Sharp Asymptotics of Kernel Ridge Regression Beyond the Linear Regime

Hong Hu HONGHU@G.HARVARD.EDU and Yue M. Lu YUELU@SEAS.HARVARD.EDU
John A. Paulson School of Engineering and Applied Sciences, Harvard University

Abstract

The generalization performance of kernel ridge regression (KRR) exhibits a multi-phased pattern that crucially depends on the scaling relationship between the sample size $n$ and the underlying dimension $d$. This phenomenon is due to the fact that KRR sequentially learns functions of increasing complexity as the sample size increases; when $d^{k-1} \ll n \ll d^k$, only polynomials with degree less than $k$ are learned. In this paper, we present sharp asymptotic characterization of the performance of KRR at the critical transition regions with $n \approx d^k$, for $k \in \mathbb{Z}^+$. Our asymptotic characterization provides a precise picture of the whole learning process and clarifies the impact of various parameters (including the choice of the kernel function) on the generalization performance. In particular, we show that the learning curves of KRR can have a delicate “double descent” behavior due to specific bias-variance trade-offs at different polynomial scaling regimes.

Keywords: Kernel ridge regression, kernel method, double-descent, sharp asymptotics.

1. Introduction

Consider kernel ridge regression (KRR), where we seek to learn a function $h : \mathbb{R}^d \mapsto \mathbb{R}$ from a reproducing kernel Hilbert space (RKHS) associated with a positive semi-definite kernel $K(\cdot, \cdot)$ by solving the following optimization problem:

$$
\hat{h} = \arg\min_h \frac{1}{n} \sum_{i=1}^{n} [y_i - h(x_i)]^2 + \lambda \|h\|_K^2.
$$

Here, $\{x_i, y_i\}_{i=1}^{n}$ is a collection of training samples, $\| \cdot \|_K$ is the RKHS norm and $\lambda > 0$ is the regularization parameter. The performance of KRR can be characterized by the training error

$$
\mathcal{E}_{\text{train}} = \frac{1}{n} \left[ \sum_{i=1}^{n} (y_i - \hat{h}(x_i))^2 + \lambda \|\hat{h}\|_K^2 \right],
$$

and the test error

$$
\mathcal{E}_{\text{test}} = \mathbb{E}_{\text{new}}[\mathbb{E}(y_{\text{new}} | x_{\text{new}}) - \hat{h}(x_{\text{new}})]^2,
$$

where $(x_{\text{new}}, y_{\text{new}}) \sim \mathcal{P}$ denotes an independent test sample, and $\mathbb{E}_{\text{new}}$ denotes the expectation with respect to $(x_{\text{new}}, y_{\text{new}})$ while keeping the training samples $\{x_i, y_i\}_{i=1}^{n}$ fixed.

Kernel ridge regression is a classical method for supervised learning (Schölkopf et al., 2002). Due to its connection to modern overparameterized neural networks (Neal, 1996; Williams, 1996; Daniely et al., 2016; Jacot et al., 2018; Belkin et al., 2018; Du et al., 2019), there has been a strong resurgence of interest in studying the performance of KRR, especially in various high-dimensional settings. See, e.g., Rakhlin and Zhai (2019); Liang et al. (2020a,b); Bordelon et al. (2020); Canatar et al. (2021); Ghorbani et al. (2021); Mei et al. (2021).
One intriguing phenomenon revealed by several recent works (Liang et al., 2020a; Ghorbani et al., 2021; Mei et al., 2021) is that the generalization performance of KRR exhibits a hierarchical and multi-phased pattern that crucially depends on the scaling relationship between the sample size $n$ and the underlying dimension $d$. We illustrate this phenomenon in Fig. 1 (top part), where we plot the test error $\mathcal{E}_{\text{test}}$ against the ratio $\log n / \log d$. The test error can be clearly partitioned into several consecutive “stationary” phases that are separated by more drastic transitions in between. More precisely, $\mathcal{E}_{\text{test}}$ appears to remain unchanged when $d^{k-1} \ll n \ll d^k$, for $k \in \mathbb{Z}^+$, while transitions occur at $n \approx d^k$. An explanation of this phenomenon was given in Ghorbani et al. (2021): It is shown that, when $d^{k-1} \ll n \ll d^k$, $\mathcal{E}_{\text{test}}$ is approximately equal to the approximation error of the function $h$ by all the polynomials with degree less than $k$. This means that KRR sequentially
learns functions of increasing complexity as the sample size increases; when $d^{k-1} \ll n \ll d^k$, only polynomials with degree less than $k$ are learned.

What is the performance of KRR near the critical regions, exactly where the transitions happen? This is the focus of the current paper. More precisely, we “zoom into” each transition region by assuming $n \asymp d^k$, and derive sharp asymptotics of KRR for different values of $k$. Such asymptotic characterization provides a precise picture of the whole learning process and clarifies the impact of various parameters (including the choice of the kernel function) on the generalization performance. As a preview of our results, we plot in the lower part of Fig. 1 the theoretical predictions of $E_{\text{test}}$ in the regimes $n \asymp d^k$, for $k = 1, 2, 3$, for a specific choice of the kernel function. It can be seen that the learning curves of KRR can exhibit delicate non-monotonic behavior due to bias-variance trade-offs: as the sample size $n$ increases, $E_{\text{test}}$ can first increase and then decrease again after crossing certain deterministic thresholds. Under the names of “double descent” or “multiple descent”, such phenomenon has been observed and analyzed in various other problems and models in learning (Mei and Montanari, 2019; d’Ascoli et al., 2020; Adlam and Pennington, 2020; Nakkiran et al., 2021).

Some of the asymptotic predictions given in the paper were first derived in Bordelon et al. (2020); Canatar et al. (2021) (see also Dietrich et al. (1999) for a related earlier work), via non-rigorous statistical physics methods and a “Gaussian equivalence conjecture” (see Sec 2.4). One of the technical contributions of this paper is to rigorously establish this conjecture, which allows us to characterize the exact performance KRR in the polynomial scaling regime.

When the current work was under review at COLT ’22, we became aware of the recent paper Misiakiewicz (2022) that also studies the exact asymptotics of KRR in the polynomial scaling regime. The target function considered in that paper is different from ours. On one hand, the expansion coefficients (i.e., $\alpha_{k,d}$ in (5) below) of low-degree components can be arbitrary, which is more general than ours; on the other hand, they require high-degree coefficients to be independent random variables. In comparison, we consider a target function (as detailed in Sec. 2.1) whose coefficients are dependent. In terms of the distribution of $\{x_i\}$, our work focuses on the uniform distribution over $d$-dimensional sphere. In addition to this case, Misiakiewicz (2022) also considers the uniform distribution over the hypercube $\{-1,1\}^d$.

2. Main Results

2.1. Model

We start by describing the statistical model under which we analyze the performance of KRR. Let $S^{d-1}(\sqrt{d})$ denotes the $d$-dimensional sphere with radius $\sqrt{d}$. We assume that the input data vectors $x_i \overset{i.i.d.}{\sim} \tau_{d-1}$, where $\tau_{d-1}$ denotes the uniform distribution over $S^{d-1}(\sqrt{d})$. The labels $\{y_i\}$ are generated from a generalized linear teacher model

$$y_i = g(x_i^\top \xi / \sqrt{d}) + z_i,$$

where $g$ is an unknown teacher function, $\xi \in S^{d-1}(\sqrt{d})$ is the teacher weight vector, and $z_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma_z^2)$ denotes independent additive noise. We consider an inner-product kernel on $S^{d-1}(\sqrt{d})$, represented as

$$K(x, x') = f_d(x^\top x' / \sqrt{d}),$$

where $f_d$ is a transformation function that can depend on $d$. It is known that any inner-product PSD kernel $K \in L^2(S^{d-1}(\sqrt{d}) \times S^{d-1}(\sqrt{d}), \tau_{d-1}^{\otimes 2})$ can be expanded as (Schölkopf et al., 2002, Lemma
There exist constants \( C \) (A.2).
\[ C > \]
There exists (A.3) Both the number of training samples \( n \) as \( d \).

4.20):
\[
K(x, x') = \sum_{k=0}^{\infty} \hat{\mu}_{k,d} \sum_{i=1}^{N_k} Y_{ki}(x)Y_{ki}(x')\tag{4},
\]
where \( \hat{\mu}_{k,d} \geq 0 \) is the eigenvalue of the \( k \)th eigenspace (we will also denote the normalized eigenvalue as \( \hat{\mu}_{k,d} := N_k \hat{\mu}_{k,d} \)). \( \{Y_{ki}(x)\}_{i=1}^{N_k} \) are the associated eigenfunctions, which is a set of orthonormal degree-\( k \) spherical harmonics. We have
\[
\int Y_{ki}(x)Y_{\ell j}(x)\tau_{d-1}(dx) = \mathbb{I}_{k} \mathbb{I}_{ij},
\]
where \( \mathbb{I}_{ab} = 1 \) if \( a = b \) and \( \mathbb{I}_{ab} = 0 \) otherwise. Moreover, \( N_k \) is the corresponding geometric multiplicity of the \( k \)th eigenspace, which coincides with the dimension of the subspace spanned by all degree-\( k \) spherical harmonics. (We collect a list of related concepts and properties of spherical harmonics in Appendix A.) Note that both \( N_k \) and \( \{Y_{ki}(x)\}_{i=1}^{N_k} \) can depend on \( d \). However, To lighten the notation, we will omit this dependence when doing so causes no confusion. Finally, we denote by \( \tau_{d-1,1} \) the distribution of the scalar random variable \( x^\top e_1 \), where \( x \sim \tau_{d-1} \) and \( e_1 \) is the first standard basis vector.

2.2. Technical Assumptions
Our main results are proved under the following assumptions.

(A.1) Both the number of training samples \( n \) and the input dimension \( d \) go to infinity, while
\[
\frac{n^g}{d^\mu K!} \rightarrow \delta_K \in (0, \infty), \text{ for } K \in \mathbb{Z}^+.
\]

(A.2) \( f_d(x) = f(x/\sqrt{d}) \), where \( f(z) \) is well-defined on \([-1,1]\) and satisfies: (1) \( f(z) \leq C_f \), for some \( C_f > 0 \) and (2) there exists some \( \nu \in (0,1] \) such that \( f(z) \in C^\infty[-\nu, \nu] \).

(A.3) There exists \( C > 0 \) such that \( \hat{\mu}_{k,d} \geq C \), for all \( 0 \leq k \leq K \) and large enough \( d \).

(A.4) There exist constants \( C_g, K_g > 0 \) such that \( g(x) \leq C_g (1 + |x|^{K_g}) \) for any \( x \in \mathbb{R} \).

Remark 1 Assumption (A.2) put two constraints on the kernel functions we consider. The first condition ensures that the expansion (4) is valid and \( \sum_{k=0}^{\infty} \mu_{k,d} < \infty \) holds uniformly over \( d \), which directly follows from the properties (36) and (37) given in Appendix A. The boundedness condition \( \sum_{k=0}^{\infty} \mu_{k,d} < \infty \) is convenient as it makes all the quantities of interests such as the training and test errors of size \( O(1) \), when \( \lambda \in (0, \infty) \). On the other hand, the second condition requires that \( f(z) \) is smooth in some neighbourhood of 0. This guarantees that for any fixed \( k \), \( \mu_{k,d} \rightarrow \frac{f^{(k)}(0)}{k!} \), as \( d \rightarrow \infty \) (see Lemma 1 in Appendix B), where \( f^{(k)}(0) \) denotes the \( k \)th derivative of \( f(z) \) at \( z = 0 \).

Below are two concrete examples of kernels that satisfy Assumption (A.2).

Example 1: Polynomial kernel. In this case, \( f(z) = (z + b)^k \), where \( b \geq 0 \) is a fixed constant and \( k \in \mathbb{Z}^+ \). It is a classical type of kernel, widely applied in several machine learning problems such as support vector machine (SVM).

Example 2: Random feature model (Rahimi and Recht, 2008). The random feature model is a computationally efficient random approximation of kernel function, which is based on the following feature map:

\[
x \mapsto \frac{1}{\sqrt{p}} [\sigma(\mathbf{r}_1^\top x), \sigma(\mathbf{r}_2^\top x), \ldots, \sigma(\mathbf{r}_p^\top x)]^\top,
\]
where \(\{r_i\}_{i=1}^p\) is a set of independent random feature vectors and \(\sigma(x)\) is an activation function satisfying \(\mathbb{E}\sigma(G)^2 < \infty\), with \(G \sim \mathcal{N}(0, 1)\). The associated random kernel function is as follows:

\[
K_p(x, x') = \frac{1}{p} \sum_{u=1}^p \sigma(r_u^\top x) \cdot \sigma(r_u^\top x').
\]

In particular, when \(r_u \overset{i.i.d.}{\sim} \mathcal{N}(0, I/d)\) and \(p \to \infty\), \(K_p(x, x') \to f(\frac{x^\top x'}{d})\). Here, \(f(z) = \mathbb{E}[\sigma(X) \cdot \sigma(Y)]\), with

\[
\begin{pmatrix} X \\ Y \end{pmatrix} \sim \mathcal{N}(0, \Sigma), \quad \Sigma = \begin{bmatrix} 1 & z \\ z & 1 \end{bmatrix}.
\]

The smoothness of \(f\) near 0 can be directly checked by taking derivatives of \(f(z)\).

In fact, we can also let \(f(z)\) depend on \(d\), as long as: (1) \(f_d \in L^2([-\sqrt{d}, \sqrt{d}], \tau_{d-1,1})\), (2) \(\sum_{k=0}^{\infty} \mu_{k,d} < \infty\) for large enough \(d\), and (3) for any fixed \(k\), \(\mu_{k,d} \to \mu_k\) as \(d \to \infty\).

**Remark 2** Assumption (A.3) guarantees that the RKHS associated with the kernel \(K\) is not degenerate: the condition that \(\mu_k > 0\) for \(0 \leq k \leq K\) is satisfied as long as all the degree-\(k\) \((k \leq K)\) polynomials are in the RKHS. This is equivalent to requiring \(f^{(k)}(0) > 0\), for all \(0 \leq k \leq K\).

**Remark 3** Assumption (A.4) implies that for all \(d \in \mathbb{Z}^+\), \(g \in L^2([-\sqrt{d}, \sqrt{d}], \tau_{d-1,1})\). Therefore, we have the following expansion:

\[
g(x) = \sum_{k=0}^{\infty} \alpha_{k,d} q_k(x), \quad (5)
\]

where \(q_k(x)\) is the degree-\(k\) ultraspherical polynomial in \(L^2([-\sqrt{d}, \sqrt{d}], \tau_{d-1,1})\) (more details about these polynomials can be found in Appendix A) and \(\{\alpha_{k,d}\}_{k=0}^{\infty}\) satisfies \(\sum_{k=0}^{\infty} \alpha_{k,d}^2 < \infty\). Note that \(q_k(x)\) depends on \(d\), but for notational simplicity, we will suppress the dependence.

In fact, \(g(x) \leq C \exp(C|x|)\), for some \(C > 0\) will suffice to guarantee the \(L^2\)-integrability of \(g\). Here, we put a stronger assumption to ensure that all the moments of \(g(x)\) exists, which helps simplify several parts of the proof.

### 2.3. Main Results and Insights

We are now ready to state our main theorem.

**Theorem 1** Under Assumption (A.1)-(A.4), we have the following asymptotic characterization of the training and test errors.

1. Training error:

\[
\mathcal{E}_{\text{train}} \overset{p}{\to} \lambda \left[ \frac{\alpha^2_K R_*}{1 + \mu_K \delta_K R_*} + \left( \sigma_z^2 + \sum_{k > K} \alpha_k^2 \right) R_* \right], \quad (6)
\]

where \(R_*\) is the unique non-negative solution of:

\[
\frac{1}{R} = \tilde{\lambda} + \frac{\mu_K}{1 + \delta_K \mu_K R}, \quad (7)
\]
with $\mu_k = \frac{f^{(k)}(0)}{k!}$, $\alpha_k = \int g(x) H_k(x) \tau_G(dx)$ and $\tilde{\lambda} = \lambda + \sum_{k > K} \mu_k$. Here, $H_k(x)$ is the degree-$k$ Hermite polynomial, $\tau_G(dx)$ is the standard Gaussian measure and $R_* = R(\tilde{\lambda}; \mu, \delta)$. where

$$R(\lambda; \mu, \delta) = -\frac{(\lambda + \mu - \mu \delta)}{1 + \mu \delta R_*} + \sqrt{\left(\frac{\lambda + \mu - \delta \mu}{1 + \mu \delta R_*}\right)^2 + 4 \lambda \mu \delta}. \quad (8)$$

2. Test error:

$$E_{\text{test}} \to \frac{1}{\theta - 1} \left[ \frac{\theta \alpha_K^2}{(1 + \mu \delta R_*)^2} + \theta \sum_{k > K} \alpha_k^2 + \sigma_z^2 \right], \quad (9)$$

where $\theta = \frac{(1 + \mu \delta R_*^2)}{\delta R_* R_*^2}$. In both (6) and (9), $\to$ denotes convergence in probability as $d \to \infty$.

Remark 4 It turns out that $R_*$ coincides with the Stieltjes transform of the Marchenko-Pastur (MP) law, with aspect ratio parameter $1/\delta$ and variance $\mu$. The MP law corresponds to the limiting empirical eigenvalue distributions of the Wishart ensemble.

Bias-Variance Decomposition. The formulas in (6) and (9) can be viewed from the perspective of bias-variance decomposition. Conditioning on the input data vectors $\{x_i\}$, we consider the following average squared bias and variance of an estimator $h$ (Hastie et al., 2009, Sec.7.3):

$$B_h := E_{\text{new}}[E_x h(x_{\text{new}}) - E(y_{\text{new}} | x_{\text{new}})]^2 \quad \text{and} \quad V_h := E_{\text{new}}[\text{Var}_x (h(x_{\text{new}}))]^2.$$

Then $E_{\text{test}}$ in (9) can be decomposed as $E_{\text{test}} = B_h + V_h$ and it holds that

$$B_h \to \frac{\theta}{\theta - 1} \left[ \frac{\alpha_K^2}{(1 + \mu \delta R_*)^2} + \sum_{k > K} \alpha_k^2 \right], \quad (10)$$

$$V_h \to \frac{\sigma_z^2}{\theta - 1}. \quad (11)$$

[These can be directly verified via the same proof strategy underlying our proof of (9).] From (11), we can regard $\theta$ as an inflation factor of the variance. By its definition, $\theta$ only depends on $\{\mu_k\}_{k \geq 0}$ but not on $\{\alpha_k\}_{k \geq 0}$ or $\sigma_z^2$. Therefore, $\theta$ reflects the influence of the kernel function on the learning performance. On the other hand, from (10) we can further decompose the bias term $B_h$ as $B_h = \sum_{k = 0}^{\infty} B_k$, where

$$B_k = \begin{cases} 0 & k < K, \\ \frac{\theta}{\theta - 1} \frac{\alpha_K^2}{(1 + \mu \delta R_*)^2} + \sum_{\ell > K} \frac{\alpha_\ell^2}{\theta - 1} & k = K, \\ \alpha_k^2 & k > K. \end{cases}$$

It can be seen that $B_k$ is equal to the average squared bias when $\alpha_k$ is the only non-zero coefficient in (5). In this sense, each $B_k$ can be understood as the contribution of degree-$k$ components to the total squared bias. Moreover, the contributions from different components are linear. Similar results also hold for the training error (6).
Hierarchical learning process. Based on the characterizations (9), we can now have a better understanding of the hierarchical learning process illustrated in Fig. 1. Consider the limit: \( \delta_K \to 0 \) and \( \delta_K \to \infty \). By (8), we can get for any fixed \( \tilde{\lambda} > 0 \) and \( \mu_K > 0 \),

\[
R_* \to \begin{cases} \frac{(\tilde{\lambda} + \mu_K)^{-1}}{\lambda^{-1}} & \delta_K \to 0 \\ \mu_K & \delta_K \to \infty \end{cases}
\]

and \( \theta \to \infty \) under both limits. Therefore, \( \lim_{\delta_K \to 0} B_K = \alpha_K^2 \) and \( \lim_{\delta_K \to \infty} B_K = 0 \). Recall that \( \alpha_K^2 \) is the energy of the degree-\( k \) component of the teacher function, so this justifies that KRR learns the degree-\( k \) components in phase-\( k \). Moreover we can also identify the roles played by the components of different degrees. From (9), we can see that at phase-\( k \): (i) all the low-degree \( (\ell < k) \) components of the kernel function and the teacher function do not exert any influence; (ii) high-degree \( (\ell > k) \) components of the kernel function act as an additional regularization term, as manifested in \( \tilde{\lambda} \); and (iii) high-degree components of the teacher function act as additive noise.

Non-monotonicity of \( \mathcal{E}_{\mathrm{test}} \). In Fig. 1, we show that \( \mathcal{E}_{\mathrm{test}} \) can be non-monotonic with respect to the sample complexity. Based on our asymptotic characterization, this phenomenon can be explained as follows. In Fig. 1, we choose \( f(z) = \frac{a^2}{20} + \frac{a^2}{2} + z + 1 \), \( g(x) = \frac{a^2}{20} + \frac{a^2}{2} + x^2 + x \), \( \sigma_z = 0.5 \) and \( \lambda = 10^{-4} \approx 0 \). This corresponds to the ridgeless limit of KRR. Let us take \( \lambda \to 0 \) in the asymptotic characterization and suppose \( \mu_k = 0 \) for all \( k > K \). In this case, we can show from (10) and (11) that \( B_h \to \alpha_K^2 \max\{1 - \delta_K, 0\} \) and \( \mathcal{V}_h \to \frac{\sigma_k^2}{\delta_K - 1} \min\{\delta_K, 1\} \). We can find that \( B_h \) is monotonically decreasing and the non-monotonicity of \( \mathcal{E}_{\mathrm{test}} \) stems from the non-monotonicity of \( \mathcal{V}_h \). The peak at the interpolation threshold \( \delta_K = 1 \) due to the explosion of the variance. In Fig. 1, this corresponds to the peak in the Transition-3. On the other hand, we can find that the peak at Transition-2 is less notable and there is no peak at Transition-1. The reason is that when \( K = 1, 2 \), higher-degree components of kernel function do not vanish and they act as regularization terms (manifested by \( \tilde{\lambda} = \lambda + \sum_{k > K} \mu_k \)), which reduces the variance.

2.4. Gaussian Equivalence Conjecture

A key technical insight behind our proof of Theorem 1 is the rigorous establishment of a so-called Gaussian equivalence conjecture. This conjecture was implicitly used (without proof) in several earlier works (Dietrich et al., 1999; Bordelon et al., 2020; Canatar et al., 2021) that study the generalization performance of kernel methods using non-rigorous statistical physics methods.

For simplicity, let us assume that the kernel and teacher functions are both band-limited: there exists \( L > 0 \) such that \( \mu_k = \alpha_k = 0 \), for all \( k > L \). First, based on the expansions (4) and (5), we can obtain an equivalent formulation of (1) as a linear regression in the feature space with the following feature map:

\[
x_a \mapsto \gamma_a = [\tilde{Y}_{01}(x_a), \tilde{Y}_{11}(x_a), \ldots, \tilde{Y}_{1N_1}(x_a), \ldots, \tilde{Y}_{L1}(x_a), \ldots, \tilde{Y}_{LN_L}(x_a)]^T
\]

where \( \tilde{Y}_{kl}(\cdot) := \sqrt{\mu_k, d}Y_{kl}(\cdot) \). Then (1) is equivalent to:

\[
\hat{\theta} = \arg\min_{\theta} \sum_{a=1}^{n} [y_a - \theta^T \gamma_a]^2 + \lambda \|\theta\|^2
\]
where \( y_a = \beta^\top \Lambda \gamma_a + z_a \), with

\[
\beta = [Y_0(\xi), Y_1(\xi), \ldots, Y_{1N_1}(\xi), \ldots, \ldots, Y_L(\xi), \ldots Y_{LN_L}(\xi)]^\top
\]

and

\[
\Lambda = \text{diag}\{\frac{\alpha_{0,d}}{\sqrt{\mu_{0,d}}}, \frac{\alpha_{1,d}}{\sqrt{\mu_{1,d}}}, \ldots, \frac{\alpha_{1,d}}{\sqrt{\mu_{1,d}}}, \ldots, \frac{\alpha_{L,d}}{\sqrt{\mu_{L,d}}}, \ldots, \frac{\alpha_{L,d}}{\sqrt{\mu_{L,d}}}\}.
\]

If the entries of \( \gamma_a \) are independent Gaussian random variables, then we reach the setting that has been analyzed in several recent papers (Dicker, 2016; Dobriban and Wager, 2018; Hastie et al., 2019; Wu and Xu, 2020; Richards et al., 2021). The main challenge here is that different entries of \( \gamma_a \) are not independent and that there is no linear transformation that can decouple this dependence. On the other hand, however, different entries \( \gamma_a \) are still uncorrelated: recall that \( \mathbb{E} Y_{ki}(x) Y_{lj}(x) = \mu_{k,d} \delta_{k,l} \delta_{ij} \), since \( \{Y_{ki}(x)\}_{k,i} \) are orthonormal with respect to \( \tau_{d-1} \). Thus, the so-called Gaussian equivalence conjecture states that the learning performance of the original KRR problem will remain asymptotically unchanged if we replace each \( \gamma_a \) by a Gaussian vector \( g_a \) with the same mean and covariance matrix.

### 2.5. Limitations of the Current Work

Finally, we point out several important limitations of our results. First, we have assumed that the input vectors \( x \) are uniformly distributed over \( S^{d-1}(\sqrt{d}) \). Although this is a convenient model for theoretical analysis, the spherical symmetry of the model might impose too strong an assumption on the input data. It will be desirable to explore other more general data distributions such as those considered in Liang et al. (2020b,a); Mei et al. (2021). Second, we have assumed that the labels \( \{y_i\} \) in the training set are generated by a specific teacher-student model, which is essentially a generalized linear model. On the contrary, in Liang et al. (2020b,a); Mei et al. (2021), there is no such constraint and a generic non-parametric model for the labels \( \{y_i\} \) is considered. Since current proof crucially hinges on the fact that the distribution of \( x_i \) is isotropic and that \( h(x) \) only depends on the projection \( x_i^\top \xi \), handling more general function classes may require substantial changes to our current proof technique. Finally, we only analyze the inner-product kernels here. It will be interesting to consider other types of kernels, e.g., radial kernel \( K(x, x') = k(\|x - x'\|/\sqrt{d}) \) and translation invariant kernel \( K(x, x') = k(x - x') \). In the current setting, since \( x_i \overset{i.i.d.}{\sim} \tau_{d-1} \), it is easy to see that radial kernels can be viewed as inner-product kernels. For more general settings, we conjecture that some versions of Gaussian equivalence may still hold. The extensions to the above more general cases are left as interesting future work.

### 3. Proof of Main Results

#### 3.1. Notations

Before delving into the formal proof, let us first list some notations that will be used throughout our proof in the following sections.

For \( n \in \mathbb{Z}^+ \), we denote by \([n]\) the set \( \{1, 2, \cdots, n\} \). For a vector \( x \in \mathbb{R}^n \), we use \( \|x\| \) to denote its \( \ell_2 \) norm and for a matrix \( X \in \mathbb{R}^{m \times n} \), we use \( \|X\| \) to denote its operator norm and \( \|X\|_F \) as its Frobenius norm.

For convenience of stating some results regarding deterministic or probabilistic upper bounds, we will adopt the following notations. \( f(d) \lesssim g(d) \) means that there exists \( C > 0 \) such that \( |f(d)| \leq C g(d) \)
where \(K\) and \(g(d)\) means that there exists \(c > 0\) such that \(|f(d)| \geq c|g(d)|\). Also for two non-negative random variables, \(X \leq Y\) means that for any \(\tau > 0\) and \(\varepsilon > 0\), \(\Pr(X \leq d^\tau Y) \leq \varepsilon\) for all large enough \(d\).

Our proof will frequently utilize the expansions of \(K(\cdot, \cdot)\) and \(g(\cdot)\) under spherical harmonics \(\{Y_k(x)\}_{k,i}\) and ultraspherical polynomials \(\{q_k\}_k\). For any vector \(a \in \mathbb{R}^d\),

\[
Y_k(a) := [Y_{k1}(a), Y_{k2}(a), \ldots, Y_{kN_k}(a)]^\top,
\]

and for any matrix \(A = [a_1, a_2, \ldots, a_n]^\top \in \mathbb{R}^{n \times d}\), \(Y_k(A) := [Y_k(a_1), Y_k(a_2), \ldots, Y_k(a_n)]^\top\). In particular, for the input matrix \(X = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^{n \times d}\), we denote \(Y_k := Y_k(X)\). In the kernel expansion, the degree-\(k\) component will be denoted as \(K_k := \tilde{\mu}_{k,d} Y_k Y_k^\top\) and likewise for the teacher model, we have \(g_k := \alpha_{k,d} q_k(x)\). We also denote \(\delta_k = n/N_k\) as the sampling ratio with respect to the degree-\(k\) component and \(D_k = \sqrt{\mu_{k,d} \delta_k} I_{N_k}\).

We use the following short-hand notations for the partial sum: \(K_{\leq k} = \sum_{t=0}^k K_{t}, N_{\leq k} = \sum_{t=0}^k N_t, g_{\leq k} = \sum_{t=0}^k g_t + z\) and block matrix: \(Y_{\leq k} = [Y_0, \ldots, Y_k]\), \(Y_{\leq k}(\xi) = [Y_0(\xi)^\top, \ldots, Y_k(\xi)^\top]^\top\) and \(D_{\leq k} = \text{diag}\{D_0, \ldots, D_k\}\). The quantities like \(K_{> k}\) or \(Y_{> k}\) are defined in the same way.

Also since we are focusing on asymptotic results and under our main assumptions, \(\mu_{k,d} \to \mu_k\) and \(\alpha_{k,d} \to \alpha_k\) as \(d \to \infty\), we will drop the dependence of \(\mu_{k,d}\) and \(\alpha_{k,d}\) on \(d\) in our proof, when it is clear from the context.

### 3.2. Proof for the Asymptotic Formula of the Training Error

We first study the asymptotics of the training error. It can be proved (Schölkopf et al., 2002, Theorem 4.2) that the optimal solution of (1) is:

\[
\hat{h}(x) = \sum_{i=1}^n K(x, x_i)\hat{w}_i.
\]

Here, \(\hat{w} = (\lambda I + K)^{-1}y\) is the optimal solution of

\[
\min_w (y - Kw)^2 + \lambda w^\top Kw,
\]

where \(K \in \mathbb{R}^{n \times n}\) is the kernel matrix, with \([K]_{ij} = K(x_i, x_j)\). Therefore, \(E_{\text{train}}\) has an explicit form:

\[
E_{\text{train}} = \frac{\lambda}{n} y^\top R y,
\]

where \(R = (\lambda I + K)^{-1}\) is the resolvent matrix of \(K\).

#### 3.2.1. A Special Case

We first present the proof for a special case. Consider the following kernel function \(K(\cdot, \cdot)\):

\[
K(x, x') = \frac{\mu_{K,d}}{N_K} \sum_{i=1}^{N_K} Y_{Ki}(x) Y_{Ki}(x').
\]

(16)
and teacher function $g(\cdot)$:

$$g(x) = \alpha_K, a q_K(x),$$

(17)

where $K \in \mathbb{Z}^+$ is defined as in Assumption (A.1). Comparing (16) and (17) with (4) and (5), we can find that (16) and (17) correspond to a special model that only retains the degree-$K$ component, while discarding all the low-degree and high-degree parts. Although this may appear to be a substantial simplification of the original model, it turns out that this simplified setting already captures some main technical ingredients in the general proof.

We can make some simplifications utilizing the rotational invariance of the input vectors $\{x_i\}_{i=1}^n$. Since $x_i \sim \tau_{d-1}$, we have the following representation:

$$x_i = (\eta_i, [(d - \eta_i^2)/(d - 1)]^{1/2} v_i^T)^T,$$

(18)

where $\eta_i \sim \tau_{d-1,1}$, $v_i \sim \tau_{d-2}$ and they are independent. Also by rotational invariance, we can assume without loss of generality that $\xi = \sqrt{d} e_1$. Then substituting $\xi = \sqrt{d} e_1$, (17) and (18) into (2), we get

$$y = \alpha_{K, a} q_K(\eta) + z,$$

(19)

where $q_K(\cdot)$ is applied pointwise on $\eta$. On the other hand, the kernel function can be written compactly as:

$$K(x_i, x_j) = \frac{\mu_{K, a}}{\sqrt{N_k}} q_K(\frac{x_i^T x_j}{\sqrt{d}}),$$

$$= \frac{\mu_{K, a}}{\sqrt{N_k}} q_K(\frac{\eta_i \eta_j}{\sqrt{d}} + \frac{v_i v_j}{\sqrt{d-1}} \sqrt{\frac{d}{d-1}} \left(1 - \frac{\eta_i^2}{d}\right) \left(1 - \frac{\eta_j^2}{d}\right))$$

(20)

where in the second step, we use (18). Correspondingly, the kernel matrix $K(= K_K)$ becomes:

$$K = \frac{\mu_{K, a}}{\sqrt{N_k}} q_K \left(\frac{\eta_1^T + \sqrt{\frac{d}{d-1}} \text{diag} \left\{ (1 - \eta_i^2/d)^{1/2} \right\} V V^T \text{diag} \left\{ (1 - \eta_i^2/d)^{1/2} \right\}}{\sqrt{d-1}} \right)$$

(21)

where $\eta = (\eta_1, \eta_2, \ldots, \eta_n)^T$ and $V = (v_1, v_2, \ldots, v_n)^T$.

From (19) we know $y$ is a (noisy) function of $\eta$. Therefore, to compute $E_{\text{train}} = \frac{\lambda}{n} y^T R y$, we need to handle the (weak) correlation between $\eta$ and $K$. However, the formulation in (21) is not amenable for analysis, as $K$ depends on $\eta$ in a convoluted way. To this end, we can apply Proposition 1, Lemma 4 and Lemma 7 in Lu and Yau (2022) (with a slightly different scaling) to get

$$\left| \frac{1}{n} y^T (R - \tilde{R}) y \right| \lesssim \frac{1}{\sqrt{d}},$$

(22)

where $\tilde{R} := (\lambda I + \tilde{K})^{-1}$, with

$$\tilde{K} = \frac{\mu_{K, a}}{\sqrt{N_k}} q_K (V V^T) + \frac{\mu_{K, a}}{N_k} v_K(\eta) v_K(\eta)^T,$$

(23)

$v_\ell(\eta) := (q_\ell(\eta_1), \ldots, q_\ell(\eta_n))^T$ and $q_K(x) := q_{K,d-1}(x)$. The approximation $\tilde{K}$ is much easier to handle, as it depends on $\eta$ only through a rank-1 matrix. Define $\tilde{R} := (\lambda I + \tilde{K})^{-1}$, where

$$\tilde{K} := \frac{\mu_{K, a}}{\sqrt{N_k}} \tilde{q}_K (V V^T).$$

By Sherman–Morrison formula, we can get:

$$\frac{1}{n} y^T \tilde{R} y = \frac{\alpha_{K, a}^2 + 2\alpha_K b - \delta_K \mu_{K, a} b^2}{1 + \delta_K \mu_{K, a} a} + c,$$
Proposition 1

There exists $L$ some and (2) the high-degree components $(\hat{K})$. We have the following decomposition for $\hat{R}_{K}$ to be chosen. Then we can follow the same strategy in Sec. 3.2.1 to obtain $\hat{R}_{K} = (\hat{\lambda}I + \hat{K})^{-1}$ and $\hat{\lambda} := \lambda + \sum_{k > K} \mu_k$ is an equivalent regularization parameter.

Proof 

We have the following decomposition for $\frac{1}{n} y^\top R y$: 

$$\frac{1}{n} y^\top R y = \frac{1}{n} y^\top (R - \tilde{R}_{\leq K}) y - \frac{1}{n} y^\top \tilde{R}_{\leq K} y \geq K y \geq K$$ 

then

$$\frac{1}{n} y^\top \tilde{R}_{\leq K} y \geq K y \geq K, \quad \tilde{R}_{\leq K} = (\hat{\lambda}I + \hat{K})^{-1}. \quad \tilde{R}_{\leq K} = (\hat{\lambda}I + \hat{K})^{-1}. \quad \text{The first three terms in the above display are approximation errors.}$$

In Lemma 4, Lemma 8 and Lemma 9, we show that they all decay to zero as $d \to \infty$, with the desired rate. This completes the proof.

3.2.2. General Case

To extend the proof to the general setting [c.f. (4) and (2)], we need to take into account all the terms in the expansion of $K(\cdot, \cdot)$ and $g(\cdot)$, not just the degree-$K$ component as in (16) and (17). The bridge is the following result, which shows that: (1) the low-degree parts ($k < K$) can be truncated and (2) the high-degree components ($k > K$) of kernel function act as a regularization term.

**Proposition 1** There exists $\tau > 0$ such that

$$\frac{1}{n} y^\top R y = \frac{1}{n} y^\top \tilde{R}_{K} y \geq K \approx \frac{1}{d^\tau}$$

where $\tilde{R}_{K} = (\hat{\lambda}I + \hat{K})^{-1}$ and $\hat{\lambda} := \lambda + \sum_{k > K} \mu_k$ is an equivalent regularization parameter.

Proof 

We have the following decomposition for $\frac{1}{n} y^\top R y$:

$$\frac{1}{n} y^\top R y = \frac{1}{n} y^\top (R - \tilde{R}_{\leq K}) y - \frac{1}{n} y^\top \tilde{R}_{\leq K} y \geq K y \geq K$$

where $\tilde{R}_{\leq K} = (\hat{\lambda}I + \hat{K})^{-1}$. The first three terms in the above display are approximation errors. In Lemma 4, Lemma 8 and Lemma 9, we show that they all decay to zero as $d \to \infty$, with the desired rate. This completes the proof.

Proposition 1 brings us closer to the special case analyzed previously in Sec. 3.2.1. In particular, it implies that all the low-degree components in $K(\cdot, \cdot)$ and $g(\cdot)$ can be dropped, without causing any non-vanishing error and all the higher-degree components of $K(\cdot, \cdot)$ can be equivalently treated as a regularization term. The remaining thing is to handle the higher-degree components contained in $y \geq K$. Recall that in the simplified setting (17), only the $K$th degree component is involved.

To proceed, we first apply a truncation over $y \geq K$. Let $y_{\geq K} = \sum_{k = K}^{L} \alpha_k g_k (X \xi / \sqrt{d}) + z$, for some $L \geq K$ to be chosen. Then we can follow the same strategy in Sec. 3.2.1 to obtain

$$\frac{1}{n} y_{\geq K}^\top \tilde{R}_{K} y_{\geq K} \geq K \approx \frac{1}{d^\tau}.$$
To complete the proof, we just need to show the above approximation by \( \hat{y}_{\geq K} \) can be made arbitrarily precise. In particular, by Lemma 2, for any \( \varepsilon > 0 \), we can always find an \( L \in \mathbb{Z}^+ \) such that for all large enough \( d \), \( \sum_{k=L+1}^{\infty} \alpha_{k,d}^2 < \frac{\varepsilon}{2} \) and \( \mathbb{P}(\frac{1}{n}\|y_{\geq K} - \hat{y}_{\geq K}\|^2 \geq \varepsilon) \leq \frac{C}{n^2} \), where \( C > 0 \) is some constant. These two bounds together with (27) imply that for any \( \varepsilon > 0 \),

\[
\mathbb{P}\left\{ \left| \frac{1}{n} y_{\geq K}^T \tilde{R}_K y_{\geq K} - \left[ \frac{\alpha_K^2 R_s^*}{1 + \delta_K \mu_K R_s^*} + \left( \sigma_z^2 + \sum_{k=K+1}^{\infty} \alpha_k^2 R_s^* \right) \right] \right| > \varepsilon \} \rightarrow 0,
\]
as \( d \rightarrow \infty \) and the proof is finished.

### 3.3. Proof for the Asymptotic Formula of the Test Error

Next we analyze the asymptotics of the test error. We can decompose \( \mathcal{E}_{\text{test}} \) as:

\[
\mathcal{E}_{\text{test}} = \mathbb{E}_{\text{new}} \mathbb{E}(y_{\text{new}} | x_{\text{new}})^2 - 2\mathbb{E}_{\text{new}} \mathbb{E}(y_{\text{new}} | x_{\text{new}}) \hat{h}(x_{\text{new}}) + \mathbb{E}_{\text{new}} \hat{h}(x_{\text{new}})^2.
\]

(28)

In the following, we deal with them individually.

#### 3.3.1. PART I

It can be directly calculated from (2) and (5) that \( \mathbb{E}_{\text{new}} \mathbb{E}(y_{\text{new}} | x_{\text{new}})^2 = \sum_{k=0}^{\infty} \alpha_k^2 d^2 \). Then by Lemma 2, as \( d \rightarrow \infty \)

\[
\mathbb{E}_{\text{new}} \mathbb{E}(y_{\text{new}} | x_{\text{new}})^2 \rightarrow \sum_{k=0}^{\infty} \alpha_k^2.
\]

(29)

#### 3.3.2. PART II

Following the similar strategy as in Sec. 3.2, we can get

\[
\mathbb{E}_{\text{new}} \mathbb{E}(y_{\text{new}} | x_{\text{new}}) \hat{h}(x_{\text{new}}) = \frac{1}{n} \tilde{g}^T \tilde{R} y \rightarrow_{\text{p}} \sum_{k<K} \alpha_k^2 + \frac{\mu_K \delta_K \mu_K R_s^*}{1 + \mu_K \delta_K R_s^*},
\]

(30)

where \( \tilde{g} = \sum_{k=0}^{\infty} \mu_k \delta_k g_k \). The proof is deferred to Appendix E.

#### 3.3.3. PART III

This part of proof follows the same strategy as Part I and Part II. In particular, we can get

\[
\mathbb{E}_{\text{new}} \hat{h}(x_{\text{new}})^2 \rightarrow_{\text{p}} \sum_{k<K} \alpha_k^2 + \frac{(\delta_K \mu_K \alpha_K R_s^*)^2}{(1 + \delta_K \mu_K R_s^*)^2} + \frac{\alpha_K^2}{\theta - 1}(1 + \delta_K \mu_K R_s^*)^2 + \frac{\sigma_z^2}{\theta - 1} \sum_{k>K} \alpha_k^2.
\]

(31)

The details are relegated to Appendix F.

### 3.4. Finish the Proof

The final step is to substitute (29), (30) and (31) back to (28) and get (9).
References

Ben Adlam and Jeffrey Pennington. The neural tangent kernel in high dimensions: Triple descent and a multi-scale theory of generalization. In International Conference on Machine Learning, pages 74–84. PMLR, 2020.

Mikhail Belkin, Siyuan Ma, and Soumik Mandal. To understand deep learning we need to understand kernel learning. arXiv preprint arXiv:1802.01396, 2018.

Patrick Billingsley. Probability and measure. John Wiley & Sons, 2008.

Blake Bordelon, Abdulkadir Canatar, and Cengiz Pehlevan. Spectrum dependent learning curves in kernel regression and wide neural networks. In International Conference on Machine Learning, pages 1024–1034. PMLR, 2020.

Abdulkadir Canatar, Blake Bordelon, and Cengiz Pehlevan. Spectral bias and task-model alignment explain generalization in kernel regression and infinitely wide neural networks. Nature communications, 12(1):1–12, 2021.

Xiuyuan Cheng and Amit Singer. The spectrum of random inner-product kernel matrices. Random Matrices: Theory and Applications, 2(04):1350010, 2013.

Feng Dai and Yuan Xu. Approximation theory and harmonic analysis on spheres and balls, volume 23. Springer, 2013.

Amit Daniely, Roy Frostig, and Yoram Singer. Toward deeper understanding of neural networks: The power of initialization and a dual view on expressivity. In Advances In Neural Information Processing Systems, pages 2253–2261, 2016.

Stéphane d’Ascoli, Maria Refinetti, Giulio Biroli, and Florent Krzakala. Double trouble in double descent: Bias and variance (s) in the lazy regime. In International Conference on Machine Learning, pages 2280–2290. PMLR, 2020.

Lee H Dicker. Ridge regression and asymptotic minimax estimation over spheres of growing dimension. Bernoulli, 22(1):1–37, 2016.

Rainer Dietrich, Manfred Opper, and Haim Sompolinsky. Statistical mechanics of support vector networks. Physical review letters, 82(14):2975, 1999.

Edgar Dobriban and Stefan Wager. High-dimensional asymptotics of prediction: Ridge regression and classification. The Annals of Statistics, 46(1):247–279, 2018.

Simon Du, Jason Lee, Haochuan Li, Liwei Wang, and Xiyu Zhai. Gradient descent finds global minima of deep neural networks. In International conference on machine learning, pages 1675–1685. PMLR, 2019.

Behrooz Ghorbani, Song Mei, Theodor Misiakiewicz, and Andrea Montanari. Linearized two-layers neural networks in high dimension. The Annals of Statistics, 49(2):1029–1054, 2021.

Trevor Hastie, Robert Tibshirani, and Jerome H Friedman. The elements of statistical learning: data mining, inference, and prediction, volume 2. Springer, 2009.
Trevor Hastie, Andrea Montanari, Saharon Rosset, and Ryan J Tibshirani. Surprises in high-dimensional ridgeless least squares interpolation. *arXiv preprint arXiv:1903.08560*, 2019.

Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in neural information processing systems*, pages 8571–8580, 2018.

Tengyuan Liang, Alexander Rakhlin, and Xiyu Zhai. On the multiple descent of minimum-norm interpolants and restricted lower isometry of kernels. In *Conference on Learning Theory*, pages 2683–2711. PMLR, 2020a.

Tengyuan Liang, Alexander Rakhlin, et al. Just interpolate: Kernel “ridgeless” regression can generalize. *Annals of Statistics*, 48(3):1329–1347, 2020b.

Yue M. Lu and Horng-Tzer Yau. An equivalence principle for the spectrum of random inner-product kernel matrices. *arXiv preprint*, 2022.

Song Mei and Andrea Montanari. The generalization error of random features regression: Precise asymptotics and double descent curve. *arXiv preprint arXiv:1908.05355*, 2019.

Song Mei, Theodor Misiakiewicz, and Andrea Montanari. Generalization error of random feature and kernel methods: hypercontractivity and kernel matrix concentration. *Applied and Computational Harmonic Analysis*, 2021.

Theodor Misiakiewicz. Spectrum of inner-product kernel matrices in the polynomial regime and multiple descent phenomenon in kernel ridge regression. *arXiv preprint arXiv:2204.10425*, 2022.

Preetum Nakkiran, Gal Kaplun, Yamini Bansal, Tristan Yang, Boaz Barak, and Ilya Sutskever. Deep double descent: Where bigger models and more data hurt. *Journal of Statistical Mechanics: Theory and Experiment*, 2021(12):124003, 2021.

Radford M Neal. Priors for infinite networks. In *Bayesian Learning for Neural Networks*, pages 29–53. Springer, 1996.

Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *Advances in neural information processing systems*, pages 1177–1184, 2008.

Alexander Rakhlin and Xiyu Zhai. Consistency of interpolation with laplace kernels is a high-dimensional phenomenon. In *Conference on Learning Theory*, pages 2595–2623. PMLR, 2019.

Dominic Richards, Jaouad Mourtada, and Lorenzo Rosasco. Asymptotics of ridge (less) regression under general source condition. In *International Conference on Artificial Intelligence and Statistics*, pages 3889–3897. PMLR, 2021.

Bernhard Schölkopf, Alexander J Smola, Francis Bach, et al. *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

Roman Vershynin. *High-dimensional Probability: An Introduction with Applications in Data Science*. Cambridge University Press, 2018.
Appendix A. Spherical Harmonics and Ultraspherical Polynomials

In this section, we give a brief overview of some properties of the spherical harmonics and ultraspherical polynomials that are frequently used in our analysis. A detailed coverage of these topics can be found in Dai and Xu (2013).

Spherical harmonics are homogeneous harmonic polynomials restricted on $S^{d-1}(\sqrt{d})$. In other words, a polynomial $P(x)$, $x \in S^{d-1}(\sqrt{d})$ is a spherical harmonic if and only if (1) $P(tx) = t^d P(tx)$, for any $t \in \mathbb{R}$, (2) $\Delta P = 0$, where $\Delta$ is the Laplace operator. Let $\mathcal{H}_{k,d}$ be the space of all degree-$k$ spherical harmonics in $d$ dimension. Then $\dim(\mathcal{H}_{k,d}) = N_k$, where

$$N_k = \begin{cases} 1 & k = 0 \\ \frac{d+2k-2}{k} & k \geq 2 \\ \frac{d+k-3}{k-1} & k = 1 \end{cases}$$ (32)

From (32), we can find that $|N_k/(\binom{d}{k}) - 1| \leq \frac{C_k}{d}$, where $C_k > 0$ is some constant that only depends on $k$, i.e., $N_k$ is approximately equal to the combinatorial number up to an $O(\frac{1}{d})$ correction. Any orthonormal basis of $\mathcal{H}_{k,d}$, $k \geq 0$ is denoted by $\{Y_{ki}(x)\}_{i=1}^{N_k}$ and they satisfy

$$\int_{S^{d-1}(\sqrt{d})} Y_{ki}(x) Y_{kj}(x) \tau_{d-1}(dx) = \mathbb{I}_{i=j}. \quad (33)$$

where $\tau_{d-1}$ is the uniform distribution over $S^{d-1}(\sqrt{d})$.

Ultraspherical polynomials $\{q_k\}_{k=0}^{\infty}$ are orthonormal polynomials on $L^2([-\sqrt{d}, \sqrt{d}], \tau_{d-1,1})$, i.e.,

$$\int_{-\sqrt{d}}^{\sqrt{d}} q_k(x) q_\ell(x) \tau_{d-1,1}(dx) = \mathbb{I}_{k=\ell}$$

where $\tau_{d-1,1}$ is the distribution of $x^\top e_1$, with $x \sim \tau_{d-1}$ and it also has the explicit form: $\tau_{d-1,1}(dx) = \frac{\omega_d}{\sqrt{\omega_{d-1}}} \sqrt{1-x^2} \frac{dx}{d^2}$, where $\omega_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the surface area of $S^{d-1}$. The moments of measure $\tau_{d-1,1}$ equal to

$$\mathbb{E}_{\tau_{d-1,1}} X^m = \begin{cases} 0 & m = 2k+1 \\ \prod_{0 \leq i < k} (1+2i/d) & m = 2k \end{cases} \quad (34)$$

Based on (34), we can explicitly write out the first three $q_k(x)$ via the Gram-Schmidt procedure:

$$q_0(x) = 1, \quad q_1(x) = x, \quad q_2(x) = \frac{1}{\sqrt{2}} \sqrt{\frac{d+2}{d-1}} (x^2 - 1).$$
In particular, for any $k \geq 0$, $q_k(x)$ and $\{Y_{ki}(x)\}_{i=1}^{N_k}$ have the following correspondence: for any $x, x' \in S^{d-1}(\sqrt{d})$,

$$q_k(x^T x'/\sqrt{d}) = \frac{1}{\sqrt{N_k}} \sum_{i=1}^{N_k} Y_{ki}(x)Y_{ki}(x'),$$

(35)

which is also known as the addition theorem. As a result, the expansion (4) can also be written as:

$$f_d(x^T x'/\sqrt{d}) = \sum_{k=0}^{\infty} \sqrt{N_k} \mu_{k,d} q_k(x^T x'/\sqrt{d}).$$

(36)

Also we can deduce that for any $x \in S^{d-1}(\sqrt{d})$,

$$\frac{1}{\sqrt{N_k}} \sum_{i=1}^{N_k} Y_{ki}(x)^2 = q_k(\sqrt{d}) = \sqrt{N_k}.$$  

(37)

Indeed, for any $x \in S^{d-1}(\sqrt{d})$,

$$q_k(\sqrt{d}) = q_k(||x||^2/\sqrt{d})
= \int_{S^{d-1}(\sqrt{d})} q_k(||x||^2/\sqrt{d}) \tau_{d-1}(dx)
\equiv \frac{1}{\sqrt{N_k}} \sum_{i=1}^{N_k} \int_{S^{d-1}(\sqrt{d})} Y_{ki}(x)^2 \tau_{d-1}(dx)
\equiv \sqrt{N_k},$$

where (a) follows from (35) and (b) follows from (33).

The ultraspherical polynomials are closely related with the Hermite polynomials $\{H_k\}_{k=0}^{\infty}$, which are the orthonormal polynomials on $L^2(\mathbb{R}, \tau_G)$, where $\tau_G$ denotes the standard Gaussian measure. From (34), we can see that for any fixed $k$, $\lim_{d \to \infty} \mathbb{E}_{\tau_{d-1,1}} X^m = \mathbb{E}_{\tau_G} X^m$, where $\tau_G$ denotes the standard Gaussian measure. By Theorem 30.1 in (Billingsley, 2008), $\tau_{d-1,1}$ converges weakly to $\tau_G$. Therefore, as $d \to \infty$, we can get $q_{k,d}(x) \to H_k(x)$ pointwise on $\mathbb{R}$.

Appendix B. Convergence of Expansion Coefficients

**Lemma 1** Suppose $f_d(x) = f(\frac{x}{\sqrt{d}})$, where $f(z)$ is defined on $[-1, 1]$ satisfying $f(z) \leq C_f$ and $f(z) \in C^\infty[-v, v]$, for some $C_f > 0$ and $v \in (0, 1]$. Then for any fixed $k \geq 0$,

$$\mu_{k,d} \to \mu_k = \frac{f^{(k)}(0)}{k!},$$

as $d \to \infty$.

**Proof** First, we analyze the special case $v = 1$, i.e., $f(z) \in C^\infty[-1, 1]$. From (36), we have

$$\mu_{k,d} = \sqrt{N_k} \int_{-\sqrt{d}}^{\sqrt{d}} f(\frac{x}{\sqrt{d}}) q_k(x) \tau_{d-1,1}(dx),$$

(38)
where \( \tau_{d-1,1}(dx) = \frac{\omega_{d-2}}{\sqrt{d(\omega_{d-1})}} (1 - x^2/d)^{\frac{d-3}{2}} dx \), with \( \omega_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} \). Then we can utilize the Rodrigues’ formula for \( q_k(x) \):

\[
q_k(x) = \sqrt{N_k} C_{k,d} \sqrt{d} \left( 1 - \frac{x^2}{d} \right)^{\frac{d-3}{2}} \left( \frac{d}{dx} \right)^k \left( 1 - \frac{x^2}{d} \right)^{k + \frac{d-3}{2}}
\]

where \( C_{k,d} = \left( -\frac{1}{2} \right)^k \frac{\Gamma(d/2)}{\Gamma(k + \frac{d-1}{2})} \). Then

\[
\int_{-\sqrt{d}}^{\sqrt{d}} f\left( \frac{x}{\sqrt{d}} \right) q_k(x) \tau_{d-1,1}(dx)
= \sqrt{N_k} C_{k,d} \sqrt{d} \int_{-\sqrt{d}}^{\sqrt{d}} f\left( \frac{x}{\sqrt{d}} \right) \cdot \left( 1 - \frac{x^2}{d} \right)^{\frac{d-3}{2}} \frac{d}{dx} \left( 1 - \frac{x^2}{d} \right)^{k + \frac{d-3}{2}} \sqrt{d} \omega_{d-1} \left( 1 - \frac{x^2}{d} \right)^{\frac{d-3}{2}} dx
= \sqrt{N_k} C_{k,d} \frac{\omega_{d-2}}{\omega_{d-1}} \int_{-1}^{1} f(z) \cdot \frac{d}{dz} \left( 1 - z^2 \right)^{k} \left( 1 - z^2 \right)^{k + \frac{d-3}{2}} f(k)(z) dz
\]

\[
= \sqrt{N_k} C_{k,d} (-1)^k \frac{\omega_{d-2}}{\omega_{d-1}} \int_{-1}^{1} (1 - z^2)^{k + \frac{d-3}{2}} f(k)(z) dz
= \frac{N_k}{2^k \prod_{i=0}^{k-1} (\frac{d-1}{2} + i)} \int_{-1}^{1} (1 - z^2)^{k + \frac{d-3}{2}} f(k)(z) dz \quad \text{(39)}
\]

where in (a) we make a change of variable: \( \frac{x}{\sqrt{d}} \to z \) and in (b) we use integration by parts for \( k \) times. After combining (38) and (39), we get

\[
\mu_{k,d} = \frac{N_k}{\prod_{i=0}^{k-1} (d - 1 + 2i)} \int_{-1}^{1} \frac{\omega_{d-2}}{\omega_{d-1}} (1 - z^2)^{k} \left( 1 - z^2 \right)^{k + \frac{d-3}{2}} f(k)(z) dz.
\]

As \( d \to \infty \), \( \frac{N_k}{\prod_{i=0}^{k-1} (d - 1 + 2i)} \to \frac{1}{k!} \). Note that \( \frac{\omega_{d-2}}{\omega_{d-1}} (1 - z^2)^{\frac{d-3}{2}} \) is the density of distribution of \( \frac{\mathbf{x}^T \mathbf{e}_1}{\sqrt{d}} \), where \( \mathbf{x} \sim \tau_{d-1,1} \), so

\[
\int_{-1}^{1} (1 - z^2)^{k + \frac{d-3}{2}} f(k)(z) dz = \mathbb{E} \left[ f(k) \left( \frac{\mathbf{x}^T \mathbf{e}_1}{\sqrt{d}} \right) \left( 1 - \frac{(\mathbf{x}^T \mathbf{e}_1)^2}{d} \right)^k \right]
\]

\[
\to f(k)(0) \quad \text{(40)}
\]

where the last step follows from dominated convergence theorem, due to the assumption that \( f(z) \in C^\infty[-1, 1] \). Therefore, we get \( \mu_{k,d} \to \frac{f^{(k)}(0)}{k!} \).

Then we analyze the general case: \( f(z) \in C^\infty[-\nu, \nu] \), for some \( \nu \in (0, 1] \). To utilize the results for \( \nu = 1 \), we need the following truncation argument. For any \( \epsilon \in (0, 1] \) and \( k \), it holds that

\[
\sqrt{N_k} \int_{-\sqrt{d}}^{\sqrt{d}} \left| f\left( \frac{x}{\sqrt{d}} \right) q_k(x) I_{|x|/\sqrt{d} \geq \epsilon} \right| \tau_{d-1,1}(dx) = \sqrt{N_k} \mathbb{E}_{Z} \left| f(Z) q_k(\sqrt{d}Z) I_{|Z| \geq \epsilon} \right|
\]

\[
\leq \sqrt{N_k} C_m^2 \mathbb{P}(|Z| \geq \epsilon)
\]

\[
\leq \sqrt{d} k (1 - \epsilon^2)^{-\frac{d-3}{2}}
\]

\[
\text{(41)}
\]
where \( Z \sim \frac{\mathbf{x}^T \mathbf{e}_1}{\sqrt{d}}, \mathbf{x} \sim \tau_{d-1} \) and in (a), we use Cauchy-Schwarz inequality, with \( \mathbb{E}q_k(\sqrt{d}Z)^2 = 1 \) and \( f(z) \leq C_f \). Clearly, in (41), \( \sqrt{d^k(1 - \varepsilon^2)^{\frac{d-3}{2}}} \to 0 \) as \( d \to \infty \), so this implies that for any \( \varepsilon \in (0, 1] \) and \( k \), as \( d \to \infty \),

\[
\sqrt{N_k} \int_{-\sqrt{d}}^{\sqrt{d}} |f(\frac{t}{\sqrt{d}}) - \tilde{f}(\frac{t}{\sqrt{d}})| \cdot |q_k(x)| \cdot \tau_{d-1,1}(dx) \to 0,
\]

where \( \tilde{f}(z) = f(z)\mathbb{1}_{|z| \leq \varepsilon} \). From (42) we conclude that for any bounded function \( r(z) \) on \([-1, 1]\), if for some \( \varepsilon \in (0, 1] \), \( r(z) = f(z) \) on \([\frac{\varepsilon}{2}, \varepsilon]\), then as \( d \to \infty \)

\[
|m_{\mu,k,d} - m_{\mu,k}d| \to 0,
\]

where \( m_{\mu,k,d}(r) := \sqrt{N_k} \int_{-\sqrt{d}}^{\sqrt{d}} r(\frac{t}{\sqrt{d}})q_k(x)\tau_{d-1,1}(dx) \).

In light of (43) and the results we have established for the smooth functions [c.f. (40)], it remains to choose a proper smoothed approximation of \( f(z) \) on \([-1, 1]\), which agrees with \( f(z) \) in some neighborhood of 0. One such choice is:

\[
\tilde{f}(z) := \int f(z - t)\mathbb{1}_{|z - t| \leq \varepsilon} \cdot m_\varepsilon(t) dt,
\]

where \( \varepsilon = \frac{1}{3} \min\{\varepsilon, 1 - \varepsilon\} \) and \( m_\varepsilon(t) = \frac{1}{\varepsilon} m(\frac{t}{\varepsilon}) \), with

\[
m(s) = \begin{cases} ce^{-\frac{1}{s^{1-\varepsilon}}} & |s| < 1 \\ 0 & |s| \geq 1 \end{cases}
\]

and \( c \) is a normalizing constant such that \( \int m(s) ds = 1 \). It can be directly verified that \( \tilde{f}(z) \in C^\infty[-1, 1] \) and \( \tilde{f}(z) = f(z) \), when \( |z| \leq \varepsilon - \varsigma \). Then applying (43) and (40), we obtain that

\[
\mu_{\mu,k,d} \to \mu_{\mu,k,d}(\tilde{f}) := \sqrt{N_k} \int_{-\sqrt{d}}^{\sqrt{d}} \tilde{f}(\frac{t}{\sqrt{d}})q_k(x)\tau_{d-1,1}(dx) \to \frac{\tilde{f}(k)(0)}{k!} = \frac{f(k)(0)}{k!}.
\]

\[\Box\]

**Lemma 2** For any \( k \geq 0 \), as \( d \to \infty \)

\[
\alpha_{\mu,k,d} \to \alpha_k = \int g(x)H_k(x)\tau_G(dx)
\]

where \( H_k(x) \) is the degree-k Hermite polynomial and \( \tau_G \) denotes the standard Gaussian measure. Also for any \( \varepsilon > 0 \), there exists \( L \in \mathbb{Z}^+ \) and \( C > 0 \), such that for any large enough \( d \),

\[
\mathbb{E}g_{>L,i}^2 = \sum_{k=L+1}^{\infty} \alpha_{\mu,k,d}^2 < \varepsilon
\]

and

\[
\mathbb{P}\left(\frac{1}{n}\|g_{>L}\|^2 > \varepsilon\right) \leq \frac{C}{ne^{\varepsilon^2}},
\]

where \( g_{>L,i} \) is the \( i \)th coordinate of \( g_{>L} \), \( i \in [n] \).
Proof From (34), we get for any fixed \( j \in \mathbb{Z}^+ \), there exists \( C_j > 0 \) such that for any \( d \in \mathbb{Z}^+ \),

\[
|E_{\tau_{d-1,1}} X_j^d - E_{\tau_d} X_j^d| \leq \frac{C_j}{d}.
\]

(44)

Also by Assumption (A.4), \( g(x) \leq C_g (1 + |x|^{K_g}) \), so there exists \( C > 0 \) such that

\[
\lim_{R \to \infty} \sup_{d \in \mathbb{Z}^+} E_{\tau_{d-1,1}} [g(X)^2 1_{X \geq R}] \leq \lim_{R \to \infty} \sup_{d \in \mathbb{Z}^+} E_{\tau_{d-1,1}} \left( C_g^2 (1 + |X|^{K_g})^2 1_{X \geq R} \right)
\]

\[
\leq \lim_{R \to \infty} \sup_{d \in \mathbb{Z}^+} \left( C_g^4 (1 + |X|^{K_g})^4 + \frac{C}{d} \right) \cdot E_{\tau_{d-1,1}} 1_{X \geq R}
\]

\[
= \lim_{R \to \infty} \sup_{d \geq R^2} \left( C_g^4 (1 + |X|^{K_g})^4 + \frac{C}{d} \right) \cdot E_{\tau_{d-1,1}} 1_{X \geq R}
\]

\[
= 0
\]

where in the last step, we use the fact that \( \tau_{d-1,1} \) converges weakly to \( \tau_G \), as \( d \to \infty \). By Lemma C.5 in Cheng and Singer (2013), we have

\[
\int g(x)^2 |\tau_{d-1}(x) - \tau_G(x)| dx \to 0.
\]

Then by Lemma C.1 in Cheng and Singer (2013), we get for any fixed \( k \geq 0, \alpha_{k,d} \to \alpha_k \) and by Lemma C.2 in Cheng and Singer (2013), for any \( \varepsilon > 0 \), there exists a fixed \( L \in \mathbb{Z}^+ \) such that for any large enough \( d \) and \( i \in [n] \), \( \mathbb{E} g_{L,i}^2 = \sum_{k=L+1}^{\infty} \alpha_{k,d}^2 < \varepsilon \). Then

\[
\mathbb{P}\left( \frac{1}{n} \| g_{\leq L} \|^2 > \varepsilon \right) \leq \mathbb{P}\left( \frac{1}{n} \left( \| g_{\leq L} \|^2 - \mathbb{E}\| g_{\leq L} \|^2 \right) > \frac{\varepsilon}{2} \right)
\]

\[
\leq \frac{4 \text{Var}(g_{\leq L,i}^2)}{n \varepsilon^2}
\]

\[
\leq C_1 \frac{\mathbb{E} g_{i}^4 + \mathbb{E} g_{\leq L,i}^4}{n \varepsilon^2}
\]

\[
\leq C_2 \frac{1}{n \varepsilon^2},
\]

where \( C_1, C_2 \) are two constants and in the last step, we use \( \mathbb{E} g_i^4, \mathbb{E} g_{\leq L,i}^4 < \infty \), which follows from Assumption (A.4) and (44).

\[\Box\]

Appendix C. Spectral Norm Bounds

The following is a concentration result for the spectral norm of kernel matrix.

Lemma 3 Let \( Y = [y_1, y_2, \ldots, y_n] \) be a matrix with \( n \) independent rows \( \{y_i\}_{i=1}^n \) satisfying \( \mathbb{E} y_i = 0 \) and \( \mathbb{E} y_i y_i^\top = I_N \) and \( \|y_i\|^2 = N \). For any \( t > 0 \), we have

\[
\mathbb{P}\left( \frac{1}{n} Y Y^\top > 1 + t \right) \leq 2N \exp \left( - \frac{\delta}{8} \min\{t^2, t\} \right)
\]

(45)
where \( \delta = n/N \). Also there exists \( c > 0 \) such that for \( \delta \geq (\log N)^2 \)

\[
P(\lambda_{\min}(\frac{1}{n}Y^T Y) \leq 1/2) \leq c \exp(- (\log N)^2/c).
\] (46)

**Proof** Since \( \|\frac{1}{n}YY^T\| = \|\frac{1}{n}Y^T Y\| \), it is equivalent to prove all the results for the sample covariance matrix \( \frac{1}{n}Y^T Y \). Denote \( X_i = \frac{1}{n}(y_i y_i^T - I) \). We have

\[
\|X_i\| \leq \frac{1}{n}(\|y_i y_i^T\| + \|I\|) = \frac{N + 1}{n}
\]

and

\[
\|\sum_{i=1}^n E X_i^2\| = \frac{1}{n^2} \|\sum_{i=1}^n E(y_i y_i^T - I)\|^2 = \frac{1}{n^2} n(n(N - 1)I) = \frac{N - 1}{n}.
\]

By matrix Bernstein’s inequality (Vershynin, 2018, Theorem 5.4.1), for any \( t > 0 \)

\[
P\left(\|\frac{1}{n}Y^T Y - I\| \geq t\right) = P\left(\|\sum_{i=1}^n X_i\| \geq t\right)
\leq 2N \exp\left(- \frac{t^2}{4n^2 N(1 + t)}\right)
\leq 2N \exp\left(- \frac{\delta}{8} \min\{t^2, t\}\right).
\] (47)

Therefore, for any \( t > 0 \),

\[
P\left(\|\frac{1}{n}Y^T Y\| \geq 1 + t\right) \leq P\left(\|\frac{1}{n}Y^T Y - I\| \geq t\right)
\leq 2N \exp\left(- \frac{\delta}{8} \min\{t^2, t\}\right)
\]

which proves (45). Finally, since \( \lambda_{\min}(\frac{1}{n}Y^T Y) \geq 1 - \|\frac{1}{n}Y^T Y - I\| \),

\[
P(\lambda_{\min}(\frac{1}{n}Y^T Y) \leq 1/2) \leq P(\|\frac{1}{n}Y^T Y - I\| \geq 1/2)
\leq 2N \exp\left(- \frac{\delta}{87}\right)
\]

where we use (47). Therefore, when \( \delta \geq (\log N)^2 \), \( P(\lambda_{\min}(\frac{1}{n}Y^T Y) \leq 1/2) \leq c \exp(- (\log N)^2/c) \), for some \( c > 0 \). 

**Lemma 4** There exists \( \tau > 0 \) such that

\[
\|R - \tilde{R}_{\leq K}\| \lesssim \frac{1}{\tau^2}\n\]

where \( \tilde{R}_{\leq K} = (\tilde{\lambda}I + K_{\leq K})^{-1} \) and \( \tilde{\lambda} := \lambda + \sum_{k > K} \mu_k \).

20
Proof By (72) in Ghorbani et al. (2021), for any fixed $k \in \mathbb{Z}^+$, there exists $C > 0$ such that for all large enough $d$,

$$
\mathbb{E}\|K_k - \mu_k I\| \leq C \left[ p^{3/2} n^{1/2p} \sqrt{n/d^k} + \left( \frac{p}{d^k} \right)^{1/p} \right] 
$$

(49)

where $p \in \mathbb{Z}^+$ need to satisfy $2p \leq -\log \left( \frac{Cn^p}{d^k} \right)$. Here we choose $p = 2K$. Since $n \asymp d^K$ by Assumption (A.1), when $k > K$, $2p \leq -\log \left( \frac{Cn^p}{d^k} \right)$ is satisfied for all large $d$. Then substituting $p = 2K$ in (49), we get there exists $C > 0$, such that for any fixed $k > K$ and large enough $d$,

$$
\mathbb{E}\|K_k - \mu_k I\| \leq C \left[ d^{-\frac{1}{2}(k-K)+\frac{1}{4}} + d^{-\frac{k-K}{2K}} \right]. 
$$

(50)

On the other hand, following the steps leading to (55) in Ghorbani et al. (2021), we can get for any $L \geq 2K+3$,

$$
\mathbb{E}\|K \geq L - \sum_{k \geq L} \mu_k I\|^2 \lesssim \frac{1}{d} 
$$

(51)

Combining (50) and (51), we can get there exists $\tau > 0$, such that

$$
\|K > K - \sum_{k > K} \mu_k I\| \lesssim \frac{1}{d^\tau}. 
$$

(52)

Therefore, combine (52) with the fact $\|\tilde{R} \leq K\|, \|R\| \leq \frac{1}{\lambda}$, we have

$$
\|R - \tilde{R} \leq K\| = \|\tilde{R} \leq K(K > K - \sum_{k > K} \mu_k I)R\|
\lesssim \frac{1}{d^\tau}. 
$$

Lemma 5 For any positive semi-definite matrix $M \in \mathbb{R}^{n \times n}$ satisfying

$$
1 \lesssim \lambda_{\min}(M) \leq \lambda_{\max}(M) \lesssim 1, 
$$

we have

$$
\left\| \frac{1}{\sqrt{n}} MY < K \right\| \lesssim 1 
$$

(54)

and

$$
\left\| (D_{< K}^2 + \frac{1}{n} Y_{< K}^\top M Y_{< K})^{-1} \right\| \lesssim 1. 
$$

(55)

Here, $\lambda_{\min}(\cdot)$ and $\lambda_{\max}(\cdot)$ are the smallest and largest eigenvalue of $M$ and

$$
D_{< K} := \text{diag}\{D_0, D_1, \ldots, D_{K-1}\}. 
$$

On the other hand, $(\lambda I + K_K)^{-1}$ and $(\lambda I + K > K)^{-1}$ both satisfy (53), for any $\lambda > 0$.
Proof Denote $R_K = (\lambda I + K_K)^{-1}$ and $R_{>K} = (\lambda I + K_{>K})^{-1}$. By Lemma 3, we have

$$\|\frac{1}{\sqrt{n}}MY_\prec K\| \lesssim 1,$$

so

$$\|\frac{1}{\sqrt{n}}MY_\prec K\| \lesssim 1$$

and we can also get $1 \lesssim \lambda_{\min}(R_K)$. On the other hand, by (46) we also have $1 \lesssim \lambda_{\min}(\frac{1}{n}Y_\prec K^TY_\prec K)$, since $n/N_\prec K \gtrsim \log(N_\prec K)^2$. As a result,

$$\|D^{-2} + \frac{1}{n}Y_\prec K^TY_\prec K\| \lesssim 1,$$

where the last step follows from $1 \lesssim \lambda_{\min}(R_K)$ and $1 \lesssim \lambda_{\min}(\frac{1}{n}Y_\prec K^TY_\prec K)$.

Finally, we verify that both $R_K$ and $R_{>K}$ satisfy (53). Clearly, $\lambda_{\max}(R_K), \lambda_{\max}(R_{>K}) \leq \frac{1}{\lambda} \lesssim 1$. On the other hand, since $\|\frac{1}{n}Y_\prec K^TY_\prec K\| \lesssim 1$ by Lemma 3 and $\delta_K \lesssim 1$, we get $1 \lesssim \lambda_{\min}(R_K)$. For $\lambda_{\min}(R_{>K})$, we can apply (52) and obtain that $\|K_{>K}\| \lesssim 2 \sum_{k>K} \mu_k \lesssim 1$, which implies that $1 \lesssim \lambda_{\min}(R_{>K})$. 

Appendix D. Auxiliary Results for Analyzing Training Error

Lemma 6 For any $I \subseteq \{0, 1, 2, \cdots\}$, we have $\|\sum_{k \in I} g_k\| \lesssim \sqrt{n}$. Also $\|z\| \lesssim \sqrt{n}$.

Proof Recall that $g_k = \frac{\alpha_k}{\sqrt{N_k}}Y_k^TY_k(\xi)$. By rotational invariance, we can assume that $\xi \sim \tau_{d-1}$. Therefore,

$$\mathbb{E}\|\sum_{k \in I} g_k\|^2 = \mathbb{E}\sum_{k \in I} \frac{\alpha_k^2}{N_k} \text{Tr}(Y_k^TY_k)$$

$$= n \sum_{k \in I} \alpha_k^2.$$

Since $\sum_{k=0}^{\infty} \alpha_k^2 \lesssim 1$, we get by Chebyshev’s inequality, $\|\sum_{k \in I} g_k\| \lesssim \sqrt{n}$. In a similar way, we can get $\|z\| \lesssim \sqrt{n}$.

Lemma 7 For any positive semidefinite matrix $M \in \mathbb{R}^{n \times n}$, we have

$$(\lambda I + K_\prec K + M)^{-1}Y_\prec K = R_M Y_\prec K(D^{-2}_\prec K + \frac{1}{n}Y_\prec K^TR_M Y_\prec K)^{-1} \cdot D^{-2}_\prec K,$$

where $R_M = (\lambda I + M)^{-1}$ and $D_K := \text{diag}\{D_0, D_1, \cdots, D_{K-1}\}$. 

22
Proof By the matrix inversion formula, we have
\[(\lambda I + K_{<K} + M)^{-1} = (\lambda I + \frac{1}{n}Y_{<K}D_{<K}^2Y_{<K}^T + M)^{-1}\]
\[= R_M - \frac{1}{n}R_MY_{<K}D_{<K}(I + \frac{1}{n}D_{<K}Y_{<K}^TR_MY_{<K}D_{<K})^{-1}D_{<K}Y_{<K}^TR_M\]
\[= R_M - \frac{1}{n}R_MY_{<K}(D_{<K} - \frac{1}{n}Y_{<K}^TR_MY_{<K})^{-1}Y_{<K}^TR_M.\]

Note that due to Assumption (A.3), \(D_{<K}^{-2}\) is well-defined. Then
\[\left(\lambda I + K_{<K} + M\right)^{-1}Y_{<K} = R_MY_{<K}[I - (D_{<K}^2 - \frac{1}{n}Y_{<K}^TR_MY_{<K})^{-1}(\frac{1}{n}Y_{<K}^TR_MY_{<K})]\]
\[= R_MY_{<K}(D_{<K}^2 - \frac{1}{n}Y_{<K}^TR_MY_{<K})^{-1}D_{<K}^{-2}.\]

\[\square\]

Lemma 8 It holds that
\[\frac{1}{n}|y^T\tilde{R}_{\leq K}y - (g_{\geq K}^T + z^T)\tilde{R}_{\leq K}(g_{\geq K} + z)| \lessapprox \frac{1}{d}.\] (57)
where \(\tilde{R}_{\leq K} = (\tilde{\lambda}I + K_{\leq K})^{-1}\) and \(\tilde{\lambda} := \lambda + \sum_{k> K} \mu_k.\)

Proof We first show
\[\left|\frac{1}{\sqrt{n}}\tilde{R}_{\leq K}g_{<K}\right| \lessapprox \frac{1}{d}.\] (58)

By (56), we have
\[\frac{1}{\sqrt{n}}\tilde{R}_{\leq K}g_{<K} = \frac{1}{\sqrt{n}}\tilde{R}_{\leq K}Y_{<K}\tilde{Y}_{<K}(\xi)\]
\[= \frac{1}{\sqrt{n}}\tilde{R}_KY_{<K}(D_{<K}^{-2} + \frac{1}{n}Y_{<K}^T\tilde{R}_KY_{<K})^{-1}D_{<K}^{-2}\tilde{Y}_{<K}(\xi),\] (59)
where \(\tilde{R}_K = (\tilde{\lambda}I + K_K)^{-1}\) and \(\tilde{Y}_{<K}(\xi) = [\tilde{Y}_0(\xi)^T, \cdots, \tilde{Y}_{K-1}(\xi)^T]^T.\) Substituting (54) and (55) in Lemma 5 into (59), we have
\[\left|\frac{1}{\sqrt{n}}\tilde{R}_{\leq K}g_{<K}\right| \lessapprox \left\|\frac{1}{\sqrt{n}}\tilde{R}_KY_{<K}\right\| \cdot \left\|D_{<K}^{-2} + \frac{1}{n}Y_{<K}^T\tilde{R}_KY_{<K}\right\|^{-1} \cdot \left\|D_{<K}^{-2}\right\| \cdot \left\|\tilde{Y}_{<K}(\xi)\right\|\]
\[\lessapprox \frac{1}{d}\]
which is (58). Since
\[\frac{1}{n}|y^T\tilde{R}_{\leq K}y - (g_{\geq K}^T + z^T)\tilde{R}_{\leq K}(g_{\geq K} + z)|\]
\[= 2\left|\frac{1}{n}y^T\tilde{R}_{\leq K}g_{<K} + \frac{1}{n}g_{<K}^T\tilde{R}_{\leq K}g_{<K}\right|\]
and \(\frac{1}{\sqrt{n}}\|y\| \lessapprox 1, \frac{1}{\sqrt{n}}\|g_{<K}\| \lessapprox 1\) by Lemma 6, we can obtain (57), after applying (58) with Cauchy-Schwarz inequality. \[\square\]
Lemma 9 It holds that
\[
\frac{1}{n} |\langle g_{\geq K}^\top + z^\top, (\tilde{R}_K - \tilde{R}_{\leq K}) \cdot (g_{\geq K} + z) \rangle| \lesssim \frac{1}{\sqrt{d}}
\] (60)
where \( \tilde{R}_K = (\tilde{\lambda} I + K_{\geq K})^{-1} \) and \( \tilde{R}_{\leq K} = (\tilde{\lambda} I + K_{\leq K})^{-1} \), with \( \tilde{\lambda} := \lambda + \sum_{k > K} \mu_k \).

Proof By the matrix inversion formula,
\[
\tilde{R}_K - \tilde{R}_{\leq K} = \frac{1}{n} \tilde{R}_K Y_{< K} (D_{< K}^{-2} + \frac{1}{n} Y_{< K}^\top \tilde{R}_K Y_{< K})^{-1} Y_{< K}^\top \tilde{R}_K,
\]
so
\[
\frac{1}{n} \langle g_{\geq K}^\top + z^\top, (\tilde{R}_K - \tilde{R}_{\leq K}) \cdot (g_{\geq K} + z) \rangle
= \frac{1}{n^2} \langle g_{\geq K}^\top + z^\top, \tilde{R}_K Y_{< K} (D_{< K}^{-2} + \frac{1}{n} Y_{< K}^\top \tilde{R}_K Y_{< K})^{-1} Y_{< K}^\top \tilde{R}_K (g_{\geq K} + z) \rangle.
\] (61)
It remains to control \( \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K g_{\geq K} \|, \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K z \| \) and \( \| (D_{< K}^{-2} + \frac{1}{n} Y_{< K}^\top \tilde{R}_K Y_{< K})^{-1} \| \lesssim 1 \) in (61). First, by Lemma 5 we have \( \| (D_{< K}^{-2} + \frac{1}{n} Y_{< K}^\top \tilde{R}_K Y_{< K})^{-1} \| \lesssim 1 \). By the independence between \( \frac{1}{n} Y_{< K}^\top \tilde{R}_K \) and \( z \), we have \( \mathbb{E}_z \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K z \|^2 = \frac{1}{n^2} \text{Tr} (Y_{< K}^\top \tilde{R}_K^2 Y_{< K}) \). Meanwhile, using Lemma 5, we can get \( \frac{1}{n} \text{Tr} (Y_{< K}^\top \tilde{R}_K^2 Y_{< K}) \lesssim \frac{N_{< K}}{n} \lesssim \frac{1}{d} \). Hence, \( \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K z \| \lesssim \frac{1}{\sqrt{d}} \).

Finally, we show \( \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K g_{\geq K} \| \lesssim d^{-1/4} \). Recall that
\[
g_{\geq K} = \sum_{k \geq K} \frac{\alpha_k}{\sqrt{N_k}} Y_k Y_k(\xi)
\]
and by rotational invariance, we can assume that \( \xi \sim \tau_{d-1} \). Therefore, conditioning on \( X \) and taking expectation over \( \xi \sim \tau_{d-1} \), we have
\[
\mathbb{E}_\xi \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K g_{\geq K} \|^2 = \frac{1}{n^2} \text{Tr} \left[ (\tilde{R}_K Y_{< K} Y_{< K}^\top \tilde{R}_K) \cdot \left( \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^\top \right) \right]
\leq \frac{1}{n^2} \| \tilde{R}_K Y_{< K} Y_{< K}^\top \tilde{R}_K \|_F \cdot \| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^\top \|_F
= \frac{1}{n^2} \sqrt{\text{Tr} (Y_{< K}^\top \tilde{R}_K Y_{< K})^2} \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F
\leq \frac{1}{n^2} \sqrt{\sum_{k \geq K} \| Y_k Y_k^\top \|^2} \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F
\leq \frac{1}{n^2} \sqrt{N_{< K}} \| \frac{1}{n} Y_{< K} Y_{< K}^\top \| \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F,
\] (62)
where \( N_{< K} := \sum_{k=0}^{K-1} N_k \). The right-hand side of (62) can be controlled as follows. From (45), we can get
\[
\mathbb{P}(\| \frac{1}{n} Y_{< K} Y_{< K}^\top \| \geq 2) \leq 2N_{< K} \exp \left( - \frac{\delta_{< K}}{8} \right),
\]
and by rotational invariance, we can assume that \( \xi \sim \tau_{d-1} \). Therefore, conditioning on \( X \) and taking expectation over \( \xi \sim \tau_{d-1} \), we have
\[
\mathbb{E}_\xi \| \frac{1}{n} Y_{< K}^\top \tilde{R}_K g_{\geq K} \|^2 = \frac{1}{n^2} \text{Tr} \left[ (\tilde{R}_K Y_{< K} Y_{< K}^\top \tilde{R}_K) \cdot \left( \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^\top \right) \right]
\leq \frac{1}{n^2} \| \tilde{R}_K Y_{< K} Y_{< K}^\top \tilde{R}_K \|_F \cdot \| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^\top \|_F
= \frac{1}{n^2} \sqrt{\text{Tr} (Y_{< K}^\top \tilde{R}_K Y_{< K})^2} \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F
\leq \frac{1}{n^2} \sqrt{\sum_{k \geq K} \| Y_k Y_k^\top \|^2} \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F
\leq \frac{1}{n^2} \sqrt{N_{< K}} \| \frac{1}{n} Y_{< K} Y_{< K}^\top \| \cdot \| \sum_{k \geq K} \alpha_k^2 \frac{Y_k Y_k^\top}{N_k} \|_F,
\] (62)
where \( N_{< K} := \sum_{k=0}^{K-1} N_k \). The right-hand side of (62) can be controlled as follows. From (45), we can get
\[
\mathbb{P}(\| \frac{1}{n} Y_{< K} Y_{< K}^\top \| \geq 2) \leq 2N_{< K} \exp \left( - \frac{\delta_{< K}}{8} \right),
\]
where $\delta_{<K} = \frac{n}{N_{<K}}$. Also $\| \frac{1}{n} Y_{<K} Y^T_{<K} \| \leq \text{Tr} (\frac{1}{n} Y_{<K} Y^T_{<K}) = N_{<K}$. Therefore,

$$
E\| \frac{1}{n} Y_{<K} Y^T_{<K} \|^2 = E\| \frac{1}{n} Y_{<K} Y^T_{<K} \|^2_2 \| \frac{1}{n} Y_{<K} Y^T_{<K} \|_2 + E\| \frac{1}{n} Y_{<K} Y^T_{<K} \|^2_2 \| \frac{1}{n} Y_{<K} Y^T_{<K} \|_2 < 2 + E\| \frac{1}{n} Y_{<K} Y^T_{<K} \|^2_2 I \| \frac{1}{n} Y_{<K} Y^T_{<K} \|_2 < 2 \leq N_{<K}^2 \exp(-\delta_{<K}^K) + 4 
$$

(63)

where in the second step, we use the deterministic bound $\| \frac{1}{n} Y_{<K} Y^T_{<K} \| \leq \frac{1}{n} \text{Tr} (Y_{<K} Y^T_{<K}) = N_{<K}$ and in the last step we use the fact that $N_{<K} \leq d^{K-1}$ and $\delta_{<K} \geq d$. On the other hand, $\| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y^T_k \|_F$ can be controlled as:

$$
E\| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y^T_k \|^2_2 = \sum_{k,\ell \geq K} \frac{\alpha_k^2 \alpha_\ell^2}{N_k N_\ell} \text{Tr} [Y^T_k Y_k Y^T_\ell Y_\ell] 
= \sum_{k,\ell \geq K} \frac{\alpha_k^2 \alpha_\ell^2}{N_k N_\ell} [N_k n + n(n-1)\delta_{k\ell}] N_\ell 
= n \sum_{k,\ell \geq K} \alpha_k^2 \alpha_\ell^2 + n(n-1) \sum_{k \geq K} \frac{\alpha_k^4}{N_k} 
\leq C_K n \cdot \left( \sum_{k \geq K} \alpha_k^2 \right)^2 
\lesssim n,
$$

(64)

where $C_K$ is a constant that only depends on $K$, in the second step, we use Lemma 12 of Ghorbani et al. (2021) and the second to last step follows from $N_k \gg n$, when $k > K$. Combining (62), (63) and (64), we can get

$$
E\| \frac{1}{n} Y^T_{<K} \tilde{R}_{Kg_{\geq K}} \|^2 = E_X E_\xi \| \frac{1}{n} Y^T_{<K} \tilde{R}_{Kg_{\geq K}} \|^2 
\leq \frac{1}{n \lambda^2} \frac{N_{<K} E\| \frac{1}{n} Y_{<K} Y^T_{<K} \|_2^2 \cdot E\| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y^T_k \|^2_2}{E_1} 
\lesssim \sqrt{\frac{N_{<K}}{n}} 
\lesssim d^{-1/2}.
$$

Then by Chebyshev’s inequality, we get $\| \frac{1}{n} Y^T_{<K} \tilde{R}_{Kg_{\geq K}} \| \lesssim d^{-1/4}$.

Substituting $\| \frac{1}{n} Y^T_{<K} \tilde{R}_{Kg_{\geq K}} \| \lesssim d^{-1/4}$, $\| \frac{1}{n} Y^T_{<K} \tilde{R}_{Kz} \| \lesssim d^{-1/2}$ and $\| (D_{<K}^{-2} + \frac{1}{n} Y^T_{<K} \tilde{R}_K Y_{<K})^{-1} \| \lesssim 1$ back to (61), we reach at the desired result. 

25
Appendix E. Proof of (30)

By (13) and (3), \( \hat{h}(x_{\text{new}}) \) can be written as

\[
\hat{h}(x_{\text{new}}) = f \left( \frac{x_{\text{new}}^\top X \right) \]

so we can get

\[
\mathbb{E}_{\text{new}} \left[ \mathbb{E}(y_{\text{new}} \mid x_{\text{new}}) \hat{h}(x_{\text{new}}) \right] = \mathbb{E}_{\text{new}} \left[ \mathbb{E}(y_{\text{new}} \mid x_{\text{new}}) f \left( \frac{x_{\text{new}}^\top X \right) \right]
\]

\[
= \mathbb{E}_{\text{new}} \left[ \left( \sum_{k=0}^{\infty} \frac{\alpha_k}{\sqrt{N_k}} Y_k(\xi)^\top Y_{\hat{h}}(x_{\text{new}}) \right) \cdot \left( \sum_{k=0}^{\infty} \frac{\mu_k}{N_k} Y_k(x_{\text{new}})^\top Y_k^\top \right) \right]
\]

\[
= \frac{1}{n} \tilde{g}^\top \tilde{R} y,
\]

where \( \tilde{g} = \sum_{k=0}^{\infty} \mu_k \delta_k g_k \) and in the second step we use the expansion of \( g(\cdot) \) and \( f(\cdot) \) under spherical harmonics. Comparing (66) and (15), we can see that \( \mathbb{E}_{\text{new}}[\mathbb{E}(y_{\text{new}} \mid x_{\text{new}}) \hat{h}(x_{\text{new}})] \) takes a similar form as \( \mathcal{E}_{\text{train}} \). We will apply a similar proof strategy here.

First, consider the truncation of \( y \): \( \hat{y} = \sum_{k=0}^{L} g_k + z \), where \( L \geq K \) is some constant to be chosen. The next result shows that \( \frac{1}{n} \tilde{g}^\top \tilde{R} \hat{y} \) can be approximated by dropping the low-degree and high-degree terms in the expansions of \( K(\cdot, \cdot) \) and \( g(\cdot) \).

**Proposition 2** There exists \( \tau > 0 \) such that

\[
\left| \frac{1}{n} \tilde{g}^\top \tilde{R} \hat{y} - \left( \sum_{k<K} \alpha_k^2 + \frac{1}{n} \tilde{g}_K^\top \tilde{R}_K \tilde{y}_{\geq K} \right) \right| \lesssim \frac{1}{d^\tau}
\]

where \( \tilde{g}_k = \mu_k \delta_k g_k \), \( \tilde{y}_{\geq K} = \sum_{k=K}^{L} g_k + z \) and \( \tilde{R}_K = (\tilde{\lambda} I + K)^{-1} \), with \( \tilde{\lambda} = \lambda + \sum_{k>K} \mu_k \).

**Proof** We make the following decomposition of \( \frac{1}{n} \tilde{g}^\top \tilde{R} \hat{y} \):

\[
\frac{1}{n} \tilde{g}^\top \tilde{R} \hat{y} = \sum_{k<K} \alpha_k^2 + \frac{1}{n} \tilde{g}_K^\top \tilde{R}_K \tilde{y}_{\geq K} + \frac{1}{n} \tilde{g}_{>K}^\top \tilde{R} \hat{y} + \left( \frac{2}{n} \tilde{g}_{>K}^\top \tilde{R} g_{<K} - \sum_{k<K} \alpha_k^2 \right) + \left( -\frac{2}{n} \tilde{g}_{<K}^\top \tilde{R} \hat{y}_{\geq K} + \frac{1}{n} \tilde{g}_K^\top \tilde{R}_K \hat{y}_{\geq K} \right) + \frac{1}{n} \tilde{g}_K^\top (\tilde{R} - \tilde{R}_K) \hat{y}_{\geq K}.
\]

The last four terms correspond to the approximation error. In Lemma 10-Lemma 13, we show they all decay to 0 with rate no slower than \( \frac{1}{d^\tau} \) for some \( \tau > 0 \), so we prove the desired result.

By Proposition 2, it boils down to compute \( \frac{1}{n} \tilde{g}_K^\top \tilde{R}_K \hat{y}_{\geq K} \). To this end, we are back to the setting in Sec. 3.2.1. Similar as obtaining (25), we can get

\[
\frac{1}{n} \tilde{g}_K^\top \tilde{R}_K \hat{y}_{\geq K} = \frac{1}{n} \mu_K \delta_K \tilde{g}_K^\top \tilde{R}_K \left( \sum_{k=K}^{L} g_k + z \right)
\]

\[
\Rightarrow \mathbb{P} \left[ \frac{\mu_K \delta_K \alpha_k^2 \tilde{R}_K}{1 + \mu_K \delta_K \tilde{R}_K} \right]
\]

26
where $\hat{R}_K = \frac{\text{Tr} [\dot{M} + \mu_K \dot{Y}_K(V)Y_K(V)^T]^{-1}}{n}$ is defined in a completely analogous way as in (25) and the only difference is that $\dot{\lambda}$ is replaced by $\dot{\lambda}$ here. Finally, by the same proof of Theorem 1 in Lu and Yau (2022), we can get $\hat{R}_K \overset{P}{\to} R_*$. Therefore, for any $L \geq K$,

$$
\frac{1}{n} \tilde{g}^\top R \tilde{g} \overset{P}{\to} \sum_{k<K} \alpha_k^2 + \frac{\mu_K \delta_k \alpha_k^2 R_*}{1 + \mu_K \delta_k R_*},
$$

(67)

The final step is to show the approximation error $|\frac{1}{n} \tilde{g}^\top R (y - \hat{y})|$ can be made arbitrarily small. Indeed, by Lemma 2, for any $\varepsilon > 0$, there exists $L \geq K$ and $C > 0$ such that for all large enough $d$, $P(\frac{1}{n} \|y - \hat{y}\|^2 > \varepsilon) \leq \frac{C}{n^2 \varepsilon^2}$. Also from (91) in the proof of Lemma 12, we have $\frac{1}{\sqrt{n}} \|R\hat{g}_{<K}\| \leq 1$ and from Lemma 6 with the fact that $\delta_k \leq 1$, for $k \geq K$, we can get $\frac{1}{\sqrt{n}} \|R\hat{g}_{\geq K}\| \leq 1$. These together imply that for any $\varepsilon > 0$, there exists $L \geq K$ and $C > 0$ such that for all large enough $d$,

$$
P(\frac{1}{n} \tilde{g}^\top R (y - \hat{y}) > \varepsilon) \leq \frac{C}{n^2 \varepsilon^2}.
$$

(68)

Combining (68), (67) and (66), we get

$$
\mathbb{E}_{\text{new}}[y_{\text{new}} \hat{h}(x_{\text{new}})] = \frac{1}{n} \tilde{g}^\top R y \overset{P}{\to} \sum_{k<K} \alpha_k^2 + \frac{\mu_K \delta_k \alpha_k^2 R_*}{1 + \mu_K \delta_k R_*}.
$$

(69)

Appendix F. Proof of (31)

Recall that $\hat{h}(x_{\text{new}}) = f \left( \frac{x_{\text{new}}^\top X}{\sqrt{d}} \right) R y$ and for any $i, j \in [n],$

$$
\mathbb{E}_{\text{new}}[f \left( \frac{x_{\text{new}}^\top X}{\sqrt{d}} \right) f \left( \frac{x_{\text{new}}^\top x_i}{\sqrt{d}} \right)] = \mathbb{E}_{\text{new}}[\sum_{k=0}^{\infty} \frac{\mu_k}{N_k} Y_k(x_i^\top)Y_k(x_{\text{new}}) \times \sum_{k=0}^{\infty} \frac{\mu_k}{N_k} Y_k(x_{\text{new}})^\top Y_k(x_j)]
$$

$$
= \sum_{k=0}^{\infty} \frac{\mu_k^2}{N_k} Y_k(x_i)^\top Y_k(x_j).
$$

Therefore, we can get

$$
\mathbb{E}_{\text{new}} \hat{h}(x_{\text{new}})^2 = \mathbb{E}_{\text{new}} \left[ y^\top R f \left( \frac{X_{\text{new}}^\top X}{\sqrt{d}} \right) f \left( \frac{X_{\text{new}}^\top X}{\sqrt{d}} \right) R y \right]
$$

$$
= \frac{1}{n} y^\top R \left( \sum_{k=0}^{\infty} \mu_k \delta_k K_k \right) R y,
$$

(70)

where $K_k = \frac{\mu_k}{N_k} Y_k Y_k^\top$ and $\delta_k = n/N_k$.

Similar as before, the first step is to apply a truncation argument to simplify the right hand-side of (70). Specifically, by Lemma 14, we have

$$
\left| \frac{1}{n} y^\top R \left( \sum_{k=0}^{\infty} \mu_k \delta_k K_k \right) R y - \left[ \sum_{k=0}^{K-1} \alpha_k^2 + \frac{1}{n} y^\top R (\mu_K \delta_K K_K) R y \right] \right| \leq \frac{1}{\sqrt{d}}.
$$

(71)
This shows that all the high-degree components of kernel function can be neglected. while the low-degree components can be equivalent to a single constant \( \sum_{k=0}^{K-1} \alpha_k^2 \). Based on (71), the remaining task is to compute \( \frac{1}{n} y^T R(\mu K \delta K K_K) R y \). To this end, we introduce the following function:

\[
\Gamma_d(\epsilon) = \frac{1}{n} y^T (\lambda I + K + \epsilon \mu K \delta K K_K)^{-1} y, \quad (72)
\]

where \( \epsilon \in [-\epsilon_0, \epsilon_0] \), with \( \epsilon_0 = \frac{1}{2}(\mu K \delta K)^{-1} \). It can be directly checked that

\[
\Gamma_d'(0) = -\frac{1}{n} y^T (\mu K \delta K K_K) R y, \quad (73)
\]

so in order to compute \( \lim_{d \to \infty} \frac{1}{n} y^T R(\mu K \delta K K_K) R y \), it suffices to compute \( \lim_{d \to \infty} \Gamma_d'(0) \). Also \( \Gamma_d(\epsilon) \) is well-defined for \( \epsilon \in [-\epsilon_0, \epsilon_0] \), because \( K + \epsilon \mu K \delta K K_K \succeq 0 \) for any \( \epsilon \in [-\epsilon_0, \epsilon_0] \). In addition, since \( \mu K \in (0, \infty) \) and \( \delta K \in (0, \infty) \) under our main assumptions, we have \( 0 < \epsilon_0 \leq C_0 \), for some \( C_0 \) not depending on \( d \).

From (72) we can find that \( \Gamma_d(\epsilon) \) takes the same form as \( \hat{\xi}_{\text{train}} \) [c.f. (15)]. Therefore, repeating the same procedure in proving (6), we can obtain

\[
\Gamma_d(\epsilon) \overset{p}{\to} \frac{\alpha_k^2 R(\tilde{\lambda}, \epsilon)}{1 + \delta K \mu K (1 + \epsilon \mu K \delta K) R(\tilde{\lambda}, \epsilon)} + \left( \sigma_k^2 + \sum_{k > K} \alpha_k^2 \right) R(\tilde{\lambda}, \epsilon) := \Gamma(\epsilon), \quad (74)
\]

where \( R(\tilde{\lambda}, \epsilon) \) is the unique non-negative solution of

\[
\frac{1}{\tilde{R}} = \tilde{\lambda} + \frac{\mu K (1 + \epsilon \mu K \delta K)}{1 + \delta K \mu K (1 + \epsilon \mu K \delta K)} \tilde{R}. \quad (75)
\]

Note that (75) is a quadratic equation. For any fixed \( \tilde{\lambda} > 0 \), it allows for an explicit solution:

\[
R(\tilde{\lambda}, \epsilon) = R(\tilde{\lambda}; \mu K (1 + \epsilon \mu K \delta K), \delta K), \quad \text{where } R(\tilde{\lambda}; \mu, \delta) \text{ is defined in (8).} \]

It can be directly verified that \( R(\tilde{\lambda}, \epsilon) \) is smooth with respect to \( \epsilon \). In particular, we can compute its partial derivative with respect to \( \epsilon \) at 0:

\[
R'(\epsilon)(\tilde{\lambda}, 0) = -\frac{1}{\theta - 1}, \quad (76)
\]

where \( \theta = \frac{(1 + \mu K \delta K R_s)^2}{\delta K \mu K R_s^2} \). For notational simplicity, in the following, we denote by \( R'_{\epsilon=0} \) := \( R'(\tilde{\lambda}, 0) \). On the other hand, since \( R(\tilde{\lambda}, \epsilon) \) is smooth, \( \Gamma(\epsilon) \) in (74) is also smooth with respect to \( \epsilon \) and

\[
\Gamma'(0) = \frac{\alpha_k^2 R'_{\epsilon=0}}{[1 + \delta K \mu K R_s]^2} - \frac{(\delta K \mu K \alpha K R_s)^2}{(1 + \delta K \mu K R_s)^2} + \left( \sigma_k^2 + \sum_{k > K} \alpha_k^2 \right) R'_{\epsilon=0}, \quad (77)
\]

The next step is to show that \( \Gamma_d'(0) \overset{p}{\to} \Gamma'(0) \). Denote \( R(\epsilon) := [\lambda I + K + \epsilon (\mu K \delta K K_K)]^{-1} \). It can be directly verified that

\[
\Gamma_d'(\epsilon) = \frac{2}{n} y^T R(\epsilon) \cdot (\mu K \delta K K_K) \cdot R(\epsilon) \cdot (\mu K \delta K K_K) \cdot R(\epsilon) y \geq 0,
\]

so \( \Gamma_d(\epsilon) \) is a convex function. Therefore, for any \( \epsilon \in (-\epsilon_0, \epsilon_0) \) and \( \varsigma \in [0, (\epsilon_0 - |\epsilon|)/2] \),

\[
\frac{\Gamma_d(\epsilon - \varsigma) - \Gamma_d(\epsilon)}{-\varsigma} - \Gamma'(\epsilon) \leq \frac{\Gamma_d(\epsilon + \varsigma) - \Gamma_d(\epsilon)}{\varsigma} - \Gamma'(\epsilon), \quad (78)
\]
On the other hand, since \( \Gamma(\epsilon) \) is smooth, for any \( \varrho > 0 \), there exists \( c > 0 \) such that for any \( \varsigma \in [-c, c] \), it holds that \(|\epsilon| + |\varsigma| < \epsilon_0\) and

\[
\left| \Gamma'(\epsilon) - \frac{\Gamma(\epsilon + \varsigma) - \Gamma(\epsilon)}{\varsigma} \right| \leq \frac{\varrho}{2}.
\]

Combining (78) and (79), we have for any \( \varsigma \in [-c, c] \),

\[
\frac{\Gamma_d(\epsilon - \varsigma) - \Gamma(\epsilon - \varsigma)}{-\varsigma} = \frac{\Gamma_d(\epsilon) - \Gamma(\epsilon)}{\varrho} \leq \frac{\Gamma_d'(\epsilon) - \Gamma'(\epsilon)}{-\varsigma} \leq \frac{\Gamma(\epsilon + \varsigma) - \Gamma(\epsilon + \varsigma)}{\varsigma} + \frac{\varrho}{2}.
\]

Since \( \Gamma_d(\epsilon) \to \Gamma(\epsilon) \) for any \( \epsilon \in (-\epsilon_0, \epsilon_0) \), taking \( d \to \infty \) in (80), we get

\[
P(\left| \Gamma_d'(\epsilon) - \Gamma'(\epsilon) \right| > \varrho) \to 0.
\]

Moreover, here \( \varrho > 0 \) can be made arbitrarily small, so setting \( \epsilon = 0 \), we prove

\[
\Gamma_d'(0) \xrightarrow{P} \Gamma'(0).
\]

Finally, putting (70), (71), (73), (77) and (81) together, we reach at:

\[
\mathbb{E}_{\text{new}} \hat{h}(\mathbf{x}_{\text{new}})^2 \to P \sum_{k<K} \alpha_k^2 + \frac{(\delta_K \mu_K \alpha_K R_{\epsilon})^2}{(1 + \delta_K \mu_K R_{\epsilon})^2} - \frac{\alpha_K^2 R'_{\epsilon=0}}{(1 + \delta_K \mu_K R_{\epsilon})^2} - \left( \sigma_z^2 + \sum_{k>K} \alpha_k^2 \right) R'_{\epsilon=0},
\]

where \( R'_{\epsilon=0} = -\frac{1}{\varrho-1} \), which is defined in (76).

**Appendix G. Auxiliary Results for Analyzing Test Error**

**Lemma 10**  It holds that

\[
\left\| \frac{1}{\sqrt{n}} \tilde{g}_{> K} \right\| \lesssim \frac{1}{d}
\]

where \( \tilde{g}_{> K} := \sum_{k> K} \tilde{g}_k \), with \( \tilde{g}_k = \mu_k \delta_k g_k \).

**Proof**  Since \( \mathbb{E} \tilde{g}_k^2 g_k = \mathbb{E} \alpha^2_k \), we have

\[
\mathbb{E} \left\| \tilde{g}_{> K} \right\|^2 = \mathbb{E} \left\| \sum_{k> K} \mu_k \delta_k g_k \right\|^2
= n \sum_{k> K} \mu_k^2 \delta_k^2 \alpha_k^2
\leq n \delta_{K+1} \sum_{k> K} \mu_k^2 \alpha_k^2
\leq \frac{n}{d^2},
\]

where the last step follows from \( \sum_{k=0}^{\infty} \mu_k < \infty; \sum_{k=0}^{\infty} \alpha_k^2 < \infty \). Therefore, we have \( \left\| \tilde{g}_{> K} \right\| \lesssim \frac{\sqrt{n}}{d} \), which is the desired result.  \( \blacksquare \)
Lemma 11  It holds that
\[ \left| \frac{1}{n} \tilde{g}_<^T R g_< - \sum_{k<K} \alpha_k^2 \right| \lesssim \frac{1}{d} \tag{83} \]
where \( \tilde{g}_< = \sum_{k<K} \mu_k \delta_k g_k \).

**Proof** From Lemma 7,
\[ \frac{1}{n} D_{<K}^2 Y_<^T (\lambda I + K)^{-1} Y_< = (D_{<K}^2 + \frac{1}{n} Y_<^T R_{\geq K} Y_<)^{-1} (\frac{1}{n} Y_<^T R_{\geq K} Y_<) \]
\[ = I - (D_{<K}^2 + \frac{1}{n} Y_<^T R_{\geq K} Y_<)^{-1} D_{<K}^2. \]
Therefore,
\[ \frac{1}{n} \tilde{g}_<^T R g_< = \frac{1}{n} \tilde{Y}_< (\xi^T) D_{<K}^2 Y_<^T (\lambda I + K)^{-1} Y_< \tilde{Y}_<(\xi) \]
\[ = \sum_{k<K} \alpha_k^2 - \tilde{Y}_<(\xi^T) \left( (D_{<K}^2 + \frac{1}{n} Y_<^T R_{\geq K} Y_<)^{-1} D_{<K}^2 \tilde{Y}_<(\xi) \right). \tag{84} \]
By Lemma 5, we have \( \| (D_{<K}^2 + \frac{1}{n} Y_<^T R_{\geq K} Y_<)^{-1} \| \lesssim 1 \). Also we have \( \| D_{<K}^2 \| \lesssim \frac{1}{d} \).
Therefore,
\[ \left| \tilde{Y}_<(\xi^T) (D_{<K}^2 + \frac{1}{n} Y_<^T R_{\geq K} Y_<)^{-1} D_{<K}^2 \tilde{Y}_<(\xi) \right| \lesssim \frac{1}{d} \sum_{k<K} \alpha_k^2. \tag{85} \]
Combining (84) and (85) together with \( \sum_{k<K} \alpha_k^2 \lesssim 1 \) (which follows from Assumption (A.4)), we reach at (83).

Lemma 12  For any \( L \geq K \), it holds that
\[ \frac{1}{n} | \tilde{g}_<^T R \hat{y}_{\geq K} | \lesssim \frac{1}{\sqrt{d}} \tag{86} \]
and
\[ \frac{1}{n} | \tilde{g}_k^T R g_\leq | \lesssim \frac{1}{\sqrt{d}} \tag{87} \]
where \( \tilde{g}_k = \mu_k \delta_k g_k \), \( \hat{y}_{\geq K} = \sum_{k=K}^L g_k + z \) and \( R = (\lambda I + K)^{-1} \).

**Proof** In the following, we present the proof for (86). The proof for (87) is analogous and will be omitted for brevity.
To prove (86), it suffices to show for any fixed \( k \geq K \),
\[ \frac{1}{n} | \tilde{g}_<^T R g_k | \lesssim \frac{1}{\sqrt{d}} \tag{88} \]
and
\[ \frac{1}{n} | \tilde{g}_k^T R z | \lesssim \frac{1}{\sqrt{d}} \tag{89} \]
The second bound (89) is easy to obtain. By the independence between \( z \) and \( \tilde{g}^T K R \), we have

\[
\mathbb{E}_z (\tilde{g}^T K R z)^2 = \| R \tilde{g}_K \|^2. \tag{90}
\]

Since \( \tilde{g}_K = Y_K D_K^2 Y_K (\xi) \), we have

\[
\frac{1}{\sqrt{n}} \| R \tilde{g}_K \| = \frac{1}{\sqrt{n}} \| (\lambda I + K)^{-1} Y_K D_K^2 Y_K (\xi) \|
\]

\[
= \frac{1}{\sqrt{n}} \| R_{\geq K} Y_K (D_K^2 + \frac{1}{n} Y_K^T R_{\geq K} Y_K)^{-1} Y_K (\xi) \|
\]

\[
\lesssim 1,
\]

(91)

where the second step follows from Lemma 7 and the last step follows from Lemma 5 and the fact that \( \| Y_K (\xi) \| \lesssim 1 \). Then combining (90) and (91), we have

\[
\frac{1}{n} | \tilde{g}^T K R z | \lesssim \frac{1}{\sqrt{n}} \| R \tilde{g}_K \|
\]

\[
\lesssim \frac{1}{\sqrt{n}}
\]

which implies (89), since \( d \lesssim n \).

Now we analyze (88). Note that (88) can be equivalently expressed as:

\[
\frac{1}{n} \| \tilde{Y}_K (\xi)^T D_K Y_K^T R Y_K (\xi) \| \lesssim \frac{1}{\sqrt{n}}. \tag{92}
\]

Here \( \tilde{Y}_K (\xi) \) and \( \tilde{Y}_K (\xi) \) are independent of the sandwiched matrix \( D_K Y_K^T R Y_K \). However, the entries of \( \tilde{Y}_K (\xi) \) and \( \tilde{Y}_K (\xi) \) are not independent, although they are uncorrelated. The key to prove (92) is to handle the weak correlation among different entries of \( \tilde{Y}_K (\xi) \) and \( \tilde{Y}_K (\xi) \). As we know, there are different choices of the orthonormal basis \( \{ Y_k (\xi) \}_{k \geq 0} \), which are all equivalent. To ease our analysis, we will work with the following specific type of \( Y_k (\xi) \):

\[
Y_k (\xi) = [ Y_{k,S} (\xi)^T, Y_{k,\setminus S} (\xi)^T ]^T, \tag{93}
\]

where \( Y_{k,S}(\xi^T) \) is a \( (\xi^j) \)-dimensional vector and its entries are \( \{ v_k \xi_{i_1} \xi_{i_2} \cdots \xi_{i_k} \} \). Here, the normalizing constant \( \nu_k = \| \mathbb{E}(\xi^2_1 \xi^2_2 \cdots \xi^2_k) \|^{-\frac{1}{2}} \), with \( \xi \sim \tau_{d-1} \). It can be easily checked that when \( \xi \sim \tau_{d-1} \) and \( \{ i_1, i_2, \cdots, i_k \} \), \( \{ j_1, j_2, \cdots, j_k \} \) are two different sets of indices, it holds that \( \mathbb{E}(\xi_{i_1} \xi_{i_2} \cdots \xi_{i_k} : \xi_{j_1} \xi_{j_2} \cdots \xi_{j_k}) = 0 \). To see this, we first represent \( \xi \) by: \( \xi = \sqrt{d} \theta / \| \theta \| \), where \( \theta \sim \mathcal{N}(0, I_d) \). Since \( \{ i_1, i_2, \cdots, i_k \} \neq \{ j_1, j_2, \cdots, j_k \} \), there exists at least one \( u \in \{ j_1, j_2, \cdots, j_k \} \) such that \( u \notin \{ i_1, i_2, \cdots, i_k \} \). Then we have:

\[
\mathbb{E}[\xi_{i_1} \xi_{i_2} \cdots \xi_{i_k} : \xi_{j_1} \xi_{j_2} \cdots \xi_{j_k}] = \mathbb{E}\mathbb{E}[\xi_{i_1} \xi_{i_2} \cdots \xi_{i_k} : \xi_{j_1} \xi_{j_2} \cdots \xi_{j_k} | \{ \theta_j \}_{j \neq u}]
\]

\[
= \mathbb{E}\mathbb{E}\left[ \varphi\left( \{ \theta_j \}_{j \neq u} \right) \frac{\theta_u}{\sum_{j \neq u} \theta_j^2 + \theta_u^2} \right] | \{ \theta_j \}_{j \neq u}
\]

\[
= 0,
\]

31
where \( \varphi \) is a function of \( \{\theta_j\}_{j \neq u} \) and the last step follows from the fact that \( \theta_u \sim \mathcal{N}(0,1) \) and \( \varphi \left( \{\theta_j\}_{j \neq u} \right) \theta \rightarrow \frac{\varphi \left( \{\theta_j\}_{j \neq u} \right) \theta}{\sum_{j \neq u} \theta_j^2 + \theta^2} \) is an odd function, for any fixed \( \{\theta_j\}_{j \neq u} \). Therefore, we have \( \mathbb{E}[Y_{k,S}(\xi)Y_{k,S}(\xi)^\top] = I \).

In the following, we make use of the following notations: (i) for any \( X, Y_{<K,S}(X) := [Y_{0,S}(X), \ldots, Y_{K-1,S}(X)] \) and \( Y_{<K}\hspace{1pt}S(X) := [Y_{0\hspace{1pt}S}(X), \ldots, Y_{K-1\hspace{1pt}S}(X)] \), (ii) for any \( k, x, \tilde{Y}_{k,S}(x) := \frac{\alpha_k}{\sqrt{N_k}} Y_{k,S}(x) \) and \( \bar{Y}_{k,S}(x) := \frac{\alpha_k}{\sqrt{N_k}} Y_{k,S}(x) \). The proof of (92) will be done in two steps.

(I) The first step is to show the following,

\[
\frac{1}{\sqrt{n}} \left| \bar{Y}_{<K}(\xi^\top) MY_{k,S} \tilde{Y}_{k,S}(\xi) - \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right| \lesssim \frac{1}{\sqrt{d}}, \tag{94}
\]

where \( M = \frac{1}{\sqrt{n}} D_{<K}^2 Y_{<K,R}^T R \) and \( M_S = \frac{1}{\sqrt{n}} D_{<K,S}^2 Y_{<K,S,R}^T R \). Here, \( D_{<K} \) is the minor of \( D_{<K,S} \), corresponding to \( Y_{<K,S} \) (in other words, if \( I \subseteq \{1, 2, \ldots, \sum_{k=0}^{K-1} N_k\} \) is the set of all row indices of \( Y_{<K,S} \) in \( Y_{<K} \), then \( D_{<K,S} = (D_{<K,i,j})_{i,j \in I} \)). In fact, (94) states that after applying a truncation on \( Y_{k,S} \) and \( \bar{Y}_{k,S}(\xi) \), the resultant approximation error vanishes as \( d \rightarrow \infty \). Then the subsequent analysis can be done over \( \frac{1}{\sqrt{n}} \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \), which is easier to handle due to the symmetric structure of \( \bar{Y}_{k,S}(\xi) \).

We now prove (94). We have

\[
\begin{align*}
&\frac{1}{\sqrt{n}} \left| \bar{Y}_{<K}(\xi^\top) MY_{k,S} \tilde{Y}_{k,S}(\xi) - \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right| \\
\leq &\frac{1}{\sqrt{n}} \left| \bar{Y}_{<K}(\xi^\top) MY_{k,S} \tilde{Y}_{k,s}(\xi) - \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right| \\
&+ \frac{1}{\sqrt{n}} \left| \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) - \bar{Y}_{<K,S}(\xi^\top) M_S Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right| \\
= &\left| \bar{Y}_{<K,S}(\xi^\top) M_S \frac{1}{\sqrt{n}} Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right| + \left| \bar{Y}_{<K,S}(\xi^\top) M_S \frac{1}{\sqrt{n}} Y_{k,S,S} \tilde{Y}_{k,S}(\xi) \right|.
\end{align*}
\tag{95}
\]

Here, \( M_{\setminus S} \) is defined via the same way as \( M_S \). Next we show both terms on the right-hand side of (95) vanish as \( d \rightarrow \infty \). First, for any \( k \),

\[
\begin{align*}
\mathbb{E} \|Y_{k,S}(\xi)\|^2 &= \mathbb{E} \text{Tr} \left[ Y_{k,S}(\xi)Y_{k,S}(\xi)^\top \right] \\
&= N_k - \binom{d}{k} \\
&\lesssim N_{k-1},
\end{align*}
\]

where we have used the fact that \( N_k = \binom{d}{k} [1 + O(1/d)] \). Therefore, by Chebyshev’s inequality,

\[
\| \bar{Y}_{k,S}(\xi) \| = \frac{\alpha_k}{\sqrt{N_k}} \| Y_{k,S}(\xi) \| \\
\lesssim d^{-1/2}, \tag{96}
\]
Similarly, for any $k$, we can show $\|\frac{1}{\sqrt{n}} Y_{k, \mathcal{S}} \tilde{Y}_{k, \mathcal{S}} (\xi)\| \lesssim d^{-1/2}$ as follows. By the independence between $Y_{k, \mathcal{S}}$ and $Y_{k, \mathcal{S}} (\xi)$, we have

\[
E\|Y_{k, \mathcal{S}} Y_{k, \mathcal{S}} (\xi)\|^2 = \mathbb{E} \text{Tr} \left[ Y_{k, \mathcal{S}} Y_{k, \mathcal{S}} (\xi) Y_{k, \mathcal{S}} (\xi)^T Y_{k, \mathcal{S}}^T \right] \\
= \mathbb{E} \text{Tr} \left[ Y_{k, \mathcal{S}} Y_{k, \mathcal{S}}^T \right] \\
= n \left[ N_k - \binom{d}{k} \right].
\]

Therefore, similar as (96) we can get

\[
\|\frac{1}{\sqrt{n}} Y_{k, \mathcal{S}} \tilde{Y}_{k, \mathcal{S}} (\xi)\| \lesssim d^{-1/2}. \tag{97}
\]

On the other hand, by Lemma 7 we have

\[
M = \frac{1}{\sqrt{n}} D_{<K}^2 Y_{<K}^T R \\
= (D_{<K}^2 + \frac{1}{n} Y_{<K}^T R_{\geq K} Y_{<K})^{-1} (\frac{1}{\sqrt{n}} Y_{<K}^T R_{\geq K})
\]

and by Lemma 5, we have $\|M\| \lesssim 1$. Since $M_{\mathcal{S}}$ and $M_{\mathcal{S}} \mathcal{S}$ are both sub-matrices of $M$, we get

\[
\|M_{\mathcal{S}}\|, \|M_{\mathcal{S}} \mathcal{S}\| \leq \|M\| \lesssim 1. \tag{98}
\]

Now substituting (96), (97), (98) back to (95) and using Lemma 6, we reach at (94).

(II) In the second step, we are going to show

\[
\frac{1}{\sqrt{n}} \tilde{Y}_{<K, \mathcal{S}} (\xi)^T M_{\mathcal{S}} Y_{k, \mathcal{S}} \tilde{Y}_{k, \mathcal{S}} (\xi) \lesssim \sqrt{\frac{1}{d}}. \tag{99}
\]

By Lemma 3 and Lemma 5 we have

\[
\|\frac{1}{\sqrt{n}} M Y_k\| = \|D_{<K}^{-2} + \frac{1}{n} Y_{<K}^T R_{\geq K} Y_{<K})^{-1} (\frac{1}{\sqrt{n}} Y_{<K}^T R_{\geq K} \frac{1}{\sqrt{n}} Y_k)\| \\
\lesssim \sqrt{\frac{N_k}{n}}
\]
Since $M_SY_{k,S}$ is a sub-matrix of $MY_k$, we get $\| \frac{1}{\sqrt{n}} M_S Y_{k,S} \| \lesssim \sqrt{\frac{N_k}{n}}$. Now we have for any $k \geq K$,

$$
\frac{1}{\sqrt{n}} | \tilde{Y}_{K,S}(\xi^T)M_S Y_{k,S} \tilde{Y}_{k,S}(\xi) | \leq \sum_{t<K} \frac{1}{\sqrt{N_t N_k}} Y_{t,S}(\xi^T) \frac{1}{\sqrt{n}} M_{S,t} Y_{k,S} Y_{t,S}(\xi) \\
\lesssim \sum_{t<K} \frac{1}{\sqrt{N_t N_k}} \sqrt{N_t} \| \frac{1}{\sqrt{n}} M_{S,t} Y_{k,S} \|_F \\
\leq \sum_{t<K} \frac{1}{\sqrt{N_t N_k}} \sqrt{N_t} \| \frac{1}{\sqrt{n}} M_S Y_{k,S} \| \\
\lesssim \sum_{t<K} \sqrt{\frac{N_t}{n}} \\
\lesssim \frac{1}{\sqrt{d}}
$$

where (a) follows from (111) in Lemma 15 and in (b) we use $\| \frac{1}{\sqrt{n}} M_S Y_{k,S} \| \lesssim \sqrt{\frac{N_k}{n}}$.

Combining (94) and (99), we reach at (92). Hence, the proof of (88) is completed. 

Lemma 13  It holds that

$$
\frac{1}{n} | g_K^T (R - \tilde{R}_K) \hat{y}_{\geq K} | \lesssim \frac{1}{d^f}
$$

where $\tilde{g}_K = \mu_K \delta_K g_K$, $g_{\geq K} = \sum_{k \geq K} g_k$, $R = (\lambda I + K)^{-1}$ and $\tilde{R}_K = (\tilde{\lambda} I + K_{\leq K})^{-1}$, with $\tilde{\lambda} = \lambda + \sum_{k \geq K} \mu_k$.

Proof  We have the following decomposition:

$$
\frac{1}{n} | g_K^T (R - \tilde{R}_K) \hat{y}_{\geq K} | \leq \frac{1}{n} | g_K^T (R - \tilde{R}_{\leq K}) \hat{y}_{\geq K} | + \frac{1}{n} | g_K^T (\tilde{R}_{\leq K} - \tilde{R}_K) \hat{y}_{\geq K} |.
$$

Since $\delta_k \lesssim 1$, when $k \geq K$, it follows directly from Lemma 4 and Lemma 6 that $\frac{1}{n} | g_K^T (R - \tilde{R}_{\leq K}) \hat{y}_{\geq K} | \lesssim \frac{1}{d^f}$. On the other hand, following the same proof of Lemma 9, we get $\frac{1}{n} | g_K^T (\tilde{R}_{\leq K} - \tilde{R}_K) \hat{y}_{\geq K} | \lesssim \frac{1}{\sqrt{d}}$. Combining these two bounds together, we reach at the desired result.

Lemma 14  It holds that

$$
\left| \frac{1}{n} y^T R \left( \sum_{k=0}^{\infty} \mu_k \delta_k K_k \right) R y - \sum_{k=0}^{K-1} \alpha_k^2 + \frac{1}{n} y^T R (\mu_K \delta_K K_K) R y \right| \lesssim \frac{1}{\sqrt{d}}. \quad (100)
$$
Proof We first show some high-degree components can be discarded:

$$\left| \frac{1}{n} y^T \left( \sum_{k > K} \mu_k \delta_k K_k \right) R y \right| \lesssim \frac{1}{d}. \quad (101)$$

From (52) in the proof of Lemma 4, we have \( \| \sum_{k > K} K_k \| \lesssim 1 \). On the other hand, since \( \sup_{k \geq 0} \mu_k \leq f(\sqrt{d}) \lesssim 1 \) and \( \sup_{k > K} \delta_k \lesssim \frac{1}{d} \), we get \( \| \sum_{k > K} \mu_k \delta_k K_k \| \lesssim \frac{1}{d} \). Combine this bound with Lemma 6 and the fact that \( \| R \| \lesssim 1 \), we verify (101).

Next we show

$$\left| \frac{1}{n} y^T \left( \sum_{k > 0} K_k \right) R y \right| \lesssim \frac{1}{\sqrt{d}}. \quad (102)$$

To start, we rewrite \( \frac{1}{n} y^T \left( \sum_{k = 0}^{K-1} \mu_k \delta_k K_k \right) R y \) as:

$$\frac{1}{n} y^T \left( \sum_{k = 0}^{K-1} \mu_k \delta_k K_k \right) R y = \left( \frac{1}{n} R Y < K D^2 < K \right) \cdot \left( \frac{1}{n} D^2 < K R^T y < K \right). \quad (103)$$

The vector \( \phi \) defined on the right-hand side of (103) can be decomposed as:

$$\phi = \frac{1}{n} D^2 < K Y^T < K R g_k + \frac{1}{n} D^2 < K Y^T < K R y_k \lesssim K = Y < K (\xi) - (D^{-2} < K + \frac{1}{n} Y^T < K R y_k) Y < K \lesssim K = Y < K (\xi) - (D^{-2} < K Y^T < K R y_k) + \frac{1}{n} D^2 < K Y^T < K R y_k \lesssim K, \quad (104)$$

where \( Y_k (\xi) = \frac{\alpha_k}{\sqrt{\mu_k}} Y_k (\xi) \), \( R y_k \geq K = (\lambda I + K > K) \) and in reaching the second step we use Lemma 7. To proceed, let us analyze the norms of vectors \( Y < K (\xi), \phi_1 \) and \( \phi_2 \) on the right-hand side of (104). First,

$$\| \tilde{Y} < K (\xi) \|^2 = \sum_{k = 0}^{K-1} \alpha_k^2. \quad (105)$$

Also it is easy to verify \( \| \phi_1 \| \lesssim \frac{1}{d} \) as follows. From (52), we have \( \| K > K \| \lesssim 1 \). Then combine this with Lemma 5 we have \( \| (D^{-2} < K + \frac{1}{n} Y^T < K R > K Y < K) \| \lesssim 1 \). Also note that \( \| D^{-2} < K \| \lesssim \frac{1}{d} \) and \( \| \tilde{Y} < K (\xi) \|^2 = \sum_{k = 0}^{K-1} \alpha_k^2 < \infty \), so

$$\| \phi_1 \| \lesssim \frac{1}{d} \quad (106)$$

Lastly, let us show

$$\| \phi_2 \| \lesssim \frac{1}{\sqrt{d}} \quad (107)$$

Note that \( \phi_2 \) can be written as:

$$\phi_2 = \sum_{k > K} \Psi Y_k \tilde{Y}_k (\xi) + \Psi z$$
where $\Psi = \frac{1}{n} D_{<K}^2 Y_{<K}^T R$. Then
\[
\mathbb{E}_{\xi,z}\left\| \phi_2 \right\|^2 = \text{Tr} \left[ \Psi \left( \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^T \right) \Psi^T \right] + \sigma_z^2 \text{Tr} \left( \Psi \Psi^T \right). \tag{108}
\]

We first control the spectral norm of $\Psi$. From Lemma 7, we can get
\[
\Psi = \frac{1}{n} (D_{<K}^2 + \frac{1}{n} Y_{<K}^T R_{\geq K} Y_{<K})^{-1} Y_{<K}^T R_{\geq K}
\]
By Lemma 3, we have
\[
\mathbb{P}(\left\| \frac{1}{n} Y_{<K} Y_{<K}^T \right\| > 2) \leq 2 N_{<K} \exp \left( - \frac{n}{8N_{<K}} \right)
\]
\[
\leq c \exp(-d/c),
\]
for some $c > 0$ and we have already shown $\left\| (D_{<K}^2 + \frac{1}{n} Y_{<K}^T R_{\geq K} Y_{<K})^{-1} \right\| \lesssim 1$, so we get
\[
\left\| \Psi \right\| \lesssim \frac{1}{\sqrt{n}}. \tag{109}
\]
On the other hand, same as (52), we can show $\left\| \sum_{k > K} \frac{\alpha_k^2}{N_k} Y_k Y_k^T - \sum_{k > K} \frac{\alpha_k^2}{N_k} I \right\| \lesssim \frac{1}{d^\tau}$, for some $\tau > 0$, so combined with $\left\| \frac{\alpha_k^2}{N_k} Y_k Y_k^T \right\| \lesssim 1$, we can get
\[
\left\| \sum_{k \geq K} \frac{\alpha_k^2}{N_k} Y_k Y_k^T \right\| \lesssim 1. \tag{110}
\]
Combining (109) and (110) with (108), we get:
\[
\left\| \phi_2 \right\|^2 \lesssim \frac{N_{<K}}{n} \lesssim \frac{1}{d^\tau}.
\]
After combining (105), (106) and (107) with (104) and (103), we get (102). Finally, the proof is completed by combing (101) with (102).

**Appendix H. Concentration of a Quadratic Form**

**Lemma 15** For any finite integer $k, \ell \geq 0$, let
\[
F_{k,\ell}(x) = Y_{k,S}(x)^T M Y_{\ell,S}(x),
\]
where $Y_{k,S}$ is defined in (93), $x \sim \tau_{d-1}$ and $M \in \mathbb{R}^{m \times p}$ is a deterministic matrix, with $m = \binom{d}{k}$ and $p = \binom{d}{\ell}$. It holds that
\[
\mathbb{E}_{x} F_{k,\ell}(x)^2 \leq C_{k,\ell} \min\{N_k, N_\ell\} \left\| M \right\|_F^2, \tag{111}
\]
where $C_{k,\ell} > 0$ is some constant that only depends on $k$ and $\ell$. 

36
Proof. Note that since \( x \) can be represented as: \( x = \frac{\theta}{\|\theta\|/\sqrt{d}} \), where \( \theta \sim \mathcal{N}(0, I_d) \) and by concentration of norm of Gaussian vector [e.g., Theorem 3.1.1 in Vershynin (2018)], there exists \( c > 0 \), such that for any \( d \in \mathbb{Z}^+ \), \( \mathbb{P}(\|\theta\|/\sqrt{d} < 1/2) \leq c^{-d} \). Hence, for \( x = \frac{\theta}{\|\theta\|/\sqrt{d}} \sim \mathcal{N}(0, I_d) \), we can get
\[
Y_{k,S}(x)^\top MY_{\ell,S}(x) \lesssim Y_{k,S}(\theta)^\top MY_{\ell,S}(\theta).
\]
Therefore, it suffices to prove (111) for \( x \sim \mathcal{N}(0, I_d) \). In the following, we set \( x \sim \mathcal{N}(0, I_d) \). We will prove (111) by induction. When \( k = \ell = 0 \), we trivially have \( \mathbb{E}[Y_{0,S}(x)^\top MY_{0,S}(x)]^2 = M^2 \).

Now suppose we have shown for any \( M_1 \in \mathbb{R}^{m_1 \times p_1} \) and \( M_2 \in \mathbb{R}^{m_2 \times p_2} \), with \( m_1 = \binom{d}{k-1} \), \( p_1 = \binom{d}{k} \) and \( m_2 = \binom{d}{\ell} \) and \( p_2 = \binom{d}{\ell-1} \), it holds that
\[
\begin{align*}
\mathbb{E}[F_{k-1,\ell}(x)]^2 & \leq C_{k-1,\ell} \min\{N_{k-1}, N_{\ell}\} \|M_1\|_F^2, \quad \text{(112)} \\
\mathbb{E}[F_{k,\ell-1}(x)]^2 & \leq C_{k,\ell-1} \min\{N_k, N_{\ell-1}\} \|M_2\|_F^2. \quad \text{(113)}
\end{align*}
\]

Based on these two bounds, we are going to show for any \( M \in \mathbb{R}^{m \times p} \), with \( m = \binom{d}{k} \), \( p = \binom{d}{\ell} \),
\[
\mathbb{E}[F_{k,\ell}(x)]^2 \leq C_{k,\ell} \min\{N_k, N_{\ell}\} \|M\|_F^2. \quad \text{(114)}
\]

In particular, if \( k = 0 \) (or \( \ell = 0 \)), we just use (113) or (112) for the induction.

We will bound \( \mathbb{E}F_{k,\ell}(x) \) and \( \text{Var}F_{k,\ell}(x) \), separately. The expectation \( \mathbb{E}F_{k,\ell}(x) \) is easy to deal with. When \( k \neq \ell \), \( \mathbb{E}F_{k,\ell}(x) = 0 \); when \( k = \ell \),
\[
\mathbb{E}F_{k,k}(x) = \mathbb{E}\text{Tr}[MY_{k,k,S}(x)Y_{k,k,S}(x)^\top] = v_k^2 \text{Tr}M
\]

where \( v_k \) is the normalizing constant defined in (93). Therefore,
\[
\mathbb{E}F_{k,k}(x)^2 \leq v_k^4 \left( \sum_{u=1}^m |M_{uu}| \right)^2 \leq C_k N_k \left( \sum_{u=1}^m M_{uu}^2 \right) \leq C_k N_k \|M\|_F^2. \quad \text{(115)}
\]

where \( C_k \) is a constant that only depends on \( k \). Next, we compute the variance of \( F_{k,\ell}(x) \). Taking derivative of \( F_{k,\ell}(x) \) with respect to each \( x_i \), we have
\[
\frac{\partial F_{k,\ell}(x)}{\partial x_i} = \frac{u_k}{u_{k-1}} Y_{k-1,S}(x)^\top M_i^{\text{row}} Y_{\ell,S}(x) + \frac{u_{\ell}}{u_{\ell-1}} Y_{k,S}(x)^\top M_i^{\text{col}} Y_{\ell-1,S}(x)
\]

where \( M_i^{\text{row}} \) and \( M_i^{\text{col}} \) are formed by concatenating a subset of rows (columns) from \( M \) and some zero rows (columns). As a result,
\[
\|\nabla F_{k,\ell}(x)\|^2 \leq 2 \left( \frac{u_k}{u_{k-1}} \right)^2 \sum_{i=1}^d \left[ Y_{k-1,S}(x)^\top M_i^{\text{row}} Y_{\ell,S}(x) \right]^2 + 2 \left( \frac{u_{\ell}}{u_{\ell-1}} \right)^2 \sum_{i=1}^d \left[ Y_{k,S}(x)^\top M_i^{\text{col}} Y_{\ell-1,S}(x) \right]^2.
\]
Then by (112) and (113), we have

\[ \mathbb{E}\|\nabla F_{k,\ell}(x)\|^2 \leq C_{k,\ell} \left[ \min\{N_{k-1}, N_{\ell}\} \sum_{i=1}^{d} \|M_i^{\text{row}}\|_F^2 + \min\{N_k, N_{\ell-1}\} \sum_{i=1}^{d} \|M_i^{\text{col}}\|_F^2 \right] \]

\[ \leq C_{k,\ell} \left[ k \min\{N_{k-1}, N_{\ell}\} \|M\|_F^2 + \ell \min\{N_k, N_{\ell-1}\} \|M\|_F^2 \right] \]

\[ \leq C_{k,\ell} \min\{N_k, N_\ell\} \|M\|_F^2. \]

Using Gaussian Poincaré inequality, we can get

\[ \text{Var} F_{k,\ell}(x) \leq \mathbb{E}\|\nabla F_{k,\ell}(x)\|^2 \]

\[ \leq C_{k,\ell} \min\{N_k, N_\ell\} \|M\|_F^2. \] (116)

Finally, combining (116) and (115), we get

\[ \mathbb{E}[F_{k,\ell}(x)^2] = [\mathbb{E} F_{k,\ell}(x)]^2 + \text{Var} F_{k,\ell}(x) \]

\[ \leq C_{k,\ell} (\delta_{k\ell} N_k \|M\|_F^2 + \min\{N_k, N_{\ell}\} \|M\|_F^2) \]

\[ \leq 2C_{k,\ell} \min\{N_k, N_{\ell}\} \|M\|_F^2 \]

which is (114).