

Mehler’s Formula, Branching Process, and Compositional Kernels of Deep Neural Networks

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Abstract

We utilize a connection between compositional kernels and branching processes via Mehler’s formula to study deep neural networks. This new probabilistic insight provides us a novel perspective on the mathematical role of activation functions in compositional neural networks. We study the unscaled and rescaled limits of the compositional kernels and explore the different phases of the limiting behavior, as the compositional depth increases. We investigate the memorization capacity of the compositional kernels and neural networks by characterizing the interplay among compositional depth, sample size, dimensionality, and non-linearity of the activation. Explicit formulas on the eigenvalues of the compositional kernel are provided, which quantify the complexity of the corresponding reproducing kernel Hilbert space. On the methodology front, we propose a new random features algorithm, which compresses the compositional layers by devising a new activation function.

1 Introduction

Kernel methods and deep neural networks are arguably two representative methods that achieved the state-of-the-art results in regression and classification tasks (Shankar et al., 2020). However, unlike the kernel methods where both the statistical and computational aspects of learning have been understood reasonably well, there are still many theoretical puzzles around the generalization, computation and representation aspects of deep neural networks (Zhang et al., 2017). One hopeful direction to resolve some of the puzzles in neural networks is through the lens of kernels (Rahimi and Recht, 2008, 2009; Cho and Saul, 2009; Belkin et al., 2018b). Such a connection can be readily observed in a two-layer infinite-width network with random weights, see the pioneering work by Neal (1996a) and Rahimi and Recht (2008, 2009). For deep networks with hierarchical structures and randomly initialized weights, compositional kernels (Daniely et al., 2017b,b; Poole et al., 2016) are proposed to rigorously characterize such a connection, with promising empirical performances (Cho and Saul, 2009). A list of simple algebraic operations on kernels (Stitson et al., 1999; Shankar et al., 2020) are introduced to incorporate specific data structures that contain bag-of-features, such as images and time series.

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In this paper, we continue to study deep neural networks and their dual compositional kernels, furthering the aforementioned mathematical connection, based on the foundational work of (Rahimi and Recht, 2008, 2009) and (Daniely et al., 2017b,a). We focus on a standard multilayer perceptron architecture with Gaussian weights and study the role of the activation function and its effect on composition, data memorization, spectral properties, algorithms, among others. Our main results are based on a simple yet elegant connection between *compositional kernels* and *branching processes* via Mehler’s formula. This new connection, in turn, opens up the possibility of studying the mathematical role of activation functions in compositional deep neural networks, utilizing the probabilistic tools in branching processes. Specifically, the new probabilistic insight allows us to answer the following questions:

Limits and phase transitions. Given an activation function, one can define the corresponding compositional kernel (Daniely et al., 2017b,a). How to classify the activation functions according to the limits of their dual compositional kernels, as the compositional depth increases? What properties of the activation functions govern the different phases of such limits? How do we properly rescale the compositional kernel such that there is a limit unique to the activation function? The above questions will be explored in Section 3.

Memorization capacity of compositions: tradeoffs. Deep neural networks and kernel machines can have a good out-of-sample performance even in the interpolation regime (Zhang et al., 2017; Belkin et al., 2018b), with perfect memorization of the training dataset. What is the memorization capacity of the compositional kernels? What are the tradeoffs among compositional depth, number of samples in the dataset, input dimensionality, and properties of the activation functions? Section 4 studies such interplay explicitly.

Spectral properties of compositional kernels. Spectral properties of the kernel (and the corresponding integral operator) affect the statistical rate of convergence, for kernel regressions (Caponnetto and Vito, 2006). What is the spectral decomposition of the compositional kernels? How do the eigenvalues of the compositional kernel depend on the activation function? Section 5 is devoted to answering the above questions.

New randomized algorithms. Given a compositional kernel with a finite depth associate with an activation, can we devise a new "compressed" activation and new randomized algorithms, such that the deep neural network (with random weights) with the original activation is equivalent to a shallow neural network with the "compressed" activation? Such algorithmic questions are closely related to the seminal Random Fourier Features (RFF) algorithm in Rahimi and Recht (2008, 2009), yet different. Section 6 investigates such algorithmic questions by considering compositional kernels and, more broadly, the inner-product kernels. Differences to the RFF are also discussed in detail therein.

Borrowing the insight from branching process, we start with studying the role of activation function in the compositional kernel, memorization capacity, and spectral properties, and conclude with the converse question of designing new activations and random nonlinear features algorithm based on kernels, thus contributing to a strengthened mathematical understanding of activation functions, compositional kernel classes, and deep neural networks.

1.1 Related Work

The connections between neural networks (with random weights) and kernel methods have been formalized by researchers using different mathematical languages. Instead of aiming to provide a complete list, here we only highlight a few that directly motivate our work. Neal (1996b,a)

advocated using Gaussian processes to characterize the neural networks with random weights from a Bayesian viewpoint. For two-layer neural networks, such correspondence has been strengthened mathematically by the work of [Rahimi and Recht \(2008, 2009\)](#). By Bochner’s Theorem, [Rahimi and Recht \(2008\)](#) showed that any positive definite translation-invariant kernel could be realized by a two-layer neural network with a specific distribution on the weights, via the trigonometric activation. Such insights also motivated the well-known random features algorithm, random kitchen sinks ([Rahimi and Recht, 2009](#)). One highlight of such an algorithm is that in the first layer weights, sampling is employed to replace the optimization. Later, several works extended along the line, see, for instance, [Kar and Karnick \(2012\)](#) on the rotation-invariant kernels, [Pennington et al. \(2015\)](#) on the polynomial kernels, and [Bach \(2016\)](#) on kernels associated to ReLU-like activations (using spherical harmonics). Recently, [Mei and Montanari \(2019\)](#) investigated the precise asymptotics of the random features model using random matrix theory. For deep neural networks, compositional kernels are proposed to carry such connections further. [Cho and Saul \(2009\)](#) introduced the compositional kernel as the inner-product of compositional features. [Daniely et al. \(2017b,a\)](#) described the compositional kernel through the language of the computational skeleton, and introduced the duality between the activation function and compositional kernel. We refer the readers to [Poole et al. \(2016\)](#); [Yang \(2019\)](#); [Shankar et al. \(2020\)](#) for more information on the connection between kernels and neural networks.

One might argue that neural networks with static random weights may not fully explain the success of neural networks, noticing that the evolution of the weights during training is yet another critical component. On this front, [Chizat and Bach \(2018b\)](#); [Mei et al. \(2018\)](#); [Sirignano and Spiliopoulos \(2018\)](#); [Rotskoff and Vanden-Eijnden \(2018\)](#) employed the mean-field characterization to describe the distribution dynamics of the weights, for two-layer networks. [Rotskoff and Vanden-Eijnden \(2018\)](#); [Dou and Liang \(2019\)](#) studied the favorable properties of the dynamic kernel due to the evolution of the weight distribution. [Nguyen and Pham \(2020\)](#) carried the mean-field analysis to multi-layer networks rigorously. On a different tread ([Jacot et al., 2019](#); [Du et al., 2018](#); [Chizat and Bach, 2018a](#); [Woodworth et al., 2019](#)), researchers showed that under specific scaling, training over-parametrized networks could be viewed as a kernel regression with perfect memorization of the training data, using a tangent kernel ([Jacot et al., 2019](#)) built from a linearization around its initialization. For a more recent resemblance between the kernel learning and the deep learning on the empirical side, we refer the readers to [Belkin et al. \(2018b\)](#).

2 Preliminary

Mehler’s formula. We will start with reviewing some essential background on the Hermite polynomials that is of direct relevance to our paper.

Definition 2.1 (Hermite polynomials). *The probabilists’ Hermite polynomials $He_k(x)$ for non-negative integers $k \in \mathbb{Z}^{\geq 0}$ follows the recursive definition with $He_0(x) = 1$ and*

$$He_{k+1}(x) = xHe_k(x) - He'_k(x) . \quad (2.1)$$

We define the normalized Hermite polynomials as

$$h_k(x) := \frac{1}{\sqrt{k!}} He_k(x), \text{ with } \mathbb{E}_{\mathbf{g} \sim \mathcal{N}(0,1)}[h_k^2(\mathbf{g})] = 1 . \quad (2.2)$$

The set $\{h_k : k \in \mathbb{Z}^{\geq 0}\}$ forms an orthogonal basis of L^2_ϕ under the Gaussian measure $\phi \sim \mathcal{N}(0, 1)$ as

$$\mathbb{E}_{\mathbf{g} \sim \mathcal{N}(0,1)}[h_k(\mathbf{g})h_{k'}(\mathbf{g})] = \mathbb{1}_{k=k'} . \quad (2.3)$$

Proposition 2.2 (Mehler's formula). *Mehler's formula establishes the following equality on Hermite polynomials: for any $\rho \in (-1, 1)$ and $x, y \in \mathbb{R}$*

$$\frac{1}{\sqrt{1-\rho^2}} \exp\left(-\frac{\rho^2(x^2+y^2)-2\rho xy}{2(1-\rho^2)}\right) = \sum_{k=0}^{\infty} \rho^k h_k(x)h_k(y) . \quad (2.4)$$

Branching process. Now we will describe the branching process and compositions of probability generating functions (PGF).

Definition 2.3 (Probability generating function). *Given a random variable Y on non-negative integers with the following probability distribution*

$$\mathbb{P}(Y = k) = p_k, \quad \forall k \in \mathbb{Z}^{\geq 0} , \quad (2.5)$$

define the associated generating function as

$$G_Y(s) := \mathbb{E}[s^Y] = \sum_{k \geq 0} p_k s^k . \quad (2.6)$$

It is clear that $G_Y(0) = 0$, $G_Y(1) = 1$ and $G_Y(s)$ is non-decreasing and convex on $s \in [0, 1]$.

Definition 2.4 (Galton-Watson branching process). *The Galton-Watson (GW) branching process is defined as a Markov chain $\{Z_L : L \in \mathbb{Z}^{\geq 0}\}$, where Z_L denotes the size of the L -th generation of the initial family. Let Y be a random variable on non-negative integers describing the number of direct children, that is, it has k children with probability p_k with $\sum_{k \geq 0} p_k = 1$. Begin with one individual $Z_0 \equiv 1$, and let it reproduce according to the distribution of Y , and then each of these children then reproduce independently with the same distribution as Y . The generation sizes $\{Z_L : L \in \mathbb{Z}^{\geq 0}\}$ are then defined by*

$$Z_{L+1} = \sum_{i=1}^{Z_L} Y_i^{(L)} \quad (2.7)$$

where $Y_i^{(L)}$ denotes the number of children for the i -th individual in generation L .

Proposition 2.5 (Extinction criterion, Proposition 5.4 in [Lyons and Peres \(2016\)](#)). *Given $p_1 \neq 1$ (in Definition 2.3), the extinction probability $\xi := \lim_{L \rightarrow \infty} \mathbb{P}(Z_L = 0)$ satisfies*

- (i) $\xi = 1$ if and only if $\mu := G'_Y(1) \leq 1$.
- (ii) ξ is the unique fixed point of $G_Y(s) = s$ in $[0, 1]$.

Multi-layer Perceptrons. We define the fully-connected Multi-Layer Perceptrons (MLPs) now, which is among the standard architectures in deep neural networks.

Definition 2.6 (Activation function). *Throughout the paper, we will only consider the activation functions $\sigma(\cdot) \in L^2_\phi: \mathbb{R} \rightarrow \mathbb{R}$ that are L^2 -integrable under the Gaussian measure ϕ . The Hermite expansion of $\sigma(\cdot)$ is denoted as*

$$\sigma(x) := \sum_{k \geq 0} a_k h_k(x) . \quad (2.8)$$

We will explicitly mention the following two assumptions when they are assumed. Otherwise, we will work with the activation $\sigma(\cdot)$ in Definition 2.6.

Assumption 1 (Normalized activation function). *Assume that the activation function $\sigma(\cdot) \in L^2_\phi(1)$ is normalized under the Gaussian measure ϕ , in the following sense*

$$\mathbb{E}_{\mathbf{g} \sim \mathcal{N}(0,1)}[\sigma^2(\mathbf{g})] = 1 , \quad (2.9)$$

with the Hermite coefficients satisfying

$$\sum_{k \geq 0} a_k^2 = 1. \quad (2.10)$$

Assumption 2 (Centered activation function). *Assume that the activation function $\sigma(\cdot) \in L^2_\phi$ is centered under the Gaussian measure ϕ , in the following sense*

$$\mathbb{E}_{\mathbf{g} \sim \mathcal{N}(0,1)}[\sigma(\mathbf{g})] = 0, \quad (2.11)$$

or equivalently the Hermite coefficient $a_0 = 0$.

Definition 2.7 (Fully-connected MLPs with random weights). *Given an activation function $\sigma(\cdot)$, the number of layers L , and the input vector $x^{(0)} := x \in \mathbb{R}^{d_0}$, we define a multi-layer feed-forward neural network which inductively computes the output for each intermediate layer*

$$x^{(\ell+1)} = \sigma \left(W^{(\ell)} x^{(\ell)} / \|x^{(\ell)}\| \right) \in \mathbb{R}^{d_{\ell+1}} , \text{ for } 0 \leq \ell < L , \text{ with} \quad (2.12)$$

$$W^{(\ell)} \in \mathbb{R}^{d_{\ell+1} \times d_\ell}, \quad W^{(\ell)} \sim \mathcal{MN}(\mathbf{0}, \mathbf{I}_{d_{\ell+1}} \otimes \mathbf{I}_{d_\ell}) . \quad (2.13)$$

Here \mathbf{I}_{d_ℓ} denotes the identity matrix of size d_ℓ , and \otimes denotes the Kronecker product between two matrices. The activation $\sigma(\cdot)$ is applied to each component of the vector input, and the weight matrix $W^{(\ell)}$ in the ℓ -th layer is sampled from a multivariate Gaussian distribution $\mathcal{MN}(\cdot, \cdot)$. For a vector v and a scalar s , the notation v/s denotes the component-wise division of v by scalar s . We remark that the scaling in (2.12) matches the standard weight initialization scheme in practice, since in the current setting $\|x^\ell\| \asymp \sqrt{d_\ell}$ and (2.13) is effectively saying that each row $W_{i \cdot}^{(\ell)} / \sqrt{d_\ell} \sim \mathcal{N}(0, 1/d_\ell \cdot \mathbf{I}_{d_\ell})$.

3 Compositional Kernel and Branching Process

3.1 Warm up: Duality

We start by describing a simple duality between the activation function in multi-layer perceptrons (that satisfies Assumption 1) and the probability generating function in branching processes. This simple yet essential duality allows us to study deep neural networks, and compare different activation functions borrowing tools from branching processes. This duality can be readily established via the Mehler's formula (Proposition 2.2). To the best of our knowledge, this probabilistic interpretation (Lemma 3.3) is new to the literature.

Lemma 3.1 (Duality: activation and generating functions). *Let $\sigma(\cdot) \in L^2_\phi(1)$ be an activation function under Assumption 1, with the corresponding Hermite coefficients $\{a_k : k \in \mathbb{Z}^{\geq 0}\}$ satisfying $\sum_{k \geq 0} a_k^2 = 1$. Define the corresponding random variable Y_σ with*

$$\mathbf{P}(Y_\sigma = k) = a_k^2, \quad \forall k \in \mathbb{Z}^{\geq 0}. \quad (3.1)$$

We denote the PGF of Y_σ (from Definition 2.3) as $G_\sigma(\cdot) : [-1, 1] \rightarrow [-1, 1]$ to be the dual generating function of the activation $\sigma(\cdot)$. Then, for any $x, z \in \mathbb{R}^d$, with $\rho := \langle x/\|x\|, z/\|z\| \rangle \in [-1, 1]$, we have

$$\mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma(\boldsymbol{\theta}^\top x / \|x\|) \sigma(\boldsymbol{\theta}^\top z / \|z\|) \right] = G_\sigma(\rho). \quad (3.2)$$

Based on the above Lemma 3.1, it is easy to define the compositional kernel associated with a fully-connected MLP, with activation $\sigma(\cdot)$. The compositional kernel approach of studying deep neural networks has been proposed in Daniely et al. (2017b,a). To see why, let us recall the MLP with random weights defined in Definition 2.7. Then, for any fixed data input $x, z \in \mathbb{R}^{d_0}$, the following holds almost surely for random weights $W^{(\ell)}$

$$\lim_{d_{\ell+1} \rightarrow \infty} \langle x^{(\ell+1)} / \|x^{(\ell+1)}\|, z^{(\ell+1)} / \|z^{(\ell+1)}\| \rangle = G_\sigma \left(\langle x^{(\ell)} / \|x^{(\ell)}\|, z^{(\ell)} / \|z^{(\ell)}\| \rangle \right). \quad (3.3)$$

Motivated by the above equation, one can introduce the asymptotic **compositional kernel** defined by a deep neural network with activation $\sigma(\cdot)$, in the following way.

Definition 3.2 (Compositional kernel). *Let $\sigma(\cdot) \in L^2_\phi(1)$ be an activation function that satisfies Assumption 1. Define the L -layer compositional kernel $K_\sigma^{(L)}(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ to be the (infinite-width) compositional kernel associated with the fully-connected MLPs (from Definition 2.7), such that for any $x, z \in \mathcal{X}$, we have*

$$K_\sigma^{(L)}(x, z) := \underbrace{G_\sigma \circ \dots \circ G_\sigma}_{\text{composite } L \text{ times}} \left(\langle x/\|x\|, z/\|z\| \rangle \right). \quad (3.4)$$

Since the kernel only depends on the inner-product $\rho = \langle x/\|x\|, z/\|z\| \rangle$, when there is no confusion, we denote for any $\rho \in [-1, 1]$

$$K_\sigma^{(L)}(\rho) = \underbrace{G_\sigma \circ \dots \circ G_\sigma}_{\text{composite } L \text{ times}}(\rho). \quad (3.5)$$

We will now point out the following connection between the compositional kernel for deep neural network and the Galton-Watson branching process. Later, we will study the (rescaled) limits, phase transitions, memorization capacity, and spectral decomposition of such compositional kernels.

Lemma 3.3 (Duality: MLP and Branching Process). *Let $\sigma(\cdot) \in L^2_\phi(1)$ be an activation function that satisfies Assumption 1, and $G_\sigma(\cdot)$ be the dual generating function as in Lemma 3.1. Let $\{Z_{\sigma,L} : L \in \mathbb{Z}^{\geq 0}\}$ be the Galton-Watson branching process with offspring distribution Y_σ . Then for any $L \in \mathbb{Z}^{\geq 0}$, the compositional kernel has the following interpretation using the Galton-Watson branching process*

$$K_\sigma^{(L)}(\rho) = \mathbb{E}[\rho^{Z_{\sigma,L}}] . \quad (3.6)$$

The above duality can be extended to study other network architectures. For instance, in the residual network, the duality can be defined as follows: for $x, z \in \mathbb{S}^{d-1}$, $r \in [0, 1]$, and a centered activation function $\sigma(\cdot)$ (Assumption 2), define the dual residual PGF G_σ^{res} as

$$\begin{aligned} G_\sigma^{\text{res}}(\langle x, z \rangle) &:= \mathbb{E}_{\{\theta_j \sim \mathcal{N}(0, \mathbf{I}_d), i \in [d]\}} \left[\sum_{i=1}^d \left(\sqrt{1-r} \sigma(\theta_j^\top x) / \sqrt{d} + \sqrt{r} x_j \right) \left(\sqrt{1-r} \sigma(\theta_j^\top z) / \sqrt{d} + \sqrt{r} z_j \right) \right] \\ &= (1-r) \mathbb{E}_{\theta \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma(\theta^\top x) \sigma(\theta^\top z) \right] + r \langle x, z \rangle = (1-r) G_\sigma^{\text{mlp}}(\langle x, z \rangle) + r \langle x, z \rangle . \end{aligned}$$

Later in the next section, we can see the cost and benefits of adding a linear component to the PGF in the compositional behavior of it.

3.2 Limits and phase transitions

In this section, we will study the properties of the compositional kernel, in the lens of branching process, utilizing the duality established in the previous section. One important result in branching process is the Kesten-Stigum Theorem (Kesten and Stigum, 1966), which can be employed to assert the rescaled limit and phase transition of the compositional kernel.

Theorem 3.4 (Rescaled non-trivial limits and phase transitions: compositional kernels). *Let $\sigma(\cdot) \in L^2_\phi(1)$ be an activation function that satisfies Assumption 1, with $\{a_k : k \in \mathbb{Z}^{\geq 0}\}$ be the corresponding Hermite coefficients that satisfy $\sum_{k \geq 0} a_k^2 = 1$. Define two quantities that depend on $\sigma(\cdot)$,*

$$\mu := \sum_{k \geq 0} a_k^2 k, \quad \mu_\star := \sum_{k > 2} a_k^2 k \log k . \quad (3.7)$$

Recall the MLP compositional kernel $K_\sigma^{(L)}(\cdot) : \mathbb{R} \rightarrow \mathbb{R}$ with activation $\sigma(\cdot)$ in Definition 3.2, and the dual PGF $G_\sigma(\cdot)$ in Lemma 3.1. For any $t \geq 0$, the following results hold, depending on the value of μ and μ_\star :

(i) $\mu \leq 1$. Then, if $a_1^2 \neq 1$, we have

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(e^{-t}) = 1 \quad \text{for } t \geq 0; \quad (3.8)$$

and, if $a_1^2 = 1$, we have $K_\sigma^{(L)}(e^{-t}) = e^{-t}$ for all $L \in \mathbb{Z}^{\geq 0}$;

(ii) $\mu > 1$ and $\mu_\star < \infty$. Then, there exists $0 \leq \xi < 1$ with $G_\sigma(\xi) = \xi$ and a unique positive random variable W_σ (that depends on σ) with a continuous density on \mathbb{R}^+ . And, the non-trivial rescaled limit is

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(e^{-t/\mu^L}) = \xi + (1 - \xi) \cdot \mathbb{E}[e^{-tW_\sigma}] ; \quad (3.9)$$

(iii) $\mu > 1$ and $\mu_\star = \infty$. Then, for any positive number $m > 0$, we have

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(e^{-t/m^L}) = \begin{cases} 1, & \text{if } t = 0 \\ 0, & \text{if } t > 0 \end{cases} . \quad (3.10)$$

The above shows that when looking at the compositional kernel at the rescaled location e^{-t/μ^L} for a fixed $t > 0$, the limit can be characterized by the moment generating function associated with a negative random variable $M_{-W_\sigma}(t) = \mathbb{E}[e^{-tW_\sigma}]$ individual to the activation function σ . The intuition behind such a rescaled location is that the limiting kernels witness an abrupt change of value at $K_\sigma^{(L)}(\rho)$ near $\rho = 1$ for large L (see the below Corollary 3.5). In the case $\mu > 1$, the proper rescaling in Theorem 3.4 stretches out the curve and zooms in the narrow window of width $O(1/\mu^L)$ local to $\rho = 1$ to inspect the detailed behavior of the compositional kernel $K_\sigma^{(L)}(\rho)$. Conceptually, the above Theorem classifies the rescaled behavior of the compositional kernel into three phases according to μ and μ_\star , functionals of the activation $\sigma(\cdot)$. One can also see that the unscaled limit for the compositional kernel has the following simple behavior.

Corollary 3.5 (Unscaled limits and phase transitions). *Under the same setting as in Theorem 3.4, the following results hold:*

(i) $\mu \leq 1$. Then, for all $\rho \in [0, 1]$, if $a_1^2 \neq 1$, we have

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(\rho) = 1; \quad (3.11)$$

and $K_\sigma^{(L)}(\rho) = \rho$ for all $L \in \mathbb{Z}^{\geq 0}$ if $a_1^2 = 1$;

(ii) $\mu > 1$. Then, there exists a unique $0 \leq \xi < 1$ with $G_\sigma(\xi) = \xi$

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(\rho) = \begin{cases} 1, & \text{if } \rho = 1 \\ \xi, & \text{if } \rho \in [0, 1) \end{cases} . \quad (3.12)$$

Under additional assumptions of $G_\sigma(\cdot)$ on $(-1, 0)$ such as no fixed points or non-negativity, we can extend the above results to $[-1, 1]$

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(\rho) = \begin{cases} 1, & \text{if } \rho = 1 \\ \xi, & \text{if } \rho \in (-1, 1) \end{cases} . \quad (3.13)$$

Under the additional Assumption 2 on $\sigma(\cdot)$, for non-linear activation $\sigma(\cdot)$, we have $\mu > 1$ and $\xi = 0$. Therefore, the unscaled limit for non-linear compositional kernel is

$$\lim_{L \rightarrow \infty} K_\sigma^{(L)}(\rho) = \begin{cases} 1, & \text{if } \rho = 1 \\ 0, & \text{if } \rho \in (-1, 1) \end{cases} . \quad (3.14)$$

We remark that the fact (ii) in the above corollary is not new and has been observed by [Daniely et al. \(2017b\)](#). On the one hand, they use the fact (ii) to shed light on why more than five consecutive fully connected layers are rare in practical architectures. On the other hand, the phase transition at $\mu = 1$ corresponds to the edge-of-chaos and exponential expressivity of deep nets studied in [Poole et al. \(2016\)](#), using physics language.

4 Memorization Capacity of Compositions: Tradeoffs

One advantage of deep neural networks (DNN) is their exceptional data memorization capacity. Empirically, researchers observed that DNNs with large depth and width could memorize large datasets ([Zhang et al., 2017](#)), while maintaining good generalization properties. Pioneered by Belkin, a list of recent work contributes to a better understanding of the interpolation regime ([Belkin et al., 2018a, 2019, 2018c](#); [Liang and Rakhlin, 2018](#); [Hastie et al., 2019](#); [Bartlett et al., 2019](#); [Liang et al., 2020](#); [Feldman, 2019](#); [Nakkiran et al., 2020](#)). With the insights gained via branching process, we will investigate the memorization capacity of the compositional kernels corresponding to MLPs, and study the interplay among the *sample size*, *dimensionality*, *properties of the activation*, and the *composition depth* in a non-asymptotic way.

In this section, we denote $\mathcal{X} = \{x_i \in \mathbb{S}^{d-1} : i \in [n]\}$ as the dataset with each data point lying on the unit sphere. Specifically, we consider the following scaling regimes on the sample size n relative to the dimensionality d :

1. Small correlation: We consider the scaling regime $\frac{\log n}{d} \rightarrow 0$, where the dataset \mathcal{X} is generated from a probabilistic model with uniform distribution on the sphere. We name it “small correlation” since in such a case we have that $\sup_{i \neq j} |\rho_{ij}|$ is vanishing small, where $\rho_{ij} = \langle x_i, x_j \rangle$.
2. Large correlation: We consider the scaling regime $\frac{\log n}{d} \rightarrow \infty$, where the dataset \mathcal{X} forms a certain packing set of the sphere. We call it “large correlation” as $\sup_{i \neq j} |\rho_{ij}|$ can be close to 1.

For the results in this section, we make the Assumptions [1](#) and [2](#) on the activation function $\sigma(\cdot)$, which are guaranteed by a simple rescaling and centering of any L^2 activation function. Let $\mathbf{K}^{(L)} \in \mathbb{R}^{n \times n}$ be the empirical kernel matrix for the compositional kernel at depth L , with

$$\mathbf{K}^{(L)}[i, j] = K_{\sigma}^{(L)}(\langle x_i, x_j \rangle) . \quad (4.1)$$

For kernel ridge regression, the spectral properties of the empirical kernel matrix affect the memorization capacity: when $\mathbf{K}^{(L)}$ has full rank, the regression function without explicit regularization can interpolate the training dataset. Specifically, the following spectral characterization on the empirical kernel matrix determines the rate of convergence in terms of optimization to the min-norm interpolated solution, thus further determines memorization.

Definition 4.1 (κ -memorization). *We call that a symmetric kernel matrix $\mathbf{K} = [K(x_i, x_j)]_{1 \leq i, j \leq n} \in \mathbb{R}^{n \times n}$ associated with the dataset $\mathcal{X} = \{x_i\}_{i \in [n]}$ has a κ -memorization property if the eigenvalues $\lambda_i(\mathbf{K})$, with $i \in [n]$, of \mathbf{K} are well behaved in the following sense*

$$1 - \kappa \leq \lambda_i(\mathbf{K}) \leq 1 + \kappa, \quad i \in [n]. \quad (4.2)$$

4.1 Small correlation regime

To study the small correlation regime, we consider a typical instance of the dataset that are generated i.i.d. from a uniform distribution on the sphere.

Theorem 4.2 (Memorization capacity, small correlation regime). *Consider a dataset with random instance $\mathcal{X} = \{x_i\}_{i \in [n]} \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(\mathbb{S}^{d-1})$. And, consider the regime $\frac{\log n}{d(n)} \rightarrow 0$. For any $0 < \kappa < 1$ and sufficiently large n , with the compositional depth*

$$L \geq c_1 \cdot \frac{\log(n\kappa^{-1}) + \log \frac{\log n}{d}}{\log a_1^{-2}} \quad (4.3)$$

the empirical kernel matrix is well conditioned in the sense that it κ -memorizes the dataset \mathcal{X} with probability at least $1 - \exp(-c_2 n)$, where c_1 and c_2 are constants that do not depend on n and d .

In the small correlation regime, the above Theorem 4.2 states that in order for us to memorize a size n -dataset \mathcal{X} , the depth L for the compositional kernel $K_\sigma^{(L)}$ scales with three quantities: the linear component in the activation function a_1^{-2} , a factor $\log(n\kappa^{-1})$, and the logarithm of the regime scaling $\log(\frac{\log n}{d})$. Two remarks are in order. First, as the quantity $\frac{\log n}{d}$ becomes larger, we need a larger depth for the compositional kernel to achieve the same memorization. However, such an effect is mild since the regime scaling enters logarithmically in a form $\log(\frac{\log n}{d})$. In other words, for i.i.d. data on the unit sphere with $\frac{\log n}{d} \rightarrow 0$, it is indeed easy for a shallow compositional kernel (with depth at most $\log n$) to memorize the data. Second, $a_1^{-2} = 1 + (\sum_{k \geq 2} a_k^2)/a_1^2$ can be interpreted as the amount of non-linearity in the activation function. Therefore, when the non-linear component is larger, we will need fewer compositions for memorization. A simple contrast should be mentioned for comparison: memorization is only possible for linear models when $d \geq n$, whereas with composition and non-linearity, $d \gg \log n$ is enough for memorization.

4.2 Large correlation regime

To study the large correlation regime, we consider a natural instance of the dataset that falls under such a setting. The construction is based on the sphere packing.

Definition 4.3 (r -polarized packing). *For a compact subset $V \subset \mathbb{R}^d$, we say $\mathcal{X} = \{x_i\}_{i \in [n]} \subset V$ is a r -polarized packing of V if for all $x_i \neq x_j \in \mathcal{X}$, we have $\|x_i - x_j\| > r$ and $\|x_i + x_j\| > r$. We define the polarized packing number of V as $\mathcal{P}_r(V)$, that is*

$$\mathcal{P}_r(V) = \max\{n: \text{exists } r\text{-polarized packing of } V \text{ of size } n\} . \quad (4.4)$$

Theorem 4.4 (Memorization capacity, large correlation regime). *Consider a size- n dataset $\mathcal{X} = \{x_i \in \mathbb{S}^{d-1} : i \in [n]\}$ that forms a certain maximal polarized packing set of the sphere \mathbb{S}^{d-1} . And, consider the regime $\frac{\log n}{d(n)} \rightarrow \infty$ and recall the μ defined in Theorem 3.4. For any $0 < \kappa < 1$ and sufficiently large n , with the compositional depth*

$$L \geq c_3 \cdot \frac{\exp(2 \frac{\log n}{d}) \log(n\kappa^{-1})}{\mu - 1} \quad (4.5)$$

the empirical kernel matrix is well conditioned in the sense that it κ -memorizes the dataset \mathcal{X} , where c_3 is a constant that does not depend on n and d .

In the large correlation regime, to memorize a dataset, the behavior of the compositional depth is rather different from the small correlation regime. The depth L in Theorem 4.4 scales with three quantities: the non-linearity measured in $\mu - 1$, a factor $\log(n\kappa^{-1})$ same as before, and the exponential of the regime scaling $\exp(2\frac{\log n}{d})$. Few remarks are in order. First, in this large correlation regime $n \gg \exp(d)$, memorization is indeed possible. However, the compositional depth needed, $\exp(2\frac{\log n}{d})$, increases exponentially as a function of the regime scaling $\frac{\log n}{d}$. The above is in contrast to the small correlation regime, where the dependence on the regime scaling is logarithmic as $\log(\frac{\log n}{d})$. In other words, for hard dataset instances on the sphere with $\frac{\log n}{d} \rightarrow \infty$, one needs a very deep compositional kernel to achieve memorization. Second, unlike in the small correlation regime, the role of non-linearity enters in a different form here: the larger the non-linear component is, the larger the $\mu - 1 = \sum_{k \geq 2} a_k^2(k - 1)$ is, which mitigates the compositional depth. To sum up, with non-linearity and composition, even in the $d \ll \log n$ regime with a hard data instance, memorization is possible but with a very deep neural network.

5 Spectral Decomposition of Compositional Kernels

In this section, we investigate the spectral decomposition of the compositional kernel function. We study the case where the base measure is a uniform distribution on the unit sphere, denote by τ_{d-1} . Let S_{d-1} be the surface area of \mathbb{S}^{d-1} . To state the results, we will need some background on the spherical harmonics. We consider the dimension $d \geq 2$, and will use $k \in \mathbb{Z}^{\geq 0}$ to denote an integer.

Definition 5.1 (Spherical harmonics, Chapter 2.8.4 in [Atkinson and Han \(2012\)](#)). *Let \mathbf{Y}_k^d be the space of k -th degree spherical harmonics in dimension d , and let $\{Y_{k,j}(x) : j \in [N_{k,d}]\}$ be an orthonormal basis for \mathbf{Y}_k^d , with*

$$\int Y_{k,i}(x)Y_{k,j}(x)d\tau_{d-1}(x) = \mathbb{1}_{i=j} . \quad (5.1)$$

Then, the sets form an orthogonal basis for the space $L^2_{\tau_{d-1}}$ of L^2 -integrable functions on \mathbb{S}^{d-1} with the base measure τ_{d-1} , noted below

$$L^2_{\tau_{d-1}} = \bigoplus_{k=0}^{\infty} \mathbf{Y}_k^d . \quad (5.2)$$

Moreover, the dimensionality $\dim \mathbf{Y}_k^d = N_{k,d}$ are the coefficients of the generating function

$$\sum_{k=0}^{\infty} N_{k,d} s^k = \frac{1+s}{(1-s)^{d-1}}, \quad |s| < 1 . \quad (5.3)$$

Definition 5.2 (Legendre polynomial, Chapter 2.7 in [Atkinson and Han \(2012\)](#)). *Define the Legendre polynomial of degree k with dimension d to be*

$$P_{k,d}(t) = (-1)^k \frac{\Gamma(\frac{d-1}{2})}{2^k \Gamma(k + \frac{d-1}{2})} (1-t^2)^{-\frac{d-3}{2}} \left(\frac{d}{dt} \right)^k (1-t^2)^{k+\frac{d-3}{2}} . \quad (5.4)$$

The following orthogonality holds

$$\int_{-1}^1 P_{k,d}(t)P_{\ell,d}(t)(1-t^2)^{\frac{d-3}{2}} dt = \begin{cases} 0, & \text{if } k \neq \ell \\ \frac{S_{d-1}}{N_{k,d}S_{d-2}}, & \text{if } k = \ell \end{cases} . \quad (5.5)$$

Recall that the compositional kernel $K_\sigma^{(L)}(\cdot)$ and the random variable $Z_{\sigma,L}$, which denotes the size of the L -th generation, as in Lemma 3.3. Then, we have the following theorem describing the spectral decomposition of the compositional kernel function and the associated integral operator.

Theorem 5.3 (Spectral decomposition of compositional kernel). *Consider any $x, z \in \mathbb{S}^{d-1}$. Then, the following spectral decomposition holds for the compositional kernel $K_\sigma^{(L)}$ with any fixed depth $L \in \mathbb{Z}^{\geq 0}$:*

$$K_\sigma^{(L)}(\langle x, z \rangle) = \sum_{k=0}^{\infty} \lambda_k \sum_{j=1}^{N_{k,d}} Y_{k,j}(x) Y_{k,j}(z) , \quad (5.6)$$

where the eigenfunctions $Y_{k,j}(\cdot)$ form an orthogonal basis of $L_{\tau_{d-1}}^2$, and the eigenvalues λ_k satisfy the following formula

$$\lambda_k := \frac{S_{d-2}}{S_{d-1}} \Gamma\left(\frac{d-1}{2}\right) \sum_{\ell \geq 0} \mathbf{P}(Z_{\sigma,L} = k + \ell) \frac{(k + \ell)!}{\ell!} \frac{1 + (-1)^\ell}{2^{k+1}} \frac{\Gamma(\frac{\ell+1}{2})}{\Gamma(k + \frac{\ell+d}{2})} . \quad (5.7)$$

The associated integral operator $\mathcal{T}_\sigma^{(L)} : L_{\tau_{d-1}}^2 \rightarrow L_{\tau_{d-1}}^2$ with respect to the kernel $K_\sigma^{(L)}$ is defined as

$$(\mathcal{T}_\sigma^{(L)} f)(x) := \int K_\sigma^{(L)}(\langle x, z \rangle) f(z) d\tau_{d-1}(z) \quad \text{for any } f \in L_{\tau_{d-1}}^2 . \quad (5.8)$$

From Theorem 5.3, we know that the eigenfunctions of the operator $\mathcal{T}_\sigma^{(L)}$ are the spherical harmonic basis $\{Y_{k,j} : k \in \mathbb{Z}^{\geq 0}, j \in [N_{k,d}]\}$, with $N_{k,d}$ identical eigenvalues λ_k such that

$$\mathcal{T}_\sigma^{(L)} Y_{k,j} = \lambda_k Y_{k,j} . \quad (5.9)$$

The above spectral decompositions are important because it helps us study the generalization error (in the fixed dimensional setting) of regression methods with the compositional kernel $K_\sigma^{(L)}$. More specifically, understanding the eigenvalues of the compositional kernels means that we can employ the classical theory on reproducing kernel Hilbert spaces regression (Caponnetto and Vito, 2006) to quantify generalization error. In the case when dimensionality grows with the sample size, several attempts have been made to understand the generalization properties of the inner-product kernels (Liang and Rakhlin, 2018; Liang et al., 2020) in the interpolation regime, which includes these compositional kernels as special cases.

6 Kernels to Activations: New Random Features Algorithms

Given any L_ϕ^2 activation function $\sigma(\cdot)$ (as in Definition 2.6), we can define a sequence of positive definite (PD) compositional kernels $K_\sigma^{(L)}$, with $L \geq 0$, whose spectral properties have been studied in

the previous section, utilizing the duality established in Section 3.1. Such compositional kernels are non-linear functions on the inner-product $\langle x, z \rangle$ (rotation-invariant), and we will call them the *inner-product kernels* (Kar and Karnick, 2012). In this section, we will investigate the *converse question*: given an arbitrary PD inner-product kernel, can we identify an activation function associated with it? We will provide a positive answer in this section. Direct algorithmic implications are new random features algorithms that are distinct from the well-known random Fourier features and random kitchen sinks algorithms studied in Rahimi and Recht (2008, 2009).

Define an inner-product kernel $K(\cdot, \cdot) : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$, with $d \geq 2$,

$$K(x, z) := f(\langle x, z \rangle) , \quad (6.1)$$

where $f : [-1, 1] \rightarrow \mathbb{R}$ is a continuous function. Denote the expansion of f under the Legendre polynomials $P_{k,d}$ (see Definition 5.2) as

$$f(t) = \sum_{k=0}^{\infty} \alpha_k P_{k,d}(t) . \quad (6.2)$$

To define the activations given an arbitrary PD inner-product kernel, we require the following theorem due to Schoenberg (1942).

Proposition 6.1 (Theorem 1 in Schoenberg (1942)). *For a fixed $d \geq 2$, the inner-product kernel $K(\cdot, \cdot)$ in (6.1) is positive definite on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$ if and only if $\alpha_k \geq 0$ for all $k \in \mathbb{Z}^{\geq 0}$ in Equation (6.2).*

Now, we are ready to state the activation function σ_f defined based on the inner-product kernel function f .

Theorem 6.2 (Kernels to activations). *Consider any positive definite inner product kernel $K(x, z) := f(\langle x, z \rangle)$ on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$ associated with the continuous function $f : [-1, 1] \rightarrow \mathbb{R}$. Assume without loss of generality that $f(1) = 1$, and recall the definition of $N_{k,d}$ in (5.3). Due to Proposition 6.1, the Legendre coefficients $\{\alpha_k : k \in \mathbb{Z}^{\geq 0}\}$, defined in Equation (6.2), of f are non-negative.*

One can define the following dual activation function $\sigma_f : [-1, 1] \rightarrow \mathbb{R}$

$$\sigma_f(t) = \sum_{k=0}^{\infty} \sqrt{\alpha_k N_{k,d}} P_{k,d}(t) . \quad (6.3)$$

Then, the following statements hold:

$$(i) \quad \sigma_f(\cdot) \text{ is } L^2 \text{ in the following sense } \int_{-1}^1 \left(\sigma_f(t) \right)^2 \frac{S_{d-2}}{S_{d-1}} (1-t^2)^{\frac{d-3}{2}} dt = 1 .$$

$$(ii) \quad \text{For any } x, z \in \mathbb{S}^{d-1}$$

$$\mathbb{E}_{\xi \sim \tau_{d-1}} \left[\sigma_f(\xi^\top x) \sigma_f(\xi^\top z) \right] = f(\langle x, z \rangle) = K(x, z) , \quad (6.4)$$

where ξ is sampled from a uniform distribution on the sphere \mathbb{S}^{d-1} .

The above theorem naturally induces a new random features algorithm for kernel ridge regression, described below. Note that the kernel K can be any compositional kernel, which is positive definite and of an inner-product form.

Algorithm 1: New random features algorithm for positive definite inner-product kernels $K(x, z) = f(\langle x, z \rangle)$ based on Theorem 6.2.

Result: Given a normalized dataset $\mathcal{X} = \{x_i \in \mathbb{S}^{d-1}, i \in [n]\}$, an integer m , and a positive definite inner-product kernel $K(x, z) = f(\langle x, z \rangle)$, return a randomized non-linear feature matrix $\Phi \in \mathbb{R}^{n \times m}$ for kernel ridge regression.

Step 1: Calculate the Legendre coefficients of $f(t) = \sum_{k=0}^{\infty} \alpha_k P_{k,d}(t)$;

Step 2: Obtain the dual activation function $\sigma_f(t) = \sum_{k=0}^{\infty} \sqrt{\alpha_k N_{k,d}} P_{k,d}(t)$, $t \in [-1, 1]$;

Step 3: Sample m -i.i.d. isotropic Gaussian vectors $t_j \sim \mathcal{N}(0, \mathbf{I}_d)$, and then define the non-linear feature matrix

$$\Phi[i, j] = \sigma_f(\langle x_i, \theta_j / \|\theta_j\| \rangle), \quad i \in [n], j \in [m] . \quad (6.5)$$

The feature matrix satisfies $\lim_{m \rightarrow \infty} (1/m \cdot \Phi \Phi^\top)[i, \ell] = f(\langle x_i, x_\ell \rangle)$ for all $i, \ell \in [n]$ a.s..

It is clear from Theorem 5.3 that all compositional kernels $K_\sigma^{(L)}$ are positive definite, though the converse statement is not true. A notable example is the kernel $P_{k,d}(\langle x, z \rangle) : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \rightarrow \mathbb{R}$, which is PD kernel but with negative Taylor coefficients, thus cannot be a compositional kernel. For the special case of compositional kernels with depth L and activation $\sigma(\cdot)$, it turns out one can define a new "compressed" activation $\sigma^{(L)}(\cdot) \in L_\phi^2$ to represent the depth- L compositional kernel. We propose the following algorithm:

Algorithm 2: New random features algorithm for compositional kernels $K_\sigma^{(L)}$.

Result: Given a normalized dataset $\mathcal{X} = \{x_i \in \mathbb{S}^{d-1}, i \in [n]\}$, an integer m , and a compositional kernel $K_\sigma^{(L)}(x, z) = K_\sigma^{(L)}(\langle x, z \rangle)$, return a randomized non-linear feature matrix $\Psi \in \mathbb{R}^{n \times m}$ for kernel ridge regression.

Step 1: Calculate the Taylor coefficients of $K_\sigma^{(L)}(t) = \sum_{k=0}^{\infty} \alpha_k t^k$ with $\alpha_k = \mathbf{P}(Z_{\sigma,L} = k)$;

Step 2: Obtain the "compressed" activation function

$$\sigma^{(L)}(t) = \sum_{k=0}^{\infty} \sqrt{\alpha_k} h_k(t), \quad t \in \mathbb{R} ; \quad (6.6)$$

Step 3: Sample m -i.i.d. isotropic Gaussian vectors $\theta_j \sim \mathcal{N}(0, \mathbf{I}_d)$, and then define the non-linear feature matrix

$$\Psi[i, j] = \sigma^{(L)}(\langle x_i, \theta_j \rangle), \quad i \in [n], j \in [m] . \quad (6.7)$$

The feature matrix satisfies $\lim_{m \rightarrow \infty} (1/m \cdot \Psi \Psi^\top)[i, l] = K_\sigma^{(L)}(\langle x_i, x_l \rangle)$ for all $i, l \in [n]$ a.s..

First, let us discuss the relationship between our random features algorithms above and that in Rahimi and Recht (2008, 2009). Rahimi and Recht (2008) employed the duality between the PD shift-invariant kernel $k(x - z)$ and a positive measure that corresponds to the inverse Fourier transform of k : the random features are constructed based on the specific positive measure where sampling could be a non-trivial task. In contrast, we utilize the duality between the PD inner-

product kernel and an activation function, where the random features are always generated based on the uniform distribution on the sphere (or the isotropic Gaussian), but with different activations $\sigma(\cdot)$. It is clear that sampling uniformly from the sphere can be easily done by sampling $\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)$, and returning $\boldsymbol{\theta}/\|\boldsymbol{\theta}\|$.

We now conclude this section by stating another property of Algorithm 2, implied by the Mehler's formula. It turns out that under a certain high dimensional scaling regime, say $d(n) \asymp n^{\frac{2}{\iota+1}}$ for some fixed integer $\iota \in \mathbb{Z}^{>0}$, the compressed activation $\sigma^{(L)}$ in (6.6) can be truncated without loss using only the low degree components $k \leq \iota$. For notation simplicity, in the statement below, we drop the superscript (L) in the kernel and the compressed activation.

Theorem 6.3 (Empirical kernel matrix: truncation and implicit regularization). *Consider the compositional kernel function $K_\sigma(t) = \sum_{k=0}^{\infty} \alpha_k t^k$ as in Algorithm 2, and the dataset $\mathbf{X} = [x_1^\top, \dots, x_n^\top]^\top \in \mathbb{R}^{n \times d}$ with column $x_i \stackrel{iid}{\sim} \text{Unif}(\mathbb{S}^{d-1})$. Consider the high dimensional regime where the dimensionality $d(n)$ scales with n , satisfying*

$$d(n) \gtrsim n^{\frac{2}{\iota+1} + \delta},$$

for some fixed integer $\iota \in \mathbb{Z}^{>0}$ and any fixed small $\delta > 0$. Define a truncated activation based on (6.6), at degree level ι

$$\sigma_{\leq \iota}(t) := \sum_{k=0}^{\iota} \sqrt{\alpha_k} h_k(t) . \quad (6.8)$$

Then the empirical kernel matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ satisfies the following decomposition

$$\mathbf{K} = \underbrace{\left(\sum_{k>\iota} \alpha_k \right) \cdot \mathbf{I}_n}_{\text{implicit regularization}} + \underbrace{\mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} [\sigma_{\leq \iota}(\mathbf{X}\boldsymbol{\theta}) \sigma_{\leq \iota}(\mathbf{X}\boldsymbol{\theta})^\top]}_{\text{degree truncated random features}} + \underbrace{\mathbf{R}}_{\text{remainder}} \quad (6.9)$$

with the remainder matrix $\mathbf{R} \in \mathbb{R}^{n \times n}$ satisfies

$$\|\mathbf{R}\|_{\text{op}} \rightarrow 0, \text{ as } n, d(n) \rightarrow \infty. \quad (6.10)$$

A direct consequence of the above theorem is that, the empirical kernel matrix \mathbf{K} shares the same eigenvalues and empirical spectral density as the matrix $(\sum_{k>\iota} \alpha_k) \cdot \mathbf{I}_n + \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} [\sigma_{\leq \iota}(\mathbf{X}\boldsymbol{\theta}) \sigma_{\leq \iota}(\mathbf{X}\boldsymbol{\theta})^\top]$, asymptotically. The implicit regularization matrix is contributed by the high degree components of the activation function collectively.

7 Numerical Investigation

In this section, we will explore numerically the theory established in the previous sections. We will experiment with four common activations used in practice as a proof of concept, namely ReLU, GeLU, Swish, and Sigmoid, and four PGFs associated with non-negative discrete probability distributions including Poisson(λ), Binomial(n, p), Geometric(p), and Uniform($0, n$). To execute the theory numerically, we introduce a simple and general Algorithm 3 for estimating the Hermite coefficients of *any* activation function $\sigma(\cdot)$, with provable guarantees. The numerical stability of this algorithm to estimate the Hermite coefficients can be seen in Figure 7. The truncation level considered is $T = 20$. We will use this level throughout the rest of the experiments in this section.

Algorithm 3: Algorithm for estimating the Hermite coefficients of an activation $\sigma(\cdot)$.

Result: Given an activation function $\sigma(t) = \sum_{k=0}^{\infty} a_k h_k(t) \in L^2_{\phi}$ and a truncation level T , return an estimate of the Hermite coefficients $\{a_k\}_{k=0}^T$.

Step 1: Generate M inputs $\{x_i\}_{i=1}^M$ from a standard normal $\mathcal{N}(0, 1)$;

Step 2: For each $k = 0, 1, 2, \dots, T$, calculate

$$a_k = \frac{1}{M} \sum_{i=1}^M \sigma(x_i) h_k(x_i) .$$

The coefficients satisfy $\lim_{M \rightarrow \infty} \hat{a}_k = a_k$ a.s..

Activations	ReLU	GeLU	Sigmoid	Swish
$\sigma(t)$	$\max(0, t)$	$t \cdot \Phi(t)$	$1/(1 + e^{-t})$	$t/(1 + e^{-t})$
PGFs	Poisson(λ)	Binomial(n, p)	Geometric(p)	Uniform($0, n$)
$G(s)$	$\exp\{\lambda(s - 1)\}$	$(1 - p + ps)^n$	$(1 - p)/(1 - ps)$	$(1 - s^{n+1})/(n(1 - s))$

Table 1: Examples of common activation functions and PGFs.

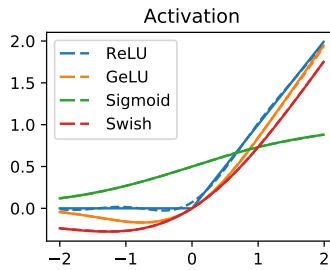


Figure 1: Plot of the numerical stability of Algorithm 3 in approximating activation functions. Solid lines represent the activations, and the dashed lines represent the approximations of the activation functions.

7.1 Duality: Activations and PGFs

According to Lemma 3.1, there is a duality between activation functions $\sigma(\cdot)$ (normalized as in 1) and PGFs $G_\sigma(\cdot)$ (of a discrete non-negative probability distribution). In the first two plots in Figure 2, we start from a probability distribution, and construct its corresponding activation function. Reversely, in the last two plots in Figure 2, we start from an activation function, and approximate (using Algorithm 3) its corresponding PGF.

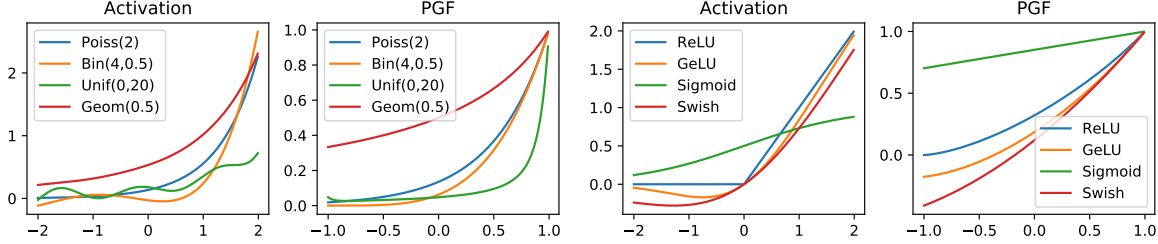


Figure 2: Duality between activations and PGFs.

7.2 Kernel limits

In this section, we will illustrate the compositional behavior of the kernels, both in the unscaled (Corollary 3.5) and rescaled (Theorem 3.4) cases. We start with Figure 3 on the compositional behavior of unscaled kernels $K_\sigma^{(L)}(\rho)$ as a function of $\rho \in [-1, 1]$, without centering the activation functions. According to Corollary 3.5, we know that the unscaled limits of compositional kernels are determined strictly by a phase transition of μ at 1. On the interval $(-1, 1)$, ReLU and Sigmoid's composite kernels converge to 1, while GeLU and Swish's converge to their corresponding extinction probability. In Figure 4 we plot the compositional behavior of the $K_\sigma^{(L)}(\rho)$ for centered activations σ : For centered ReLU, GeLU, Swish, the limit approaches 0 for $\rho \in [-1, 1)$, and approaches 1 at $\rho = 1$. For centered Sigmoid, $a_1 \approx 1$, which explains the resemblance to the linear kernel.

On the other hand, for rescaled kernels $K_\sigma^{(L)}(e^{-t/\mu^L})$ as a function of $t \in [0, \infty)$, non-trivial limits that depend on $\sigma(\cdot)$ exist, when $\mu_\star < \infty$. In the un-centered and rescaled case (Theorem 3.4), we have that ReLU and Sigmoid's compositional kernels converge to 1, while GeLU and Swish's ones approach a non-trivial limit, shown in Figure 5. If we center the activations, all rescaled kernels will approach non-trivial limits as seen in Figure 6.

In terms of the convergence speed of kernels to their unscaled limit, Theorem 4.2 explains how fast the curve flattens around 0, and Theorem 4.4 on the rate it flattens around 1. The convergence speed, in fact, determines the memorization capacity of composition kernels. To flatten around 0, we need the number of compositions to scale with $\frac{1}{\log a_1^{-2}}$, while to flatten around 1, we need the compositional depth to scale with $\frac{1}{\mu-1}$. For example, Sigmoid has $\mu \approx 1.03$ and $a_1^2 \approx 0.99$, thus explaining slow convergence compared to the other activations. Table 2 summarizes the crucial quantities that determine the compositional behavior for each activation.

Activation	ReLU		GeLU		Sigmoid		Swish	
μ	0.95	1.39	1.08	1.47	0.15	1.03	1.07	1.22
μ_\star	0.48	0.69	0.39	0.89	0.01	0.05	0.28	0.31
a_1^2	0.50	0.74	0.59	0.71	0.15	0.99	0.80	0.70
ξ	1.00	0.00	0.76	0.00	1.00	0.00	0.66	0.00

Table 2: Approximations of μ , μ_\star (from Theorem 3.4), and a_1 (from Definition 2.6). For each activation, there are two columns: values for un-centered activation (left) and values for centered activation (right).

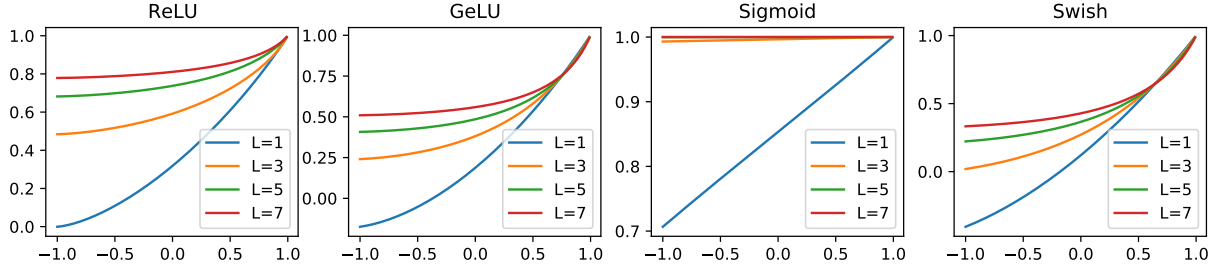


Figure 3: Compositional behavior of unscaled kernels.

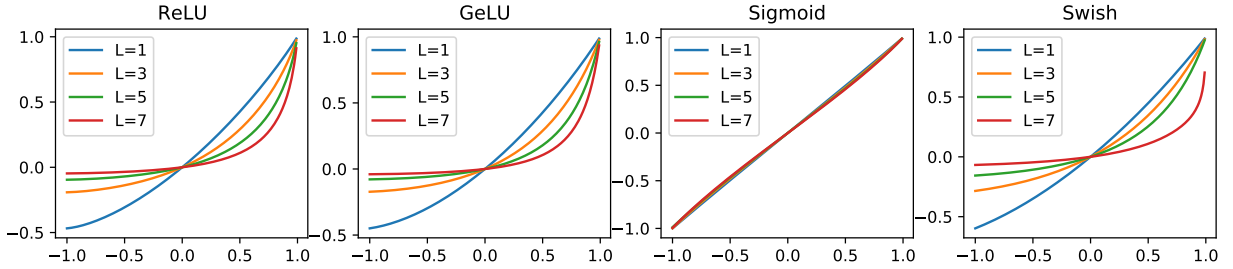


Figure 4: Compositional behavior of unscaled kernels with centered activations.

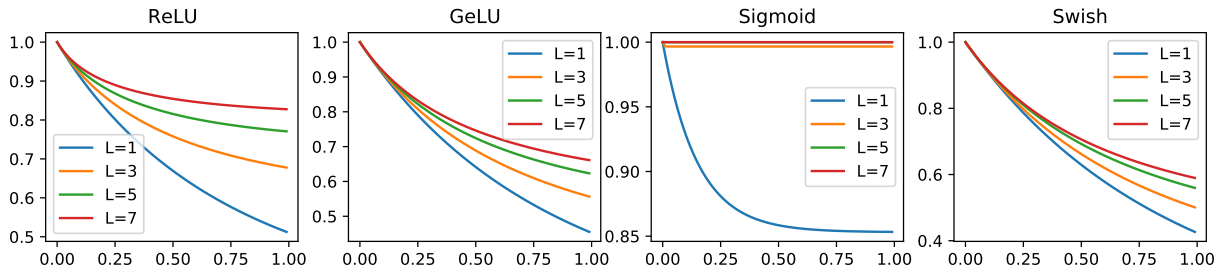


Figure 5: Compositional behavior of rescaled kernels.

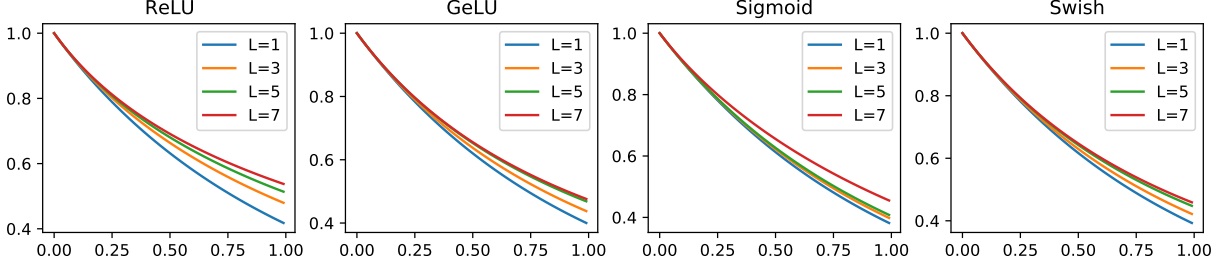


Figure 6: Compositional behavior of rescaled with centered activations.

7.3 Applications to datasets: new random features algorithm

In this section, we will investigate the "compressed" activations obtained from compositional kernels to generate random features, as in Algorithm 2. In Figure 7, we plot the shape of the compressed activations. We will test the validity of the new random features Algorithm 2 on two datasets, MNIST and CIFAR10. For each dataset, we run multi-class logistic regression (a simple one-layer neural network) with 10 categories, using the random features generated by Algorithm 2. For each dataset, we consider four activations and three compositional depths, in total 12 experiments. We run vanilla stochastic gradient descent as the training algorithm. The results are plotted in Figure 8 and the numerical results are displayed in Table 8. We remark that the generalization gap, that is the difference between training accuracy and test accuracy, is smaller for $L = 3$ than for $L = 1$ in the case of using the activation functions ReLU, GeLU, and Swish.

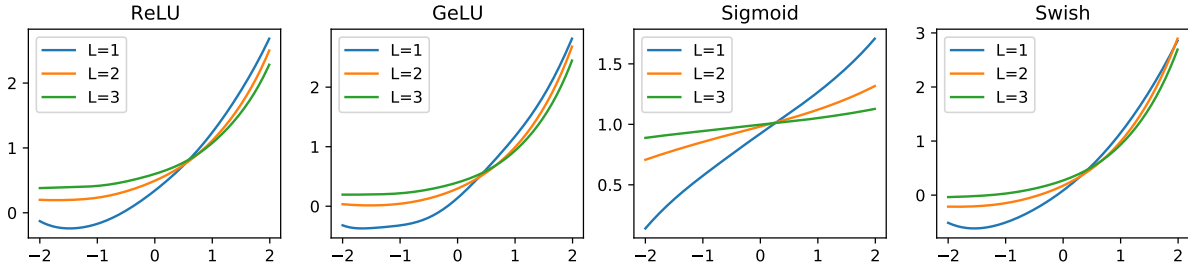


Figure 7: Compressed activation functions as in Algorithm 2.

8 Proofs

8.1 Proofs in Section 3

Proof of Lemma 3.1. By properties of the normal distribution, we have

$$\mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma(\boldsymbol{\theta}^\top \mathbf{x} / \|\mathbf{x}\|) \sigma(\boldsymbol{\theta}^\top \mathbf{z} / \|\mathbf{z}\|) \right] = \mathbb{E}_{(\tilde{\mathbf{x}}, \tilde{\mathbf{z}}) \sim \mathcal{N}_p} [\sigma(\tilde{\mathbf{x}}) \sigma(\tilde{\mathbf{z}})], \quad (8.1)$$

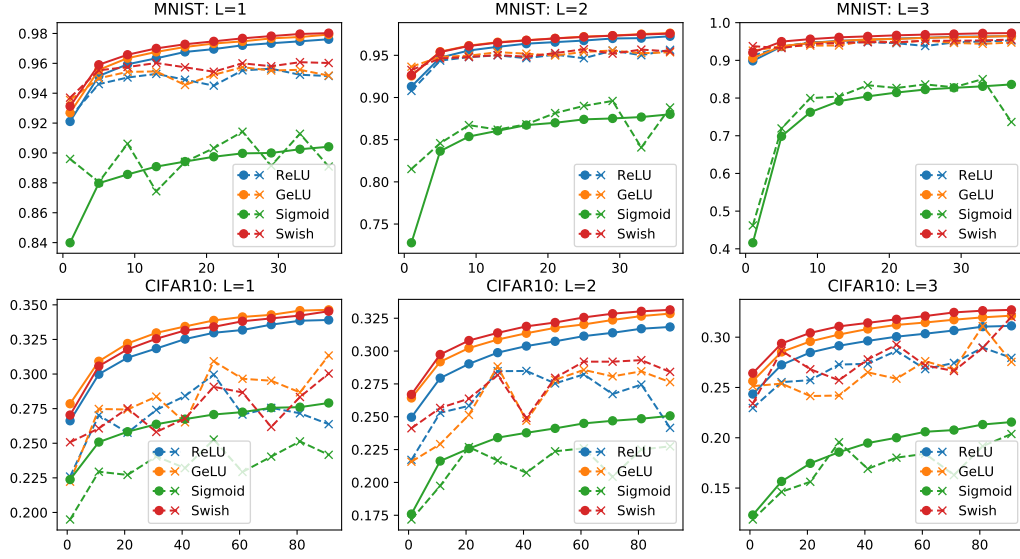


Figure 8: Accuracy percentage of MNIST and CIFAR10 based on various activation functions and depths. Solid lines represent the training accuracy and dashed lines represent the testing accuracy. We used 40 epochs for MNIST and 100 epochs for CIFAR10. The number of random features was set to $m = 1024$ (yielding 10×1024 trainable parameters), and the learning rate was set to 0.1.

Activation		ReLU			GeLU			Sigmoid			Swish		
Depth		1	2	3	1	2	3	1	2	3	1	2	3
MNIST	Train	0.98	0.97	0.96	0.98	0.98	0.96	0.90	0.88	0.84	0.98	0.98	0.97
	Test	0.95	0.96	0.95	0.95	0.95	0.95	0.89	0.89	0.74	0.96	0.95	0.96
CIFAR10	Train	0.34	0.32	0.31	0.35	0.33	0.32	0.28	0.25	0.22	0.35	0.33	0.33
	Test	0.26	0.24	0.28	0.31	0.28	0.28	0.24	0.23	0.20	0.30	0.28	0.32

Table 3: Accuracy percentage based on activation and depths.

where \mathcal{N}_ρ denotes the standard bivariate normal distribution with correlation $\rho = \langle x/\|x\|, z/\|z\| \rangle$. Expand the above expression explicitly and use Mehler's formula in Proposition 2.2 to obtain

$$\mathbb{E}_{(\tilde{x}, \tilde{z}) \sim \mathcal{N}_\rho} [\sigma(\tilde{x}) \sigma(\tilde{z})] = \int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(\tilde{x}) \sigma(\tilde{z}) \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left\{-\frac{\tilde{x}^2 + \tilde{z}^2 - 2\rho\tilde{x}\tilde{z}}{2(1-\rho^2)}\right\} d\tilde{x} d\tilde{z} \quad (8.2)$$

$$= \int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(\tilde{x}) \sigma(\tilde{z}) \frac{1}{2\pi} \exp\left\{-\frac{\tilde{x}^2 + \tilde{z}^2}{2}\right\} \sum_{k \geq 0} \rho^k h_k(\tilde{x}) h_k(\tilde{z}) \quad (8.3)$$

$$= \sum_{k \geq 0} \rho^k \mathbb{E}_{\tilde{x} \sim \mathcal{N}(0,1)} [\sigma(\tilde{x}) h_k(\tilde{x})] \mathbb{E}_{\tilde{z} \sim \mathcal{N}(0,1)} [\sigma(\tilde{z}) h_k(\tilde{z})] \quad (8.4)$$

$$= \sum_{k \geq 0} a_k^2 \rho^k = G_\sigma(\rho) . \quad (8.5)$$

□

Proof of Lemma 3.3. We can prove by induction on L . For $L = 0$, it follows from the definition that

$$K_\sigma^{(0)}(\rho) = \rho = \mathbb{E}[\rho^{Z_{\sigma,0}}]. \quad (8.6)$$

For $L \geq 1$, we have by induction

$$\begin{aligned} K_\sigma^{(L)}(\rho) &= K_\sigma^{(L-1)}(K_\sigma(\rho)) = K_\sigma^{(L-1)}(G(\rho)) \\ &= \mathbb{E}[G(\rho)^{Z_{\sigma,L-1}}] = \mathbb{E}[\mathbb{E}[\rho^{Y_\sigma}]^{Z_{\sigma,L-1}}] \\ &= \mathbb{E}[\rho^{\sum_{i=1}^{Z_{\sigma,L-1}} Y_\sigma^{(L-1)}}] = \mathbb{E}[\rho^{Z_{\sigma,L}}] . \end{aligned}$$

□

We will use the following facts about branching process and composition of PGFs.

Proposition 8.1 (Composition of PGFs). *The PGF associated with the size of the L -th generation Z_L in a branching process satisfies*

$$\mathbb{E}[s^{Z_L}] = \underbrace{G \circ \dots \circ G}_{\text{composite } L \text{ times}}(s) =: G^{(L)}(s) \quad (8.7)$$

where $G(s)$ is the PGF of Y in Definition 2.4.

Theorem 8.2 (Kesten and Stigum (1966), See also Theorem 12.3 in Lyons and Peres (2016)). *Consider the setting in Theorem 3.4. On the one hand if $\mu_\star < \infty$ then there exist a random variable $W_\sigma > 0$*

$$\lim_{L \rightarrow \infty} Z_{\sigma,L}/\mu^L = W_\sigma, \text{ a.s. conditional on non-extinction} . \quad (8.8)$$

Here $\mathbb{E}[W_\sigma] = 1$, and $\mathbf{Var}[W_\sigma] = \frac{\mathbf{Var}[Y_\sigma]}{\mathbb{E}[Y_\sigma](\mathbb{E}[Y_\sigma]-1)}$. On the other hand if $\mu_\star = \infty$ then for any constant $m > 0$, we have

$$\lim_{L \rightarrow \infty} Z_{\sigma,L}/m^L = \infty, \text{ a.s. conditional on non-extinction} . \quad (8.9)$$

Proposition 8.3 (Properties of PGF). *Consider the function $G_\sigma(\cdot)$ defined in Lemma 3.1. Let ξ be smallest fixed point with $G_\sigma(\xi) = \xi$, in $[0, 1]$. If $a_1^2 = 1$, then $G_\sigma(\cdot)$ is linear with $G_\sigma(\rho) = \rho$. For $a_1 \neq 1$, we have*

1. (Extinction). $\xi = 1$ if and only if $G'(1) \leq 1$.
2. (Fixed Points). $G_\sigma(\cdot)$ has only two fixed points ξ and 1 on $[0, 1]$.
3. (Compositional limit). $\lim_{L \rightarrow \infty} G_\sigma^{(L)}(\rho) = \xi$ for any $\rho \in [0, 1]$.

Proof. Note that $G_\sigma(\cdot)$ has a fixed point at 1 and it is continuous. Therefore, ξ is well defined. The first two properties *extinction* and *fixed points* are just a restatement of Proposition 2.5. Let's prove the third property *compositional limit*. There are two cases $\xi = 1$ and $\xi < 1$.

If $\xi = 1$, then $G'_\sigma(1) \leq 1$. Hence, by convexity, we have $G_\sigma(\rho) \geq \rho \geq 0$ for any $\rho \in [0, 1]$. Therefore, $\{G_\sigma^{(L)}(\rho) : L \in \mathbb{Z}^{\geq 0}\}$ is a non-decreasing sequence, for any $\rho \in [0, 1]$, and it's limit converges to the unique fixed point $\xi = 1$ of $G_\sigma(\cdot)$ on $[0, 1]$.

If $\xi < 1$, then $G'_\sigma(1) = \mu > 1$. First, let's look at $\rho \in [\xi, 1]$. By convexity, we have $G_\sigma(\rho) \leq \rho$ for any $\rho \in [\xi, 1]$. Moreover, $G_\sigma(\cdot)$ is non-decreasing on $[\xi, 1]$. Therefore, we have $\xi = G_\sigma(\xi) \leq G_\sigma(\rho) \leq \rho$ for any $\rho \in [\xi, 1]$. Then, we have that $\{G_\sigma^{(L)}(\rho) : L \in \mathbb{Z}^{\geq 0}\}$ is a non-increasing sequence, for any $\rho \in [\xi, 1]$, and it's limit converges to the unique fixed point ξ of G_σ on $[\xi, 1]$.

Now, let's look at $\rho \in [0, \xi]$. By continuity of $G_\sigma(\cdot)$ and property *fixed points*, we have that $G_\sigma(\rho) > \rho$ for any $\rho \in [0, \xi]$. If for any L we have that $G_\sigma^{(L)} \in [\xi, 1]$, then the result follows as a consequence of the case $\rho \in [\xi, 1]$. If $\xi > G_\sigma^{(L)}(\rho) > \rho$ for all $L \in \mathbb{Z}^{\geq 0}$, then the result follows by the same monotonicity argument as in the case $\rho \in [\xi, 1]$. \square

Remark 8.4. *Under the same notation as Proposition 8.3, we will state three sufficient conditions for which the compositional limit property of G_σ extends for $\rho \in (-1, 1)$:*

1. (Reduction to positive side). $G_\sigma(\cdot)$ is non-negative; for example, an even function $G_\sigma(\cdot)$. In this case, after the first iteration we will be in the realm of $[0, 1]$, that is $G_\sigma(\rho) \in [0, 1]$, and the result follows by the compositional limit property applied to $G_\sigma(\rho)$.
2. (Extension of fixed points). $G_\sigma(\cdot)$ has only two fixed points ξ and 1; for example, a convex function $G_\sigma(\cdot)$. In this case, the result follows because the proof of compositional limit property for $\rho \in [0, \xi]$ relies solely on the fixed points property. Therefore, we can extend the part in which $\rho \in (0, \xi]$ to $\rho \in (-1, \xi)$.
3. (Centered Activation) $G_\sigma(0) = 0$; for example, an odd function $G_\sigma(\cdot)$. In this case, the result follows because $\xi = 0$ and the contraction behavior of $G_\sigma(\cdot)$, see Lemma 8.6 and equation (8.22).

Proof of Theorem 3.4. Recall that $K_\sigma^{(L)} = G_\sigma^{(L)}$.

- (i) Since $e^{-t} \in (0, 1]$, the conclusion follows by applying Proposition 8.3's compositional limit and extinction properties.

(ii) By applying Lemma 3.3 and Kesten-Stigum Theorem 8.2, we have conditional on non-extinction that

$$\lim_{L \rightarrow \infty} K_{\sigma}^{(L)}(e^{-t/\mu^L}) = \lim_{L \rightarrow \infty} \mathbb{E}[e^{-tZ_{\sigma,L}/\mu^L}] \quad (8.10)$$

$$= \mathbb{E}[\lim_{L \rightarrow \infty} e^{-tZ_{\sigma,L}/\mu^L}] \quad (8.11)$$

$$= \mathbb{E}[e^{-tW_{\sigma}}], \quad (8.12)$$

where interchanging limit and expectation follows by the Bounded Convergence Theorem. The proof completes by recalling that the extinction probability is ξ .

(iii) Analogous as above, if $t \neq 0$, then for any $m > 0$

$$\lim_{L \rightarrow \infty} K_{\sigma}^{(L)}(e^{-t/m^L}) = \lim_{L \rightarrow \infty} \mathbb{E}[e^{-tZ_{\sigma,L}/m^L}] \quad (8.13)$$

$$= \mathbb{E}[\lim_{L \rightarrow \infty} e^{-tZ_{\sigma,L}/m^L}] \quad (8.14)$$

$$= \mathbb{E}[0]. \quad (8.15)$$

$$= 0. \quad (8.16)$$

The case $t = 0$ follows immediately from the fact that $G_{\sigma}(1) = 1$.

□

Proof of Corollary 3.5. The conclusions are a reformulation of Proposition 8.3's *compositional limit* and *extinction* properties, with the addition of Remark 8.4.

□

8.2 Proofs in Section 4

Proposition 8.5 (Diagonal-dominance). *If for some $0 < \kappa < 1$, we have for all $i \in [n]$*

$$\sum_{j: j \in [n], j \neq i} K(x_i, x_j) \leq \kappa \quad (8.17)$$

then \mathbf{K} is diagonally dominant and satisfies the κ -memorization property.

We define

$$F_{\sigma}(\rho) := \sum_{k \geq 0} a_{k+1}^2 \rho^k = \frac{G_{\sigma}(\rho)}{\rho} \quad (8.18)$$

where one can see that F has the properties $F_{\sigma}(\rho) = 1$, $F'_{\sigma}(0) = a_1^2$ and $F'_{\sigma}(1) = \mu - 1$.

Lemma 8.6 (Contraction rate). *Let $\mathcal{X} = \{x_i\}_{i \in [n]}$ be a dataset of size n with no repetition of data points, and define $\rho_{ij} = \langle x_i / \|x_i\|, x_j / \|x_j\| \rangle$. Let $\delta := \sup_{i < j} |\rho_{ij}| < 1$. Then the kernel matrix $\mathbf{K} = [K_{\sigma}^{(L)}(\rho_{ij})]_{1 \leq i, j \leq n}$ will κ -memorizes \mathcal{X} for any compositional depth L that satisfies*

$$L \geq \left\lceil \frac{\log n + \log \kappa^{-1} - \log \delta^{-1}}{\log F_{\sigma}(\delta)^{-1}} \right\rceil, \quad (8.19)$$

Proof. We have the following inequality for any ρ such that $\rho \in (0, \delta]$

$$F_\sigma(\rho) \leq \sum_{k \geq 0} a_{k+1}^2 \rho^k \leq F_\sigma(\delta) \leq 1. \quad (8.20)$$

Hence, we obtain the sequence of inequalities

$$|G_\sigma(\rho_{ij})| \leq G(|\rho_{ij}|) \leq |\rho_{ij}| F_\sigma(\delta) \leq \delta, \quad (8.21)$$

and therefore

$$|K_\sigma^{(L)}(\rho_{ij})| = |G_\sigma^{(L)}(\rho_{ij})| \leq \delta F_\sigma(\delta)^L. \quad (8.22)$$

One can easily verify that the lower bound on L suffices to ensure (8.17). \square

8.2.1 Small correlation

Consider the small correlation regime 1, when the correlation $\sup_{1 \leq i < j \leq n} |\rho_{ij}| = o(1)$ as $\frac{\log(n)}{d} \rightarrow 0$. We consider a typical instance of the data where such small correlation is guaranteed with high probability, due to the following lemma.

Lemma 8.7 (Concentration: small correlation regime). *Suppose $x_i \stackrel{iid}{\sim} \text{Unif}(\mathbb{S}^{d-1})$, with $i \in [n]$, then for all $i \neq j$*

$$|\langle x_i, x_j \rangle| \leq c_0 \sqrt{\frac{\log n}{d}} \quad (8.23)$$

with probability at least $1 - n^{-c_1}$, where c_0 and c_1 are constants that do not depend on n and d .

Proof of Lemma 8.7. We include a short proof here since the term $\sqrt{\log n}$ is not obvious (the obvious argument results in a $\log n$ term). Let $g_i \stackrel{iid}{\sim} \mathcal{N}(0, \mathbf{I}_d)$, then $x_i \stackrel{d}{=} g_i / \|g_i\|$ in distribution. It is clear that $\langle x_i, x_j \rangle = \langle x_i, g_j \rangle / \|g_j\|$. Let's bound $\langle x_i, g_j \rangle$ and $\|g_j\|$ separately. First, since $\langle x_i, g_j \rangle | x_i \sim \mathcal{N}(0, 1)$, then standard Gaussian tail bound claims that

$$\mathbf{P}(|\langle x_i, g_j \rangle| > \delta \mid x_i) < 2 \exp(-\delta^2/2) \quad (8.24)$$

for any $\delta > 0$. Marginalize over x_i , we have $\mathbf{P}(|\langle x_i, g_j \rangle| > \delta) < 2 \exp(-\delta^2/2)$. Therefore w.p. at least $1 - n^{-c_1}$, uniformly over $i \neq j$,

$$|\langle x_i, g_j \rangle| \leq c_2 \sqrt{\log n}. \quad (8.25)$$

It is clear that $\|g_j\|^2 \sim \chi_d^2$, standard χ^2 tail bound informs us w.p. at least $1 - n^{-c_1}$, uniformly over j

$$\|g_j\| \geq \sqrt{d} \left(1 - c_2 \sqrt{\frac{\log n}{d}}\right). \quad (8.26)$$

Put things together, we complete the proof. \square

Proof of Theorem 4.2. Consider $\delta = c_0 \sqrt{\frac{\log n}{d}}$. Therefore, with high probability, we have

$$\sup_{1 \leq i < j \leq n} |\rho_{ij}| \leq \delta. \quad (8.27)$$

By applying Lemma 8.6, we have

$$L \geq \left\lceil \frac{\log n + \log \kappa^{-1} - \log \delta^{-1}}{\log F_\sigma(\delta)^{-1}} \right\rceil, \quad (8.28)$$

and invoke the following inequality, which is sharp around 0, we have

$$F_\sigma(\delta) \leq a_1^2 + (1 - a_1^2)\delta. \quad (8.29)$$

Therefore, for sufficiently large n , we have

$$L \geq \left\lceil \frac{\log n + \log \kappa^{-1} - \log \delta^{-1}}{\log(a_1^2 + (1 - a_1^2)\delta)^{-1}} \right\rceil \quad (8.30)$$

$$\geq c_1 \cdot \frac{\log \frac{n \log n}{d} + \log \kappa^{-1}}{\log a_1^{-2}}, \quad (8.31)$$

for some constant c_1 that does not depends on n and d . □

8.2.2 Large correlation

We will be in large correlation regime 2, when the correlation $\sup_{1 \leq i < j \leq n} |\rho_{ij}| = 1 - o(1)$ as $\frac{\log n}{d} \rightarrow \infty$. We consider a typical instance of the data where such large correlation arises in the sphere packing/covering setup.

Definition 8.8 (r-covering). *For a compact subset $V \subset \mathbb{R}^d$, we say $\mathcal{X} = \{x_i\}_{i \in [n]} \subset V$ is a r -covering of V if for any $x \in V$, there exists $x_i \in \mathcal{X}$ such that $\|x - x_i\| \leq r$. We define the covering number of V as $\mathcal{N}_r(V)$, that is*

$$\mathcal{N}_r(V) = \min\{n: \text{exists } r\text{-covering of } V \text{ of size } n\}. \quad (8.32)$$

Definition 8.9 (r-packing). *For a subset $V \subset \mathbb{R}^d$, we say $\mathcal{X} = \{x_i\}_{i \in [n]} \subset V$ is a r -packing of V if for all $x_i \neq x_j \in \mathcal{X}$, we have $\|x_i - x_j\| > r$. We define the packing number of V as $\mathcal{K}_r(V)$, that is*

$$\mathcal{K}_r(V) = \max\{n: \text{exists } r\text{-packing of } V \text{ of size } n\}. \quad (8.33)$$

Lemma 8.10 (Metric entropy on the sphere). *Denote by $S_{d-1} := \frac{2\pi^{d/2}}{\Gamma(d/2)}$ to be the surface area of \mathbb{S}^{d-1} . Then, we have for all $r \leq 1$ the following bounds on the packing and covering numbers of a sphere*

$$\left(\frac{1}{r}\right)^{d-1} \leq \frac{(d-1)S_{d-1}}{S_{d-2}} \left(\frac{1}{r}\right)^{d-1} \leq \mathcal{N}_r(\mathbb{S}^{d-1}) \leq \mathcal{K}_r(\mathbb{S}^{d-1}) \leq \left(\frac{1+r/2}{r/2}\right)^d \leq \left(\frac{3}{r}\right)^d. \quad (8.34)$$

Proof of Lemma 8.10. The upper bound follows since

$$\mathcal{K}_r(\mathbb{S}^{d-1}) \leq \mathcal{K}_r(\mathbb{B}^d) \leq \frac{\text{vol}(\mathbb{B}^d + \frac{r}{2}\mathbb{B}^d)}{\text{vol}(\frac{r}{2}\mathbb{B}^d)} = \left(\frac{1+r/2}{r/2}\right)^d. \quad (8.35)$$

Moreover, recall that every minimal r -packing is a maximal r -covering, thus, $\mathcal{N}_r \leq \mathcal{K}_r$.

Now, for the lower bound, let's calculate the surface area of the hyper-spherical cap of a covering ball of radius r defined in the following way

$$\text{Cap}_r(x_0) := \{x | x \in \mathbb{S}^{d-1}, \|x - x_0\| \leq r\} \quad (8.36)$$

for any $x_0 \in \mathbb{S}^{d-1}$. By Pythagora's theorem, one can calculate the height of the cap as $h = \frac{r^2}{2}$. The bottom of the cap is a $d-2$ dimensional sphere of radius $f(h) := \sqrt{1 - (1-h)^2}$. Therefore, the surface area of the cap $\text{Cap}_r(x_0)$ is

$$S_{d-1,r} := \int_0^h S_{d-2} [f(x)]^{d-2} \sqrt{1 + [f'(x)]^2} dx \quad (8.37)$$

$$= S_{d-2} \int_0^h x^{\frac{d-3}{2}} (2-x)^{\frac{d-3}{2}} dx \quad (8.38)$$

$$\leq S_{d-2} \frac{1}{d-1} (2x)^{\frac{d-1}{2}} \Big|_0^h = \frac{S_{d-2}}{d-1} r^{d-1}. \quad (8.39)$$

Therefore, we have

$$\mathcal{N}_r(\mathbb{S}^{d-1}) \geq \frac{S_{d-1}}{S_{d-1,r}} \geq \frac{(d-1)S_{d-1}}{S_{d-2}} \cdot r^{-(d-1)}. \quad (8.40)$$

By Gautschi's inequality, for $d \geq 3$, we have

$$\frac{(d-1)S_{d-1}}{S_{d-2}} = (d-1)\sqrt{\pi} \cdot \frac{\Gamma(\frac{d-2}{2} + \frac{1}{2})}{\Gamma(\frac{d-2}{2} + 1)} > (d-1)\sqrt{\pi} \cdot \left(\frac{d-2}{2} + 1\right)^{\frac{1}{2}-1} \geq 1. \quad (8.41)$$

□

Lemma 8.11 (Polarized metric entropy on the sphere). *For all $r \leq 1$ and $d \geq 3$, we have the following bounds on the packing polarization number of the sphere*

$$\left(\frac{1}{3r}\right)^{d-1} \leq \frac{1}{2} \left(\frac{1}{2r}\right)^{d-1} \leq \frac{1}{2} \mathcal{K}_{2r}(\mathbb{S}^{d-1}) \leq \mathcal{P}_r(\mathbb{S}^{d-1}) \leq \mathcal{K}_r(\mathbb{S}^{d-1}) \leq \left(\frac{3}{r}\right)^d. \quad (8.42)$$

Proof. By definition, any r -packing polarization set is a r -packing set. Therefore, the upper bounds $\mathcal{P}_r \leq \mathcal{K}_r$ follows. Now, consider any $2r$ -maximal packing set $\mathcal{X} = \{x_1, \dots, x_n\}$ of the sphere. Define the polar neighborhood of x_i of radius r as

$$\text{PS}(x_i) := \{x \in \mathbb{S}^{d-1} : \|x - x_i\| \leq r \text{ or } \|x + x_i\| \leq r\} \quad (8.43)$$

Consider a simple graph \mathcal{G} with vertices \mathcal{X} and edges (x_i, x_j) if $x_j \in \text{PS}(x_i)$ or $x_i \in \text{PS}(x_j)$. We claim that each vertex has at most one edge. Otherwise, consider a vertex x_i adjacent to both x_k and x_ℓ . Then, we must have

$$\|x_\ell + x_i\| \leq r \quad \text{and} \quad \|x_k + x_i\| \leq r, \quad (8.44)$$

Thus, $\|x_\ell - x_k\| \leq 2r$, which contradicts the definition of a packing set. Therefore, we would need to remove at most $\lfloor \frac{n}{2} \rfloor$ vertices of the graph \mathcal{G} to get a graph $\mathcal{G}' \subset \mathcal{G}$ with no edges. Therefore, the graph \mathcal{G}' has at least $\frac{n}{2}$ vertices and the vertices form an r -polarized packing set. The rest of the conclusions follow by Lemma 8.10. \square

Corollary 8.12 (Polarized metric entropy: large correlation regime). *Suppose that the n data points $\mathcal{X} = \{x_i\}_{i \in [n]}$ form a maximum r -polarized packing set of \mathbb{S}^{d-1} with $r = r(n, d)$ as a function of (n, d) . Then, we have*

$$1 - 18.2 \cdot \exp\left\{-2 \frac{\log n}{d}\right\} < \max_{i \neq j} |\langle x_i, x_j \rangle| < 1 - 0.06 \cdot \exp\left\{-2 \frac{\log n}{d-1}\right\} \quad (8.45)$$

Proof. By theorem Lemma 8.11 Equation (8.42), we have

$$\frac{1}{3} \exp\left\{-\frac{\log n}{d-1}\right\} \leq r(n, d) \leq 3 \exp\left\{-\frac{\log n}{d}\right\}. \quad (8.46)$$

Let $\mathcal{X} = \{x_i\}_{i \in [n]}$ a maximum r -polarized packing set of \mathbb{S}^{d-1} . Denote the polarization completion of the set \mathcal{X} by $\tilde{\mathcal{X}}$, that is

$$\tilde{\mathcal{X}} = \{\tilde{x}_i\}_{i \in [2n]} := \{x_i\}_{i \in [n]} \cup \{-x_i\}_{i \in [n]}. \quad (8.47)$$

Observe the following simple relationship that allows us to work with the set $\tilde{\mathcal{X}}$ in this proof

$$\max_{i \neq j} |\langle x_i, x_j \rangle| = \max_{i \neq j} \langle \tilde{x}_i, \tilde{x}_j \rangle. \quad (8.48)$$

By definition, we know $\min_{i \neq j} \|\tilde{x}_i - \tilde{x}_j\| > r(n, d)$. Furthermore, we claim that

$$\min_{i \neq j} \|\tilde{x}_i - \tilde{x}_j\| \leq 2.01 \cdot r(n, d). \quad (8.49)$$

Therefore, the conclusion's upper bound follows because

$$\langle \tilde{x}_i, \tilde{x}_j \rangle = \frac{2 - \|\tilde{x}_i - \tilde{x}_j\|^2}{2} < 1 - \frac{[r(n, d)]^2}{2}. \quad (8.50)$$

The claim (8.49) can be proved by contradiction. Suppose the claim is not true, then we have $\min_{i \neq j} \|\tilde{x}_i - \tilde{x}_j\| > 2.01 \cdot r(n, d)$. In an annulus around some \tilde{x}_i ,

$$\{x \in \mathbb{S}^{d-1} : r(n, d) < \|x - \tilde{x}_i\| \leq 1.005 \cdot r(n, d)\}, \quad (8.51)$$

one can add another point x' , such that

$$\min_{j \in [2n] \setminus \{i\}} \|x' - \tilde{x}_j\| \geq \min_{j \in [2n] \setminus \{i\}} \|\tilde{x}_j - \tilde{x}_i\| - \|\tilde{x}_i - x'\| > 1.005 \cdot r(n, d) > r(n, d). \quad (8.52)$$

The above contradicts with the maximal cardinality nature of the polarized $r(n, d)$ -packing set. Thus, we know

$$\max_{i \neq j} \langle \tilde{x}_i, \tilde{x}_j \rangle \geq 1 - \frac{2.01^2}{2} [r(n, d)]^2 > 1 - 18.2 \cdot \exp \left\{ -2 \frac{\log n}{d} \right\} . \quad (8.53)$$

□

Proof of Theorem 4.4. Consider the choice $\delta = 0.06 \cdot \exp(-\frac{2 \log n}{d-1})$. By Lemma 8.12, we have

$$\sup_{1 \leq i < j \leq n} |\rho_{ij}| \leq 1 - \delta. \quad (8.54)$$

Therefore, by applying Lemma 8.6, we have

$$L \geq \left\lceil \frac{\log n + \log \kappa^{-1} - \log \delta^{-1}}{\log F_\sigma(\delta)^{-1}} \right\rceil. \quad (8.55)$$

We have the following Taylor expansion near 1 for $\delta = 1 - o(1)$

$$F_\sigma(\delta) = 1 - (\mu - 1)\delta + o(\delta). \quad (8.56)$$

Therefore, for sufficiently large n ,

$$L \geq \left\lceil \frac{\log n + \log \kappa^{-1} - \log \delta^{-1}}{\log(1 - (\mu - 1)\delta + o(\delta))^{-1}} \right\rceil \quad (8.57)$$

$$\geq c_3 \cdot \frac{\delta^{-1}(\log n + \log \kappa^{-1})}{(\mu - 1)}, \quad (8.58)$$

for some constant c_3 that does not depend on n and d .

□

8.3 Proofs in Section 5

Proof of Theorem 5.3. First, we know for all $t \in [-1, 1]$

$$|K_\sigma^{(L)}(t)| \leq 1 , \quad (8.59)$$

which implies

$$\int_{-1}^1 |K_\sigma^{(L)}(t)| (1 - t^2)^{\frac{d-3}{2}} dt < \infty . \quad (8.60)$$

Therefore, one can apply the Funk–Hecke formula (Theorem 2.22 in [Atkinson and Han \(2012\)](#)) to obtain

$$\int K_\sigma^{(L)}(\langle x, z \rangle) Y_{k,j}(z) d\tau_{d-1}(z) = \lambda_k Y_{k,j}(x) \quad (8.61)$$

with

$$\lambda_k = \frac{S_{d-2}}{S_{d-1}} \int_{-1}^1 K_\sigma^{(L)}(t) P_{k,d}(t) (1-t^2)^{\frac{d-3}{2}} dt . \quad (8.62)$$

Recall that $K_\sigma^{(L)}(t) = \sum_\ell \mathbf{P}(Z_{\sigma,L} = \ell) t^\ell$. Let us calculate the following expression explicitly through the Rodrigues representation formula (Theorem 2.23 and Proposition 2.26 in [Atkinson and Han \(2012\)](#)) for the Legendre polynomial, for $\ell \geq k$

$$\int_{-1}^1 t^\ell P_{k,d}(t) (1-t^2)^{\frac{d-3}{2}} dt = \frac{\Gamma(\frac{d-1}{2})}{2^k \Gamma(k + \frac{d-1}{2})} \cdot \int_{-1}^1 \left[\left(\frac{d}{dt} \right)^k t^\ell \right] (1-t^2)^{k + \frac{d-3}{2}} dt \quad (8.63)$$

$$= \frac{\Gamma(\frac{d-1}{2})}{2^k \Gamma(k + \frac{d-1}{2})} \frac{\ell!}{(\ell-k)!} \int_{-1}^1 t^{\ell-k} (1-t^2)^{k + \frac{d-3}{2}} dt \quad (8.64)$$

$$= \frac{\Gamma(\frac{d-1}{2})}{2^k \Gamma(k + \frac{d-1}{2})} \frac{\ell!}{(\ell-k)!} [1 + (-1)^{\ell-k}] \int_0^1 s^{\frac{\ell-k}{2}} (1-s)^{k + \frac{d-3}{2}} \frac{ds}{2s^{\frac{1}{2}}} \quad (8.65)$$

$$= \frac{\Gamma(\frac{d-1}{2})}{\Gamma(k + \frac{d-1}{2})} \frac{\ell!}{(\ell-k)!} \frac{1 + (-1)^{\ell-k}}{2^{k+1}} \frac{\Gamma(\frac{\ell-k+1}{2}) \Gamma(k + \frac{d-1}{2})}{\Gamma(\frac{\ell+k+d}{2})} . \quad (8.66)$$

Plug in $K_\sigma^{(L)}(t) = \sum_\ell \mathbf{P}(Z_{\sigma,L} = \ell) t^\ell$, we obtain the formula for λ_k . Due to the orthogonality of Legendre polynomial under measure $(1-t^2)^{\frac{d-3}{2}}$ (5.5), we know

$$K_\sigma^{(L)}(t) = \sum_{k \geq 0} \lambda_k N_{k,d} P_{k,d}(t) \quad (8.67)$$

and by the Addition Theorem 2.9 in [Atkinson and Han \(2012\)](#), we know

$$N_{k,d} P_{k,d}(\langle x, z \rangle) = \sum_{j=1}^{N_{k,d}} Y_{k,j}(x) Y_{k,j}(z) . \quad (8.68)$$

Put things together, we have

$$K_\sigma^{(L)}(\langle x, z \rangle) = \sum_{k \geq 0} \lambda_k \sum_{j=1}^{N_{k,d}} Y_{k,j}(x) Y_{k,j}(z) . \quad (8.69)$$

□

8.4 Proofs in Section 6

Proof of Theorem 6.2. We denote $f \in L^1_{(d-3)/2} : [-1, 1] \rightarrow \mathbb{R}$ as L^1 integrable in the following sense

$$\int_{-1}^1 |f(t)| (1-t^2)^{\frac{d-3}{2}} < \infty . \quad (8.70)$$

Note that for $d \geq 2$, continuous function is L^1 integrable since $C([-1, 1]) \subset L^1_{(d-3)/2}$. Due to Equation (2.66) (variant of Funk-Hecke Formula) in [Atkinson and Han \(2012\)](#), we know that for any $g \in L^1_{(d-3)/2}$, $x, z \in \mathbb{S}^{d-1}$ and $k \geq 0$

$$\int_{\mathbb{S}^{d-1}} g(\xi^\top x) P_{k,d}(\xi^\top z) d\tau_{d-1}(\xi) = \frac{\beta_k}{N_{k,d}} \cdot P_{k,d}(x^\top z) \quad (8.71)$$

with β_k being the coefficients of g under Legendre polynomials

$$g(t) = \sum_{k \geq 0} \beta_k P_{k,d}(t) . \quad (8.72)$$

Let's first plug in $g = P_{k,d}$, then for any $\alpha_k \geq 0$

$$\int_{\mathbb{S}^{d-1}} P_{k,d}(\xi^\top x) P_{k,d}(\xi^\top z) d\tau_{d-1}(\xi) = \frac{1}{N_{k,d}} \cdot P_{k,d}(x^\top z) \quad (8.73)$$

$$\int_{\mathbb{S}^{d-1}} \left(\sqrt{\alpha_k N_{k,d}} P_{k,d}(\xi^\top x) \right) \left(\sqrt{\alpha_k N_{k,d}} P_{k,d}(\xi^\top z) \right) d\tau_{d-1}(\xi) = \alpha_k \cdot P_{k,d}(x^\top z) . \quad (8.74)$$

Then plug in $g = P_{\ell,d}$, $\ell \neq k$, we know

$$\int_{\mathbb{S}^{d-1}} P_{\ell,d}(\xi^\top x) P_{k,d}(\xi^\top z) d\tau_{d-1}(\xi) = 0 . \quad (8.75)$$

Therefore we know

$$\mathbb{E}_{\xi \sim \tau_{d-1}} \left[\sigma_f(\xi^\top x) \sigma_f(\xi^\top z) \right] = \sum_{k, \ell \geq 0} \mathbb{E}_{\xi \sim \tau_{d-1}} \left[\left(\sqrt{\alpha_k N_{k,d}} P_{k,d}(\xi^\top x) \right) \left(\sqrt{\alpha_\ell N_{\ell,d}} P_{\ell,d}(\xi^\top z) \right) \right] \quad (8.76)$$

$$= \sum_{k=0}^{\infty} \int_{\mathbb{S}^{d-1}} \left(\sqrt{\alpha_k N_{k,d}} P_{k,d}(\xi^\top x) \right) \left(\sqrt{\alpha_k N_{k,d}} P_{k,d}(\xi^\top z) \right) d\tau_{d-1}(\xi) \quad \text{Equation (8.75)} \quad (8.77)$$

$$= \sum_{k=0}^{\infty} \alpha_k P_{k,d}(\langle x, z \rangle) = f(\langle x, z \rangle) \quad \text{Equation (8.74)} . \quad (8.78)$$

□

Proof of Theorem 6.3. The proof relies on the Mehler's formula in Proposition 2.2. It is straightforward to verify that the diagonal element of \mathbf{R} is zero. Let's focus on the off-diagonal components $\mathbf{R}[i, l]$ with $i, l \in [n]$, $i \neq l$. Define the following notation

$$\sigma_{>l}(t) := \sum_{k>l} \sqrt{\alpha_k} h_k(t) , \quad (8.79)$$

and observe that

$$\mathbf{R}[i, l] = \mathbf{K}[i, l] - \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma_{\leq l}(x_i^\top \boldsymbol{\theta}) \sigma_{\leq l}(x_l^\top \boldsymbol{\theta}) \right] \quad (8.80)$$

$$= 2 \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma_{>l}(x_i^\top \boldsymbol{\theta}) \sigma_{\leq l}(x_l^\top \boldsymbol{\theta}) \right] + \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} \left[\sigma_{>l}(x_i^\top \boldsymbol{\theta}) \sigma_{>l}(x_l^\top \boldsymbol{\theta}) \right] . \quad (8.81)$$

By Mehler's formula and the derivations in Lemma 3.1, we know that for $f, g \in L^2_\phi$ and $\rho_{il} := \langle x_i, x_l \rangle$

$$\begin{aligned} \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} [f(x_i^\top \boldsymbol{\theta}) g(x_l^\top \boldsymbol{\theta})] &= \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x}) g(\tilde{z}) \frac{1}{2\pi \sqrt{1 - \rho_{il}^2}} \exp \left\{ -\frac{\tilde{x}^2 + \tilde{z}^2 - 2\rho_{il}\tilde{x}\tilde{z}}{2(1 - \rho_{il}^2)} \right\} d\tilde{x} d\tilde{z} \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x}) g(\tilde{z}) \frac{1}{2\pi} \exp \left\{ -\frac{\tilde{x}^2 + \tilde{z}^2}{2} \right\} \sum_{k \geq 0} \rho_{il}^k h_k(\tilde{x}) h_k(\tilde{z}) \\ &= \sum_{k \geq 0} \rho_{il}^k \mathbb{E}_{\tilde{x} \sim \mathcal{N}(0,1)} [f(\tilde{x}) h_k(\tilde{x})] \mathbb{E}_{\tilde{z} \sim \mathcal{N}(0,1)} [g(\tilde{z}) h_k(\tilde{z})] . \end{aligned}$$

Plug in $f(\cdot) = \sigma_{>l}(\cdot)$ and $g(\cdot) = \sigma_{\leq l}(\cdot)$, we know that the first term in (8.81) is zero. Plug in with $f(\cdot) = g(\cdot) = \sigma_{>l}(\cdot)$, we know that that the second term in (8.81) satisfies

$$\mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{N}(0, \mathbf{I}_d)} [\sigma_{>l}(x_i^\top \boldsymbol{\theta}) \sigma_{>l}(x_l^\top \boldsymbol{\theta})] = \sum_{k > l} \rho_{il}^k \alpha_k \quad (8.82)$$

and hence $|\mathbf{R}[i, l]| \leq |\rho_{il}|^{l+1}$. Now use concentration results on $|\rho_{il}|$ derived in Lemma 8.7, and recall that for small $\delta > 0$, $d(n) > n^{\frac{2}{l+1} + \delta}$, we have

$$\|\mathbf{R}\|_{\text{op}} \leq n \cdot \max_{i, l \in [n], i \neq l} |\rho_{il}|^{l+1} \lesssim n \cdot \left(\frac{\log n}{d} \right)^{\frac{l+1}{2}} \leq \left(\frac{\log n}{n^\delta} \right)^{\frac{l+1}{2}} = o(1) . \quad (8.83)$$

□

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