phi = 1/\gamma_0, \quad \psi = \gamma_1/\gamma_0, \quad \eta = 1 = \mathbb{E}[\sigma(\xi)^2], \quad \zeta = b_2^2. \]

[PW17] Theorem 1 characterizes \( G(z) \equiv -m_M(z) \) as the root of a quartic equation. Defining three \( z \)-dependent quantities \( P, P_\phi, P_\psi \) by

\[ G(z) = \frac{\psi}{z} P + \frac{1 - \psi}{z}, \quad P_\phi = 1 + (P - 1) \phi, \quad P_\psi = 1 + (P - 1) \psi, \]

this quartic equation is expressed as

\[ P = 1 + (1 - \zeta) t P_\phi P_\psi + \frac{\zeta t P_\phi P_\psi}{1 - \zeta t P_\phi P_\psi}, \quad \text{where} \quad t = \frac{1}{z \psi}, \]

[4] In [PW17], the \( 1/\sqrt{d_0} \) scaling is in \( W_1 \) rather than \( X \), but these are clearly the same. We consider \( \sigma_w = \sigma_x = 1 \) and \( \eta = 1 \) in the results of [PW17].
and dividing both sides by $-\zeta$, this may be rearranged as
\[ m_K(z) = \int \frac{1}{[(1 - b_0^2) + b_0^2 x][1 - \gamma_1 - \gamma_1 zm_K(z)] - z} \, d\mu_0(x). \]

Applying the identity $1 - \gamma_1 - \gamma_1^2zm_K(\gamma_1z) = -zm_M(z)$ from rearranging \([65]\), and applying also $\zeta = b_0^2$ in \([66]\),
\[ m_K(\gamma_1z) = \int \frac{1}{[(1 - \zeta) + \zeta x][\gamma_0zm_M(z)] - \gamma_1zm_0(x). \]

When $X$ has i.i.d. $\mathcal{N}(0,1/d_0)$ entries, the limit spectrum of $X^\top X$ is the Marcenko-Pastur law $\mu_0 = \rho^{\text{MP}}_{\gamma_0}$. The Stieltjes transform $m(z)$ of this law $\mu_0 = \rho^{\text{MP}}_{\gamma_0}$ is characterized by the quadratic equation
\[ 1 = m(z)[1 - \gamma_0 - \gamma_0zm(z) - z] \]
(which is the specialization of \([63]\) when $\mu$ is the point distribution at 1). Defining
\[ g(a,b) = \int \frac{1}{ax - b} \, d\mu_0(x) = \frac{1}{a} m \left( \frac{b}{a} \right), \]
we obtain then that $g(a,b)$ satisfies the quadratic equation
\[ 1 = g(a,b)[a - \gamma_0a - \gamma_0m(b/a) - b] = g(a,b)[(a - b) - \gamma_0a - \gamma_0\sigma g(a,b)], \]
Applying this with $a = -\zeta zm_M(z)$ and $b = (1 - \zeta)zm_M(z) + \gamma_1z$, the quantity \([70]\) is exactly $g(a,b)$. Thus this equation holds for $g(a,b) = m_K(\gamma_1z)$ and these settings of $(a,b)$, i.e.
\[ 1 = m_K(\gamma_1z)\left( -zm_M(z) - \gamma_1z + \gamma_0\zeta zm_M(z) + \gamma_0\zeta zm_M(z) [(1 - \zeta)zm_M(z) + \gamma_1z] m_K(\gamma_1z) \right). \]

From the relation \([65]\), we see that this is a quartic equation in $m_M(z)$. Note that the definitions of $P_\psi$ and $P_\phi$ in \([67]\) may be equivalently written as
\[
\begin{align*}
P_\psi &= \psi P + 1 - \psi = zG(z) = -zm_M(z), \\
P_\phi &= 1 + \frac{\phi}{\psi}(zG(z) - 1) = \frac{1}{\gamma_1}(-zm_M(z) - 1 + \gamma_1) = -\gamma_1zm_K(\gamma_1z)
\end{align*}
\]
where we have used $G(z) = -m_M(z)$, $\psi/\phi = 1$ from \([66]\), and the relation \([65]\). Applying now $\gamma_1z = (\psi/\phi)z = 1/(\phi t)$ and $\gamma_0 = 1/\phi$, the equation \([71]\) becomes
\[
\begin{align*}
1 &= -\phi t P_\phi \left( P_\psi - \frac{1}{\phi t} - \frac{\zeta}{\phi} P_\psi + \frac{\zeta}{\phi} P_\phi \left( -(1 - \zeta)P_\psi + \frac{1}{\phi t} \right) \phi t P_\phi \right) \\
&= -\phi t P_\phi P_\psi + P_\phi + (1 - P_\phi)\zeta_t P_\phi P_\psi + \zeta(1 - \zeta)\phi(t P_\phi P_\psi)^2.
\end{align*}
\]
This may be rearranged as
\[
(1 - P_\phi - \phi)(1 - \zeta t P_\phi P_\psi) = -\phi(1 - \zeta t P_\phi P_\psi) - \phi t P_\phi P_\psi + \zeta(1 - \zeta)\phi(t P_\phi P_\psi)^2,
\]
and dividing both sides by $-\phi(1 - \zeta t P_\phi P_\psi)$ yields
\[
\frac{1}{\phi}(P_\phi - 1) + 1 = 1 + \frac{t P_\phi P_\psi - \zeta(1 - \zeta)(t P_\phi P_\psi)^2}{1 - \zeta t P_\phi P_\psi} = 1 + (1 - \zeta)t P_\phi P_\psi + \frac{\zeta t P_\phi P_\psi}{1 - \zeta t P_\phi P_\psi}.
\]
Identifying the left side as $P$ by \([67]\), we obtain \([68]\) as desired.
J  Additional simulation results

J.1  Pairwise orthogonality of training samples

All pairwise inner-products $\{x_\alpha^\top x_\beta : 1 \leq \alpha < \beta \leq n\}$, for (a) 5000 CIFAR-10 training samples, (b) 5000 CIFAR-10 training samples with the first 10 PCs removed, and (c) i.i.d. Gaussian training data of the same dimensions. Results for (b) were reported in Section 4.2, and results for (a) are reported below in Appendix J.2. CIFAR-10 training samples were mean-centered and normalized to satisfy $x_\alpha^\top 1 = 0$ and $\|x_\alpha\|^2 = 1$ in (a) and (b).

The pairwise inner-products in (a) span a typical range of $[-0.5, 0.5]$. Those in (b) span a range of about $[-0.2, 0.2]$, and those in (c) about $[-0.02, 0.02]$. Thus, with 10 PCs removed, these inner-products for CIFAR-10 are larger than for i.i.d. Gaussian inputs by a factor of 10. We found in Section 4.2 that the inner-products of (b) are sufficiently small for the observed spectra to match the theoretical limits of Theorems 3.4 and 3.7.

J.2  CK and NTK spectra for CIFAR-10 without removal of leading PCs

Same plots as Figure 2 for CIFAR-10 training samples, without the removal of the 10 leading PCs. We observe a close agreement of the observed CK spectrum with the limit spectrum of Theorem 3.4. However, there is a greater discrepancy of the NTK spectrum with the limit spectrum of Theorem 3.7 in this setting.
J.3 Observed and limit CK spectra for all layers

Simulated spectra of the CK matrices $X^\top_\ell X_\ell$ at all intermediate layers $\ell = 1, \ldots, 5$, corresponding to the i.i.d. Gaussian training data example of Figure J.4. Numerical computations of the limit spectra from Theorem 3.4 are overlaid in red. We observe a merging of the two bulk spectral components and an extension of the spectral support with increase in layer number.

The same as above, corresponding to the CIFAR-10 training samples in Appendix J.2 (Results with 10 PCs removed look the same.) A close agreement with the limit spectrum described by Theorem 3.4 is observed at each layer.
Spectra of the CK matrices at all three layers, corresponding to the trained 3-layer network of Section 4.3. The limit spectra at random initialization of weights are depicted in red, and the two largest eigenvalues of each matrix are depicted by blue arrows.