Exact Gap between Generalization Error and Uniform Convergence in Random Feature Models

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Abstract

Recent work showed that there could be a large gap between the classical uniform convergence bound and the actual test error of zero-training-error predictors (interpolators) such as deep neural networks. To better understand this gap, we study the uniform convergence in the nonlinear random feature model and perform a precise theoretical analysis on how uniform convergence depends on the sample size and the number of parameters. We derive and prove analytical expressions for three quantities in this model: 1) classical uniform convergence over norm balls, 2) uniform convergence over interpolators in the norm ball (recently proposed by Zhou et al. (2020)), and 3) the risk of minimum norm interpolator. We show that, in the setting where the classical uniform convergence bound is vacuous (diverges to \(\infty\)), uniform convergence over the interpolators still gives a non-trivial bound of the test error of interpolating solutions. We also showcase a different setting where classical uniform convergence bound is non-vacuous, but uniform convergence over interpolators can give an improved sample complexity guarantee. Our result provides a first exact comparison between the test errors and uniform convergence bounds for interpolators beyond simple linear models.

1. Introduction

Uniform convergence—the supremum difference between the training and test errors over a certain function class—is a powerful tool in statistical learning theory for understanding the generalization performance of predictors. Bounds on uniform convergence usually take the form of \(\sqrt{\text{complexity}/n}\) (Vapnik, 1995), where the numerator represents the complexity of the function class, and \(n\) is the sample size. If such a bound is tight, then the predictor is not going to generalize well whenever the function class complexity is too large.

However, it is shown in recent theoretical and empirical work that overparametized models such as deep neural networks could generalize well, even in the interpolating regime in which the model exactly memorizes the data (Zhang et al., 2016; Belkin et al., 2019a). As interpolation (especially for noisy training data) usually requires the predictor to be within a function class with high complexity, this challenges the classical methodology of using uniform convergence to bound generalization. For example, Belkin et al. (2018c) showed that interpolating noisy data with kernel machines requires exponentially large norm in fixed dimensions. The large norm would effectively make the uniform convergence bound \(\sqrt{\text{complexity}/n}\) vacuous. Nagarajan & Kolter (2019a) empirically measured the spectral-norm bound in Bartlett et al. (2017) and find that for interpolators, the bound increases with \(n\), and is thus vacuous at large sample size. Towards a more fine-grained understanding, we ask the following

**Question:** How large is the gap between uniform convergence and the actual generalization errors for interpolators?

In this paper, we study this gap in the random features model from Rahimi & Recht (2007). This model can be interpreted as a linearized version of two-layer neural networks (Jacot et al., 2018) and exhibit some similar properties to deep neural networks such as double descent (Belkin et al., 2019a). We consider two types of uniform convergence in this model:

- \(U\) : The classical uniform convergence over a norm ball of radius \(\sqrt{A}\).
- \(T\) : The modified uniform convergence over the same norm ball of size \(\sqrt{A}\) but only include the interpolators, proposed in Zhou et al. (2020).
Our main theoretical result is the exact asymptotic expressions of two versions of uniform convergence $U$ and $T$ in terms of the number of features, sample size, as well as other relevant parameters in the random feature model. Under some assumptions, we prove that the actual uniform convergence concentrates to these asymptotic counterparts. To further compare these uniform convergence bounds with the actual generalization error of interpolators, we adopt

- $R$ : the generalization error (test error) of the minimum norm interpolator.

from Mei & Montanari (2019). To make $U$, $T$, $R$ comparable with each other, we choose the radius of the norm ball $\sqrt{A}$ to be slightly larger than the norm of the minimum norm interpolator. Our limiting $U$, $T$ (with norm ball of size $\sqrt{A}$ as chosen above), and $R$ depend on two main variables: $\psi_1 = \lim_{d \to \infty} N/d$ representing the number of parameters, and $\psi_2 = \lim_{d \to \infty} n/d$ representing the sample size. Our formulae for $U$, $T$ and $R$ yield three major observations.

1. **Sample Complexity in the Noisy Regime:** When the training data contains label noise (with variance $\tau^2$), we find that the norm required to interpolate the noisy training set grows linearly with the number of samples $\psi_2$ (green curve in Figure 1(c)). As a result, the standard uniform convergence bound $U$ grows with $\psi_2$ at the rate $U \sim \psi_2^{1/2}$, leading to a vacuous bound on the generalization error (Figure 1(b)).

In contrast, in the same setting, we show the uniform convergence over interpolators $T \sim 1$ is a constant for large $\psi_2$, and is only order one larger than the actual generalization error $R \sim 1$. Further, the excess versions scale as $T - \tau^2 \sim 1$ and $R - \tau^2 \sim \psi_2^{-1}$.

2. **Sample Complexity in the Noisy Regime:** When the training set does not contain label noise, the generalization error $R$ decays faster: $R \sim \psi_2^{-2}$. In this setting, we find that the classical uniform convergence $U \sim \psi_2^{-1/2}$ and the uniform convergence over interpolators $T \sim \psi_2^{-1}$. This shows that, even when the classical uniform convergence already gives a non-vacuous bound, there still exists a sample complexity separation among the classical uniform convergence $U$, the uniform convergence over interpolators $T$, and the actual generalization error $R$.

3. **Dependence on Number of Parameters:** In addition to the results on $\psi_2$, we find that $U$, $T$ and $R$ decay to its limiting value at the same rate $1/\psi_1$. This shows that both $U$ and $T$ correctly predict that as the number of features $\psi_1$ grows, the risk $R$ would decrease.

These results provide a more precise understanding of uniform convergence versus the actual generalization errors, under a natural model that captures a lot of essences of nonlinear overparametrized learning.

1.1. Related work

**Classical theory of uniform convergence.** Uniform convergence dates back to the empirical process theory of Glivenko (1933) and Cantelli (1933). Application of uniform convergence to the framework of empirical risk minimization usually proceeds through Gaussian and Rademacher complexities (Bartlett & Mendelson, 2003; Bartlett et al., 2005) or VC and fat shattering dimensions (Vapnik, 1995; Bartlett, 1998).

**Modern take on uniform convergence.** A large volume of recent works showed that overparametrized interpola-
Random features model and kernel machines. A number of papers studied the generalization error of kernel machines (Caponnetto & De Vito, 2007; Jactot et al., 2020b; Wainwright, 2019) and random features models (Rahimi & Recht, 2009; Rudi & Rosasco, 2017; Bach, 2015; Ma et al., 2020) in the non-asymptotic settings, in which the generalization error bound depends on the RKHS norm. However, these bounds cannot characterize the generalization error for interpolating solutions. In the last three years, a few papers (Belkin et al., 2018c; Liang et al., 2020; 2019) showed that interpolating solutions of kernel ridge regression can also generalize well in high dimensions. Recently, a few papers studied the generalization error of random features model in the proportional asymptotic limit in various settings (Hastie et al., 2019; Louart et al., 2018; Mei & Montanari, 2019; Montanari et al., 2019; Gerace et al., 2020; d’Ascoli et al., 2020; Yang et al., 2020; Adlam & Pennington, 2020; Dhifallah & Lu, 2020; Hu & Lu, 2020), where they precisely characterized the asymptotic generalization error of interpolating solutions, and showed that double-descent phenomenon (Belkin et al., 2019a; Advani et al., 2020) exists in these models. A few other papers studied the generalization error of random features models in the polynomial scaling limits (Ghorbani et al., 2019; 2020; Mei et al., 2021), where other interesting behaviors were shown.

Precise asymptotics for the Rademacher complexity of some underparameterized learning models was calculated using statistical physics heuristics in Abbaras et al. (2020). In our work, we instead focus on the uniform convergence of overparameterized random features model.

2. Problem formulation

In this section, we present the background needed to understand the insights from our main result. In Section 2.1 we define the random feature regression task that this paper focuses on. In Section 2.2, we informally present the limiting regime our theory covers.

2.1. Model setup

Consider a dataset \((x_i, y_i)_{i \in [n]}\) with \(n\) samples. Assume that the covariates follow \(x_i \sim_{iid} \text{Unif}(\mathbb{S}^{d-1}(\sqrt{d}))\), and responses satisfy \(y_i = f_d(x_i) + \epsilon_i\), with the noises satisfying \(\epsilon_i \sim_{iid} \mathcal{N}(0, \tau^2)\) which are independent of \((x_i)_{i \in [n]}\). We will consider both the noisy \((\tau^2 > 0)\) and noiseless \((\tau^2 = 0)\) settings.

We fit the dataset using the random features model. Let \(\{\theta_j\}_{j \in [N]} \sim_{iid} \text{Unif}(\mathbb{S}^{d-1}(\sqrt{d}))\) be the random feature vectors. Given an activation function \(\sigma : \mathbb{R} \rightarrow \mathbb{R}\), we define the random features function class \(\mathcal{F}_{RF}(\Theta)\) by

\[
\mathcal{F}_{RF}(\Theta) \equiv \left\{ f(x) = \sum_{j=1}^{N} a_j \sigma(\langle x, \theta_j \rangle / \sqrt{d}) : a \in \mathbb{R}^N \right\}.
\]

Generalization error of the minimum norm interpolator. Denote the population risk and the empirical risk of a predictor \(a \in \mathbb{R}^N\) by

\[
R(a) = \mathbb{E}_{x,y} \left( y - \sum_{j=1}^{N} a_j \sigma(\langle x, \theta_j \rangle / \sqrt{d}) \right)^2, \quad (1)
\]

\[
\hat{R}_n(a) = \frac{1}{n} \sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{N} a_j \sigma(\langle x_i, \theta_j \rangle / \sqrt{d}) \right)^2, \quad (2)
\]

and the regularized empirical risk minimizer with vanishing regularization by

\[
a_{\min} = \lim_{\lambda \to 0^+} \arg \min_a \left[ \hat{R}_n(a) + \lambda \|a\|_2^2 \right].
\]

In the overparameterized regime \((N > n)\), under mild conditions, we have \(\min_a \hat{R}_n(a) = \hat{R}_n(a_{\min}) = 0\). In this regime, \(a_{\min}\) can be interpreted as the minimum \(\ell_2\) norm interpolator.

A quantity of interest is the generalization error of this predictor, which gives (with a slight abuse of notation)

\[
R(N, n, d) \equiv R(a_{\min}). \quad (3)
\]
Uniform convergence bounds. We denote the uniform convergence bound over a norm ball and the uniform convergence over interpolators in the norm ball by

\[ U(A, N, n, d) \equiv \sup_{\langle \psi_1, \beta \rangle} \left( R(\beta) - \tilde{R}_n(\beta) \right), \quad (4) \]

\[ T(A, N, n, d) \equiv \sup_{\langle \psi_1, \beta \rangle} \left( R(\beta) \right). \quad (5) \]

Here the scaling factor \( N/d \) of the norm ball is such that the norm ball converges to a non-trivial RKHS norm ball with size \( \sqrt{A} \) as \( \psi_1 \to \infty \) (limit taken after \( N/d \to \psi_1 \)). Note that in order for the maximization problem in (5) to have a non-empty feasible region, we need \( \tilde{R}_n(\alpha_{\min}) = 0 \) and need to take \( A \geq (N/d)\|\alpha_{\min}\|^2 \): we will show that in the region \( N \gg n \) with sufficiently large \( A \), this happens with high probability.

By construction, for any \( A \geq (N/d)\|\alpha_{\min}\|^2 \), we have \( U(A) \geq T(A) \geq \tilde{R}(\alpha_{\min}) \) (see Figure 2). So a natural problem is to quantify the gap among \( U(A), T(A) \), and \( \tilde{R}(\alpha_{\min}) \), which is our goal in this paper.

![Figure 2. Illustration of uniform convergence \( U \) (c.f. eq. (4)), uniform convergence over interpolators \( T \) (c.f. eq. (5)), and minimum norm interpolator \( R(\alpha_{\min}) \). We take \( \psi_1 = (x, \beta) \) for some \( \|\beta\|^2 = 1 \), and take the ReLU activation function \( \sigma(x) = \max\{x, 0\} \). Solid lines are our theoretical predictions \( U \) and \( T \) (cf. (6) & (7)). Points with error bars are obtained from simulations with the number of features \( N = 500 \), number of samples \( n = 300 \), and covariate dimension \( d = 200 \). The error bar reports \( 1/\sqrt{20} \times \) standard deviation over 20 instances. See Appendix B for details.](image)

2.2. High dimensional regime

We approach this problem in the limit \( d \to \infty \) with \( N/d \to \psi_1 \) and \( n/d \to \psi_2 \) (c.f. Assumption 3). We further assume the setting of a linear target function \( f_d \) and a non-linear activation function \( \sigma \) (c.f. Assumptions 1 and 2). In this regime, our main result Theorem 1 will show that, the uniform convergence \( U \) and the uniform convergence over interpolators \( T \) will converge to deterministic functions, i.e., writing here informally,

\[ U(A, N, n, d) \overset{d \to \infty}{\longrightarrow} U(A, \psi_1, \psi_2), \quad (6) \]

\[ T(A, N, n, d) \overset{d \to \infty}{\longrightarrow} T(A, \psi_1, \psi_2), \quad (7) \]

where \( U \) and \( T \) will be defined in Definition 2 (which depends on the definition of some other quantities that are defined in Appendix A and heuristically presented in Remark 1). In addition to \( U \) and \( T \), Theorem 1 of Mei & Montanari (2019) implies the following convergence

\[ \tilde{R}(\alpha_{\min}) \overset{d \to \infty}{\longrightarrow} R(\psi_1, \psi_2). \quad (9) \]

The precise algebraic expression of equation (8) and (9) was given in Definition 1 of Mei & Montanari (2019), and we include in Appendix A for completeness. We will sometimes refer to \( U, T, A, R \) without explicitly mark their dependence on \( A, \psi_1, \psi_2 \) for notational simplicity.

Kernel regime. Rahimi & Recht (2007) have shown that, as \( N \to \infty \), the random feature space \( RF(\Theta) \) (equipped with proper inner product) converges to the RKHS (Reproducing Kernel Hilbert Space) induced by the kernel

\[ H(x, x') = \mathbb{E}_{w \sim \text{Unif}(0, 1)} \sigma(x \cdot w) \sigma(x' \cdot w). \]

We expect that, if we take limit \( \psi_1 \to \infty \) after \( N, d, n \to \infty \), the formula of \( U \) and \( T \) will coincide with the corresponding asymptotic limit of \( U \) and \( T \) for kernel ridge regression with the kernel \( H \). This intuition has been mentioned in a few papers (Mei & Montanari, 2019; d’Ascoli et al., 2020; Jacot et al., 2020a). In this spirit, we denote

\[ U_{\infty}(A, \psi_2) \equiv \lim_{\psi_1 \to \infty} U(A, \psi_1, \psi_2), \quad (10) \]

\[ T_{\infty}(A, \psi_2) \equiv \lim_{\psi_1 \to \infty} T(A, \psi_1, \psi_2), \quad (11) \]

\[ A_{\infty}(\psi_2) \equiv \lim_{\psi_1 \to \infty} A(\psi_1, \psi_2), \quad (12) \]

\[ R_{\infty}(\psi_2) \equiv \lim_{\psi_1 \to \infty} R(\psi_1, \psi_2). \quad (13) \]

We will refer to the quantities \( \{U_{\infty}, T_{\infty}, A_{\infty}, R_{\infty}\} \) as the \{uniform convergence in norm ball, uniform convergence over interpolators in norm ball, minimum \( \ell_2 \) norm of interpolators, and generalization error of interpolators\} of kernel ridge regression.

Low norm uniform convergence bounds. There is a question of which norm \( A \) to choose in \( U \) and \( T \) to compare with \( R \). In order for \( U \) and \( T \) to serve as proper bounds for \( \tilde{R}(\alpha_{\min}) \), we need to take at least \( A \geq \psi_1\|\alpha_{\min}\|^2 \). Therefore, we will choose

\[ A = \alpha \psi_1\|\alpha_{\min}\|^2, \quad (14) \]
for some $\alpha > 1$ (e.g., $\alpha = 1.1$). Note $\psi_1 \|a_{\min}\|_2^2 \rightarrow A(\psi_1, \psi_2)$ as $d \rightarrow \infty$. So for a fixed $\alpha > 1$, we further define

$$U^{(\alpha)}(\psi_1, \psi_2) \equiv U(\alpha A(\psi_1, \psi_2), \psi_1, \psi_2),$$

$$T^{(\alpha)}(\psi_1, \psi_2) \equiv T(\alpha A(\psi_1, \psi_2), \psi_1, \psi_2),$$

and their kernel version,

$$U^{(\alpha)}_\infty(\psi_2) \equiv \lim_{\psi_1 \rightarrow \infty} U^{(\alpha)}(\psi_1, \psi_2),$$

$$T^{(\alpha)}_\infty(\psi_2) \equiv \lim_{\psi_1 \rightarrow \infty} T^{(\alpha)}(\psi_1, \psi_2).$$

This definition ensures that $R(\psi_1, \psi_2) \leq T^{(\alpha)}(\psi_1, \psi_2) \leq U^{(\alpha)}(\psi_1, \psi_2)$ and $R_\infty(\psi_2) \leq T^{(\alpha)}_\infty(\psi_2) \leq U^{(\alpha)}_\infty(\psi_2)$.

3. Asymptotic power laws and separations

In this section, we evaluate the algebraic expressions derived in our main result (Theorem 1) as well as the quantities $U^{(\alpha)}$, $T^{(\alpha)}$, $A$, and $R$, before formally presenting the theorem. We examine their dependence with respect to the noise level $\tau^2$, the number of features $\psi_1 = \lim_{d \rightarrow \infty} N/d$, and the sample size $\psi_2 = \lim_{d \rightarrow \infty} n/d$, and we further infer their asymptotic power laws for large $\psi_1$ and $\psi_2$.

3.1. Norm of the minimum norm interpolator

Since we are considering uniform convergence bounds over the norm ball of size $\alpha$ times $A_\infty(\psi_2)$ (the norm of the minimum norm interpolator), let’s first examine how $A_\infty(\psi_2)$ scale with $\psi_2$. As we shall see, $A_\infty(\psi_2)$ behaves differently in the noiseless ($\tau^2 = 0$) and noisy ($\tau^2 > 0$) settings, so here we explicitly mark the dependence on $\tau^2$, i.e., $A_\infty(\psi_2; \tau^2)$.

The inferred asymptotic power law gives (c.f. Figure 1(c))

$$A_\infty(\psi_2; \tau^2 > 0) \sim \psi_2,$$

$$A_\infty(\psi_2; \tau^2 = 0) \sim 1,$$

where $X_1(\psi) \sim X_2(\psi)$ for large $\psi$ means that

$$\lim_{\psi \rightarrow \infty} \log(X_1(\psi))/\log(X_2(\psi)) = 1.$$

In words, when there is no label noise ($\tau^2 = 0$), we can interpolate infinite data even with a finite norm. When the responses are noisy ($\tau^2 > 0$), interpolation requires a large norm that is proportional to the number of samples.

On a high level, our statement echoes the finding of Belkin et al. (2018c), where they study a binary classification problem using the kernel machine, and prove that an interpolating classifier requires RKHS norm to grow at least exponentially with $n^{1/d}$ for fixed dimension $d$. Here instead we consider the high dimensional setting and we show a linear grow in $\psi_2 = \lim_{d \rightarrow \infty} n/d$.

3.2. Kernel regime with noiseless data

We first look at the noiseless setting ($\tau^2 = 0$) and present the asymptotic power law for the uniform convergence $U^{(\alpha)}_\infty$ over the low-norm ball, the uniform convergence over interpolators $T^{(\alpha)}_\infty$ in the low norm ball, and the minimum norm risk $R_\infty$ from (17) (18) (13), respectively.

In this setting, the inferred asymptotic power law of $U^{(\alpha)}_\infty(\psi_2)$, $T^{(\alpha)}_\infty(\psi_2)$, and $R_\infty(\psi_2)$ gives (c.f. Figure 1(a))

$$U^{(\alpha)}_\infty(\psi_2; \tau^2 = 0) \sim \psi_2^{-1},$$

$$T^{(\alpha)}_\infty(\psi_2; \tau^2 = 0) \sim \psi_2^{-1},$$

$$R_\infty(\psi_2; \tau^2 = 0) \sim \psi_2^{-2}.$$

As we can see, all the three quantities converge to 0 in the large sample limit, which indicates that uniform convergence is able to explain generalization in this setting. Yet uniform convergence bounds do not correctly capture the convergence rate (in terms of $\psi_2$) of the generalization error.

3.3. Kernel regime with noisy data

In the noisy setting (fix $\tau^2 > 0$), the Bayes risk (minimal possible risk) is $\tau^2$. We study the excess risk and the excess version of uniform convergence bounds by subtracting the Bayes risk $\tau^2$. The inferred asymptotic power law gives (c.f. Figure 1(b))

$$U^{(\alpha)}(\psi_2; \tau^2) - \tau^2 \sim \psi_2^{1/2},$$

$$T^{(\alpha)}(\psi_2; \tau^2) - \tau^2 \sim 1,$$

$$R_\infty(\psi_2; \tau^2) - \tau^2 \sim \psi_2^{-1}.$$

In the presence of label noise, the excess risk $R_\infty - \tau^2$ vanishes in the large sample limit. In contrast, the classical uniform convergence $U_\infty$ becomes vacuous, whereas the uniform convergence over interpolators $T_\infty$ converges to a constant, which gives a non-vacuous bound of $R_\infty$.

The decay of the excess risk of minimum norm interpolators even in the presence of label noise is no longer a surprising phenomenon in high dimensions (Liang et al., 2019; Ghorbani et al., 2019; Bartlett et al., 2020). A simple explanation of this phenomenon is that the nonlinear part of the activation function $\sigma$ has an implicit regularization effect (Mei & Montanari, 2019).

The divergence of $U^{(\alpha)}_\infty$ in the presence of response noise is partly due to $A_\infty(\psi_2)$ blows up linearly in $\psi_2$ (c.f. Section 3.1). In fact, we can develop a heuristic intuition that $U_\infty(A; \psi_2; \tau^2) \sim A/\psi_2^{1/2}$. Then the scaling $U^{(\alpha)}(\psi_2; \tau^2 > 0) \sim A_\infty(\psi_2; \tau^2 > 0)/\psi_2^{1/2} \sim \psi_2^{1/2}$ can be explained away by the power law of $A_\infty(\psi_2; \tau^2 > 0) \sim \psi_2$. In other words, the complexity of the function space of interpolators grows faster than the sample size $n$, which
leads to the failure of uniform convergence in explaining generalization. This echoes the findings in Nagarajan \\& Kolter (2019a).

To illustrate the scaling $U_\infty(A, \psi_2) \sim A/\psi_2^{1/2}$. We fix all other parameters $(\mu_1, \mu_*, \tau, F_1)$, and examine the dependence of $U_\infty$ on $A$ and $\psi_2$. We choose $A = A(\psi_2)$ according to different power laws $A(\psi_2) \sim \psi_2^{p}$ for $p = 0, 0.25, 0.5, 0.75, 1$. The inferred asymptotic power law gives $U_\infty(A(\psi_2), \psi_2) \sim \psi_2^{p-0.5}$ (c.f. Figure 3). This provides an evidence for the relation $U\infty(A, \psi_2) \sim A/\psi_2^{1/2}$.

![Figure 3](image-url) Uniform convergence $U_{\infty}(A(\psi_2), \psi_2)$ over the norm ball in the kernel regime $\psi_1 \to \infty$. The size of the norm ball $A = A(\psi_2)$ is chosen according to different power laws as shown in the legend.

3.4. Finite-width regime

Here we shift attention to the dependence of $U, T, \mathcal{R}$ on the number of features $\psi_1$. We fix the number of training samples $\psi_2$, noise level $\tau^2 > 0$, and norm level $\alpha > 1$ similar as before. Since $U_\alpha \to U_{\infty}, T_\alpha \to T_{\infty}$ and $\mathcal{R} \to \mathcal{R}_{\infty}$ as $\psi_1 \to \infty$, we look at the dependence of $U_\alpha - U_{\infty}, T_\alpha - T_{\infty}$ and $\mathcal{R}_\alpha - \mathcal{R}_{\infty}$ with respect to $\psi_1$. The inferred asymptotic law gives (c.f. Figure 4)

$$U^{(\alpha)}(\psi_1, \psi_2) - U^{(\alpha)}_{\infty}(\psi_2) \sim \psi_1^{-1},$$

$$T^{(\alpha)}(\psi_1, \psi_2) - T^{(\alpha)}_{\infty}(\psi_2) \sim \psi_1^{-1},$$

$$\mathcal{R}(\psi_1, \psi_2) - \mathcal{R}_{\infty}(\psi_2) \sim \psi_1^{-1},$$

$$A(\psi_1, \psi_2) - A_{\infty}(\psi_2) \sim \psi_1^{-1}.$$

Note that large $\psi_1$ should be interpreted as the model being heavily overparametrized (a large width network). This asymptotic power law implies that, both uniform convergence bounds correctly predict the decay of the test error with the increase of the number of features.

**Remark on power laws.** For the derivation of the power laws in this section, instead of working with the analytical formula, we adopt an empirical approach: we perform linear fits with the inferred slopes, upon the numerical evaluations (of these expressions defined in Definition 2) in the log-log scale. However, these linear fits are for the analytical formulae and do not involve randomness, and thus reliably indicate the true decay rates.

4. Main theorem

In this section, we state the main theorem that presents the asymptotic expressions for the uniform convergence bounds. We will start by stating a few assumptions, which fall into two categories: Assumption 1, 2, and 3, which specify the setup for the learning task; Assumption 4 and 5, which are technical in nature.

4.1. Modeling assumptions

The three assumptions in this subsection specify the target function, the activation function, and the limiting regime.

**Assumption 1** (Linear target function). We assume that $f_a \in L^{2}((\mathbb{S}^{d-1} \sqrt{d}))$ with $f_a(x) = (\beta(d), \mathbf{x})$, where $\beta(d) \in \mathbb{R}^d$ and

$$\lim_{d \to \infty} \|\beta(d)\|_2^2 = F_1^2.$$

We remark here that, if we are satisfied with heuristic formula instead of rigorous results, we are able to deal with non-linear target functions, where the additional nonlinear part is effectively increasing the noise level $\tau^2$. This intuition was first developed in (Mei & Montanari, 2019).

**Assumption 2** (Activation function). Let $\sigma \in C^2(\mathbb{R})$ with $|\sigma(u)|, |\sigma'(u)|, |\sigma''(u)| \leq c_0 e^{c_1 |u|}$ for some constant $c_0, c_1 < \infty$. Define $\mu_0 = \mathbb{E}[\sigma(G)], \mu_1 = \mathbb{E}[\sigma(G)\sigma(G)], \mu_2^{*} = \mathbb{E}[\sigma(G)^2] - \mu_0^2 - \mu_1^2$, where expectation is with respect to $G \sim \mathcal{N}(0, 1)$. Assume $\mu_0 = 0, 0 < \mu_1^2, \mu_2^* < \infty$.

The assumption that $\mu_0 = 0$ is not essential and can be relaxed with a certain amount of additional technical work.

**Assumption 3** (Proportional limit). Let $N = N(d)$ and $n = n(d)$ be sequences indexed by $d$. We assume that the following limits exist in $(0, \infty)$:

$$\lim_{d \to \infty} N(d)/d = \psi_1, \quad \lim_{d \to \infty} n(d)/d = \psi_2.$$

4.2. Technical assumptions

We will make some assumptions upon the properties of some random matrices that appear in the proof. These assumptions are technical and we believe they can be proved under more natural assumptions. However, proving them requires substantial technical work, and we defer them to future work. We note here that these assumptions are often implicitly required in papers that present intuitions using
heuristic derivations. Instead, we ensure the mathematical rigor by listing them. See Section 5 for more discussions upon these assumptions.

We begin by defining some random matrices which are the key quantities that are used in the proof of our main results.

**Definition 1** (Block matrix and log-determinant). Let $X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times d}$ and $\Theta = (\theta_1, \ldots, \theta_n)^T \in \mathbb{R}^{N \times d}$, where $x_i, \theta_n \sim_{\text{iid}} \text{Unif}([0,1])$, as mentioned in Section 2.1. Define

$$Z = \frac{1}{\sqrt{d}} \Theta \frac{X^T}{\sqrt{d}}, \quad Z_1 = \frac{\mu_1}{d} X \Theta^T,$$

$$Q = \Theta \Theta^T, \quad H = \frac{X X^T}{d}, \quad (19)$$

and for $q = (s_1, s_2, t_1, t_2, q) \in \mathbb{R}^5$, we define

$$A(q) = \begin{bmatrix} s_1 I_N + s_2 Q & Z^T + p Z_1 \\ Z + p Z_1 & t_1 I_n + t_2 H \end{bmatrix}.$$

Finally, we define the log-determinant of $A(q)$ by

$$G_d(\xi; q) = \frac{1}{d} \sum_{i=1}^{N+n} \log \lambda_i \left(A(q) - \xi I_{n+N}\right).$$

Here $\log$ is the complex logarithm with branch cut on the negative real axis and $\{\lambda_i(A)\}_{i \in [n+N]}$ is the set of eigenvalues of $A$.

The following assumption states that for properly chosen $A$, some specific random matrices are well-conditioned. As we will see in the next section, this ensures that the dual problems in Eq. (20) and (21) are bounded with high probability.

**Assumption 4** (Invertability). Consider the asymptotic limit as specified in Assumption 3 the activation function as in Assumption 2. We assume the following.

- Denote $U_2(\lambda) = \mu_2^2 Q + (\mu_2^*-\psi_1 \lambda) I_N - \psi_2^{-1} Z^T Z$. There exists $\varepsilon > 0$ and $\lambda_{U_2} = \lambda_{U_2}(\psi_1, \psi_2, \mu_1, \mu_2)$ such that for any fixed $\lambda \in (\lambda_{U_2}, \infty)$ with high probability, we have

$$U(\lambda) \leq -\varepsilon I_N.$$  

- Denote $\bar{T}(\lambda) = P_{null}[\mu_2^2 Q + (\mu_2^*-\psi_1 \lambda) I_N]P_{null}$, such that for any fixed $\lambda \in (\lambda_{\bar{T}}, \infty)$ with high probability we have

$$\bar{T}(\lambda) \leq -\varepsilon P_{null},$$

and $Z$ has full row rank with $\sigma_{\min}(Z) \geq \varepsilon$ (which requires $\psi_1 > \psi_2$).

The following assumption states that the order of limits and derivatives regarding $G_d$ can be exchanged.

**Assumption 5** (Exchangeability of limits). We denote

$$S_U = \{ (\mu_2^2 - \lambda \psi_1, \mu_2^2, \psi_2, 0, 0; \psi_1, \psi_2) : \lambda \in (\lambda_{U}, \infty) \},$$

$$S_T = \{ (\mu_2^2 - \lambda \psi_1, \mu_2^2, 0, 0, 0; \psi_1, \psi_2) : \lambda \in (\lambda_{T}, \infty) \},$$

where $\lambda_{U}$ and $\lambda_{T}$ are given in Assumption 4 and depend on $(\psi_1, \psi_2, \mu_1^2, \mu_2^2)$. For any fixed $(q; \psi) = (s_1, s_2, t_1, t_2, p; \psi_1, \psi_2) \in S_U \cup S_T$, in the asymptotic limit as in Assumption 3, for $k = 1, 2$, we have

$$\lim_{u \to 0^+} \lim_{d \to \infty} \mathbb{E}[\nabla^k q G_d(iu; q)] = \lim_{u \to 0^+} \nabla^k q \left( \lim_{d \to \infty} \mathbb{E}[G_d(iu; q)] \right),$$

and

$$\left\| \nabla^k q G_d(0; q) - \lim_{u \to 0^+} \lim_{d \to \infty} \mathbb{E}[\nabla^k q G_d(iu; q)] \right\| = o_{d,p}(1),$$

where $o_{d,p}(1)$ stands for convergence to 0 in probability.
4.3. From constrained forms to Lagrangian forms

Before we give the asymptotics of $U$ and $T$ as defined in Eq. (4) and (5), we first consider their dual forms which are more amenable in analysis. These are given by

\begin{align*}
\mathcal{U}(\lambda, N, n, d) & \equiv \sup_{\alpha} \left[ R(\alpha) - \tilde{R}_n(\alpha) - \psi_1 \lambda \| \alpha \|_2^2 \right], \\
\mathcal{T}(\lambda, N, n, d) & \equiv \sup_{\alpha} \inf_{\mu} \left[ R(\alpha) - \psi_1 \lambda \| \alpha \|_2^2 \\ & + 2 \langle \mu, Z \alpha - y/\sqrt{d} \rangle \right].
\end{align*}

(20)

The proposition below shows that the strong duality holds upon the constrained forms and their dual forms.

**Proposition 1 (Strong Duality).** For any $A > 0$, we have

\[ U(A, N, n, d) = \inf_{\lambda \geq 0} \mathcal{U}(\lambda, N, n, d) + \lambda A. \]

Moreover, for any $A > \psi_1 \| \alpha_{\text{min}} \|_2^2$, we have

\[ T(A, N, n, d) = \inf_{\lambda \geq 0} \mathcal{T}(\lambda, N, n, d) + \lambda A. \]

The proof of Proposition 1 is based on a classical result which states that strongly duality holds for quadratic programs with single quadratic constraint (Appendix B.1 in Boyd & Vandenberghe (2004)).

4.4. Expressions of $\mathcal{U}$ and $\mathcal{T}$

Proposition 1 transforms our task from computing the asymptotics of $U$ and $T$ to that of $\mathcal{U}$ and $\mathcal{T}$. The latter is given by the following proposition.

**Proposition 2.** Let the target function $f_d$ satisfy Assumption 1, the activation function $\sigma$ satisfy Assumption 2, and $(N, n, d)$ satisfy Assumption 3. In addition, let Assumption 4 and 5 hold. Then for $\lambda \in \Lambda_U$, with high probability the maximizer in Eq. (20) can be achieved at a unique point $\overline{\alpha}_U(\lambda)$, and we have

\[ \mathcal{U}(\lambda, N, n, d) = \overline{U}(\lambda, \psi_1, \psi_2) + o_d(1), \]

\[ \psi_1 \| \overline{\alpha}_U(\lambda) \|_2^2 = \mathcal{A}_U(\lambda, \psi_1, \psi_2) + o_d(1). \]

Moreover, for any $\lambda \in \Lambda_T$, with high probability the maximizer in Eq. (21) can be achieved at a unique point $\overline{\alpha}_T(\lambda)$, and we have

\[ \mathcal{T}(\lambda, N, n, d) = \overline{T}(\lambda, \psi_1, \psi_2) + o_d(1), \]

\[ \psi_1 \| \overline{\alpha}_T(\lambda) \|_2^2 = \mathcal{A}_T(\lambda, \psi_1, \psi_2) + o_d(1). \]

The functions $\overline{U}, \overline{T}, \mathcal{A}_U, \mathcal{A}_T$ are given in Definition 5 in Appendix A.

Remark 1. Here we present the heuristic formulae of $\overline{U}, \overline{T}, \mathcal{A}_U, \mathcal{A}_T$, and defer their rigorous definition to the appendix. Define a function $g_0(\mathbf{q}; \psi)$ by

\[ g_0(\mathbf{q}; \psi) \equiv \max_{z_1, z_2} \left[ \log \left( \left( s_2 z_1 + 1 \right) (t_2 z_2 + 1) \right) \right. \]

\[ - \mu_2^2 (1 + p)^2 z_1 z_2 - \mu_1^2 z_1 z_2 + s_1 z_1 + t_1 z_2 \]

\[ - \psi_1 \log(z_1/\psi_1) - \psi_2 \log( z_2/\psi_2) - \psi_1 - \psi_2 \]

(22)

where $\max$ stands for setting $z_1$ and $z_2$ to be stationery (which is a common symbol in statistical physics heuristics). We then take

\[ \overline{U}(\lambda, \psi) = F_1^2(1 - \mu_1^2 \gamma_{s_2} - \gamma_{p} - \gamma_{t_2}) + \tau^2(1 - \gamma_{t_1}), \]

where $\gamma_a \equiv \partial_a g_0(\mathbf{q}; \psi)|_{\mathbf{q}=(\mu_2^2 - \lambda \psi_1, \mu_1^2, \psi_2, 0, 0)}$ for the symbol $a \in \{s_1, s_2, t_1, t_2, p\}$, and

\[ \overline{T}(\lambda, \psi) = F_1^2(1 - \mu_2^2 \nu_{s_2} - \nu_p - \nu_{t_2}) + \tau^2(1 - \nu_{t_1}), \]

where we define $\nu_a \equiv \partial_a g_0(\mathbf{q}; \psi)|_{\mathbf{q}=(\mu_2^2 - \lambda \psi_1, \mu_1^2, \psi_2, 0, 0)}$ for symbols $a \in \{s_1, s_2, t_1, t_2, p\}$. Finally $\mathcal{A}_U = -\partial_\lambda \overline{U}, \mathcal{A}_T = -\partial_\lambda \overline{T}$. By a further simplification, we can express these formulae as rational functions of $(\mu_1^2, \mu_2^2, \lambda, \psi_1, \psi_2, m_1, m_2)$ where $(m_1, m_2)$ is the stationery point of the variational problem in Eq. (22) (c.f. Remark 2).

We next define $\overline{U}$ and $\overline{T}$ to be dual forms of $\mathcal{U}$ and $\mathcal{T}$.

**Definition 2** (Formula for uniform convergence bounds). For $A \in \Gamma_U \equiv \{ A_U(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_U \}$, define

\[ U(A, \psi_1, \psi_2) \equiv \inf_{\lambda \geq 0} \left[ \overline{U}(\lambda, \psi_1, \psi_2) + \lambda A \right]. \]

For $A \in \Gamma_T \equiv \{ A_T(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_T \}$, define

\[ T(A, \psi_1, \psi_2) \equiv \inf_{\lambda \geq 0} \left[ \overline{T}(\lambda, \psi_1, \psi_2) + \lambda A \right]. \]

Finally, we are ready to present the main theorem of this paper, which states that the uniform convergence bounds $U(A, N, n, d)$ and $T(A, N, n, d)$ converge to the formula presented in the definition above.

**Theorem 1.** Let the same assumptions in Proposition 2 hold. For any $A \in \Gamma_U$, we have

\[ U(A, N, n, d) = U(A, \psi_1, \psi_2) + o_d(1), \]

and for $A \in \Gamma_T$ we have

\[ T(A, N, n, d) = T(A, \psi_1, \psi_2) + o_d(1), \]

where functions $U$ and $T$ are given in Definition 2.

The proof of this theorem is contained in Section E.
5. Discussions

In this paper, we calculated the uniform convergence bounds for random features models in the proportional scaling regime. Our results exhibit a setting in which standard uniform convergence bound is vacuous while uniform convergence over interpolators gives a non-trivial bound of the actual generalization error.

Modeling assumptions and technical assumptions.  We made a few assumptions to prove the main result Theorem 1. Some of these assumptions can be relaxed. Indeed, if we assume a non-linear target function $f_d$ instead of a linear one as in Assumption 1, the non-linear part will behave like additional noises in the proportional scaling limit. However, proving this rigorously requires substantial technical work. Similar issue exists in Mei & Montanari (2019). Moreover, it is not essential to assume vanishing $\mu_0^2$ in Assumption 2.

Assumption 4 and 5 involve some properties of specific random matrices. We believe these assumptions can be proved under more natural assumptions on the activation function $\sigma$. However, proving these assumptions requires developing some sophisticated random matrix theory results, which could be of independent interest.

Relationship with non-asymptotic results.  We hold the same opinion as in Abbaras et al. (2020): the exact formulae in the asymptotic limit can provide a complementary view to the classical theories of generalization. On the one hand, asymptotic formulae can be used to quantify the tightness of non-asymptotic bounds; on the other hand, the asymptotic formulae in many cases are comparable to non-asymptotic bounds. For example, Lemma 22 in Bartlett & Mendelson (2003) coupled with the bound of Lipschitz constant of the square loss in proper regime implies that $\mathcal{U}_\infty(A,\psi_2)$ have a non-asymptotic bound that scales linearly in $A$ and inverse proportional to $\psi_2^{1/2}$ (c.f. Proposition 6 of E et al. (2020)). This coincides with the intuitions in Section 3.3.

Uniform convergence in other settings.  A natural question is whether the power law derived in Section 3 holds for models in more general settings. One can perform a similar analysis to calculate the uniform convergence bounds in a few other settings (Montanari et al., 2019; Dhifallah & Lu, 2020; Hu & Lu, 2020). We believe the power law may be different, but the qualitative properties of uniform convergence bounds will share some similar features.

Relationship with Zhou et al. (2020).  The separation of uniform convergence bounds ($U$ and $T$) is first pointed out by Zhou et al. (2020), where the authors worked with the linear regression model in the “junk features” setting. We believe random features model are more natural models to illustrate the separation: in Zhou et al. (2020), there are some unnatural parameters $\lambda_n$, $d_J$ that are hard to make connections to deep learning models, while the random features model is closely related to two-layer neural networks.

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A. Definitions of quantities in the main text

A.1. Full definitions of $\overline{U}$, $\overline{T}$, $A_U$, and $A_T$ in Proposition 2

We first define functions $m_1(\cdot), m_2(\cdot)$, which could be understood as the limiting partial Stieltjes transforms of $A(q)$ (c.f. Definition 1).

**Definition 3** (Limiting partial Stieltjes transforms). For $\xi \in \mathbb{C}_+$ and $q \in Q$ where

\[ Q = \{(s_1, s_2, t_1, t_2, p) : |s_2t_2| \leq \mu_1^2(1 + p)^2/2\}, \tag{25} \]

define functions $F_1(\cdot, \cdot; q, \psi_1, \psi_2, \mu_1, \mu_*)$, $F_2(\cdot, \cdot; q, \psi_1, \psi_2, \mu_1, \mu_*) : \mathbb{C} \times \mathbb{C} \rightarrow \mathbb{C}$ via:

\[
F_1(m_1, m_2; q, \psi_1, \psi_2, \mu_1, \mu_*) \equiv \psi_1 \left( -\xi + s_1 - \mu_2^2m_2 + \frac{(1 + t_2m_2)s_2 - \mu_1^2(1 + p)^2m_2}{(1 + s_2m_1)(1 + t_2m_2) - \mu_1^2(1 + p)^2m_1m_2} \right)^{-1}, \\
F_2(m_1, m_2; q, \psi_1, \psi_2, \mu_1, \mu_*) \equiv \psi_2 \left( -\xi + t_1 - \mu_2^2m_1 + \frac{(1 + s_2m_1)t_2 - \mu_1^2(1 + p)^2m_1}{(1 + t_2m_2)(1 + s_2m_1) - \mu_1^2(1 + p)^2m_1m_2} \right)^{-1}.
\]

Let $m_1(\cdot; q, \psi)$, $m_2(\cdot; q, \psi) : \mathbb{C}_+ \rightarrow \mathbb{C}_+$ be defined, for $\exists(\xi) \geq C$ a sufficiently large constant, as the unique solution of the equations

\[
m_1 = F_1(m_1, m_2; q, \psi_1, \psi_2, \mu_1, \mu_*), \\
m_2 = F_2(m_1, m_2; q, \psi_1, \psi_2, \mu_1, \mu_*) \tag{26}
\]

subject to the condition $|m_1| \leq \psi_1/\exists(\xi)$, $|m_2| \leq \psi_2/\exists(\xi)$. Extend this definition to $\exists(\xi) > 0$ by requiring $m_1, m_2$ to be analytic functions in $\mathbb{C}_+$.

We next define the function $g(\cdot)$ that will be shown to be the limiting log determinant of $A(q)$.

**Definition 4** (Limiting log determinants). For $q = (s_1, s_2, t_1, t_2, p)$ and $\psi = (\psi_1, \psi_2)$, define

\[
\Xi(\xi, z_1, z_2; q, \psi) \equiv \log \left( (s_2z_1 + 1)(t_2z_2 + 1) - \mu_1^2(1 + p)^2z_1z_2 - \mu_2^2z_1z_2 + s_1z_1 + t_1z_2 - \psi_1 \log(z_1/\psi_1) - \psi_2 \log(z_2/\psi_2) - \xi(z_1 + z_2) - \psi_1 - \psi_2 \right). \tag{27}
\]

Let $m_1(\xi; q, \psi)$, $m_2(\xi; q, \psi)$ be defined as the analytic continuation of solution of Eq. (26) as defined in Definition 3. Define

\[
g(\xi; q, \psi) = \Xi(\xi, m_1(\xi; q, \psi), m_2(\xi; q, \psi); q, \psi). \tag{28}
\]

We next give the definitions of $\overline{U}$, $\overline{T}$, $A_U$, and $A_T$.

**Definition 5** ($\overline{U}$, $\overline{T}$, $A_U$, and $A_T$ in Proposition 2). For any $\lambda \in \Lambda_U$, define

\[
A_U(\lambda, \psi_1, \psi_2) = -\lim_{u \rightarrow 0^+} \left[ \psi_1 \left( F_1^2 \mu_2^2 \partial_{s_1s_2} + F_1^2 \partial_{s_1p} + F_1^2 \partial_{s_1t_2} + \tau^2 \partial_{s_1t_1} \right) g(\mu; q, \psi) \right]_{q=q_U},
\]

\[
\overline{U}(\lambda, \psi_1, \psi_2) = F_1^2 + \tau^2 - \lim_{u \rightarrow 0^+} \left[ (F_1^2 \mu_2^2 \partial_{s_2s_1} + F_1^2 \partial_{t_2} + F_1^2 \partial_{t_1} + \tau^2 \partial_t) g(\mu; q, \psi) \right]_{q=q_U},
\]

\[
A_T(\lambda, \psi_1, \psi_2) = -\lim_{u \rightarrow 0^+} \left[ \psi_1 \left( F_1^2 \mu_2^2 \partial_{s_1s_2} + F_1^2 \partial_{s_1p} + F_1^2 \partial_{s_1t_2} + \tau^2 \partial_{s_1t_1} \right) g(\mu; q, \psi) \right]_{q=q_T},
\]

\[
\overline{T}(\lambda, \psi_1, \psi_2) = F_1^2 + \tau^2 - \lim_{u \rightarrow 0^+} \left[ (F_1^2 \mu_2^2 \partial_{s_2s_1} + F_1^2 \partial_{t_2} + F_1^2 \partial_{t_1} + \tau^2 \partial_t) g(\mu; q, \psi) \right]_{q=q_T},
\]

where $q_U = (\mu_2^2 - \lambda \psi_1, \mu_2^2, 0, 0)$, $q_T = (\mu_2^2 - \lambda \psi_1, \mu_2^2, 0, 0, 0)$.

In the following, we give a simplified expression for $\overline{U}$ and $A_U$.

**Remark 2** (Simplification of $\overline{U}$ and $A_U$). Define $\zeta, \overline{\chi}$ as the rescaled version of $\mu_1^2$ and $\lambda$

\[
\zeta = \frac{\mu_2^2}{\mu_1^2}, \quad \overline{\chi} = \frac{\lambda}{\mu_2^2}.
\]
Let $m_1(\cdot; \psi) m_2(\cdot; \psi): \mathbb{C}_+ \to \mathbb{C}_+$ be defined, for $\Im(\xi) \geq C$ a sufficiently large constant, as the unique solution of the equations
\begin{align*}
m_1 &= \psi_1 \left[ -\xi + (1 - \lambda_1) - m_2 + \frac{\zeta(1 - m_2)}{1 + \zeta m_1 - \zeta m_1 m_2} \right]^{-1}, \\
m_2 &= -\psi_2 \left[ \xi + \psi_2 - m_1 - \frac{\zeta m_1}{1 + \zeta m_1 - \zeta m_1 m_2} \right]^{-1},
\end{align*}
subject to the condition $|m_1| \leq \psi_1/\Im(\xi)$, $|m_2| \leq \psi_2/\Im(\xi)$. Extend this definition to $\Im(\xi) > 0$ by requiring $m_1, m_2$ to be analytic functions in $\mathbb{C}_+$. Let
\begin{align*}
m_1 &= \lim_{u \to \infty} m_1(iu, \psi), \\
m_2 &= \lim_{u \to \infty} m_2(iu, \psi).
\end{align*}
Define
\begin{align*}
\chi_1 &= m_1 \zeta - m_1 m_2 \zeta + 1, \\
\chi_2 &= m_1 - \psi_2 + \frac{m_1 \zeta}{\chi_1}, \\
\chi_3 &= \bar{\lambda}_1 \psi_1 + m_2 - 1 + \frac{\zeta(m_2 - 1)}{\chi_1}.
\end{align*}
Define two polynomials $E_1, E_2$ as
\begin{align*}
E_1(\psi_1, \psi_2, \bar{\lambda}, \zeta) &= \psi_1^2(\psi_2 \chi_1^4 + \psi_2 \chi_2^4), \\
E_2(\psi_1, \psi_2, \bar{\lambda}, \zeta) &= \psi_1^2(\chi_1^4 \chi_2^4 \zeta - 2 \chi_1^4 \chi_2^4 \zeta + \chi_1^4 \zeta + \psi_2 \chi_1^4 - \psi_2 m_1^2 m_2^2 \zeta^2 + 2 \psi_2 m_1^2 m_2 \zeta^2 - \psi_2 m_2^2 \zeta + \psi_2), \\
E_3(\psi_1, \psi_2, \bar{\lambda}, \zeta) &= -\chi_1^4 \chi_2^4 \zeta^2 + \psi_1 \psi_2 \chi_1^4 + \psi_1 \chi_1^4 \chi_2^2 \zeta^2 - 2 \psi_1 \chi_1^4 \chi_2^2 \zeta^2 + \psi_1 \chi_1^4 \chi_2 \zeta^2 + \psi_1 \chi_1 \chi_2^2 \zeta^2 \\
&+ \psi_2 \chi_1 \chi_2 \zeta^2 + 2 \psi_1 \psi_2 \chi_1 \zeta^2 - \psi_1 \psi_2 m_1^2 m_2 \zeta^2 + 2 \psi_1 \psi_2 m_1^2 m_2 \zeta^2 - \psi_1 \psi_2 m_2^2 \zeta^2 + \psi_1 \psi_2 \chi_2 \zeta.
\end{align*}
Then
\begin{align*}
\mathcal{U}(\bar{\lambda}, \psi_1, \psi_2) &= \frac{m_2 - 1}{\chi_1(\psi_1, \psi_2, \bar{\lambda}, \zeta) + E_1^2}, \\
\mathcal{A}_U(\bar{\lambda}, \psi_1, \psi_2) &= \frac{\tau^2 E_1(\psi_1, \psi_2, \bar{\lambda}, \zeta) + E_1^2 E_1(\psi_1, \psi_2, \bar{\lambda}, \zeta)}{E_2(\psi_1, \psi_2, \bar{\lambda}, \zeta)}.
\end{align*}

**Remark 3** (Simplification of $\mathcal{T}$ and $\mathcal{A}_T$). Define $\zeta, \bar{\lambda}$ as the rescaled version of $\mu_3^2$ and $\lambda$ given by
\begin{align*}
\zeta &= \frac{\mu_3^2}{\mu_*^2}, \quad \bar{\lambda} = \frac{\lambda}{\mu_*^2}.
\end{align*}
Let $m_1(\cdot; \psi) m_2(\cdot; \psi): \mathbb{C}_+ \to \mathbb{C}_+$ be defined, for $\Im(\xi) \geq C$ a sufficiently large constant, as the unique solution of the equations
\begin{align*}
m_1 &= \psi_1 \left[ -\xi + (1 - \lambda_1) - m_2 + \frac{\zeta(1 - m_2)}{1 + \zeta m_1 - \zeta m_1 m_2} \right]^{-1}, \\
m_2 &= -\psi_2 \left[ \xi + m_1 + \frac{\zeta m_1}{1 + \zeta m_1 - \zeta m_1 m_2} \right]^{-1},
\end{align*}
subject to the condition $|m_1| \leq \psi_1/\Im(\xi)$, $|m_2| \leq \psi_2/\Im(\xi)$. Extend this definition to $\Im(\xi) > 0$ by requiring $m_1, m_2$ to be analytic functions in $\mathbb{C}_+$. Let
\begin{align*}
m_1 &= \lim_{u \to \infty} m_1(iu, \psi), \\
m_2 &= \lim_{u \to \infty} m_2(iu, \psi).
\end{align*}
Define
\begin{align*}
\chi_4 &= m_1 + \frac{m_1 \zeta}{\chi_1(m_1, m_2, \bar{\lambda})},
\end{align*}
and

\[ \chi_1 = m_1 \zeta - m_1 m_2 \zeta + 1, \]
\[ \chi_3 = \chi_1 + m_2 - 1 + \frac{\zeta (m_2 - 1)}{\chi_1}, \]

where the definitions of \( \chi_1, \chi_3 \) are the same as in Remark 2. Define three polynomials \( E_3, E_4, E_5 \) as

\[ E_4(\psi_1, \psi_2, \zeta) = \psi_1 \left( \psi_2 \chi_1^4 + \chi_1^4 \chi_4^2 m_2^2 \zeta^3 - 2 \chi_1^2 \chi_4^2 m_2^2 \zeta^3 + \chi_1^4 \chi_4 m_2^2 \zeta - 4 \chi_1^2 \chi_4 m_2^2 \zeta^2 + 2 \chi_1^2 \chi_4^2 m_2^5 + 4 \psi_2 \chi_1 \chi_4 m_2^2 \zeta - 2 \psi_1 \chi_1 \chi_4 m_2^2 \zeta - 2 \psi_2 \chi_1 \chi_4 m_2^2 \zeta^2 ight) \]
\[ E_5(\psi_1, \psi_2, \zeta) = m_1 \left( \chi_1^2 - m_1 \chi_1 \zeta + m_1 \zeta \right) \left( m_1 \zeta - m_1 m_2 \zeta + 1 \right)^2. \]

Then

\[ \mathcal{T}(\zeta, \psi_1, \psi_2) = -\frac{m_2 - 1}{\chi_1(\psi_1, \psi_2, \zeta)} \left( \frac{\tau^2 \chi_1(\psi_1, \psi_2, \zeta) + F_1^2}{\chi_1(\psi_1, \psi_2, \zeta)} \right), \]
\[ A_T(\zeta, \psi_1, \psi_2) = -\frac{F_1^2 E_4(\psi_1, \psi_2, \zeta)}{E_5(\psi_1, \psi_2, \zeta)}, \]

\[ \zeta = \mu_1^2 / \mu_2^2, \quad \rho = F_1^2 / \tau^2. \]

Let the functions \( \nu_1, \nu_2 : \mathbb{C}_+ \to \mathbb{C}_+ \) be uniquely defined by the following conditions: (i) \( \nu_1, \nu_2 \) are analytic on \( \mathbb{C}_+ \); (ii) For \( \Im(\xi) > 0, \nu_1(\xi), \nu_2(\xi) \) satisfy the following equations

\[ \nu_1 = \psi_1 \left( -\xi - \nu_2 - \frac{\zeta \nu_1}{1 - \zeta^2 \nu_1} \right)^{-1}, \]
\[ \nu_2 = \psi_2 \left( -\xi - \nu_1 - \frac{\zeta \nu_2}{1 - \zeta^2 \nu_2} \right)^{-1}. \]

(iii) \( (\nu_1(\xi), \nu_2(\xi)) \) is the unique solution of these equations with \( |\nu_1(\xi)| \leq \psi_1 / \Im(\xi), |\nu_2(\xi)| \leq \psi_2 / \Im(\xi) \) for \( \Im(\xi) > C, \)

with \( C \) a sufficiently large constant.

Let

\[ \chi \equiv \lim_{u \to 0} \nu_1(\imath u) \cdot \nu_2(\imath u), \]

and

\[ E_0(\zeta, \psi_1, \psi_2) = -\chi^5 \zeta^6 + 3 \chi^4 \zeta^4 + (\psi_1 \psi_2 - \psi_2 - \psi_1 + 1) \chi^3 \zeta^6 - 2 \chi^3 \zeta^4 - 3 \chi^3 \zeta^2 \]
\[ + (\psi_1 + \psi_2 - 3 \psi_1 \psi_2 + 1) \chi^2 \zeta^4 + 2 \chi^2 \zeta^2 + \chi^2 + 3 \psi_1 \psi_2 \chi \zeta - \psi_1 \psi_2, \]
\[ E_1(\zeta, \psi_1, \psi_2) = \psi_2 \chi^3 \zeta^4 - \psi_2 \chi^2 \zeta^2 + \psi_1 \psi_2 \chi \zeta^2 - \psi_1 \psi_2, \]
\[ E_2(\zeta, \psi_1, \psi_2) = \chi^5 \zeta^6 - 3 \chi^4 \zeta^4 + (\psi_1 - 1) \chi^3 \zeta^6 + 2 \chi^3 \zeta^4 + 3 \chi^3 \zeta^2 + (-\psi_1 - 1) \chi^2 \zeta^4 - 2 \chi^2 \zeta^2 - \chi^2. \]
Then the expression for the asymptotic risk of minimum norm interpolator gives
\[ R(\psi_1, \psi_2) = F_1^2 E_1(\zeta, \psi_1, \psi_2) E_0(\zeta, \psi_1, \psi_2) + \tau^2 E_2(\zeta, \psi_1, \psi_2) + \tau^2. \]

The expression for the norm of the minimum norm interpolator gives
\[ A_1 = \frac{\rho}{1 + \rho} \left[ -\chi^2(\chi\zeta^4 - \chi\zeta^2 + \psi_2\zeta^2 + \chi^2 - \chi\psi_2\zeta^4 + 1) + \frac{1}{1 + \rho} \left[ \chi^2(\chi\zeta^2 - 1)(\chi^2\zeta^4 - 2\chi\zeta^2 + \zeta^2 + 1) \right] \right], \]
\[ A_0 = -\chi^5\zeta^6 + 3\chi^4\zeta^4 + (\psi_1\psi_2 - \psi_2 - \psi_1 + 1)\chi^3\zeta^6 - 2\chi^3\zeta^4 - 3\chi^3\zeta^2 + (\psi_1 + \psi_2 - 3\psi_1\psi_2 + 1)\chi^2\zeta^4 + 2\chi^2\zeta^2 + \chi^2 + 3\psi_1\psi_2\psi_2^2 - \psi_1\psi_2, \]
\[ A(\psi_1, \psi_2) = \psi_1(F_1^2 + \tau^2) A_1/\mu^2 A_0. \]

B. Experimental setup for simulations in Figure 2

In this section, we present additional details for Figure 2. We choose \( y_i = \langle x_i, \beta \rangle \) for some \( \|\beta\|^2 = 1 \), the ReLU activation function \( \sigma(x) = \max\{x, 0\} \), and \( \psi_1 = N/d = 2.5 \) and \( \psi_2 = n/d = 1.5 \).

For the theoretical curves (in solid lines), we choose \( \lambda \in [0.426, 2] \), so that \( A_U(\lambda) \in [0, 15] \), and plot the parametric curve \( (A_U(\lambda), \Upsilon(\lambda) + \lambda A_U(\lambda)) \) for the uniform convergence. For the uniform convergence over interpolators, we choose \( \lambda \in [0.21, 2] \) so that \( A_T(\lambda) \in [6.4, 15] \), and plot \( (A_T(\lambda), \Upsilon(\lambda) + \lambda A_T(\lambda)) \). The definitions of these theoretical predictions are given in Definition 5, Remark 2 and Remark 3.

For the empirical simulations (in dots), first recall that in Proposition 2, we defined
\[ a_U(\lambda) = \arg\max_a \left[ R(a) - \hat{R}_n(a) - \psi_1 \lambda \|a\|^2 \right], \]
\[ a_T(\lambda) = \arg\max_a \inf_{\mu} \left[ R(a) - \lambda \psi_1 \|a\|^2 + 2\langle \mu, \zeta a - y/\sqrt{d} \rangle \right]. \]

After picking a value of \( \lambda \), we sample 20 independent problem instances, with the number of features \( N = 500 \), number of samples \( n = 300 \), covariate dimension \( d = 200 \). We compute the corresponding \( (\psi_1 \|a_U\|^2, R(a_U) - \hat{R}_n(a_U)) \) and \( (\psi_1 \|a_T\|^2, R(a_T)) \) for each instance. Then, we plot the empirical mean and \( 1/\sqrt{20} \) times the empirical standard deviation (around the mean) of each coordinate.

C. Proof of Proposition 1

The proof of Proposition 1 contains two parts: standard uniform convergence \( U \) and uniform convergence over interpolators \( T \). The proof for the two cases are essentially the same, both based on the fact that strong duality holds for quadratic program with single quadratic constraint (c.f. Boyd & Vandenberghe (2004), Appendix A.1).

C.1. Standard uniform convergence \( U \)

Recall that the uniform convergence bound \( U \) is defined as in Eq. (4)
\[ U(A, N, n, d) = \sup_{(N/d)\|a\|^2 \leq A} \left( R(a) - \hat{R}_n(a) \right). \]

Since the maximization problem in (4) is a quadratic program with a single quadratic constraint, the strong duality holds. So we have
\[ \sup_{(N/d)\|a\|^2 \leq A^2} R(a) - \hat{R}_n(a) = \inf_{\lambda \geq 0} \sup_a \left[ R(a) - \hat{R}_n(a) - \psi_1 \lambda (\|a\|^2 - \psi_1^{-1} A) \right]. \]

Finally, by the definition of \( \Upsilon \) as in Eq. (20), we get
\[ U(A, N, n, d) = \inf_{\lambda \geq 0} \left[ \Upsilon(\lambda, N, n, d) + \lambda A \right]. \]
C.2. Uniform convergence over interpolators $T$

Without loss of generality, we consider the regime when $N > n$. Recall that the uniform convergence over interpolators $T$ is defined as in Eq. (5)

$$T(A, N, n, d) = \sup_{(N/d)\|a\|_2^2 \leq A, \hat{R}_n(a) = 0} R(a).$$

When the set $\{a \in \mathbb{R}^N : (N/d)\|a\|_2^2 \leq A, \hat{R}_n(a) = 0\}$ is empty, we have

$$T(A, N, n, d) = \inf_{\lambda \geq 0} \left[ T(\lambda, N, n, d) + \lambda A \right] = -\infty.$$ 

In the following, we assume that the set $\{a \in \mathbb{R}^N : (N/d)\|a\|_2^2 \leq A, \hat{R}_n(a) = 0\}$ is non-empty, i.e., there exists $a \in \mathbb{R}^N$ such that $\hat{R}_n(a) = 0$ and $(N/d)\|a\|_2^2 \leq A$.

Let $m$ be the dimension of the null space of $Z \in \mathbb{R}^{n \times N}$, i.e. $m = \dim(\{u : Zu = 0\})$. Note that $Z \in \mathbb{R}^{N \times n}$ and $N > n$, we must have $N - n \leq m \leq N$. We let $R \in \mathbb{R}^{N \times m}$ be a matrix whose column space gives the null space of matrix $Z$. Let $a_0$ be the minimum norm interpolating solution (whose existence is given by the assumption that $\{a \in \mathbb{R}^N : \hat{R}_n(a) = 0\}$ is non-empty)

$$a_0 = \lim_{\lambda \to 0^+} \arg \min_{a \in \mathbb{R}^N} \left[ \hat{R}_n(a) + \lambda \|a\|_2^2 \right] = \arg \min_{a \in \mathbb{R}^N : \hat{R}_n(a) = 0} \|a\|_2^2.$$ 

Then we have

$$\{a \in \mathbb{R}^N : \hat{R}_n(a) = 0\} = \{a \in \mathbb{R}^N : y = \sqrt{d}Za\} = \{Ru + a_0 : u \in \mathbb{R}^m\}.$$ 

Then $T$ can be rewritten as a maximization problem in terms of $u$:

$$\sup_{(N/d)\|a\|_2^2 \leq A, \hat{R}_n(a) = 0} R(a) = \sup_{u \in \mathbb{R}^m : \|Ru + a_0\|_2^2 \leq \psi_1^{-1}A} \left[ \langle Ru + a_0, U(Ru + a_0) \rangle - 2\langle Ru + a_0, v \rangle + E(y^2) \right]$$

$$= R(a_0) + \sup_{u \in \mathbb{R}^m : \|Ru + a_0\|_2^2 \leq \psi_1^{-1}A} \left[ \langle u, R^\top Ur \rangle + 2\langle Ru, Ua_0 - v \rangle \right].$$ 

Note that the optimization problem only has non-feasible region when $A > (N/d)\|a_0\|_2^2$. By strong duality of quadratic programs with a single quadratic constraint, we have

$$\sup_{u \in \mathbb{R}^m : \|Ru + a_0\|_2^2 \leq \psi_1^{-1}A} \left[ \langle u, R^\top Ur \rangle + 2\langle Ru, Ua_0 - v \rangle \right]$$

$$= \inf_{\lambda \geq 0} \sup_{u \in \mathbb{R}^m} \left[ \langle u, R^\top Ur \rangle + 2\langle Ru, Ua_0 - v \rangle - \lambda(\psi_1\|Ru + a_0\|_2^2 - A) \right].$$ 

The maximization over $u$ can be restated as the maximization over $a$:

$$R(a_0) + \sup_{u \in \mathbb{R}^m} \left[ \langle u, R^\top Ur \rangle + 2\langle Ru, Ua_0 - v \rangle - \lambda\psi_1\|Ru + a_0\|_2^2 \right] = \sup_{a : \hat{R}_n(a) = 0} \left[ R(a) - \lambda\psi_1\|a\|_2^2 \right].$$ 

Moreover, since $\sup_{a : \hat{R}_n(a) = 0} [R(a) - \lambda\psi_1\|a\|_2^2]$ is a quadratic programming with linear constraints, we have

$$\sup_{a : \hat{R}_n(a) = 0} \left[ R(a) - \lambda\psi_1\|a\|_2^2 \right] = \sup_{a} \inf_{\mu} \left[ R(a) - \lambda\psi_1\|a\|_2^2 + 2\langle \mu, Za - y/\sqrt{d} \rangle \right].$$
Combining all the equality above and the definition of $T$ as in Eq. (21), we have

$$T(A, N, n, d) = \sup_{(N/d)\parallel a\parallel_2^2 \leq A, \hat{R}_n(a) = 0} R(a)$$

$$= R(a_0) + \sup_{u \in \mathbb{R}^m: \parallel Ru + a_0 \parallel_2^2 \leq \psi_i^{-1} A} \left[ (u, R^T U Ru) + 2(Ru, U a_0 - v) \right]$$

$$= R(a_0) + \inf_{\lambda \geq 0} \left\{ \lambda A + \sup_{u \sim \text{Unif}(S)} \left[ (u, R^T U Ru) + 2(Ru, U a_0 - v) - \lambda \psi_i \parallel Ru + a_0 \parallel_2^2 - A \right] \right\}$$

$$= \inf_{\lambda \geq 0} \left\{ \lambda A + \sup_{a: \hat{R}_n(a) = 0} \left[ R(a) - \lambda \psi_i \parallel a \parallel_2^2 \right] \right\}$$

$$= \inf_{\lambda \geq 0} \left[ T(\lambda, N, n, d) + \lambda A \right].$$

This concludes the proof.

**D. Proof of Proposition 2**

Note that the definitions of $\overline{U}$ and $\overline{T}$ as in Eq. (20) and (21) depend on $\beta = \beta^{(d)}$, where $\beta^{(d)}$ gives the coefficients of the target function $f_d(x) = \langle x, \beta^{(d)} \rangle$. Suppose we explicitly write their dependence on $\beta = \beta^{(d)}$, i.e., $\overline{U}(\lambda, N, n, d) = \overline{U}(\beta, \lambda, N, n, d)$ and $\overline{T}(\lambda, N, n, d) = \overline{T}(\beta, \lambda, N, n, d)$, then we can see that for any fixed $\beta$, we have $\overline{U}(\beta, \lambda, N, n, d) \triangleq \overline{U}(\lambda, \psi_2 + o_d, \sqrt{d})$ and $\overline{T}(\beta, \lambda, N, n, d) \triangleq \overline{T}(\lambda, \psi_2 + o_d, \sqrt{d})$, where the randomness comes from $X, \Theta, \varepsilon, \beta$. This is by the fact that the distribution of $x_i$'s and $\theta_i$'s are rotationally invariant. As a consequence, for any fixed deterministic $\beta$, we have $\overline{U}(\lambda, N, n, d) \triangleq \overline{U}(\lambda, N, n, d)$ and $\overline{T}(\lambda, N, n, d) \triangleq \overline{T}(\lambda, N, n, d)$ where the randomness comes from $X, \Theta, \varepsilon, \beta$.

Consequently, as long as we are able to show the equation

$$\overline{U}(\beta, \lambda, N, n, d) = \overline{U}(\beta, \lambda, N, n, d), \overline{T}(\beta, \lambda, N, n, d) = \overline{T}(\beta, \lambda, N, n, d),$$

for random $\beta \sim \text{Unif}(S^{d-1}(F_1))$, this equation will also hold for any deterministic $\beta$ with $\parallel \beta \parallel_2^2 = F_2^2$. Vice versa for $\overline{T}$.

As a result, in the following, we work with the assumption that $\beta = \beta^{(d)} \sim \text{Unif}(S^{d-1}(F_1))$. That is, in proving Proposition 2, we replace Assumption 1 by Assumption 6 below.

**Assumption 6 (Linear Target Function).** We assume that $f_d \in L^2(S^{d-1}(\sqrt{d}))$ with $f_d(x) = \langle \beta^{(d)}, x \rangle$, where $\beta^{(d)} \sim \text{Unif}(S^{d-1}(F_1))$.

**D.1. Expansions**

Denote $v = (v_i)_{i \in [N]} \in \mathbb{R}^N$ and $U = (U_{ij})_{i,j \in [N]} \in \mathbb{R}^{N \times N}$ where their elements are defined via

$$v_i \equiv E_x, \sigma(\langle x, \theta_i \rangle / \sqrt{d})], \quad U_{ij} \equiv E_x[\sigma(\langle x, \theta_i \rangle / \sqrt{d}) \sigma(\langle x, \theta_j \rangle / \sqrt{d})].$$

Here, $y = \langle x, \beta \rangle + \varepsilon$, where $\beta \sim \text{Unif}(S^{d-1}(F_1)), x \sim \text{Unif}(S^{d-1}(\sqrt{d})), \varepsilon \sim \mathcal{N}(0, \tau^2), \text{and } (\theta_i)_{i \in [N]} \sim \text{iid Unif}(S^{d-1}(\sqrt{d}))$ are mutually independent. The expectations are taken with respect to the test sample $x \sim \text{Unif}(S^{d-1}(\sqrt{d}))$ and $\varepsilon \sim \mathcal{N}(0, \tau^2)$ (especially, the expectations are conditional on $\beta$ and $(\theta_i)_{i \in [N]}$).
Moreover, we denote \( y = (y_1, \ldots, y_n)^T \in \mathbb{R}^n \) where \( y_i = (x_i, \beta) + \varepsilon_i \). Recall that \((x_i)_{i \in [n]} \sim \text{iid } \text{Unif}(S^{d - 1}(\sqrt{d})) \) and \((\varepsilon_i)_{i \in [n]} \sim \text{iid } \mathcal{N}(0, \tau^2) \) are mutually independent and independent from \( \beta \sim \text{Unif}(S^{d - 1}(\sqrt{d})) \). We further denote \( Z = (Z_{ij})_{i \in [n], j \in [N]} \) where its elements are defined via \( Z_{ij} = \sigma((x_i, \theta_j)/\sqrt{d})/\sqrt{d} \).

The population risk (1) can be reformulated as
\[
R(a) = \langle a, Ua \rangle - 2\langle a, v \rangle + \mathbb{E}[y^2],
\]
where \( a = (a_1, \ldots, a_N) \in \mathbb{R}^N \). The empirical risk (2) can be reformulated as
\[
\hat{R}_n(a) = \psi_2^{-1}(a, Z^2 a) - 2\psi_2^{-1}(Z^2 y, a) + \frac{1}{n}||y||_2^2.
\]

By the Appendix A in Mei & Montanari (2019) (we include in the Appendix F for completeness), we can expand \( \sigma(x) \) in terms of Gegenbauer polynomials
\[
\sigma(x) = \sum_{k=0}^{\infty} \lambda_{d,k}(\sigma) B(d, k)Q_k^{(d)}(\sqrt{d} \cdot x),
\]
where \( Q_k^{(d)} \) is the \( k \)’th Gegenbauer polynomial in \( d \) dimensions, \( B(d, k) \) is the dimension of the space of polynomials on \( S^{d - 1}(\sqrt{d}) \) with degree exactly \( k \). Finally, \( \lambda_{d,k}(\sigma) \) is the \( k \)’th Gegenbauer coefficient. More details of this expansion can be found in Appendix F.

By the properties of Gegenbauer polynomials (c.f. Appendix F.2), we have
\[
\mathbb{E}_{x \sim \text{Unif}(S^{d - 1}(\sqrt{d}))}[xQ_k((x, \theta_i))] = 0, \quad \forall k \neq 1,
\]
\[
\mathbb{E}_{x \sim \text{Unif}(S^{d - 1}(\sqrt{d}))}[xQ_1((x, \theta_i))] = \theta_i/d, \quad k = 1.
\]

As a result, we have
\[
v_i = \mathbb{E}_{x \sim \text{Unif}(S^{d - 1}(\sqrt{d}))}[y\sigma((x, \theta_i)/\sqrt{d})] = \sum_{k=0}^{\infty} \lambda_{d,k}(\sigma) B(d, k)\mathbb{E}_x[x, \beta]Q_k^{(d)}(\sqrt{d} \cdot x) = \lambda_{d,1}(\sigma)\langle \theta_i, \beta \rangle.
\]

D.2. Removing the perturbations

By Lemma 6 and 7 as in Appendix D.6, we have the following decomposition
\[
U = \mu_1^2Q + \mu_2^2I_N + \Delta,
\]
with \( Q = \Theta \Theta^T/d, \mathbb{E}[\|\Delta\|^2_{op}] = o_d(1) \), and \( \mu_1^2 \) and \( \mu_2^2 \) are given in Assumption 2.

In the following, we would like to show that \( \Delta \) has vanishing effects in the asymptotics of \( \overline{U}, \overline{T}, \|\overline{a}_U\|_2^2 \) and \( \|\overline{a}_T\|_2^2 \).

For this purpose, we denote
\[
U_c = \mu_1^2Q + \mu_2^2I_N,
\]
\[
R_c(a) = \langle a, Ua \rangle - 2\langle a, v \rangle + \mathbb{E}[y^2],
\]
\[
\hat{R}_{c,n}(a) = \langle a, \psi_2^{-1}Z^2 a \rangle - 2\langle a, \psi_2^{-1}Z^2 y/\sqrt{d} \rangle + \mathbb{E}[y^2],
\]
\[
\overline{U}_c(\lambda, N, n, d) = \sup_a \left(R_c(a) - \hat{R}_{c,n}(a) - \psi_1\lambda\|a\|_2^2\right),
\]
\[
\overline{T}_c(\lambda, N, n, d) = \sup_a \inf_{\mu} \left[R_c(a) - \lambda\psi_1\|a\|_2^2 + 2\langle \mu, Za - y/\sqrt{d} \rangle\right].
\]
For a fixed $\lambda \in \Lambda_U$, note we have
\begin{align}
\bar{U}_c(\lambda, N, n, d) &= \sup_a \left( \langle a, (U_c - \psi_2^{-1}Z^T\lambda\mathbf{I}_N) a \rangle - 2\langle a, v - \psi_2^{-1}\frac{Z^Ty}{\sqrt{d}} \rangle \right) \\
&= \sup_a \left( \langle a, \mathbf{M} a \rangle - 2\langle a, v \rangle \right)
\end{align}
(37)
where $\mathbf{M} = U_c - \psi_2^{-1}Z^T\lambda\mathbf{I}_N$ and $v = v - \psi_2^{-1}\frac{Z^Ty}{\sqrt{d}}$. When $X, \Theta$ are such that the good event in Assumption 4 happens (which says that $\mathbf{M} \preceq -\epsilon\mathbf{I}_N$ for some $\epsilon > 0$), the inner maximization can be uniquely achieved at
\[ \bar{a}_{U,c}(\lambda) = \arg\max_a \left( \langle a, \mathbf{M} a \rangle - 2\langle a, v \rangle \right) = \mathbf{M}^{-1}v. \]
(38)
and when the good event $\{ \|\Delta\|_{op} \leq \epsilon/2 \}$ also happens, the maximizer in the definition of $U(\lambda, N, n, d)$ (c.f. Eq. (20)) can be uniquely achieved at
\[ \bar{a}_U(\lambda) = \arg\max_a \left( \langle a, (\mathbf{M} + \Delta) a \rangle - 2\langle a, v \rangle \right) = (\mathbf{M} + \Delta)^{-1}v. \]
Note we have
\[ \|\bar{a}_U(\lambda) - \bar{a}_{U,c}(\lambda)\|_2 \leq \| (\mathbf{M} + \Delta)^{-1} \Delta \|_{op} \| \bar{a}_{U,c}(\lambda) \|_2, \]
so by the fact that $\|\Delta\|_{op} = o_d, p(1)$, we have
\[ \| \bar{a}_U(\lambda) - \bar{a}_{U,c}(\lambda) \|_2 \leq \| (\mathbf{M} + \Delta)^{-1} \Delta \|_{op} \| \bar{a}_{U,c}(\lambda) \|_2 = o_d, p(1) \| \bar{a}_{U,c}(\lambda) \|_2. \]
This gives $\| \bar{a}_U(\lambda) \|_2^2 = (1 + o_d, p(1)) \| \bar{a}_{U,c}(\lambda) \|_2^2$.
Moreover, by the fact that $\|\Delta\|_{op} = o_d, p(1)$, we have
\begin{align*}
\bar{U}_c(\lambda, N, n, d) &= \sup_a \left( \langle \hat{R}(a) - \hat{R}_n(a) - \psi_1\lambda\|a\|_2^2 - \langle a, \Delta a \rangle \rangle + \mathbb{E}[y^2] - \|y\|_2^2/n \right) \\
&= \bar{U}(\lambda, N, n, d) + o_d, p(1)(\| \bar{a}_{U,c}(\lambda) \|_2^2 + 1). 
\end{align*}
As a consequence, as long as we can prove the asymptotics of $\bar{U}_c$ and $\| \bar{a}_{U,c}(\lambda) \|_2^2$, it also gives the asymptotics of $\bar{U}$ and $\| \bar{a}_U(\lambda) \|_2^2$. Vice versa for $\bar{T}$ and $\| \bar{a}_T(\lambda) \|_2^2$.

**D.3. The asymptotics of $\bar{U}_c$ and $\psi_1 \| \bar{a}_{U,c}(\lambda) \|_2^2$**

In the following, we derive the asymptotics of $\bar{U}_c(\lambda, N, n, d)$ and $\psi_1 \| \bar{a}_{U,c}(\lambda) \|_2^2$. When we refer to $\bar{a}_{U,c}(\lambda)$, it is always well defined with high probability, since it can be well defined under the condition that the good event in Assumption 4 happens. Note that this good event only depend on $X, \Theta$ and is independent of $\beta, \epsilon$.

By Eq. (37) and (38), simple calculation shows that
\[ \bar{U}_c(\lambda, N, n, d) = -\langle v, \mathbf{M}^{-1}v \rangle = -\Psi_1 - \Psi_2 - \Psi_3, \]
\[ \| \bar{a}_{U,c} \|_2^2 = \langle v, \mathbf{M}^{-2}v \rangle = \Phi_1 + \Phi_2 + \Phi_3, \]
where
\[ \Psi_1 = \langle v, \mathbf{M}^{-1}v \rangle, \quad \Psi_2 = -2\psi_2^{-1}\langle \frac{Z^Ty}{\sqrt{d}}, \mathbf{M}^{-1}v \rangle, \quad \Psi_3 = \psi_2^{-2}\langle \frac{Z^Ty}{\sqrt{d}}, \mathbf{M}^{-1}Z^Ty \rangle, \]
\[ \Phi_1 = \langle v, \mathbf{M}^{-2}v \rangle, \quad \Phi_2 = -2\psi_2^{-1}\langle \frac{Z^Ty}{\sqrt{d}}, \mathbf{M}^{-2}v \rangle, \quad \Phi_3 = \psi_2^{-2}\langle \frac{Z^Ty}{\sqrt{d}}, \mathbf{M}^{-2}Z^Ty \rangle. \]

The following lemma gives the expectation of $\Psi_i$’s and $\Phi_i$’s with respect to $\beta$ and $\epsilon$. 

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**Generalization Error of Random Features Models**
Furthermore, we have

\[ \begin{align*}
\mathbb{E}_{\epsilon, \beta}[\Psi_1] &= \mu_2^* F_1^2 \cdot \frac{1}{d} \mathrm{Tr}(M^{-1} Q) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Psi_2] &= -\frac{2F_2^2}{\psi_2} \cdot \frac{1}{d} \mathrm{Tr}(ZM^{-1} Z^T) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Psi_3] &= \frac{F_1^2}{\psi_2^2} \cdot \frac{1}{d} \mathrm{Tr}(\frac{ZM^{-1} Z^T}{2}) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_1] &= \mu_2^* F_1^2 \cdot \frac{1}{d} \mathrm{Tr}(M^{-2} Q) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_2] &= -\frac{2F_2^2}{\psi_2} \cdot \frac{1}{d} \mathrm{Tr}(ZM^{-2} Z^T) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_3] &= \frac{F_1^2}{\psi_2^2} \cdot \frac{1}{d} \mathrm{Tr}(\frac{ZM^{-2} Z^T}{2}) \times (1 + o_d(1)), \\
\end{align*} \]

Here the definitions of \( Q, H, \) and \( Z_1 \) are given by Eq. (19).

Furthermore, we have

\[ \begin{align*}
\mathbb{E}_{\epsilon, \beta}[\Psi_1] &= \mu_1^2 F_1^2 \cdot \partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Psi_2] &= F_1^2 \cdot \partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Psi_3] &= F_1^2 \cdot (\partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) - 1) + \tau^2 \cdot (\partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) - 1), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_1] &= -\mu_1^2 F_1^2 \cdot \partial_{\epsilon_2} \partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_2] &= -F_1^2 \cdot \partial_{\epsilon_2} \partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) \times (1 + o_d(1)), \\
\mathbb{E}_{\epsilon, \beta}[\Phi_3] &= -F_1^2 \cdot \partial_{\epsilon_2} \partial_{\epsilon_2} \partial_{\epsilon_2} G_d(0_+; q_U(\lambda, \psi)) \times (1 + o_d(1)), \\
\end{align*} \]

The definition of \( G_d \) is as in Definition 1, and \( \nabla^k_q G_d(0_+; q) \) for \( k \in \{1, 2\} \) stands for the \( k \)'th derivatives (as a vector or a matrix) of \( G_d(iu; q) \) with respect to \( q \) in the \( u \rightarrow 0^+ \) limit (with its elements given by partial derivatives)

\[ \nabla^k_q G_d(0_+; q) = \lim_{u \to 0^+} \nabla_q G_d(iu; q). \]

We next state the asymptotic characterization of the log-determinant which was proven in (Mei & Montanari, 2019).

**Proposition 3** (Proposition 8.4 in (Mei & Montanari, 2019)). Define

\[ \begin{align*}
\Xi(\xi, z_1, z_2; q; \psi) &\equiv \log[(s_2 z_1 + 1)(t_2 z_2 + 1) - \mu_1^2 (1 + p)^2 z_1 z_2 - \mu_2^2 z_1 z_2 \\
&\quad + s_1 z_1 + t_1 z_2 - \psi_1 \log(z_1 / \psi_1) - \psi_2 \log(z_2 / \psi_2) - \xi(z_1 + z_2) - \psi_1 - \psi_2. \\
\end{align*} \]

(39)

For \( \xi \in \mathbb{C}_+ \) and \( q \in \mathbb{Q} \) (c.f. Eq. (25)), let \( m_1(\xi; q; \psi), m_2(\xi; q; \psi) \) be defined as the analytic continuation of solution of Eq. (26) as defined in Definition 3. Define

\[ g(\xi; q; \psi) = \Xi(\xi, m_1(\xi; q; \psi), m_2(\xi; q; \psi); q; \psi). \]

(40)

Consider proportional asymptotics \( N/d \to \psi_1, N/d \to \psi_2, \) as per Assumption 3. Then for any fixed \( \xi \in \mathbb{C}_+ \) and \( q \in \mathbb{Q}, \) we have

\[ \lim_{d \to \infty} \mathbb{E}[|G_d(\xi; q) - g(\xi; q; \psi)|] = 0. \]

(41)

Moreover, for any fixed \( u \in \mathbb{R}_+ \) and \( q \in \mathbb{Q}, \) we have

\[ \lim_{d \to \infty} \mathbb{E}[|\partial_q G_d(iu; q) - \partial_q g(iu; q; \psi)|] = 0, \]

(42)

\[ \lim_{d \to \infty} \mathbb{E}[|\nabla^2_q G_d(iu; q) - \nabla^2_q g(iu; q; \psi)|_{op}] = 0. \]

(43)

**Remark 4.** Note that Proposition 8.4 in (Mei & Montanari, 2019) stated that the Eq. (42) and (43) holds at \( q = 0. \) However, by a simple modification of their proof, one can show that these equations also holds at any \( q \in \mathbb{Q}. \)
Combining Assumption 5 with Proposition 3, we have

**Proposition 4.** Let Assumption 5 holds. For any \( \lambda \in \Lambda_U \), denote \( q_U = q_U(\lambda, \psi) = (\mu_2^2 - \lambda \psi_1, \mu_1^2, \psi_2, 0, 0) \), then we have, for \( k = 1, 2 \),

\[
\|\nabla_q G_d(0^+; q_U) - \lim_{u \to 0^+} \nabla^k q(iu; q_U; \psi)\| = o_{d, \mathbb{P}}(1).
\]

As a consequence of Proposition 4, we can calculate the asymptotics of \( \Psi_1 \)'s and \( \Phi_1 \)'s. Combined with the concentration result in Lemma 2 latter in the section, the proposition below completes the proof of the part of Proposition 2 regarding the standard uniform convergence \( U \). Its correctness follows directly from Lemma 1 and Proposition 4.

**Proposition 5.** Follow the assumptions of Proposition 2. For any \( \lambda \in \Lambda_U \), denote \( q_U(\lambda, \psi) = (\mu_2^2 - \lambda \psi_1, \mu_1^2, \psi_2, 0, 0) \), then we have

\[
\mathbb{E}_{\varepsilon, \beta}[\Psi_1] \overset{p}{\to} \mu_2^2 F_1 \cdot \partial_{u_2} g(0^+; q_U(\lambda, \psi); \psi),
\]
\[
\mathbb{E}_{\varepsilon, \beta}[\Psi_2] \overset{p}{\to} F_2^2 \cdot \partial_{u_2} g(0^+; q_U(\lambda, \psi); \psi),
\]
\[
\mathbb{E}_{\varepsilon, \beta}[\Psi_3] \to F_2^2 \cdot \left( \partial_{u_2} g(0^+; q_U(\lambda, \psi); \psi) - 1 \right) + \tau^2 \left( \partial_{u_1} g(0^+; q_U(\lambda, \psi); \psi) - 1 \right),
\]
\[
\mathbb{E}_{\varepsilon, \beta}[\Phi_1] \overset{p}{\to} - \mu_2^2 F_1 \cdot \partial_{u_1} g(0^+; q_U(\lambda, \psi); \psi),
\]
\[
\mathbb{E}_{\varepsilon, \beta}[\Phi_2] \overset{p}{\to} - F_2^2 \cdot \partial_{u_1} g(0^+; q_U(\lambda, \psi); \psi),
\]
\[
\mathbb{E}_{\varepsilon, \beta}[\Phi_3] \overset{p}{\to} - F_2^2 \cdot \partial_{u_1} g(0^+; q_U(\lambda, \psi); \psi) - \tau^2 \cdot \partial_{u_1} g(0^+; q_U(\lambda, \psi); \psi),
\]

where \( \nabla^k q(iu; q_U; \psi) \) for \( k \in \{1, 2\} \) stands for the \( k \)'th derivatives (as a vector or a matrix) of \( g(iu; q_U; \psi) \) with respect to \( q \) in the \( u \to 0^+ \) limit (with its elements given by partial derivatives)

\[
\nabla^k q(iu; q_U; \psi) = \lim_{u \to 0^+} \nabla^k q(iu; q_U; \psi).
\]

As a consequence, we have

\[
\mathbb{E}_{\varepsilon, \beta}[\mathcal{U}_c(\lambda, N, n, d)] \overset{p}{\to} \mathcal{U}(\lambda, \psi_1, \psi_2), \quad \mathbb{E}_{\varepsilon, \beta}[\mathbb{I}_U, c(\lambda)] \overset{p}{\to} A_U(\lambda, \psi_1, \psi_2),
\]

where the definitions of \( \mathcal{U} \) and \( A_U \) are given in Definition 5. Here \( \overset{p}{\to} \) stands for convergence in probability as \( N/d \to \psi_1 \) and \( n/d \to \psi_2 \) (with respect to the randomness of \( X \) and \( \Theta \)).

**Lemma 2.** Follow the assumptions of Proposition 2. For any \( \lambda \in \Lambda_U \), we have

\[
\text{Var}_{\varepsilon, \beta}[\Psi_1], \text{Var}_{\varepsilon, \beta}[\Psi_2], \text{Var}_{\varepsilon, \beta}[\Psi_3] = o_d, \mathbb{P}(1),
\]
\[
\text{Var}_{\varepsilon, \beta}[\Phi_1], \text{Var}_{\varepsilon, \beta}[\Phi_2], \text{Var}_{\varepsilon, \beta}[\Phi_3] = o_d, \mathbb{P}(1),
\]

so that

\[
\text{Var}_{\varepsilon, \beta}[\mathcal{U}_c(\lambda, N, n, d)], \text{Var}_{\varepsilon, \beta}[\mathbb{I}_U, c(\lambda)] \overset{p}{\to} o_d, \mathbb{P}(1).
\]

Here, \( o_d, \mathbb{P}(1) \) stands for converges to 0 in probability (with respect to the randomness of \( X \) and \( \Theta \)) as \( N/d \to \psi_1 \) and \( n/d \to \psi_2 \) and \( d \to \infty \).
For a fixed $\lambda \in \Lambda_T$, recalling that the definition of $T_c$ as in Eq. (36), we have
\[
T_c(\lambda, N, n, d) = \sup_{a} \inf_{\mu} \left\{ R_c(a) - \lambda \psi_1 \|a\|_2^2 + 2\langle \mu, Z a - y/\sqrt{d} \rangle \right\}
\]
\[
= \sup_{a} \inf_{\mu} \left( \langle a, (U_c - \lambda \psi_1 I_N) a \rangle - 2\langle a, v \rangle + 2\langle \mu, Z a \rangle - 2\langle \mu, y/\sqrt{d} \rangle \right) + \mathbb{E}[y^2]
\]
\[
= \sup_{\sqrt{d} Z a = y} \langle a, (U_c - \lambda \psi_1 I_N) a \rangle - 2\langle a, v \rangle + \mathbb{E}[y^2]
\]
(44)
Whenever the good event in Assumption 4 happens, $(U_c - \lambda \psi_1 I_N)$ is negative definite in $\text{null}(Z)$. The optimum of the above variational equation exists. By KKT condition, the optimal $a$ and dual variable $\mu$ satisfies

- Stationary condition: $(U_c - \lambda \psi_1 I_N) a + Z^T \mu = v$.
- Primal Feasible: $Z a = y/\sqrt{d}$.

The two conditions can be written compactly as
\[
\begin{bmatrix}
U_c - \psi_1 I_N \\
Z
\end{bmatrix}
\begin{bmatrix}
a \\
\mu
\end{bmatrix}
= \begin{bmatrix}
v \\
y/\sqrt{d}
\end{bmatrix}.
\]
(45)
We define
\[
\begin{bmatrix}
U_c - \psi_1 I_N \\
Z
\end{bmatrix}
\begin{bmatrix}
a \\
\mu
\end{bmatrix}
= \begin{bmatrix}
v \\
y/\sqrt{d}
\end{bmatrix} = \nu.
\]
(46)
Under Assumption 4, $\overline{M}$ is invertible. To see this, suppose there exists vector $[a_1^T, \mu_1^T] \neq 0 \in \mathbb{R}^{N+n}$ such that $\overline{M}[a_1^T, \mu_1^T] = 0$, then
\[
(U_c - \lambda \psi_1 I_N) a_1 + Z^T \mu_1 = 0,
\]
$Z a_1 = 0$.

As in Assumption 4, let $P_{\text{null}} = I_N - Z^T Z$. We write $a_1 = P_{\text{null}} v_1$ for some $v_1 \neq 0 \in \mathbb{R}^N$. Then,
\[
(U_c - \lambda \psi_1 I_N) P_{\text{null}} v_1 + Z^T \mu_1 = 0,
\]
\[
\Rightarrow P_{\text{null}} (U_c - \lambda \psi_1 I_N) P_{\text{null}} v_1 + P_{\text{null}} Z^T \mu_1 = 0,
\]
\[
\Rightarrow P_{\text{null}} (U_c - \lambda \psi_1 I_N) P_{\text{null}} v_1 = 0,
\]
where the last relation come from the fact that $Z P_{\text{null}} = 0$. However by Assumption 4, $P_{\text{null}} (U_c - \lambda \psi_1 I_N) P_{\text{null}}$ is negative definite, which leads to a contradiction.

In the following, we assume the event in Assumption 4 happens so that $\overline{M}$ is invertible. In this case, the maximizer in Eq. (44) can be well defined as
\[
\overline{a}_{T,c}(\lambda) = [I_N, 0_{N \times n}] \overline{M}^{-1} \nu.
\]
Moreover, we can write $T_c$ as
\[
T_c(\lambda, N, n, d) = \mathbb{E}[y^2] - \nu^T \overline{M}^{-1} \nu.
\]
We further define
\[
\overline{v}_1 = [v^T, 0_{n \times 1}^T], \quad \overline{v}_2 = [0_{N \times 1}^T, y^T/\sqrt{d}]^T, \quad E = \begin{bmatrix} I_N & 0_{N \times n} \\ 0_{n \times N} & 0_{n \times n} \end{bmatrix}.
\]
Simple calculation shows that
\[
\overline{T}_c(\lambda, N, n, d) = \mathbb{E}[y^2] - \langle \overline{v}, \overline{M}^{-1} \overline{v} \rangle = F_1^2 + \tau^2 - \Psi_1 - \Psi_2 - \Psi_3,
\]
\[
\|\overline{a}_{U,c}\|_2^2 = \langle \overline{v}, \overline{M}^{-1} E \overline{M}^{-1} \overline{v} \rangle = \Phi_1 + \Phi_2 + \Phi_3,
\]
where
\[
\Psi_1 = \langle \overline{v}_1, \overline{M}^{-1} \overline{v}_1 \rangle, \quad \Phi_1 = \langle \overline{v}_1, \overline{M}^{-1} E \overline{M}^{-1} \overline{v}_1 \rangle,
\]
\[
\Psi_2 = 2\langle \overline{v}_2, \overline{M}^{-1} \overline{v}_1 \rangle, \quad \Phi_2 = 2\langle \overline{v}_2, \overline{M}^{-1} E \overline{M}^{-1} \overline{v}_1 \rangle,
\]
\[
\Psi_3 = \langle \overline{v}_2, \overline{M}^{-1} \overline{v}_2 \rangle, \quad \Phi_3 = \langle \overline{v}_2, \overline{M}^{-1} E \overline{M}^{-1} \overline{v}_2 \rangle.
\]
The following lemma gives the expectation of $\Psi_i$’s and $\Phi_i$’s with respect to $\beta$ and $\epsilon$. 
The definition of $\Psi$ is as in Definition 1, and $\nabla_q^k G_d(0_+; q)$ for $k \in \{1, 2\}$ stands for the $k$'th derivatives (as a vector or a matrix) of $G_d(iu; q)$ with respect to $q$ in the $u \to 0+$ limit (with its elements given by partial derivatives)

$$\nabla_q^k G_d(0_+; q) = \lim_{u \to 0+} \nabla_q^k G_d(iu; q).$$

The proof of Lemma 3 follows from direct calculation and is identical to the proof of Lemma 1. Combining Assumption 5 with Proposition 3, we have

**Proposition 6.** Let Assumption 5 holds. For any $\lambda \in \Lambda_T$, denote $q_T = q_T(\lambda, \psi) = (\mu_2^2 - \lambda \psi_1, \mu_1^2, 0, 0, 0)$, then we have

$$(\lambda, \psi) = (\mu_2^2 - \lambda \psi_1, \mu_1^2, 0, 0, 0), \quad \text{then we have for} \ k = 1, 2,

\|\nabla_q^k G_d(0_+; q_T) - \lim_{u \to 0+} \nabla_q^k g(iu; q_T; \psi)\| = o_{d,p}(1).$$

As a consequence of Proposition 6, we can calculate the asymptotics of $\Psi_i$'s and $\Phi_i$'s.

**Proposition 7.** Follow the assumptions of Proposition 2. For any $\lambda \in \Lambda_T$, denote $q_T = q_T(\lambda, \psi) = (\mu_2^2 - \lambda \psi_1, \mu_1^2, 0, 0, 0)$, then we have

$$\begin{align*}
\mathbb{E}_{\varepsilon, \beta}[\Psi_1] &\xrightarrow{p} \mu_2^2 F_1^2 \cdot \partial_{x_2} g(0_+; q_T(\lambda, \psi); \psi), \\
\mathbb{E}_{\varepsilon, \beta}[\Psi_2] &\xrightarrow{p} F_1^2 \cdot \partial_p g(0_+; q_T(\lambda, \psi); \psi), \\
\mathbb{E}_{\varepsilon, \beta}[\Psi_3] &\xrightarrow{p} F_1^2 \cdot \partial_{x_2} g(0_+; q_T(\lambda, \psi); \psi) + \tau^2 \cdot \partial_{x_1} g(0_+; q_T(\lambda, \psi); \psi), \\
\mathbb{E}_{\varepsilon, \beta}[\Phi_1] &\xrightarrow{p} - \mu_1^2 F_1^2 \cdot \partial_{x_1} \partial_{x_2} g(0_+; q_T(\lambda, \psi); \psi), \\
\mathbb{E}_{\varepsilon, \beta}[\Phi_2] &\xrightarrow{p} - F_1^2 \cdot \partial_{x_1} \partial_p g(0_+; q_T(\lambda, \psi); \psi), \\
\mathbb{E}_{\varepsilon, \beta}[\Phi_3] &\xrightarrow{p} - F_1^2 \cdot \partial_{x_1} \partial_{x_2} g(0_+; q_T(\lambda, \psi); \psi) - \tau^2 \cdot \partial_{x_1} \partial_{x_1} g(0_+; q_T(\lambda, \psi); \psi),
\end{align*}$$

where $\nabla_q^k g(0_+; q_T; \psi)$ for $k \in \{1, 2\}$ stands for the $k$'th derivatives (as a vector or a matrix) of $g(iu; q; \psi)$ with respect to $q$ in the $u \to 0+$ limit (with its elements given by partial derivatives)

$$\nabla_q^k g(0_+; q_T; \psi) = \lim_{u \to 0+} \nabla_q^k g(iu; q_T; \psi).$$

As a consequence, we have

$$\begin{align*}
\mathbb{E}_{\varepsilon, \beta}[T_c(\lambda, N, n, d)] &\xrightarrow{p} T(\lambda, \psi_1, \psi_2), \\
\mathbb{E}_{\varepsilon, \beta}[\mathcal{P} ||a_T(\lambda)||^2_2] &\xrightarrow{p} A_T(\lambda, \psi_1, \psi_2),
\end{align*}$$

where the definitions of $T$ and $A_T$ are given in Definition 5. Here $\xrightarrow{p}$ stands for convergence in probability as $N/d \to \psi_1$ and $n/d \to \psi_2$ (with respect to the randomness of $X$ and $\Theta$).

The Proposition above suggests that $\Psi_i$ and $\Phi_i$ concentrates with respect to the randomness in $X$ and $\Theta$. To complete the concentration proof, we need to show that $\Psi_i$ and $\Phi_i$ concentrates with respect to the randomness in $\beta$ and $\varepsilon$.

**Lemma 4.** Follow the assumptions of Proposition 2. For any $\lambda \in \Lambda_T$, we have

$$\begin{align*}
\text{Var}_{\varepsilon, \beta}[\Psi_1], \text{Var}_{\varepsilon, \beta}[\Psi_2], \text{Var}_{\varepsilon, \beta}[\Psi_3] &= o_{d,p}(1), \\
\text{Var}_{\varepsilon, \beta}[\Phi_1], \text{Var}_{\varepsilon, \beta}[\Phi_2], \text{Var}_{\varepsilon, \beta}[\Phi_3] &= o_{d,p}(1),
\end{align*}$$

where the definitions of $T$ and $A_T$ are given in Definition 5. Here $\xrightarrow{p}$ stands for convergence in probability as $N/d \to \psi_1$ and $n/d \to \psi_2$ (with respect to the randomness of $X$ and $\Theta$).
so that

$$\text{Var}_{\epsilon, \beta} \left[ T_c(\lambda, N, n, d) \right], \text{Var}_{\epsilon, \beta} \left[ \| a_{T,c}(\lambda) \|_2^2 \right] = o_{d,p}(1).$$

Here, $o_{d,p}(1)$ stands for converges to 0 in probability (with respect to the randomness of $X$ and $\Theta$) as $N/d \rightarrow \psi_1$ and $n/d \rightarrow \psi_2$ and $d \rightarrow \infty$.

Now, combining Proposition 7 and 4, we have

$$\mathcal{T}_c(\lambda, N, n, d) \xrightarrow{p} \mathcal{T}(\lambda, \psi_1, \psi_2), \quad \psi_1 \| a_{T,c}(\lambda) \|_2^2 \xrightarrow{p} A_T(\lambda, \psi_1, \psi_2).$$

The results above combined with the arguments in Appendix D.2 completes the proof for the asymptotics of $\mathcal{T}$ and $\psi_1 \| a_T(\lambda) \|_2^2$.

D.5. Proof of Lemma 1 and Lemma 2

Proof of Lemma 1. Note that by Assumption 4, the matrix $\mathcal{M} = U_c - \psi_2^{-1} Z^T Z - \psi_1 I_N$ is negative definite (so that it is invertible) with high probability. Moreover, whenever $\mathcal{M}$ is negative definite, the matrix $A(q_U)$ for $q_U = (\mu_2^2 - \lambda \psi_1, \mu_2^2, \psi_2, 0, 0)$ is also invertible. In the following, we condition on this good event happens.

From the expansion for $v_1$ in (34), we have

$$\mathbb{E}_{\beta, \epsilon} \Psi_1 = \mathbb{E}_{\beta, \epsilon} \left[ \text{Tr} \left( \mathcal{M}^{-1} \nu \nu^T \right) \right] = \frac{1}{d} \lambda_{d,1} \sigma^2 F_1^2 \cdot \left[ \text{Tr} \left( \mathcal{M}^{-1} \Theta \Theta^T \right) \right] = \frac{1}{d} \mu_1^2 F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-1} \Theta \Theta^T \right) \times (1 + o_d(1)),$n

where we used the relation $\lambda_{d,1} = \mu_1 / \sqrt{d} \times (1 + o_d(1))$ as in Eq. (66). Similarly, the second term is

$$\mathbb{E}_{\beta, \epsilon} \Psi_2 = - \frac{2}{\psi_2 \sqrt{d}} \mathbb{E}_{\beta, \epsilon} \left[ \text{Tr} \left( \mathcal{M}^{-1} \nu y^T \right) \right] = - \frac{2}{\psi_2 \sqrt{d}} \lambda_{d,1} \sigma^2 F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-1} \Theta X^T \right) = - \frac{2}{\psi_2 \sqrt{d}} \mu_1^2 F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-1} \Theta X^T \right) \times (1 + o_d(1)).$$

To compute $\Psi_3$, note we have

$$\mathbb{E}_{\beta, \epsilon} [yy^T] = F_2^2 \cdot (XX^T)/d + \tau^2 I_n.$$

This gives the expansion for $\Psi_3$

$$\mathbb{E}_{\beta, \epsilon} \Psi_3 = \psi_2^{-2} d^{-1} \mathbb{E}_{\beta, \epsilon} \text{Tr} \left( \mathcal{M}^{-1} Z^T yy^T \right) = \psi_2^{-2} d^{-1} F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-1} Z^T X X^T \right) + \psi_2^{-2} d^{-1} \text{Tr} \left( \mathcal{M}^{-1} Z \right) \tau^2.$$

Through the same algebraic manipulation above, we have

$$\mathbb{E}_{\beta, \epsilon} \Phi_1 = \frac{1}{d} \mu_2^2 F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-2} \Theta \Theta^T \right) \times (1 + o_d(1)),$n

$$\mathbb{E}_{\beta, \epsilon} \Phi_2 = - \frac{2}{\psi_2 \sqrt{d}} \mu_1 F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-2} \Theta X^T \right) \times (1 + o_d(1)),$n

$$\mathbb{E}_{\beta, \epsilon} \Phi_3 = \psi_2^{-2} d^{-2} F_1^2 \cdot \text{Tr} \left( \mathcal{M}^{-2} Z^T X X^T \right) + \psi_2^{-2} d^{-2} \tau^2 \text{Tr} \left( \mathcal{M}^{-2} Z \right).$$

Next, we express the trace of matrices products as the derivative of the function $G_d(\xi, q)$ (c.f. Definition 1). The derivatives of $G_d$ are (which can we well-defined at $q = q_U = (\mu_2^2 - \lambda \psi_1, \mu_2^2, \psi_2, 0, 0)$ with high probability by Assumption 4)

$$\partial_q G_d(0, q) = \frac{1}{d} \text{Tr}(A(q)^{-1} \partial_q A(q)), \quad \partial_q \partial_q G_d(0, q) = - \frac{1}{d} \text{Tr}(A(q)^{-1} \partial_q A(q) A(q)^{-1} \partial_q A(q)). \quad (47)$$
As an example, we consider evaluating $\partial_{x_2}G_d(0, q)$ at $q = q_U \equiv (\mu^2 - \lambda \psi_1, \mu^2, \psi_2, 0, 0)$. Using the formula for block matrix inversion, we have

$$A(\mu^2 - \lambda \psi_1, \mu^2, \psi_2, 0, 0)^{-1} = \left[ \begin{array}{cc} \mu^2 - \lambda \psi_1 & \mu^2 Q \\ Z & \psi_2 I_n \end{array} \right]^{-1} = \left[ \begin{array}{cc} (U_c - \psi_2^{-1}Z^TZ - \psi_1^{-1}I_n)^{-1} & \ldots \\ \ldots & \ldots \end{array} \right].$$

Then we have

$$\partial_{x_2}G_d(0, q_U) = \frac{1}{d} \text{Tr} \left( \begin{array}{cc} \bar{M}^{-1} & \ldots \\ \ldots & \ldots \end{array} \right) \left[ \begin{array}{cc} Q & 0 \\ 0 & 0 \end{array} \right] = \text{Tr}(\bar{M}^{-1}Q)/d.$$

Applying similar arguments to compute other derivatives, we get

1. $\text{Tr}(\bar{M}^{-1} \Theta \Theta^T)/d^2 = \text{Tr}(\bar{M}^{-1}Q)/d = \partial_{x_2}G_d(0, q_U)$.
2. $\mu_1 \cdot \text{Tr}(Z\bar{M}^{-1} \Theta X^T)/d^2 = \text{Tr}(\bar{M}^{-1}Z^TZ)/d = -\psi_2 \partial_{x_2}G_d(0, q_U)/2$.
3. $\text{Tr}(Z\bar{M}^{-1}Z^T X^T)/d^2 = \text{Tr}(Z\bar{M}^{-1}Z^T H)/d = \psi_2 \partial_{x_2}G_d(0, q_U) - \psi_2^2$.
4. $\text{Tr}(Z\bar{M}^{-1}Z^T)/d = \psi_2 \partial_{x_1}G_d(0, q_U) - \psi_2^2$.
5. $\text{Tr}(\bar{M}^{-2}Q)/d = -\partial_{x_1} \partial_{x_2}G_d(0, q_U)$.
6. $(2/d\psi_2) \cdot \text{Tr}(Z^T Z \bar{M}^{-2}) = \partial_{x_1} \partial_{x_2}G_d(0, q_U)$.
7. $\text{Tr}(\bar{M}^{-2}Z^T H Z)/(d\psi_2)^2 = -\partial_{x_1} \partial_{x_2}G_d(0, q_U)$.
8. $\text{Tr}(\bar{M}^{-2}Z^T Z)/(d\psi_2)^2 = -\partial_{x_1} \partial_{x_2}G_d(0, q_U)$.

Combining these equations concludes the proof. \hfill \Box

Proof of Lemma 2. We prove this lemma by assuming that $\beta$ follows a different distribution: $\beta \sim \mathcal{N}(0, ||F_1||^2/d)I_d)$. The case when $\beta \sim \text{Unif}(S^{d-1}(F_1))$ can be treated similarly.

By directly calculating the variance, we can show that, there exists scalers $(c_{ik}^{(d)}), k \in [K_i]$ with $c_{ik}^{(d)} = \Theta_d(1)$, and matrices $(A_{ik}, B_{ik})_{k \in [K_i]} \subseteq \{I_N, Q, Z^T H Z, Z^T Z\}$, such that the variance of $\Psi_i$’s can be expressed in form

$$\text{Var}_\varepsilon(\Psi_i) = \frac{1}{d} \sum_{k=1}^{K_i} c_{ik}^{(d)} \text{Tr}(\bar{M}^{-1} A_{ik} \bar{M}^{-1} B_{ik})/d.$$

For example, by Lemma 8, we have

$$\text{Var}_{\beta \sim \mathcal{N}(0, (||F_1||^2/d)I_d)}) (\Psi_1) = \lambda_{d,1}(\sigma)^4 \text{Var}_{\beta \sim \mathcal{N}(0, (||F_1||^2/d)I_d)}) (\beta^T \Theta^T \bar{M}^{-1} \Theta \beta) = 2 \lambda_{d,1}(\sigma)^4 F_1 \| \Theta^T \bar{M}^{-1} \Theta \|^2/d^2$$

$$= c_1^{(d)} \text{Tr}(\bar{M}^{-1} Q \bar{M}^{-1} Q)/d^2,$$

where $c_1^{(d)} = 2d^2 \lambda_{d,1}(\sigma)^4 F_1^2 = O_d(1)$. The variance of $\Psi_2$ and $\Psi_3$ can be calculated similarly.

Note that each $\text{Tr}(\bar{M}^{-1} A_{ik} \bar{M}^{-1} B_{ik})/d$ can be expressed as an entry of $\nabla^2 G_d(0; q)$ (c.f. Eq. (47)), and by Proposition 4, they are of order $O_{d,p}(1)$. This gives

$$\text{Var}_\varepsilon,\beta(\Psi_i) = o_{d,p}(1).$$

Similarly, for the same set of scalers $(c_{ik}^{(d)}), k \in [K_i]$ and matrices $(A_{ik}, B_{ik})_{k \in [K_i]}$, we have

$$\text{Var}_\varepsilon,\beta(\Phi_i) = \frac{1}{d} \sum_{k=1}^{K_i} c_{ik} \text{Tr}(\bar{M}^{-2} A_{ik} \bar{M}^{-2} B_{ik})/d.$$
D.6. Auxiliary Lemmas

The following lemma (Lemma 5) is a reformulation of Proposition 3 in (Ghorbani et al., 2019). We present it in a stronger form, but it can be easily derived from the proof of Proposition 3 in (Ghorbani et al., 2019). This lemma was first proved in (El Karoui, 2010) in the Gaussian case. (Notice that the second estimate —on $Q_k(\Theta X^T)$— follows by applying the first one whereby $\Theta$ is replaced by $W = [\Theta^\top X]^T$.

**Lemma 5.** Let $\Theta = (\theta_1, \ldots, \theta_N)^T \in \mathbb{R}^{N \times d}$ with $(\theta_a)_{a \in [N]} \sim_{iid} \text{Unif}(S^{d-1}(\sqrt{d}))$ and $X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times d}$ with $(x_i)_{i \in [n]} \sim_{iid} \text{Unif}(S^{d-1}(\sqrt{d}))$. Assume $1/c \leq n/d, N/d \leq c$ for some constant $c \in (0, \infty)$. Then,

$$
\mathbb{E} \left[ \sup_{k \geq 2} \|Q_k(\Theta X^T) - I_N\|_{op}^2 \right] = o_d(1), \\
\mathbb{E} \left[ \sup_{k \geq 2} \|Q_k(\Theta X^T)^2\|_{op} \right] = o_d(1).
$$

Notice that the second estimate —on $Q_k(\Theta X^T)$— follows by applying the first one —Eq. (48)— whereby $\Theta$ is replaced by $W = [\Theta^\top X]^T$, and we use $\|Q_k(\Theta X^T)\|_{op} \leq \|Q_k(W W^T) - I_{N+n}\|_{op}$.

The following lemma (Lemma 6) can be easily derived from Lemma 5. Again, this lemma was first proved in (El Karoui, 2010) in the Gaussian case.

**Lemma 6.** Let $\Theta = (\theta_1, \ldots, \theta_N)^T \in \mathbb{R}^{N \times d}$ with $(\theta_a)_{a \in [N]} \sim_{iid} \text{Unif}(S^{d-1}(\sqrt{d}))$. Let activation function $\sigma$ satisfies Assumption 2. Assume $1/c \leq n/d \leq c$ for some constant $c \in (0, \infty)$. Denote

$$
U = \left( \mathbb{E}_{x \sim \text{Unif}(S^{d-1}(\sqrt{d}))} [\sigma(\langle \theta_a, x \rangle/\sqrt{d})\sigma(\langle \theta_b, x \rangle/\sqrt{d})] \right)_{a,b \in [N]} \in \mathbb{R}^{N \times N}.
$$

Then we can rewrite the matrix $U$ to be

$$
U = \lambda_{d,0}(\sigma)^2 I_N + \mu_1^2 Q + \mu_2^2 (I_N + \Delta),
$$

with $Q = \Theta \Theta^T/d$ and $\mathbb{E}[\|\Delta\|_{op}^2] = o_d(1)$.

In the following, we show that, under sufficient regularity condition of $\sigma$, we have $\lambda_{d,0}(\sigma) = O(1/d)$.

**Lemma 7.** Let $\sigma \in C^2(\mathbb{R})$ with $|\sigma'(x)|, |\sigma''(x)| < c_0 e^{c_1 |x|}$ for some $c_0, c_1 \in \mathbb{R}$. Assume that $\mathbb{E}_{G \sim \mathcal{N}(0, I_d)} [\sigma(G)] = 0$. Then we have

$$
\lambda_{d,0}(\sigma) \equiv \mathbb{E}_{x \sim \text{Unif}(S^{d-1}(\sqrt{d}))} [\sigma(x_1)] = O(1/d).
$$

**Proof of Lemma 7.** Let $x \sim \text{Unif}(S^{d-1}(\sqrt{d}))$ and $\gamma \sim \chi(d)/\sqrt{d}$ independently. Then we have $\gamma x \sim \mathcal{N}(0, I_d)$, so that by the assumption, we have $\mathbb{E}[\sigma(\gamma x_1)] = 0$.

As a consequence, by the second order Taylor expansion, and by the independence of $\gamma$ and $x$, we have (for $x_1 \in [\gamma, 1]$)

$$
|\lambda_{d,0}(\sigma)| = |\mathbb{E}[\sigma(x_1)]| \leq |\mathbb{E}[\sigma(x_1)] - \mathbb{E}[\sigma(\gamma x_1)]| \leq \left| \mathbb{E}[\sigma'(x_1)x_1]\mathbb{E}[\gamma - 1] \right| + \left( 1/2 \right) \mathbb{E}[\sigma''(\xi(x_1)x_1)(\gamma - 1)^2]^{1/2} \mathbb{E}[(\gamma - 1)^2]^{1/2}.
$$

By the assumption that $|\sigma'(x)|, |\sigma''(x)| < c_0 e^{c_1 |x|}$ for some $c_0, c_1 \in \mathbb{R}$, there exists constant $K$ that only depends on $c_0$ and $c_1$ such that

$$
\sup_d \left| \mathbb{E}[\sigma'(x_1)x_1] \right| \leq K, \quad \sup_d \left( 1/2 \right) \mathbb{E} \left[ \sup_{u \in [\gamma, 1]} \sigma''(u x_1)^2 \right]^{1/2} \leq K.
$$

Moreover, by property of the $\chi$ distribution, we have

$$
\mathbb{E}[\gamma - 1] = O(d^{-1}), \quad \mathbb{E}[(\gamma - 1)^4]^{1/2} = O(d^{-1}).
$$

This concludes the proof. \qed
The following lemma is a simple variance calculation and can be found as Lemma C.5 in (Mei & Montanari, 2019). We restate here for completeness.

**Lemma 8.** Let $A \in \mathbb{R}^{n \times N}$ and $B \in \mathbb{R}^{n \times n}$. Let $g = (g_1, \ldots, g_n)^T$ with $g_i \sim_{\text{iid}} \mathbb{P}_g$, $\mathbb{E}_g[g] = 0$, and $\mathbb{E}_g[g^2] = 1$. Let $h = (h_1, \ldots, h_N)^T$ with $h_i \sim_{\text{iid}} \mathbb{P}_h$, $\mathbb{E}_h[h] = 0$, and $\mathbb{E}_h[h^2] = 1$. Further we assume that $h$ is independent of $g$. Then we have

$$\text{Var}(g^TAh) = \|A\|^2_F,$$

$$\text{Var}(g^TBg) = \sum_{i=1}^n B_{ii}^2(\mathbb{E}[g^4] - 3) + \|B\|^2_F + \text{Tr}(B^2).$$

**E. Proof of Theorem 1**

Here we give the whole proof for $U$. The proof for $T$ is the same.

For fixed $A^2 \in \Gamma_U \equiv \{A_U(\lambda, \psi_1, \psi_2) : \lambda \in \Lambda_U\}$, we denote

$$\lambda_*(A^2) = \inf_{\lambda} \left\{ \lambda : A_U(\lambda, \psi_1, \psi_2) = A^2 \right\}.$$

By the definition of $\Gamma_U$, the set $\{\lambda : A_U(\lambda, \psi_1, \psi_2) = A^2\}$ is non-empty and lower bounded, so that $\lambda_*(A^2)$ can be well-defined. Moreover, we have $\lambda_*(A^2) \in \Lambda_U$. It is also easy to see that we have

$$\lambda_*(A^2) \in \arg\min_{\lambda \geq 0} \left[ \overline{U}(\lambda, \psi_1, \psi_2) + \lambda A^2 \right]. \tag{50}$$

**E.1. Upper bound**

Note we have

$$U(A, N, n, d) = \sup_{(N/d)\|a\|_2^2 \leq A^2} \left( R(a) - \hat{R}_n(a) \right)$$

$$\leq \inf_{\lambda} \sup_{(N/d)\|a\|_2^2 \leq A^2} \left( R(a) - \hat{R}_n(a) - \psi_1\lambda(\|a\|_2^2 - \psi_1^{-1} A^2) \right)$$

$$\leq \inf_{\lambda} \left[ \overline{U}(\lambda, N, n, d) + \lambda A^2 \right]$$

$$\leq \overline{U}(\lambda_*(A^2), N, n, d) + \lambda_*(A^2)A^2.$$

Note that $\lambda_*(A^2) \in \Lambda_U$, so by Lemma 5, in the limit of Assumption 3, we have

$$U(A, N, n, d) \leq \overline{U}(\lambda_*(A^2), \psi_1, \psi_2) + \lambda_*(A^2)A^2 + o_{d,p}(1) = U(A, \psi_1, \psi_2) + o_{d,p}(1),$$

where the last equality is by Eq. (50). This proves the upper bound.

**E.2. Lower bound**

For any $A^2 > 0$, we define a random variable $\hat{\lambda}(A^2)$ (which depend on $X$, $\Theta$, $\beta$, $\varepsilon$) by

$$\hat{\lambda}(A^2) = \inf_{\lambda} \left\{ \lambda : \lambda \in \arg\min_{\lambda \geq 0} \left[ \overline{U}(\lambda, N, n, d) + \lambda A^2 \right] \right\}.$$ 

By Proposition 1, the set is always non-empty, so that $\hat{\lambda}(A^2)$ can always be well-defined.

Moreover, since $\lambda_*(A^2) \in \Lambda_U$, by Assumption 4, as we have shown in the proof in Proposition 2, we can uniquely define $\overline{a}_U(\lambda_*(A^2))$ with high probability, where

$$\overline{a}_U(\lambda_*(A^2)) = \arg\max_{a} \left[ R(a) - \hat{R}_n(a) - \psi_1\lambda_*(A^2)\|a\|_2^2 \right].$$

As a consequence, for a small $\varepsilon > 0$, the following event $E_{\varepsilon,d}$ can be well-defined with high probability

$$E_{\varepsilon,d} = \left\{ \psi_1\|\overline{a}_U(\lambda_*(A^2))\|_2^2 \geq A^2 - \varepsilon \right\} \cap \left\{ \hat{\lambda}(A^2 + \varepsilon) \leq \lambda_*(A^2) \right\}$$

$$= \left\{ A^2 - \varepsilon \leq \psi_1\|\overline{a}_U(\lambda_*(A^2))\|_2^2 \leq A^2 + \varepsilon \right\}.$$
where the last equality is by the definition of (Efthimiou & Frye, 2014; Szego, Gabor, 1939; Chihara, 2011; Ghorbani et al., 2019; Mei & Montanari, 2019) for further information on these topics.

Consequently, for small \( \varepsilon > 0 \), when the event \( \mathcal{E}_{\varepsilon,d} \) happens, we have

\[
U((A^2 + \varepsilon)^{1/2}, N, n, d) = \sup_a \left( R(a) - \hat{R}_n(a) - \psi_1 A^2 + \varepsilon \cdot \left( \|a\|^2 - \psi_1^{-1}(A^2 + \varepsilon) \right) \right)
\]
\[
\geq R(\hat{a}_U(\lambda_\ast(A^2))) - \hat{R}_n(\hat{a}_U(\lambda_\ast(A^2))) - \psi_1 \hat{\lambda}(A^2 + \varepsilon) \cdot \left( \|\hat{a}_U(\lambda_\ast(A^2))\|^2 - \psi_1^{-1}(A^2 + \varepsilon) \right)
\]
\[
\geq R(\bar{a}_U(\lambda_\ast(A^2))) - \bar{R}_n(\bar{a}_U(\lambda_\ast(A^2))) - \psi_1 \hat{\lambda}(A^2 + \varepsilon) \cdot \left( \|\bar{a}_U(\lambda_\ast(A^2))\|^2 - \psi_1^{-1}(A^2 - \varepsilon) \right)
\]
\[
= \hat{U}(\lambda_\ast(A^2), N, n, d) + \lambda_\ast(A^2) \cdot (A^2 - \varepsilon).
\]

As a consequence, by Eq. (51) and (52), we have

\[
U((A^2 + \varepsilon)^{1/2}, N, n, d) \geq \hat{U}(\lambda_\ast(A^2), \psi_1, \psi_2) + \lambda_\ast(A^2) \cdot (A^2 - \varepsilon) - \epsilon, 1 = U(A, \psi_1, \psi_2, \varepsilon, \lambda_\ast(A^2) - \epsilon, 1).
\]

where the last equality is by the definition of \( U \) as in Definition 2, and by the fact that \( \lambda_\ast(A^2) \in \arg \min_{\lambda \geq 0} \| U(\lambda, \psi_1, \psi_2) + \lambda A^2 \| \). Taking \( \varepsilon \) sufficiently small proves the lower bound. This concludes the proof of Theorem 1.

F. Technical background

In this section we introduce additional technical background useful for the proofs. In particular, we will use decompositions in (hyper-)spherical harmonics on the \( S^{d-1}(\sqrt{d}) \) and in Hermite polynomials on the real line. We refer the readers to (Efthimiou & Frye, 2014; Szego, Gabor, 1939; Chihara, 2011; Ghorbani et al., 2019; Mei & Montanari, 2019) for further information on these topics.

F.1. Functional spaces over the sphere

For \( d \geq 1 \), we let \( S^{d-1}(r) = \{ x \in \mathbb{R}^d : \|x\|_2 = r \} \) denote the sphere with radius \( r \) in \( \mathbb{R}^d \). We will mostly work with the sphere of radius \( \sqrt{d} \), \( S^{d-1}(\sqrt{d}) \) and will denote by \( \gamma_d \) the uniform probability measure on \( S^{d-1}(\sqrt{d}) \). All functions in the following are assumed to be elements of \( L^2(S^{d-1}(\sqrt{d}), \gamma_d) \), with scalar product and norm denoted as \( (\cdot, \cdot)_{L^2} \) and \( \| \cdot \|_{L^2} \):

\[
(f, g)_{L^2} = \int_{S^{d-1}(\sqrt{d})} f(x) g(x) \gamma_d(dx).
\]

For \( \ell \in \mathbb{Z}_{\geq 0} \), \( \hat{V}_{d,\ell} \) be the space of homogeneous harmonic polynomials of degree \( \ell \) on \( \mathbb{R}^d \) (i.e. homogeneous polynomials \( q(x) \) satisfying \( \Delta q(x) = 0 \)), and denote by \( V_{d,\ell} \) the linear space of functions obtained by restricting the polynomials in \( \hat{V}_{d,\ell} \) to \( S^{d-1}(\sqrt{d}) \). With these definitions, we have the following orthogonal decomposition

\[
L^2(S^{d-1}(\sqrt{d}), \gamma_d) = \bigoplus_{\ell=0}^{\infty} V_{d,\ell}.
\]

The dimension of each subspace is given by

\[
\dim(V_{d,\ell}) = B(d, \ell) = \frac{2\ell + d - 2}{\ell} \left( \frac{\ell + d - 3}{\ell - 1} \right).
\]
For each $\ell \in \mathbb{Z}_{\geq 0}$, the spherical harmonics $\{Y_{\ell j}^{(d)}\}_{1 \leq j \leq B(d,\ell)}$ form an orthonormal basis of $V_{d,\ell}$:

$$\langle Y_{k i}^{(d)}, Y_{s j}^{(d)} \rangle_{L^2} = \delta_{i j} \delta_{k s}.$$ 

Note that our convention is different from the more standard one, that defines the spherical harmonics as functions on $S^{d-1}(1)$. It is immediate to pass from one convention to the other by a simple scaling. We will drop the superscript $d$ and write $Y_{\ell j} = Y_{\ell j}^{(d)}$ whenever clear from the context.

We denote by $P_k$ the orthogonal projections to $V_{d,k}$ in $L^2(S^{d-1}(\sqrt{d}), \gamma_d)$. This can be written in terms of spherical harmonics as

$$P_k f(x) \equiv \sum_{l=1}^{B(d,k)} \langle f, Y_{kl} \rangle_{L^2} Y_{kl}(x).$$

Then for a function $f \in L^2(S^{d-1}(\sqrt{d}))$, we have

$$f(x) = \sum_{k=0}^{\infty} P_k f(x) = \sum_{k=0}^{\infty} \sum_{l=1}^{B(d,k)} \langle f, Y_{kl} \rangle_{L^2} Y_{kl}(x).$$

F.2. Gegenbauer polynomials

The $\ell$-th Gegenbauer polynomial $Q_{\ell}^{(d)}$ is a polynomial of degree $\ell$. Consistently with our convention for spherical harmonics, we view $Q_{\ell}^{(d)}$ as a function $Q_{\ell}^{(d)}: [-d, d] \to \mathbb{R}$. The set $\{Q_{\ell}^{(d)}\}_{\ell \geq 0}$ forms an orthonormal basis on $L^2([-d, d], \tilde{\gamma}_d)$ (where $\tilde{\gamma}_d$ is the distribution of $\langle x_1, x_2 \rangle$ when $x_1, x_2 \sim_{i.i.d.}$ Unif($S^{d-1}(\sqrt{d})$)), satisfying the normalization condition:

$$\langle Q_k^{(d)}, Q_j^{(d)} \rangle_{L^2(\tilde{\gamma}_d)} = \frac{1}{B(d, k)} \delta_{j k}.$$  

In particular, these polynomials are normalized so that $Q_{\ell}^{(d)}(d) = 1$. As above, we will omit the superscript $d$ when clear from the context (write it as $Q_{\ell}$ for notation simplicity).

Gegenbauer polynomials are directly related to spherical harmonics as follows. Fix $v \in S^{d-1}(\sqrt{d})$ and consider the subspace of $V_f$ formed by all functions that are invariant under rotations in $\mathbb{R}^d$ that keep $v$ unchanged. It is not hard to see that this subspace has dimension one, and coincides with the span of the function $Q_{\ell}^{(d)}(\langle v, \cdot \rangle)$.

We will use the following properties of Gegenbauer polynomials

1. For $x, y \in S^{d-1}(\sqrt{d})$

$$\langle Q_j^{(d)}(\langle x, \cdot \rangle), Q_k^{(d)}(\langle y, \cdot \rangle) \rangle_{L^2(S^{d-1}(\sqrt{d}), \gamma_d)} = \frac{1}{B(d, k)} \delta_{jk} Q_k^{(d)}(\langle x, y \rangle).$$

2. For $x, y \in S^{d-1}(\sqrt{d})$

$$Q_k^{(d)}(\langle x, y \rangle) = \frac{1}{B(d, k)} \sum_{i=1}^{B(d,k)} Y_{ki}^{(d)}(x) Y_{ki}^{(d)}(y).$$

Note in particular that property 2 implies that —up to a constant— $Q_k^{(d)}(\langle x, y \rangle)$ is a representation of the projector onto the subspace of degree-$k$ spherical harmonics

$$(P_k f)(x) = B(d, k) \int_{S^{d-1}(\sqrt{d})} Q_k^{(d)}(\langle x, y \rangle) f(y) \gamma_d(dy).$$
For a function $\sigma \in L^2([-\sqrt{d}, \sqrt{d}], \tau_d)$ (where $\tau_d$ is the distribution of $\langle x_1, x_2 \rangle / \sqrt{d}$ when $x_1, x_2 \sim_{iid} \text{Unif}(S^{d-1}(\sqrt{d}))$), denoting its spherical harmonics coefficients $\lambda_{d,k}(\sigma)$ to be

$$\lambda_{d,k}(\sigma) = \int_{[-\sqrt{d}, \sqrt{d}]} \sigma(x) Q_k^{(d)}(\sqrt{d}x) \tau_d(x),$$

(61)

then we have the following equation holds in $L^2([-\sqrt{d}, \sqrt{d}], \tau_d)$ sense

$$\sigma(x) = \sum_{k=0}^{\infty} \lambda_{d,k}(\sigma) B(d, k) Q_k^{(d)}(\sqrt{d}x).$$

(62)

### F.3. Hermite polynomials

The Hermite polynomials $\{H_k\}_{k \geq 0}$ form an orthogonal basis of $L^2(\mathbb{R}, \mu_G)$, where $\mu_G(dx) = e^{-x^2/2dx}/\sqrt{2\pi}$ is the standard Gaussian measure, and $H_k$ has degree $k$. We will follow the classical normalization (here and below, expectation is with respect to $G \sim N(0, 1)$):

$$\mathbb{E}\{H_j(G) H_k(G)\} = k! \delta_{j,k}.$$  

(63)

As a consequence, for any function $\sigma \in L^2(\mathbb{R}, \mu_G)$, we have the decomposition

$$\sigma(x) = \sum_{k=1}^{\infty} \frac{\mu_k(\sigma)}{k!} H_k(x), \quad \mu_k(\sigma) = \mathbb{E}\{\sigma(G) H_k(G)\}.$$  

(64)

The Hermite polynomials can be obtained as high-dimensional limits of the Gegenbauer polynomials introduced in the previous section. Indeed, the Gegenbauer polynomials (up to a $\sqrt{d}$ scaling in domain) are constructed by Gram-Schmidt orthogonalization of the monomials $\{x^k\}_{k \geq 0}$ with respect to the measure $\tau_d$, while Hermite polynomial are obtained by Gram-Schmidt orthogonalization with respect to $\mu_G$. Since $\tau_d \Rightarrow \mu_G$ (here $\Rightarrow$ denotes weak convergence), it is immediate to show that, for any fixed integer $k$,

$$\lim_{d \to \infty} \text{Coeff}\{Q_k^{(d)}(\sqrt{d}x) B(d, k)^{1/2}\} = \text{Coeff}\left\{\frac{1}{(k!)^{1/2}} H_k(x)\right\}.$$  

(65)

Here and below, for $P$ a polynomial, $\text{Coeff}\{P(x)\}$ is the vector of the coefficients of $P$. As a consequence, for any fixed integer $k$, we have

$$\mu_k(\sigma) = \lim_{d \to \infty} \lambda_{d,k}(\sigma)(B(d, k)k!)^{1/2},$$  

(66)

where $\mu_k(\sigma)$ and $\lambda_{d,k}(\sigma)$ are given in Eq. (64) and (61).