Risk of the Least Squares Minimum Norm Estimator under the Spike Covariance Model

Yasaman Mahdaviyeh*1 and Zacharie Naulet2

1University of Toronto
Department of Computer Science,
Vector Institute
Toronto, ON, Canada

2Université Paris-Saclay
CNRS, Laboratoire de mathématiques d’Orsay
91405, Orsay, France.

Abstract

We study risk of the minimum norm linear least squares estimator in when the number of parameters \(d\) depends on \(n\), and \(\frac{d}{n} \to \infty\). We assume that data has an underlying low rank structure by restricting ourselves to spike covariance matrices, where a fixed finite number of eigenvalues grow with \(n\) and are much larger than the rest of the eigenvalues, which are (asymptotically) in the same order. We show that in this setting risk of minimum norm least squares estimator vanishes in compare to risk of the null estimator. We give asymptotic and non asymptotic upper bounds for this risk, and also leverage the assumption of spike model to give an analysis of the bias that leads to tighter bounds in compare to previous works.

1 Introduction

One of the recent approaches to explain good performance of neural networks has focused on their ability to fit training data perfectly (interpolate) without over-fitting. It has been shown that this property is not unique to neural nets, and that simpler class of models such as kernel regression could exhibit this behaviour, too Belkin et al. (2018); Tengyuan Liang (2018). One of

*Corresponding author: yasamanmdv@cs.toronto.edu
the simpler models where interpolation has been studied recently is the least squares solution for linear regression. In this case, interpolation is only guaranteed to happen in the high dimensional setting where the number of parameters \(d\) exceeds the number of samples \(n\); therefore, the least squares solution is not necessarily unique. However, the minimum norm least squares (MNLS) solution is unique, and can be written in closed form. Also, if we minimize the squared loss using gradient descent with initial parameters set to zero, we recover the minimum norm solution (Hastie et al., 2019). This has, at least partially, motivated several works that study the risk of minimum norm least squares estimator for linear regression.

We study the risk of MNLS Estimator under the spike covariance model of Johnstone (2001), where few population eigenvalues are much larger than the rest. We expect spike covariance models to represent underlying low dimensional structure of the data, or fast decay of the eigenspectrum of the sample covariance or Gram matrix that is observed in some datasets, see for example Tengyuan Liang (2018) and Jung and Marron (2009) for plots of eigenspectrums of an image data set and microarray data respectively. Also, a few recent works have shown that decay of eigenvalues plays an important role in interpolation without over-fitting in case of linear and kernel regression (Bartlett et al., 2019; Tengyuan Liang, 2018). These factors have inspired us to study the MNLS estimator under spike covariance model.

We are especially interested in the High Dimensional Low Sample Size (HDLSS) regime introduced in Hall et al. (2005) and later studied thoroughly in Ahn et al. (2007); Jung and Marron (2009); Shen et al. (2013, 2016b,a) where \(d/n \to \infty\). This setting fits scenarios where the amount of information collected about individuals grows much faster than the number of individuals, as in collection of genetic data, for example (Jung and Marron, 2009). Combined with spike covariance model with diverging spiked eigenvalues, we are in a setting where even though increasingly more features are collected, the new features are highly correlated with existing ones, and do not add much new information, but rather reinforce existing knowledge. It is interesting to note that in this setting, intuitively, roles of \(n\) and \(d\) are almost swapped, since the large number of highly correlated features has the redundancy effect of large \(n\) and small \(n\) with diverging variance plays the role of small \(d\). This interpretation of this phenomenon can be even seen in analysis of the covariance matrices in high dimensions when the analysis is done through the Gram matrix (Hastie et al., 2019; Wang and Fan, 2017)

We rely on the characterization of limits of the eigenvalues and eigenvectors of sample covariance matrix given in this regime in Shen et al. (2016a); Koltchinskii and Lounici (2016) and other similar works to give an asymptotic bound on the risk which vanishes relative to asymptotic risk of the null estimator. Under less restrictive assumptions on the covariance matrix but stronger assumptions on the distribution of data, we also give a high probability bound on the predictive risk that depends on spectral gaps of the covariance matrix. Our analysis of the bias is novel and leads to a tighter bound on the bias in the HDLSS regime in compare to other related work. We show that consistent estimation of the spiked eigenvalues and eigenvectors leads to small risk, and thus highlight the connection between Principal Component Analysis (PCA) and linear regression.

This paper is organized as follows. First in Sections 1.1 and 1.2, we introduce the model and the main assumptions. In Section 1.3, we review current related literature, and we establish the
main technical notations in Section 1.4. We give the main theorems in Section 2: the first is an almost-sure convergence of the risk of the MNLS estimator, given in Section 2.1, while the second is a non-asymptotic bound for the risk, given in Section 2.2. Finally, we discuss the results in Section 3. The proofs for everything related to the MNLS estimator are postponed to Section 4, and to Appendix A for existing results on estimation of spike covariance matrices.

1.1 Set up and assumptions

Given \( n \) independent, identically distributed pairs of data points and labels \((X_1, Y_1) \in \mathbb{R}^d \times \mathbb{R}, \) we assume the following model

\[ Y_i = \theta^T X_i + \xi_i, \quad i = 1, \ldots, n, \]

where \( \xi_i \) are mean 0, independent and identically distributed (i.i.d.) noise, with variance \( \mathbb{E}[\xi_i^2] = \sigma^2 \). The goal is to recover the parameter \( \theta \), or rather to have accurate predictions of future observations, based upon the knowledge of \((X_1, Y_1), \ldots, (X_n, Y_n)\). It is helpful to collect the covariates \( X_i \) into the \( n \times p \) design matrix \( X \) whose rows are \( X_1, \ldots, X_n \). Similarly, we collect the responses inside the vector \( Y = (Y_1, \ldots, Y_n) \). Here we are interested in the Minimum Norm Least Squares (MNLS) estimator, defined as

\[
\hat{\theta} = \arg \min_{\theta} \| \theta \| \quad \text{s.t.} \quad X \theta = Y. \tag{1.1}
\]

This estimator can be written in closed form as

\[
\hat{\theta} = (X^T X)^\dagger X^T Y,
\]

where \((X^T X)^\dagger\) denotes the Moore-Penrose pseudo-inverse of \( X^T X \). This is quite well known, see for instance Penrose (1956). As we will see, this notion of risk depends heavily on the \( d \times d \) random matrix \( \hat{\Sigma} := n^{-1} X^T X \), that is, the sample covariance matrix. We let \( \Sigma := \mathbb{E}[\Sigma] \) denote the corresponding population covariance matrix. We write \( \hat{U} \hat{\Lambda} \hat{U}^T := \hat{\Sigma} \) the singular value decomposition of \( \hat{\Sigma} \), where \( \hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_d) \) are the singular values of \( \hat{\Sigma} \) sorted in non-increasing order, i.e. \( \hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \ldots \hat{\lambda}_d \), and \( \hat{U} = (\hat{u}_1, \ldots, \hat{u}_d) \). Under fairly weak assumptions on the distribution of \( X \), it is immediately seen that \( \hat{\Sigma} \) has rank equal to \( n \), thereby \( \hat{\lambda}_{n+1}, \ldots, \hat{\lambda}_d = 0 \). Similarly, we let \( U \Lambda U^T := \Sigma \) denote the singular value decomposition of \( \Sigma \), where \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d) \) are the singular values of \( \Sigma \) sorted in non-increasing order, and \( U = (u_1, \ldots, u_d) \) the eigenvectors. Here we assume the following on the distribution of \( X \).

**Assumption 1 (Distribution of \( X_i \), weak).** As in Shen et al. (2016a, Assumption 1), we assume that \( X_1, \ldots, X_n \) are independent, identically distributed (iid) and the random vectors \( Z_i := \Lambda^{-1/2} U^T X_i \) have iid entries with zero mean, unit variance, and finite fourth moments, i.e. \( Z_i = (Z_{i,1}, \ldots, Z_{i,d}) \) where the variables \( \{Z_{i,k}\} \) are iid with \( \mathbb{E}[Z_{i,k}] = 0, \mathbb{E}[Z_{i,k}^2] = 1, \) and \( \mathbb{E}[Z_{i,k}^4] < \infty \).

We use Assumption 1 and Assumption 3, which is introduced in next section to establish almost-sure bounds for the MNLS estimator in Section 2.1. Non-asymptotic upper bounds on the risk are obtained in Section 2.2, under the following additional structure on the distribution of \( X \).
Assumption 2 (Distribution of $X_i$, strong). The Assumption 1 holds, and in addition the random variables $(Z_{i,k})$ are sub-gaussian. That is, there exists $\nu > 0$ such that $\log \mathbb{E}[e^{\lambda Z_{i,k}}] \leq \frac{\lambda^2}{2}$ for all $\lambda \in \mathbb{R}$.

1.2 Spike model and HDLSS regime

The spike model was first studied in Johnstone (2001), where a fixed number of eigenvalues are greater than one, and the rest are one. It was motivated by some cases such as functional data analysis (Johnstone, 2001), and financial data (Baik and Silverstein, 2006), where empirically, first few eigenvalues of sample covariance matrix are much larger than the rest. A spike covariance matrix can also be thought of as a perturbation of a low rank matrix, that is $\Sigma = M + \delta I$, where $M$ is a rank $m \ll n$ matrix with large eigenvalues.

In the context of PCA, Hall et al. (2005); Ahn et al. (2007); Jung and Marron (2009); Shen et al. (2013, 2016b,a) introduce the so-called HDLSS regime as a realistic model for data, where they assume that $d \equiv d^{(n)}$ with $d^{(n)}/n \to \infty$, and that the eigenvalues of $\Sigma \equiv \Sigma^{(n)} = \sum_{j=1}^d \lambda_j^{(n)} u_j^{(n)} u_j^{(n)T}$ are such that a few of them are very large and dominate the rest of the eigenvalues. In particular, they study the spike covariance model with diverging spiked eigenvalues, where the amount of signal increases as $n \to \infty$, in the sense that for the first $\bar{m}$ eigenvalues we have $\lambda_1^{(n)} \to \infty$, ..., $\lambda_{\bar{m}}^{(n)} \to \infty$. Formally, the assumption is the following.

Assumption 3 (HDLSS). $\lim_{n \to \infty} d^{(n)}/n = \infty$, and there exists $\bar{m} \in \mathbb{N}$ and $c_1, c_2 > 0$ such that the sequence of eigenvalues $\lambda_1^{(n)} > \lambda_2^{(n)} > \cdots > \lambda_d^{(n)}$ satisfies $\lim_{n \to \infty} n\lambda_{\bar{m}}^{(n)}/d^{(n)} = \infty$, $\lim_{n \to \infty} \lambda_j^{(n)}/\lambda_{j+1}^{(n)} > 0$ for $j = 1, \ldots, \bar{m}$, while $\lim_{n \to \infty} \lambda_{\bar{m}+1}^{(n)} = c_1$ and $\lim_{n \to \infty} \lambda_{d}^{(n)} = c_2$.

Shen et al. (2016a,b) show that the first $\bar{m}$ samples eigenvalues $\hat{\lambda}_1, \ldots, \hat{\lambda}_{\bar{m}}$ of $\hat{\Sigma}$ are consistent for $\lambda_1^{(n)}, \ldots, \lambda_{\bar{m}}^{(n)}$, in the sense that $\lim_{n \to \infty} \max_{j=1,\ldots,\bar{m}} \hat{\lambda}_j/\lambda_j^{(n)} = 1$, and also $\hat{u}_1, \ldots, \hat{u}_{\bar{m}}$ are consistent for $u_1^{(n)}, \ldots, u_{\bar{m}}^{(n)}$. We mainly use these results to bound the risk of the MNLS estimator.

In the sequel, and thus to avoid the heavy notations, we drop the superscript $(n)$ and we write $d$ for $d^{(n)}$, $\Sigma$ for $\Sigma^{(n)}$, $\lambda_j$ for $\lambda_j^{(n)}$, and $u_j$ for $u_j^{(n)}$, while keeping in mind that those are considered to be sequences indexed by $n$. The same goes for $\theta^{(n)} \equiv \theta$.

The spike covariance model might seem like a very specific case to study. We borrow here Jung and Marron (2009, Example 4.1), which shows that the Assumption 3 on $\Sigma$ can be encountered even by really simple covariance designs. We refer to the aforementioned papers for more examples and thorough discussions.

Example 1. In the case where $\Sigma_{i,i} = 1$ for $i = 1, \ldots, d$ and $\Sigma_{i,j} = a$ for $i \neq j$, then the first eigenvalue of $\Sigma$ is $\lambda_1 = 1 + (d-1)a$, while $\lambda_2, \ldots, \lambda_d = 1 - a$. Then we have $\frac{d}{n\lambda_1} \to 0$, $\frac{d}{n\lambda_2} \to \infty$, $\lambda_1 = \Theta(d)$.

1.3 Related work

Here, we give a short overview of existing works that give bounds on the risk of MNLS estimator in a high dimensional regime (where interpolation could happen).
Belkin et al. (2019) study mean squared error in a finite sample and dimension setting with isotropic Gaussian data. Under fairly general setting, Hastie et al. (2019) give asymptotic risk bounds when \( \frac{d}{n} \to \alpha \in (0, \infty) \) for general covariance matrices, assuming their operator norm is bounded. Their bound in the general case depends on some results in random matrix theory, making it difficult to interpret. This is expected if there are no restrictions on structure of the covariance matrix. They also give more explicit bounds for some special covariance matrices, including an equicorrelated covariance matrix, which is a single spike model. For this covariance matrix, their results would be the same as ours if we take limit of \( \frac{d}{n} \to \infty \). They compare the risk bounds they get to signal to noise ratio (SNR) which turns out to be equal to risk of the null estimator within constant factors. Likewise, when we give the asymptotic bound, we look at the ratio of bias to risk of the null estimator.

Bartlett et al. (2019) study this (unnormalized) risk for Gaussian data in an infinite dimensional Hilbert space, with finite samples, and give conditions on the covariance matrix such that the risk is small with high probability. They call covariance matrices that meet these conditions benign. Intuitively, for a covariance matrix to be benign, the eigenvalues must decay but not too fast. Bartlett et al. (2019) break down the spectrum of covariance matrix into the larger eigenvalues and the tail, and their bound depends on where the spectrum is partitioned. Spike covariance matrices do have some properties of benign covariance matrices, even though their eigenvalues don’t decay to zero. Applying their partitioning of the spectrum to the spike covariance matrices considered here, we get spiked and non spiked eigenvalues. Indeed, their bounds can still hold under our setting; this will be discussed more thoroughly in Section 3.4.

Finally, we mention that the main novelty and essential difference with Hastie et al. (2019); Bartlett et al. (2019) resides in the way we analyze the bias the MNLS estimator. For instance, in Bartlett et al. (2019), bias is bounded by operator norm of the difference between sample and population covariance matrices, which is in turn bounded in probability using the bounds in Koltchinskii and Lounici (2016). Here, we leverage the extra structure we assume on the covariance matrix to perform a finer analysis of the bias. In particular, we rely on findings of (Shen et al., 2016a) that the first \( m \) eigenvalues and eigenvectors of \( \hat{\Sigma} \) are asymptotically consistent for their corresponding population counterparts. We emphasize that the bias depends on which subspace is not spanned by data, that is, the null space of \( X \), and the norm of the projection of the parameter \( \theta \) into the null space of \( X \). Sample covariance eigenvectors corresponding to nonzero eigenvalues form a basis for the row space of \( X \), thus characterizing them enables us to examine bias closely.

1.4 Notations

We assume that all random variables are defined on a common probability space \( (\Omega, \mathcal{F}, P) \). We write expectations under \( P \) as \( E \). The symbols \( E_\theta[f(Y) \mid X] \) means that \( Y \) is assumed to be \( X\theta + \xi \), where \( \xi \sim N(0, \sigma^2 I) \). For a matrix \( A \), we let \( \sigma_{\min}(A) \) and \( \sigma_{\max}(A) \) denote the smallest and largest singular values of \( A \) respectively. We also write \( \sigma_j(A) \) the \( j \)-th singular value of \( A \), ordered such that \( \sigma_1(A) \geq \sigma_2(A) \geq \ldots \). We denote the trace operator by \( \text{Tr} \). We rewrite the covariance matrix as \( \Sigma = \sum_{j=1}^d \lambda_j P_j \) where \( P_j \) is the projection operator onto the \( j \)-th eigenspace.
of $\Sigma$. Similarly we let $\hat{\Sigma} = \sum_{j=1}^{n} \hat{\lambda}_j \hat{P}_j$.

2 Main results

2.1 Almost-sure bounds on risk of the MNLS estimator

Let $X_{\text{new}}$ be a new sample from the same distribution as $X_1, \ldots, X_n$. The expected error (at $\theta$) of the MNLS estimator can be decomposed into the two terms

$$R_X(\hat{\theta}, \theta) := \mathbb{E}_\theta[(X_{\text{new}}^T \theta - X_{\text{new}}^T \hat{\theta})^2 \mid X] = \theta^T (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \Sigma (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \theta + \frac{\sigma^2}{n} \text{Tr}(\hat{\Sigma}^\dagger \Sigma),$$

which are called bias $B_X(\hat{\theta}, \theta)^2 := \theta^T (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \Sigma (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \theta$ and variance $V_X(\hat{\theta}, \theta) := \frac{\sigma^2}{n} \text{Tr}(\hat{\Sigma}^\dagger \Sigma)$, respectively. This is a standard derivation given in Appendix A.5. Theorem below gives an upper bound on asymptotic risk of the MNLS estimator (1.1). Note that bias is essentially variance of (noiseless) response after $\theta$ and $\Sigma$ are projected into some subspace. Intuitively, Theorem 1 below shows that if spike eigenvalues grow fast enough, then asymptotically, we incur no bias in the subspace spanned by the spike eigenvectors. More specifically, we consider the maximum risk of $\hat{\theta}$ over the classes of parameters, for $m \in \mathbb{N}$, $0 < \delta < 1$, and $L > 0$

$$A(m, \delta) := \{ \theta \in \mathbb{R}^d : \sum_{j=m+1}^{d} \|P_j \theta\|^2 \leq \delta \|\theta\|^2 \}.$$ 

**Theorem 1.** Under Assumptions 1 and 3 for all $L > 0$, for all $0 \leq \delta < 1$, it holds almost-surely as $n \to \infty$,

$$\sup_{\theta \in \mathbb{A}(\tilde{m}, \delta)} \frac{B_X(\hat{\theta}, \theta)^2}{\text{Var}(X_1^T \theta)} = O\left(\frac{1}{n} \sqrt{\frac{d}{n \lambda_1}} \right) \times \left\{ \delta + O\left(\frac{1}{n} \sqrt{\frac{d}{n \lambda_1}} \right) \right\} = o(1),$$

and, almost-surely as $n \to \infty$,

$$\sup_{\theta \in \mathbb{R}^d} V_X(\hat{\theta}, \theta) \leq \frac{\sigma^2 \tilde{m}}{n} \left\{ 1 + o(1) + O\left(\sqrt{\frac{n \lambda_1}{d}} \left(1 \sqrt{\frac{\lambda_1}{d}} \right) \right) \right\} + O\left(\frac{\sigma^2 n}{d} \right).$$

Consequently if $\lambda_1 = o\left(\frac{d \sqrt{m}}{\sigma^2 n} \right)$ and $\sigma^2 = o\left(\frac{d}{n} \right)$, then $R_X(\hat{\theta}, \theta) = o(\text{Var}(X_1^T \theta))$.

**Remark.** The previous theorem shows that in the HDLSS regime under fairly reasonable assumptions on $\theta$, the MNLS estimator always perform (asymptotically) better than the trivial null estimator, whose risk is given by $\text{Var}(X_1^T \theta)$. In particular, for $R_X(\theta, \theta)/\text{Var}(X_1^T \theta)$ to vanish (analysis of the proof of Theorem 1 show that this can vanish fast), it suffices that the parameter $\theta$ is sufficiently oriented along the directions of the spiked eigenvectors of $\Sigma$. In particular, it is enough to have $0 \leq \delta < 1$, such that $\sum_{j=m+1}^{d} \|P_j \theta\|^2 \leq \delta \|\theta\|^2$. 
2.2 Non asymptotic bounds for the MNLS estimator

The asymptotic bound of the previous section tells us that under Assumptions 1 and 3 the risk of the MNLS estimator vanishes in the limit, but the bound is not very informative on what are the essential features of the covariance matrix Σ and θ that can make the risk small. In order to get a better comprehension of the risk, we propose to investigate non-asymptotic bounds.

In order to get non-asymptotic bounds on the risk of the MNLS estimator, we require finer characterization of the spectrum of Σ. Indeed, the key assumption to understand the risk of the MNLS estimator is how the spectrum of Σ is spread, and especially the spectral gap between its eigenvalues. We now introduce the main definitions we need to characterize the spectrum of Σ.

**Definition 2** (Spectral gap). Let \( G_j := \lambda_j - \lambda_{j+1} \) denote the \( j \)-th spectral gap of Σ, and let \( \bar{G}_1 := G_1, \bar{G}_j = \min\{G_{j-1}, G_j\} \) for \( j \geq 2 \). We also define the following global measure of spectral gap. For every \( m \geq 1 \) and every \( \alpha \in \mathbb{R} \), we let \( G_m(\alpha) := \sum_{j=1}^{m} (\lambda_j^\alpha / G_j) \).

Then we can establish the following non-asymptotic upper bound on the risk. Note that the bounds on the next theorem are true under Assumption 2 only, but do not require Assumption 3 to hold, as we discuss hereafter.

**Theorem 3.** Let \( \rho_n(m) := n \left( \sqrt{d\lambda_{m+1}/n\lambda_1} + \sqrt{d\lambda_{m+1}/n\lambda_1} \right) \). Then, there exists a universal constant \( C > 0 \) such that with \( \mathbb{P} \)-probability at least \( 1 - e^{-t} \), for all \( \theta \in \mathbb{R}^d \),

\[
B_X(\hat{\theta}, \theta) \leq 2\lambda_1 \|\theta\|^2 \min_{m=1,\ldots,n} \left\{ \left( \frac{\lambda_{m+1}}{\lambda_1} + C\lambda_1 G_m \left( \frac{1}{2} \right) \right) \frac{\rho_n(m)^2 \vee t}{n} \right. \\
\times \left. \left( C\lambda_1 G_m(0) \frac{\rho_n(m)^2 \vee t}{n} + \sum_{j=m+1}^{d} \frac{\|P_j\theta\|^2}{\|\theta\|^2} \right) \right\},
\]

and, letting for simplicity \( \alpha = C \sqrt{\frac{m\lambda_1}{d}}, \beta = C \sqrt{\frac{m\lambda_1}{n}} \) and \( \delta = C \sqrt{\frac{m\lambda_1}{n}} \sqrt{\rho_n(m)} \),

\[
V_X(\hat{\theta}, \theta) \leq \min_{m=1,\ldots,n} \min_{m=1,\ldots,n} \left\{ \frac{\sigma^2}{n} \left( 1 + \frac{d\lambda_{m+1}}{n\lambda_m} \left( 1 + \alpha \right) + \beta \right) \left( 2m + \lambda_1 G_m(1) \delta \right) \\
+ \frac{\sigma^2}{1 - \alpha} \left( 2\delta m G_m(1) + \frac{n\lambda_{m+1}}{\lambda_1} \right) \frac{\lambda_1}{d\lambda_0} \right\}.
\]

**Remark.** Theorem 3 emphasizes that the HDLSS regime is only one idealized setting where the risk vanishes, and that Assumption 3 is certainly not required for this purpose. In particular, the bound in Theorem 3 is valid regardless of any assumption on Σ or θ. Though difficult to read, a careful analysis of each term tells us that the fundamental condition to meet is to have a sufficiently fast decay of \( m \mapsto \lambda_m/\lambda_1 \) as \( m \) grows to reduce the bias, but not too fast so that the variance doesn’t explode. Note that those conditions are reminiscent to Bartlett et al. (2019) findings too.

**Remark.** Theorem 3 also emphasizes that the more the parameter \( \theta \) is aligned with the dominating eigenvectors of Σ the smaller the bias will be. Note that this is not only to make the term
\[
\sum_{j=m+1}^{d} \|P_j \theta\|^2 \text{ small}, \text{ but also more importantly, the faster } m \mapsto \sum_{j=m+1}^{d} \|P_j \theta\|^2 \text{ decays, the more } \lambda_1 \|\theta\|^2 \approx \text{Var}(X_1^T \theta), \text{ which is risk of the null estimator we want at least to beat.}
\]

**Remark.** Under Assumption 2 only, i.e., sub-gaussianity of the \(X_i\)'s, the setting we investigate is quite close to the one in Bartlett et al. (2019), where the authors study the same problem under the assumption that \(X_i \sim N(0, \Sigma)\). Nevertheless, the bounds are quite different and it seems difficult to relate them. The setting in Bartlett et al. (2019) is more general, as they make no assumption about the spectral gap of \(\Sigma\). We believe that their bound can be better in situations where the spectral gap is small, as ours could deteriorate rapidly. We expect, however, our bound to be slightly better if the spectral gap gets larger. We discuss this point more thoroughly in Section 3.4. Note that if the spectral gap is small while the eigenvalues can be grouped into small blocks, such that the blocks are sufficiently separated, then one can carry a similar analysis as ours too, using the same arguments as the ones in usual PCA literature (Koltchinskii and Lounici, 2016; Shen et al., 2016a).

3 Discussion

3.1 General discussion

Although the asymptotic analysis might seem odd at first, and in particular the requirement that the risk vanish at infinity, this aims to provide some guidance on the conditions under which interpolation can lead to reasonable answers. Indeed, this is also coherent with Bartlett et al. (2019) results, the asymptotic analysis tells us that we can expect the risk to be small in situations where a few eigenvalues dominate the others and the parameter is relatively well aligned with the directions of eigenvectors corresponding to dominating eigenvalues.

3.2 The HDLSS regime and interpolation

The HDLSS regime is an idealization of the situation where a few eigenvalues of the population covariance matrix dominates the rest of them. As we point out in the Theorem 3, the risk of the MNLS estimator can vanish in other situations too, though the HDLSS regime is the prototypical example of sufficient conditions where interpolation of the data and vanishing predictive risk can coexist. Still, the requirement that \(\lambda_1, \ldots, \lambda_m \to \infty\) as \(n, d \to \infty\) might seem very unrealistic at first, even having in mind the Example 1. Indeed, this is not as idealized as it seems and occurs when over time we collect highly correlated features about individuals faster than we collect new individuals. In this situation, even though \(d/n \to \infty\), the “effective” number of features about which we collect information remains small, as they are all highly correlated. Then, the amount of information (i.e. signal) in the data indeed increases over time, which translates by saying that a certain number of eigenvalues grow as \(n, d \to \infty\) (corresponding to the directions of the effective features). In other words, collecting large number of correlated features, most of which are redundant, increases the amount of information contained in the data about the effective features. Interestingly, interpolation and good prediction are not discordant in such a situation.

\(^1\text{Indeed, this is not even necessary to have a vanishing risk, though it certainly improves the bias.}\)
3.3 What if $d/n\lambda_1$ doesn’t vanish?

One might wonder how essential it is for $d/n\lambda_1 \to 0$ to get small risk in compare to the null estimator. Considering the minimax lower bounds for linear regression given in Duchi and Wainwright (2013), along with results of Wang and Fan (2017) gives us some insight into this scenario. Under slightly stronger assumption on the distribution of data, Wang and Fan (2017) show that if for spiked eigenvalues indexed by $1 \leq j \leq \bar{m}$ we have $d/n\lambda_j = c_j < \infty$, then

$$\hat{\lambda}_j/\lambda_j = 1 + c_j + O_P\left(\lambda_j^{-1}\sqrt{\frac{d}{n}}\right).$$

On the other hand, the minimax lower bound given in Duchi and Wainwright (2013) is of the form

$$c d^2 \sigma^2 \|X\|_F^2.$$ 

Since $\|X\|_F^2 = n \sum_{i=1}^n \hat{\lambda}_i$, we have

$$c d^2 \sigma^2 \|X\|_F^2 \geq \frac{d^2 \sigma^2}{n^2 \lambda_1}.$$ 

Then using results of Wang and Fan (2017) in (3.1) (while absorbing constant terms in $c$), we get that $c d^2 \sigma^2 / n^2 \lambda_1 \approx c d^2 \sigma^2 / n^2 \lambda_1$, which diverges. We note that this doesn’t imply a a lower bound for the normalized risk since it doesn’t depend on $\|\theta\|$, unless we assume that $\|\theta\|$ remains bounded as $n, d \to \infty$ to remove dependence of $\text{Var}(X^T \theta)$ on $\|\theta\|$, the $\text{Var}(X^T \theta) \approx \lambda_1$, which means that even the normalized risk would be bounded away from zero. Furthermore, this minimax bound applies to the estimation risk, rather than the predictive risk that we are considering here, though they can be in the same order under strong but standard assumptions on design matrix.

It is also interesting that in this setting, limits of sample spiked and non spiked eigenvalues are the same asymptotically. For $m + 1 \leq j \leq n$, $\frac{n\lambda_j}{d\lambda_j} \to 1$ (Shen et al., 2016b). That is, both spiked and non spiked eigenvalues of the sample covariance matrix grow at the same rate of $\frac{d}{n}$, making them hard to distinguish which also hints at why the risk might be large in this case.

3.4 Comparison with Bartlett et al. (2019)

As already discussed in Section 1.3, the main difference with Bartlett et al. (2019) resides in the way we analyse the bias of the MNLS. Indeed, since we work in a more restricted setting, i.e. the HDLSS regime, we take benefit from the extra structure to improve on the bias. Indeed, inspection of the proof of Bartlett et al. (2019, Lemma 8) shows that they bound the bias as,

$$B^{H_{LLT}}_X(\hat{\theta}, \theta)^2 \leq \|\theta\|^2 \|\Sigma - \frac{X^TX}{n}\|.$$ 

They further bound in probability the term $\|\Sigma - n^{-1}X^TX\|$ using the general results from Koltchinskii and Lounici (2016), which requires the effective rank $r(\Sigma) \leq \frac{1}{\bar{m}} \sum_{k=1}^d \lambda_j$ to be a $o(n)$. In the HDLSS regime, the effective rank is asymptotically equal to $\bar{m} + n\rho_n(\bar{m})^2$, where
where \( \rho_n(m) \) is defined in Theorem 3. Hence the bound in Bartlett et al. (2019) gives in the HDLSS regime of Assumption 2, as \( n, d \to \infty \),

\[
B_X^{BLT} (\hat{\theta}, \theta)^2 \leq \lambda_1 \|\theta\|^2 \times O_p\left( \frac{1}{\sqrt{n}} \sqrt{\rho_n(\bar{m})} \right).
\]

In comparison, the bound in the Theorem 1 can be seen to be in the HDLSS regime, as \( n, d \to \infty \),

\[
B_X (\hat{\theta}, \theta)^2 \leq \lambda_1 \|\theta\|^2 \times O\left( \frac{1}{\sqrt{n}} \sqrt{\rho_n(\bar{m})^2} \right) \times \left\{ O\left( \frac{1}{\sqrt{n}} \sqrt{\rho_n(\bar{m})^2} \right) + \sum_{j=m+1}^d \|P_j \theta\|^2 \right\},
\]

almost-surely. Hence, the bound in this paper is sharper by several order of magnitude for the HDLSS regime (especially if \( \theta \) has most of its mass on the dominating eigenvalues directions), showing that in this regime there is an interest in exploiting the consistency of \( \hat{P}_1, \ldots, \hat{P}_m \) for \( P_1, \ldots, P_m \). As already mentioned, Bartlett et al. (2019) results don’t rely on separation of eigenvalues in contrast to our bounds, and we expect their bound to become better in situations where the spectrum of \( \Sigma \) is not separated enough.

Finally, our work complements Bartlett et al. (2019) results by showing that not only harmless interpolation in linear regression is possible in the large \( d \) small \( n \) regime, but also the bias can be significantly smaller than expected if \( \Sigma \) is well-behaved and \( \theta \) is well-aligned.

3.5 Further directions

In Theorem 1, we showed that in the setting where signal grows fast enough with \( n \), which is when spiked eigenvectors can be estimated consistently, normalized risk will vanish. We suspect that it is possible to give a non trivial lower bound for bias in the scenario briefly discussed in Section 3.3. That is, if we assume that for spiked eigenvalues \( 1 \leq j \leq m, \frac{d(n)}{\lambda_j} \to c_j \) where \( 0 < c_j < \infty \), and Gaussian data, we could use results of Wang and Fan (2017) to characterize sample spiked eigenvalues. However, to get a non trivial lower bound, we also need to know more about behaviour of non spiked sample eigenvectors (especially their projection into the spiked eigenspace), which is not explored in spike PCA literature.

4 Proofs

4.1 Preliminaries

Here we prove simultaneously the Theorems 1 and 3. Indeed, we prove the theorems by establishing bounds on the bias in Section 4.2, and the variance in Section 4.3. These bounds are not tied to the HDLSS scenario and may hold in a more general setting. The bounds mostly depends on the spectral gap of \( \Sigma \), as defined in Definition 2. In the asymptotic viewpoint of Assumption 3 and Theorem 1, however, the expression for the spectral gap simplifies quite consequently in the limit, which we emphasize in the next trivial proposition.

**Proposition 4.** Under Assumption 3, it holds \( \lim_{n \to \infty} \lambda_j / \bar{G}_j \to 1 \) for all \( j = \ldots, \bar{m} \), and consequently \( \lim_{n \to \infty} \lambda_1^{-\alpha} G_{\bar{m}}(\alpha) \leq C\bar{m} \) for a universal constant \( C > 0 \).
4.2 Upper bound on the bias of MNLS estimator

We summarize in the statement of the next lemma the results of this section. Then, the bounds for the bias in Theorems 1 and 3 follows from both the bound in Lemma 5, the results on the behaviour of \( P_j - \hat{P}_j \) in the HDLSS regime, which we recall in Appendix A.4, see the Lemma 12, and Proposition 4. We summarize the proofs of Theorems 1 and 3 in Section 4.4.

**Lemma 5 (Bias).** For any \( \theta \) and any \( X \), the following bound is true. For all \( m = 1, \ldots, d \),

\[
B_{\theta}(\hat{\theta}, \theta)^2 \leq 2\|\theta\|^2 \left( \lambda_{m+1}^1 + \left\| \sum_{j=1}^{m} \sqrt{\lambda_j} (\hat{P}_j - P_j) \right\|^2 \right) \left( \left\| \sum_{j=1}^{m} (\hat{P}_j - P_j) \right\|^2 + \sum_{j=m+1}^{d} \|P_j\theta\|^2 \right).
\]

In particular, the Lemma 12 implies that the following bounds are true.

1. If Assumptions 1 and 3 are true. Then, as \( n \to \infty \), almost-surely,

\[
B_{\theta}(\hat{\theta}, \theta)^2 \leq 2\lambda_1^1 \|\theta\|^2 \left( \lambda_{m+1}^1 + O \left( \frac{1}{n} \sqrt{\frac{d}{n \lambda_1}} \right) \right) \left( \left( \frac{1}{n} \sqrt{\frac{d}{n \lambda_1}} \right) + \frac{\sum_{j=m+1}^{d} \|P_j\theta\|^2}{\|\theta\|^2} \right).
\]

Further, remark that under Assumption 3, \( \frac{\lambda_{m+1}^1}{\lambda_1^1} = O \left( \frac{n d}{n \lambda_1} \right) = o \left( \frac{d}{n \lambda_1} \right) \).

2. Let define \( \rho_n(m) = n \left( \sqrt{\frac{d \lambda_{m+1}^1}{n \lambda_1^1}} \sqrt{\frac{d \lambda_{m+1}^1}{n \lambda_1^1}} \right) \). If Assumption 2 is true, then there is a universal constant \( C > 0 \) such that with \( \mathbb{P} \)-probability at least \( 1 - e^{-t} \)

\[
B_{\theta}(\hat{\theta}, \theta)^2 \leq 2\lambda_1^1 \|\theta\|^2 \min_{m=1, \ldots, n} \left\{ \left( \frac{\lambda_{m+1}^1}{\lambda_1^1} + C \lambda_1^1 \rho_n(m)^2 \right) \left( 1 \right) \left( \frac{2 m \vee \rho_n(m)^2 \vee t}{n} \right) \right. \\
\times \left. \left( C \lambda_1^1 \rho_n(0)^2 \left( \frac{2 m \vee \rho_n(m)^2 \vee t}{n} \right) + \sum_{j=m+1}^{d} \|P_j\theta\|^2 \right) \right\}.
\]

We now prove the Lemma 5. Remark that by linearity \( \mathbb{E}_{\theta}[\hat{\theta} \mid X] = (X^T X)^\dagger X^T X \theta \) and thus the bias can be rewritten as

\[
B_{\theta}(\hat{\theta}, \theta)^2 = \|\Sigma^{1/2}(\theta - \mathbb{E}[\hat{\theta} \mid X])\|^2 = \theta^T (I - (X^T X)^\dagger X^T X) \Sigma (I - (X^T X)^\dagger X^T X) \theta.
\]

We wish to understand \( \Sigma^{1/2}(I - (X^T X)^\dagger X^T X) \theta \). Remark that \( (X^T X)^\dagger X^T X = \sum_{j=1}^{n} \hat{P}_j \) and that \( \Sigma^{1/2} = \sum_{j=1}^{d} \sqrt{\lambda_j} P_j \). So, \( \Sigma^{1/2}(X^T X)^\dagger X^T X \theta = \sum_{j=1}^{d} \sqrt{\lambda_j} P_j \sum_{k=1}^{n} \hat{P}_k \). We decompose as follows,

\[
\Sigma^{1/2}(X^T X)^\dagger X^T X \theta - \Sigma^{1/2} \theta = \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k - I \right) \theta + \sum_{j=m+1}^{d} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k - I \right) \theta. \tag{4.1}
\]
Bound on the first term of the rhs of Equation (4.1) We rewrite each of the $P_j$ as $P_j = \hat{P}_j + (P_j - \hat{P}_j)$, and thus

$$\sum_{j=1}^{m} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k - I \right) \theta = \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \sum_{k=1}^{n} \hat{P}_k \theta + \sum_{j=1}^{m} \sqrt{\lambda_j} (P_j - \hat{P}_j) \sum_{k=1}^{n} \hat{P}_k \theta - \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \theta$$

$$= \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \theta + \sum_{j=1}^{m} \sqrt{\lambda_j} (P_j - \hat{P}_j) \sum_{k=1}^{n} \hat{P}_k \theta - \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \theta$$

$$= \sum_{j=1}^{m} \sqrt{\lambda_j} (\hat{P}_j - P_j) \left( I - \sum_{k=1}^{n} \hat{P}_k \right) \theta.$$ 

Thus, we obtain that,

$$\left\| \sum_{j=1}^{m} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k - I \right) \theta \right\| \leq \left\| \left( I - \sum_{k=1}^{n} \hat{P}_k \right) \theta \right\| \cdot \left\| \sum_{j=1}^{m} \sqrt{\lambda_j} (P_j - \hat{P}_j) \right\| .$$

But,

$$\theta - \sum_{k=1}^{n} \hat{P}_k \theta = \theta - \sum_{k=1}^{d} P_k \theta - \sum_{k=1}^{m} (\hat{P}_k - P_k) \theta - \sum_{k=1}^{n} \hat{P}_k \theta$$

$$= \sum_{k=m+1}^{d} P_k \theta - \sum_{k=1}^{m} (\hat{P}_k - P_k) \theta - \sum_{k=1}^{n} \hat{P}_k \theta$$

$$= \sum_{k=m+1}^{d} P_k \theta - \sum_{k=1}^{m} (\hat{P}_k - P_k) \theta - \sum_{k=1}^{m} \sum_{\ell=k+1}^{n} \hat{P}_k \theta$$

$$= \sum_{k=m+1}^{d} P_k \theta - \sum_{k=1}^{m} (\hat{P}_k - P_k) \theta - \sum_{k=m+1}^{d} \sum_{k=1}^{n} \hat{P}_k \theta$$

$$= \left( I - \sum_{k=m+1}^{n} \hat{P}_k \right) \sum_{k=m+1}^{d} P_k \theta - \left( I - \sum_{k=m+1}^{n} \hat{P}_k \right) \sum_{k=1}^{n} (\hat{P}_k - P_k) \theta.$$ 

Therefore,

$$\left\| \left( I - \sum_{k=1}^{n} \hat{P}_k \right) \theta \right\| \leq \left\| \sum_{k=m+1}^{d} P_k \theta \right\| + \left\| \sum_{k=1}^{m} (\hat{P}_k - P_k) \theta \right\| .$$
Bound on the second term of the rhs of Equation (4.1) For the sake of simplicity we let \( \hat{Q} := \sum_{k=1}^{n} \hat{P}_k \). Then, using that \( I = \sum_{\ell=1}^{d} P_{\ell} \) we rewrite,

\[
\left\| \sum_{j=m+1}^{d} \sqrt{\lambda_j} P_j \hat{Q} \theta \right\|^2 = \sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \theta \right\|^2 \\
= \sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \sum_{\ell=1}^{m} P_{\ell} \theta + P_j \hat{Q} \sum_{\ell=m+1}^{d} P_{\ell} \theta \right\|^2 \\
\leq 2 \sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \sum_{\ell=1}^{m} P_{\ell} \theta \right\|^2 + 2 \sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \sum_{\ell=m+1}^{d} P_{\ell} \theta \right\|^2 \tag{4.2}
\]

Regarding the second term of the rhs of the last display,

\[
\sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \left( \sum_{\ell=m+1}^{d} P_{\ell} \right) \theta \right\|^2 \leq \lambda_{m+1} \sum_{j=m+1}^{d} \left\| P_j \hat{Q} \left( \sum_{\ell=m+1}^{d} P_{\ell} \right) \theta \right\|^2 \\
= \lambda_{m+1} \left\| \left( \sum_{j=m+1}^{d} P_j \right) \hat{Q} \left( \sum_{\ell=m+1}^{d} P_{\ell} \right) \theta \right\|^2 \\
\leq \lambda_{m+1} \left\| \left( \sum_{\ell=m+1}^{d} P_{\ell} \right) \theta \right\|^2 \\
= \lambda_{m+1} \sum_{\ell=m+1}^{d} \left\| P_{\ell} \theta \right\|^2.
\]

For the first term of the rhs of Equation (4.2), we can rewrite that

\[
\hat{Q} P_{\ell} = \hat{Q} P_{\ell} + \hat{Q} (P_{\ell} - \hat{P}_{\ell}) \\
= \hat{P}_{\ell} + \hat{Q} (P_{\ell} - \hat{P}_{\ell}) \\
= P_{\ell} + (\hat{P}_{\ell} - P_{\ell}) + \hat{Q} (P_{\ell} - \hat{P}_{\ell}) \\
= P_{\ell} + (\hat{Q} - I) (P_{\ell} - \hat{P}_{\ell}),
\]

and hence,

\[
\sum_{j=m+1}^{d} \lambda_j \left\| P_j \hat{Q} \sum_{\ell=1}^{m} P_{\ell} \theta \right\|^2 \leq \lambda_{m+1} \sum_{j=m+1}^{d} \left\| \sum_{\ell=1}^{m} \left( P_j P_{\ell} + P_j (\hat{Q} - I) (P_{\ell} - \hat{P}_{\ell}) \right) \theta \right\|^2 \\
= \lambda_{m+1} \sum_{j=m+1}^{d} \left\| P_j (\hat{Q} - I) \sum_{\ell=1}^{m} (P_{\ell} - \hat{P}_{\ell}) \theta \right\|^2 \\
\leq \lambda_{m+1} \left\| \sum_{\ell=1}^{m} (P_{\ell} - \hat{P}_{\ell}) \theta \right\|^2.
\]
Combining everything,
\[
\left\| \sum_{j=m+1}^{d} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k - I \right) \theta \right\|^2 \leq 2 \left\| \sum_{j=m+1}^{d} \sqrt{\lambda_j} P_j \left( \sum_{k=1}^{n} \hat{P}_k \right) \theta \right\|^2 + 2 \left\| \sum_{j=m+1}^{d} \sqrt{\lambda_j} P_j \theta \right\|^2 \\
\leq 2\lambda_{m+1} \left\| \sum_{\ell=1}^{m} (P_{\ell} - \hat{P}_{\ell}) \theta \right\|^2 + 2\lambda_{m+1} \sum_{j=m+1}^{d} \|P_j\theta\|^2.
\]

### 4.3 Upper bound on the variance of MNLS estimator

We summarize in the statement of the next lemma the results of this section. Then, the bounds for the variance in Theorems 1 and 3 follows from both the bound in Lemma 6, the results on behaviour of $\lambda_1, \ldots, \lambda_n$, which we recall in Appendices A.2 and A.3, and the results on the behaviour of $P_j - \hat{P}_j$ in the HDLSS regime, which we recall in Appendix A.4.

**Lemma 6.** For any $\theta$ and any $X$, the following bound is true. For all $m = 1, \ldots, d$,
\[
V_X(\hat{\theta}, \theta) \leq \frac{\sigma^2 m}{n} \left( 1 + \frac{\lambda_{m+1}}{\lambda_m} \right) \max_{j=1, \ldots, m} \frac{\lambda_j}{\lambda_j} + \frac{\sigma^2}{n} \max_{j=1, \ldots, m} \frac{\lambda_j}{\lambda_j} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} \|P_j - \hat{P}_j\| \right) \left( \sum_{k=1}^{m} \lambda_k \right) \\
+ \frac{2\sigma^2 m}{n\lambda_n} \left\| \sum_{k=1}^{m} \lambda_k (P_k - \hat{P}_k) \right\| + \frac{\sigma^2 \lambda_{m+1}}{\lambda_n}.
\]

In particular, the following bounds are true.

1. If Assumptions 1 and 3 are true. Then, as $n \to \infty$, almost-surely,
\[
V_X(\hat{\theta}, \theta) \leq \frac{\sigma^2 m}{n} \left\{ 1 + o(1) + O\left( \sqrt{\frac{n \lambda_1}{d}} \left( \frac{1}{\sqrt{n}} \frac{\lambda_1}{d} \right) \right) \right\} + O\left( \frac{\sigma^2 n}{d} \right).
\]

2. $\rho_n(m) = n\left( \frac{\sqrt{\lambda_{m+1}}}{\lambda_1} \sqrt{\frac{\lambda_{m+1}}{\lambda_1}} \right)$. If Assumption 2 is true, then there is a universal constant $C > 0$ such that with $\mathbb{P}$-probability at least $1 - e^{-t}$,
\[
V_X(\hat{\theta}, \theta) \leq \min_{m=1, \ldots, n} \min_{m=1, \ldots, m} \left\{ \frac{\sigma^2}{n} \left( 1 + \frac{\lambda_{m+1}}{n \lambda_m} \left( 1 + \alpha \right) + \beta \right) \left( 2m + \lambda_1 G_m(1) \right) \delta \right. \\
\left. + \frac{\sigma^2}{1 - \alpha} \left( 2\delta m G_m(1) + \frac{n \lambda_{m+1}}{\lambda_1} \right) \frac{\lambda_1}{d \delta} \right\},
\]

where $\alpha = C \sqrt{\frac{n \delta}{d}}$, $\beta = C \sqrt{\frac{n \delta}{n}}$ and $\delta = C \sqrt{\frac{m \delta}{n}} \sqrt{n}$ $\rho_n(m)$.

In order to establish Lemma 6, we recall that $V_X(\hat{\theta}, \theta) = \sigma^2 \text{Tr}(\hat{\Sigma}^1 \Sigma)/n$. Then, we decompose $\hat{\Sigma}^1 \Sigma = \sum_{j=1}^{n} \frac{1}{\lambda_j} \hat{P}_j \sum_{k=1}^{d} \lambda_k P_k$ into four terms
\[
\hat{\Sigma}^1 \Sigma = \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k + \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k + \sum_{j=m+1}^{n} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k + \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k. \quad (4.3)
\]
We bound the trace of each of the four terms above in the paragraphs below. The final result follows by combining all these bounds.

**Bound on the first term of Equation (4.3)** To bound the first term, we use that the projectors \( \hat{P}_j \) are consistent for \( P_j \) in the operator norm when \( j = 1, \ldots, m \). Then, we can rewrite

\[
\sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k = \sum_{j=1}^{m} \frac{\lambda_j}{\lambda_j} P_j + \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} (\hat{P}_j - P_j) P_k.
\]

Since \( P_j \) has always rank 1, by taking the trace of the previous expression we obtain

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) = \sum_{j=1}^{m} \frac{\lambda_j}{\lambda_j} + \text{Tr} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \sum_{k=1}^{m} \lambda_k P_k \right)
\]

\[
\leq m \max_{j=1,...,m} \frac{\lambda_j}{\lambda_j} + \text{Tr} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \sum_{k=1}^{m} \lambda_k P_k \right).
\]

We bound the second term of the last display using von Neumann’s trace inequality. Indeed,

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) \leq m \max_{j=1,...,m} \frac{\lambda_j}{\lambda_j} + \sum_{\ell=1}^{d} \sigma_\ell \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \right) \sigma_\ell \left( \sum_{k=1}^{m} \lambda_k P_k \right).
\]

Now the matrix \( \sum_{k=1}^{m} \lambda_k P_k \) has rank no more than \( m \) so \( \sigma_\ell (\sum_{k=1}^{m} \lambda_k P_k) = 0 \) if \( \ell > m \), and \( \sigma_\ell (\sum_{k=1}^{m} \lambda_k P_k) = \lambda_\ell \) if \( 1 \leq \ell \leq m \). Further \( \max_{1 \leq \ell \leq d} \sigma_\ell (\sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j)) = \sigma_1 (\sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j)) \leq \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \| \), and thus

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) \leq m \max_{j=1,...,m} \frac{\lambda_j}{\lambda_j} + \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \| \right) \left( \sum_{k=1}^{m} \lambda_k \right)
\]

\[
\leq m \max_{j=1,...,m} \frac{\lambda_j}{\lambda_j} + \max_{j=1,...,m} \lambda_j \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \| \right) \left( \sum_{k=1}^{m} \lambda_k \right).
\]

**Bound on the second term of Equation (4.3)** Using that \( \text{Tr}(\hat{P}_j P_k) = (\hat{u}_j^T u_k)^2 \), we indeed have

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) = \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} (\hat{u}_j^T u_k)^2
\]

\[
\leq \frac{\lambda_{m+1}}{\lambda_m} \sum_{j=1}^{m} \sum_{k=m+1}^{d} (\hat{u}_j^T u_j)^2
\]

\[
\leq \frac{\lambda_{m+1}}{\lambda_m} \sum_{j=1}^{m} \| \hat{u}_j \|^2
\]

\[
= \frac{m \lambda_{m+1}}{\lambda_m}.
\]

(4.4)
Using the consistency of \( \hat{P}_j \) for \( P_j \) in the operator norm, we can get another bound. Note that the second bound is not needed, as Equation (4.4) is already smaller than the dominating term of the variance, but we give it for completeness. Indeed, using von Neumann’s trace inequality, we get

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) = \text{Tr} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \sum_{k=m+1}^{d} \lambda_k P_k \right)
\]

\[
\leq \sum_{\ell=1}^{d} \sigma_{\ell} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \right) \sigma_{\ell} \left( \sum_{k=m+1}^{d} \lambda_k P_k \right).
\]

But the matrix \( \sum_{j=1}^{m} \lambda_j^{-1}(\hat{P}_j - P_j) \) has rank no more than \( 2m \), so that \( \sigma_{\ell}(\sum_{j=1}^{m} \lambda_j^{-1}(\hat{P}_j - P_j)) = 0 \) for \( \ell > 2m \). Also, \( \max_{\ell=1, \ldots, d} \sigma_{\ell}(\sum_{k=m+1}^{d} \lambda_k P_k) = \lambda_{m+1} \), so that we have the bound

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) \leq 2m \lambda_{m+1} \sigma_{1} \left( \sum_{j=1}^{m} \frac{1}{\lambda_j} (\hat{P}_j - P_j) \right)
\]

\[
\leq 2m \lambda_{m+1} \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \|
\]

\[
\leq 2m \lambda_{m+1} \max_{j=1, \ldots, m} \frac{\lambda_j}{\lambda_j} \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \|. \quad (4.5)
\]

Combining Equations (4.4) and (4.5) it follows,

\[
\text{Tr} \left( \sum_{j=1}^{m} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) \leq \frac{m \lambda_{m+1}}{\lambda_m} \max_{1 \leq j \leq m} \frac{\lambda_j}{\lambda_j} \left( 1 \wedge \left\| \sum_{j=1}^{m} \frac{1}{\lambda_j} \| \hat{P}_j - P_j \| \right) \right).
\]

**Bound on the third term of Equation (4.3)** We use the argument that for \( j = 1, \ldots, m \) the projectors \( \hat{P}_j \) are consistent for \( P_j \), and thus in the limit the projector \( \sum_{j=m+1}^{n} \hat{P}_j \) is orthogonal to any \( P_k \) for \( k = 1, \ldots, m \). Indeed, we rewrite \( \hat{P}_k = P_k - \hat{P}_k + \hat{P}_k \) in the previous term and use von Neumann’s trace inequality to deduce that

\[
\text{Tr} \left( \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) = \text{Tr} \left( \sum_{j=m+1}^{n} \frac{1}{\lambda_j} \hat{P}_j \sum_{k=m+1}^{d} \lambda_k (P_k - \hat{P}_k) \right)
\]

\[
\leq \sum_{\ell=1}^{d} \sigma_{\ell} \left( \sum_{j=m+1}^{n} \frac{1}{\lambda_j} \hat{P}_j \right) \sigma_{\ell} \left( \sum_{k=m+1}^{d} \lambda_k (P_k - \hat{P}_k) \right).
\]

Now \( \max_{\ell=1}^{d} \sigma_{\ell}(\sum_{j=m+1}^{n} \hat{P}_j) = \sigma_{1}(\sum_{j=m+1}^{n} \hat{P}_j) = \lambda_{-1} \), and the matrix \( \sum_{k=m+1}^{d} \lambda_k (P_k - \hat{P}_k) \) has rank no more than \( 2m \), from which we deduce that \( \sigma_{\ell}(\sum_{k=m+1}^{d} \lambda_k (P_k - \hat{P}_k)) = 0 \) for \( \ell > 2m \).
Henceforth,
\[
\text{Tr} \left( \sum_{j=m+1}^{n} \sum_{k=1}^{m} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) \leq \frac{2m}{\lambda_n} \sigma_1 \left( \sum_{k=1}^{m} \lambda_k (P_k - \hat{P}_k) \right) \\
\leq \frac{2m}{\lambda_n} \left\| \sum_{k=1}^{m} \lambda_k (P_k - \hat{P}_k) \right\|
\]

**Bound on the last term of Equation (4.3)** To bound the last term, we again use that \(\text{Tr}(\hat{P}_j P_k) = (\hat{u}_j^T u_k)^2\) to deduce that
\[
\text{Tr} \left( \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \hat{P}_j P_k \right) = \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} \frac{\lambda_k}{\lambda_j} \text{Tr}(\hat{P}_j P_k) \\
\leq \frac{\lambda_{m+1}}{\lambda_n} \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} (\hat{u}_j^T u_k)^2 \\
\leq \frac{\lambda_{m+1}}{\lambda_n} \sum_{j=m+1}^{n} \sum_{k=m+1}^{d} (\hat{u}_j^T u_k)^2 \\
\leq \frac{\lambda_{m+1}}{\lambda_n} \sum_{j=m+1}^{n} ||\hat{u}_j||^2 \\
\leq \frac{n \lambda_{m+1}}{\lambda_n}.
\]

### 4.4 Summary of the proof of Theorems 1 and 3

The proofs are an immediate consequence of Lemmas 5 and 6, the only thing remaining to show is to relate \(\text{Var}(X^T_1 \theta)\) to \(\lambda_1 ||\theta||^2\) when \(\theta \in A(\bar{m}, L, \delta)\). But, we have for any \(\theta \in A(m, L, \delta)\)
\[
\frac{\lambda_1 ||\theta||^2}{\text{Var}(X^T_1 \theta)} = \frac{\lambda_1 ||\theta||^2}{\sum_{j=1}^{d} \lambda_j ||P_j \theta||^2} \leq \frac{\lambda_1 ||\theta||^2}{\sum_{j=1}^{m} \lambda_j ||P_j \theta||^2} \leq \frac{\lambda_1 ||\theta||^2}{\lambda_m \sum_{j=1}^{m} ||P_j \theta||^2} \\
\leq \frac{\lambda_1 ||\theta||^2}{\lambda_m \left( \sum_{j=1}^{d} ||P_j \theta||^2 - \sum_{j=m+1}^{d} ||P_j \theta||^2 \right)} \leq \frac{\lambda_1}{\lambda_m} \frac{1}{1 - \delta}.
\]

Remark that we also always have \(\text{Var}(X^T_1 \theta) \leq \lambda_1 ||\theta||^2\), and hence \(\frac{\lambda_1}{\lambda_1} (1 - \delta) \lambda_1 ||\theta||^2 \leq \text{Var}(X^T_1 \theta) \leq \lambda_1 ||\theta||^2\) for every \(\theta \in A(m, \delta, L)\). For the Theorem 1, simply remark that \(\lambda_1 \asymp \lambda_{\bar{m}}\) and thus \(\text{Var}(X^T_1 \theta) \asymp \lambda_1 ||\theta||^2\) under the Assumption 3.

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A Asymptotics of sample covariance matrix in the HDLSS regime

A.1 Preliminaries

Here we investigate the asymptotics of the sample covariance matrix in the HDLSS regime. Note that this has already been done for instance in Hall et al. (2005); Ahn et al. (2007); Jung and Marron (2009); Shen et al. (2013, 2016a,b) and we give those results for completeness. Along the way, we extend a bit the results of Shen et al. (2016a) under the Assumption 2 to obtain non-asymptotic bounds in the case where the entries of $Z$ are sub-gaussian.

As shown in Shen et al. (2016a), the proofs rely on analyzing the asymptotics of the dual matrix $\hat{D} := n^{-1}XX^T = n^{-1}Z\Lambda Z^T$, which can be rewritten as $\hat{D} = n^{-1}\sum_{j=1}^{d} \lambda_j \tilde{Z}_j \tilde{Z}_j^T$, where
\( \mathbf{Z}_j \in \mathbb{R}^n \) has i.i.d entries \( \mathbf{Z}_j := (Z_{1,j}, \ldots, Z_{n,j}) \). Then, we can decompose \( \hat{D} \) into spiked-part \( \hat{D}_s := n^{-1} \sum_{j=1}^{\hat{m}} \lambda_j \mathbf{Z}_j \mathbf{Z}_j^T \) and non-spiked-part \( \hat{D}_{ns} := n^{-1} \sum_{j=\hat{m}+1}^{d} \lambda_j \mathbf{Z}_j \mathbf{Z}_j^T \).

### A.2 On the behaviour of the spiked eigenvalues

The goal is to demonstrate the following lemma. The first item of the lemma is taken as it is from Shen et al. (2016a, Lemma 3). The second item is obtained using the same steps as Shen et al. (2016a, Lemma 3) by exploiting the additional structure offered by Assumption 2, and the well-known results from Vershynin (2010), which we recall for completeness in Appendix A.6.

**Lemma 7.** The following statements are true.

1. If Assumption 1 is valid, then for every fixed integer \( \hat{m} \), and every \( 1 \leq m \leq \hat{m} \), as \( n \to \infty \),
   \[
   \max_{1 \leq k \leq m} \frac{\hat{\lambda}_k - \lambda_k}{\lambda_k} \leq \frac{d \lambda_{\hat{m}+1}}{n \lambda_m} \left\{ 1 + O \left( \sqrt{\frac{n}{d}} \right) \right\} + O \left( \frac{1}{\sqrt{n}} \right), \quad \text{almost-surely.}
   \]

2. If Assumption 2 is valid and \( 0 < t \leq n \), then there is a universal constant \( C > 0 \) such that with \( \mathbb{P} \)-probability at least \( 1 - e^{-t} \), for all \( 1 \leq m \leq n \), all \( 1 \leq m \leq \hat{m} \),
   \[
   \max_{1 \leq k \leq m} \frac{\hat{\lambda}_k - \lambda_k}{\lambda_k} \leq \frac{d \lambda_{\hat{m}+1}}{n \lambda_m} \left\{ 1 + C \sqrt{\frac{n \lor t}{d}} \right\} + C \sqrt{\frac{m \lor t}{n}}.
   \]

**Proof.** We copy (Shen et al., 2016a, Lemma 3). Note that Item (1) is simply (Shen et al., 2016a, Lemma 3), or can be derived using the same steps as Item (2), and thus we only prove the Item (2). The matrix \( \hat{\Sigma} := n^{-1} \mathbf{X}^T \mathbf{X} \) has the same non-zero singular values as the dual matrix \( \hat{D} \). Then, by Weyl’s inequalities, we have for any \( 1 \leq j \leq \hat{m} \) that \( \sigma_{\min}(\hat{D}_{ns}) + \sigma_j(\hat{D}_s) \leq \sigma_j(\hat{D}) \leq \sigma_j(\hat{D}_s) + \sigma_{\max}(\hat{D}_{ns}) \). By Proposition 10, with \( \mathbb{P} \)-probability at least \( 1 - e^{-t} \),
   \[
   \max_{1 \leq j \leq m} \frac{n}{d \lambda_{\hat{m}+1}} |\sigma_j(\hat{D}) - \sigma_j(\hat{D}_s)| \leq 1 + C \sqrt{\frac{n \lor t}{d}}.
   \]

Hence, it is enough to establish the asymptotics of \( \sigma_j(\hat{D}_s) \). We proceed as in (Shen et al., 2016a, Lemma 3) and for \( k = 1, \ldots, \hat{m} \) we introduce the matrices \( \hat{D}_s^k := n^{-1} \sum_{j=k}^{\hat{m}} \lambda_j \mathbf{Z}_j \mathbf{Z}_j^T \). Then, by their equations (14) and (16), for all \( k = 1, \ldots, \hat{m} \) it holds \( \sigma_{\max}(n^{-1} \mathbf{Z}_k \mathbf{Z}_k^T) \leq \frac{\sigma_k(\hat{D}_s)}{\lambda_k} \leq \frac{1}{\lambda_k} \sigma_{\max}(\hat{D}_s^k) \). The result follows from Proposition 8.

**Proposition 8.** Under Assumption 2, if \( 0 < t \leq n \) there exists a constant \( C > 0 \) depending on \( \nu \) such that with \( \mathbb{P} \)-probability \( 1 - e^{-t} \), for all \( 1 \leq m \leq n \)
   \[
   \max_{1 \leq k \leq m} \frac{\sigma_{\max}(\hat{D}_s^k)}{\lambda_k} \leq 1 + C \sqrt{\frac{\hat{m} \lor t}{n}}, \quad \min_{1 \leq k \leq m} \sigma_{\max}(n^{-1} \mathbf{Z}_k \mathbf{Z}_k^T) \geq 1 - C \sqrt{\frac{\hat{m} \lor t}{n}}.
   \]
Proof. Those computations are standard. The result for $\sigma_{\text{max}}(n^{-1}\tilde{\mathbf{Z}}_k\tilde{\mathbf{Z}}_k^T)$ immediately follows from Proposition 14 and a union-bound. We proceed with the other bound. As in Shen et al. (2016a, Lemma 3), let define $W_i := (\sqrt{\lambda_k}Z_{i,k}, \ldots, \sqrt{\lambda_m}Z_{i,\bar{m}}) \in \mathbb{R}^{m-k}$, and $i = 1, \ldots, n$. Let also $\mathbf{W}$ be $n \times (\bar{m} - k)$ matrix whose rows are $W_i$. Then, remark that $\hat{D}_s^k = n^{-1}\mathbf{W}^T\mathbf{W}$, and thus $\hat{D}_s^k$ and $n^{-1}\mathbf{W}^T\mathbf{W}$ have the same non-zero singular values, and it is enough to bound in probability $\sigma_{\text{max}}(n^{-1}\mathbf{W}^T\mathbf{W})$. First we remark that $\mathbb{E}[n^{-1}\mathbf{W}^T\mathbf{W}] = \text{diag}(\lambda_k, \ldots, \lambda_{\bar{m}})$, and thus at least $\sigma_{\text{max}}(\mathbb{E}[n^{-1}\mathbf{W}^T\mathbf{W}]) = \lambda_k$. We now show that under Assumption 2 there is enough concentration so that the result holds in probability. For any $v \in \mathbb{R}^{m-k}$, $n^{-1}\|\mathbf{W}v\|^2 = v^T(n^{-1}\mathbf{W}^T\mathbf{W})v = \sum_{j=k}^{m} \sum_{k=1}^{n} v_i^2 \sum_{i=1}^{m} \lambda_{j,k} v_i v_k = \sum_{j=k}^{m} \sum_{k=1}^{n} \sqrt{\lambda_j} v_i \sqrt{\lambda_k} v_k \sum_{i=1}^{m} Z_{i,j} Z_{i,k}$. Indeed, letting the transformation $\mathbf{v} = (\sqrt{\lambda_k} v_k, \ldots, \sqrt{\lambda_{\bar{m}}} v_{\bar{m}})$ and letting $\mathbf{W}_s$ be the $n \times (\bar{m} - k)$ matrix whose rows are $(Z_{i,k}, \ldots, Z_{i,\bar{m}})$, then we can write,

$$\sigma_{\text{max}}(\hat{D}_s^k) = \sigma_{\text{max}}(n^{-1}\mathbf{W}^T\mathbf{W}) = \sup_{v \in \mathbb{R}^{m-k}} \frac{n^{-1}\|\mathbf{W}v\|^2}{\|v\|^2} = \sup_{v \in \mathbb{R}^{m-k}} \frac{n^{-1}\|\mathbf{W}_s\mathbf{v}\|^2}{\|\mathbf{v}\|^2},$$

and hence $\sigma_{\text{max}}(\hat{D}_s^k) \leq \sigma_{\text{max}}(n^{-1}\mathbf{W}^T\mathbf{W}_s) \sup_{v \in \mathbb{R}^{m-k}} \frac{\|\mathbf{v}\|^2}{\|\mathbf{v}\|^2} \leq \lambda_k \sigma_{\text{max}}(n^{-1}\mathbf{W}^T\mathbf{W}_s)$. The result then follows from Proposition 14 and a union bound. \(\square\)

A.3 On the behaviour of non-spiked eigenvalues

Here we consider the asymptotic behaviour of the non-spiked sample eigenvalues in the HDLSS regime. In particular, to bound the variance of the MNLS estimator, we need to understand the behaviour of $\hat{\lambda}_n$. Again, we borrow the result from Shen et al. (2016a).

Proposition 9. The following statements are true.

1. Under Assumption 1 it holds $\frac{\hat{\lambda}_n}{\lambda_{\bar{m}}} \geq 1 + O\left(\sqrt{\frac{\alpha}{d}}\right)$ almost-surely as $n \to \infty$.

2. Under Assumption 2, there exists a universal constant $C > 0$ such that with $\mathbb{P}$-probability at least $1 - e^{-t}$ it holds $\frac{n\lambda_n}{\lambda_{\bar{m}}} \geq 1 - C\sqrt{\frac{n\lambda_T}{d}}$.

Proof. Using Weyl's inequality, we obtain that $\hat{\lambda}_n = \sigma_{\text{min}}(\hat{D}) \geq \sigma_{\text{min}}(\hat{D}_{\text{ns}})$. Then the result is a consequence of the next Proposition 10. \(\square\)

Proposition 10. The following statements are true.

1. Under Assumption 1 it holds $\frac{n\sigma_{\text{max}}(\hat{D}_{\text{ns}})}{\lambda_{\bar{m}} + 1} \leq 1 + O\left(\sqrt{\frac{\alpha}{d}}\right)$ almost-surely as $n \to \infty$, and $\frac{n\sigma_{\text{min}}(\hat{D}_{\text{ns}})}{\lambda_{\bar{m}} + 1} \geq 1 + O\left(\sqrt{\frac{\alpha}{d}}\right)$ almost-surely as $n \to \infty$.

2. Under Assumption 2, there exists a universal constant $C > 0$ such that with $\mathbb{P}$-probability at least $1 - e^{-t}$ it holds $\frac{n\sigma_{\text{max}}(\hat{D}_{\text{ns}})}{\lambda_{\bar{m}} + 1} \leq 1 + C\sqrt{\frac{n\lambda_T}{d}}$, and $\frac{n\sigma_{\text{min}}(\hat{D}_{\text{ns}})}{\lambda_{\bar{m}} + 1} \geq 1 - C\sqrt{\frac{n\lambda_T}{d}}$.\(\square\)
Proof. We copy (Shen et al., 2016a, Lemma 4). It is enough to consider \( \hat{D}_{ns}^* := \frac{1}{n} \sum_{j=m+1}^{d} \tilde{Z}_j \tilde{Z}_j^T \). Indeed by the equation (22) in their paper for every \( j \geq 1 \) it holds \( \lambda_d \sigma_j(\hat{D}_{ns}^*) \leq \sigma_j(\hat{D}_{ns}) \leq \lambda_{m+1} \sigma_j(\hat{D}_{ns}^*) \). Then the result follows by Propositions 13, and 14, because \( \hat{D}_{ns}^* \) is a \((d-m) \times n\) matrix with i.i.d entries of zero mean and finite variance.

\[ \square \]

A.4 On the behaviour of the eigen-projectors

Here we mostly follow the results in Koltchinskii and Lounici (2016) instead of Shen et al. (2016a), which provides a simpler approach to bounding \( \| P_j - \hat{P}_j \| \). In particular, the following proposition is a restatement of their more general Koltchinskii and Lounici (2016, Lemma 1). Then, the main result of this section, given in Lemma 12, simply follows from the next proposition and classical random matrix theory arguments.

**Proposition 11** (Koltchinskii and Lounici (2016)). Let \( \Sigma = \sum_{j=1}^{d} \lambda_j P_j \), where \((\lambda_1, \ldots, \lambda_d)\) are the eigenvalues of \( \Sigma \) sorting in decreasing order, i.e. \( \lambda_1 \geq \cdots \geq \lambda_d \) and \( P_j \) is the projection operator onto the span of the \( j \)-th eigenvector of \( \Sigma \). Similarly, let \( \hat{\Sigma} = \sum_{j=1}^{d} \hat{\lambda}_j \hat{P}_j \). Also let \( g_j := \lambda_j - \lambda_{j+1} \) denote the \( j \)-th spectral gap of \( \Sigma \), \( \tilde{g}_1 := g_1 \), and \( \bar{g}_j := \min\{g_{j-1}, g_j\} \) for \( j = 2, \ldots, d \). Then, \( \| \hat{P}_j - P_j \| \leq \frac{4\| \hat{\Sigma} - \Sigma \|}{\bar{g}_j} \).

**Lemma 12.** The following statements are true.

1. If Assumption 1 is valid, then for every fixed integer \( m \), as \( n \to \infty \),

\[
\max_{1 \leq j \leq m} \frac{\bar{G}_j \| \hat{P}_j - P_j \|}{\lambda_1} = O\left( \sqrt{\frac{1}{n}} \sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}} \sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}} \right), \quad \text{almost-surely.}
\]

2. If Assumption 2 is valid then there is a universal constant \( C > 0 \) such that with probability at least \( 1 - e^{-t} \), for all \( m = 1, \ldots, n \),

\[
\max_{1 \leq j \leq m} \frac{\bar{G}_j \| \hat{P}_j - P_j \|}{C\lambda_1} \leq \sqrt{\frac{m^\vee t}{n}} \sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}} \sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}}.
\]

**Proof.** In order to apply Proposition 11, we need to figure out an upper bound for \( \| \hat{\Sigma} - \Sigma \| \). Remark that \( \Sigma = UA U^T \) and \( \hat{\Sigma} = n^{-1} X^T X = n^{-1} U \Lambda^{1/2} Z^T Z \Lambda^{1/2} U^T \). Then, we have the following chain of estimates, as \( \| U \| = \| U^T \| = 1 \)

\[
\| \hat{\Sigma} - \Sigma \| = \| U (n^{-1} \Lambda^{1/2} Z^T Z \Lambda^{1/2} - \Lambda) U^T \| = \left\| \Lambda^{1/2} \left( \frac{Z^T Z}{n} - I \right) \Lambda^{1/2} \right\|.
\]

We split the space \( \mathbb{R}^d \) onto two orthogonal subspaces, corresponding to projection on \( S := \text{span}(e_1, \ldots, e_m) \) and \( S_\perp := \text{span}(e_{m+1}, \ldots, e_d) \). Then, we let \( \Lambda_S \), respectively \( Z_S \), denote the
restriction of \( \Lambda \) to \( S \), respectively \( Z \). Similarly we let \( \Lambda_\perp \), respectively \( Z_\perp \) the restrictions to \( S_\perp \).

Then we rewrite by blocks,

\[
\Lambda^{1/2}\left(\frac{Z^T Z}{n} - I\right)\Lambda^{1/2} = \left(\Lambda_S^{1/2}(n^{-1}Z_S^T Z_S - I)\Lambda_S^{1/2} - n^{-1}\Lambda_\perp^{1/2}Z_\perp^T Z_\perp\Lambda_\perp^{1/2}\right).
\] (A.2)

Hence, combining the expressions Equations (A.1) and (A.2), we can bound \( \|\hat{\Sigma} - \Sigma\| \) as

\[
\|\hat{\Sigma} - \Sigma\| \leq \left\|\Lambda_S^{1/2}\left(\frac{Z_S^T Z}{n} - I\right)\Lambda_S^{1/2}\right\| + \left\|\Lambda_\perp^{1/2}\frac{Z_\perp^T Z_\perp}{n}\Lambda_\perp^{1/2}\right\| + \left\|\Lambda_\perp^{1/2}\left(\frac{Z_\perp^T Z_\perp}{n} - I\right)\Lambda_\perp^{1/2}\right\|.
\]

The rhs of the last display is bounded by,

\[
\left\|\Lambda_S^{1/2}\left(\frac{Z_S^T Z}{n} - I\right)\Lambda_S^{1/2}\right\| + 2\left\|\frac{Z_S}{\sqrt{n}}\Lambda_S^{1/2}\right\| + \left\|\frac{Z_\perp}{\sqrt{n}}\Lambda_\perp^{1/2}\right\| + \left\|\Lambda_\perp^{1/2}\frac{Z_\perp^T Z_\perp}{n}\Lambda_\perp^{1/2}\right\| + \left\|\Lambda_\perp^{1/2}\left(\frac{Z_\perp^T Z_\perp}{n} - I\right)\Lambda_\perp^{1/2}\right\|,
\]

which is in turn bounded by

\[
\|\Lambda_S^{1/2}\|^2\left\|\frac{Z_S^T Z}{n} - I\right\| + 2\|\Lambda_S^{1/2}\|\left\|\Lambda_\perp^{1/2}\right\| + \left\|\frac{Z_S}{\sqrt{n}}\right\| + \left\|\frac{Z_\perp}{\sqrt{n}}\right\| + \left\|\Lambda_\perp^{1/2}\right\|^2 + \|\Lambda_\perp\|.
\]

Since \( \|\Lambda_S^{1/2}\| = \sqrt{\lambda_1}, \|\Lambda_\perp^{1/2}\| = \sqrt{\lambda_{m+1}} \) and \( \|\lambda_\perp\| = \lambda_{m+1} \), we deduce that

\[
\|\hat{\Sigma} - \Sigma\| \leq \lambda_1\left\|\frac{Z_S^T Z}{n} - I\right\| + 2\sqrt{\lambda_1}\lambda_{m+1}\sigma_{\text{max}}\left(\frac{Z_S}{\sqrt{n}}\right)\sigma_{\text{max}}\left(\frac{Z_\perp}{\sqrt{n}}\right) + \lambda_{m+1}\sigma_{\text{max}}^2\left(\frac{Z_\perp}{\sqrt{n}}\right) + \lambda_{m+1}.
\]

We now consider only Item (2). On the event that \( \sigma_{\text{max}}(n^{-1/2}Z_S) \leq 1 + C\sqrt{m/n + \sqrt{t/c}} \) and \( \sigma_{\text{min}}(n^{-1/2}Z_S) \geq 1 - C\sqrt{m/n - \sqrt{t/c}} \), it is easily seen that \( \|n^{-1}Z_S^T Z_S - I\| \leq C\sqrt{m/n + \sqrt{t/c}} \); see for instance Vershynin (2010, Lemma 5.36). Further, by Proposition 14 this event has probability at least \( 1 - 4\exp(-t) \) for appropriate choice of \( C, c > 0 \). The other terms are also bounded using Proposition 14. In fact, using that \( 0 < t \leq n \) and \( d \geq n \), we can show that there exists a constant \( K > 0 \) depending only on \( \nu \) such that with probability at least \( 1 - e^{-t} \) (by eventually increasing the constants if needed),

\[
\|\hat{\Sigma} - \Sigma\| \leq K\lambda_1\left(\sqrt{\frac{m}{n}}\sqrt{\frac{t}{n}}\sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}} + \sqrt{\frac{d\lambda_{m+1}}{n\lambda_1}}\right).
\]

The result follows by combining the last display with Proposition 11. The proof for Item (1) is similar but uses Proposition 13 instead of Proposition 14, or could be derived from the results in Shen et al. (2016a). \( \square \)
A.5 Bias variance decomposition of risk

To show (2.1), we start with adding and subtracting $x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X]$
\[ \mathbb{E}[(x_{\text{new}}^T \theta_* - x_{\text{new}}^T \hat{\theta})^2 \mid X] = \mathbb{E}[(x_{\text{new}}^T \theta_* - x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X])^2 \mid X] + \mathbb{E}[(x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X] - x_{\text{new}}^T \hat{\theta})^2 \mid X], \]

note that expectation of cross term is zero.

Since
\[ \mathbb{E}[(x_{\text{new}}^T \theta_* - x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X])^2 \mid X] = \mathbb{E}[(x_{\text{new}}^T (\theta_* - (X^T X)^\dagger X^T X \theta_*))^2 \mid X] \]
\[ = \mathbb{E}[(x_{\text{new}}^T (I - (X^T X)^\dagger X^T X)\theta_* )^2 \mid X]. \]

Next we expand the square above. By definition
\[ \mathbb{E}[x_{\text{new}}^T x_{\text{new}}^T \mid X] = \Sigma \]
and $\frac{1}{n} X^T X = \hat{\Sigma}$. So we can write bias
\[ \mathbb{E}[(x_{\text{new}}^T \theta_* - x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X])^2 \mid X] = \text{Tr}(\theta_*^T (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \Sigma (I - \hat{\Sigma}^\dagger \hat{\Sigma}) \theta_*). \]

Similarly for variance we get
\[ \mathbb{E}[(x_{\text{new}}^T \mathbb{E}[\hat{\theta} \mid X] - x_{\text{new}}^T \hat{\theta})^2 \mid X] = \mathbb{E}[(x_{\text{new}}^T ((X^T X)^\dagger X^T (X \theta_* - Y)))^2 \mid X] \]
\[ = \mathbb{E}[(x_{\text{new}}^T ((X^T X)^\dagger X^T \xi))^2 \mid X] = \mathbb{E}[x_{\text{new}}^T (X^T X)^\dagger X^T \xi^T X (X^T X)^\dagger x_{\text{new}} \mid X] \]
\[ \leq \sigma^2 \mathbb{E}[x_{\text{new}}^T (X^T X)^\dagger X^T X (X^T X)^\dagger x_{\text{new}} \mid X] = \text{sigm}^2 \mathbb{E}[x_{\text{new}}^T (X^T X)^\dagger x_{\text{new}} \mid X] = \frac{\sigma^2}{n} \text{Tr}(\hat{\Sigma}^\dagger \Sigma), \]

where the second to last equality follows from definition of pseudo-inverse.

A.6 Random matrix facts

The following useful proposition combines famous results from Yin et al. (1988); Bai and Yin (1993) about the asymptotic behavior or large covariance matrices, see also Vershynin (2010, Theorem 2.1).

Proposition 13 (Bai-Yin’s law). Let $W$ be a $n \times p$, $n > p$, matrix with i.i.d entries $W_{i,j}$ such that $E[W_{i,j}] = 0$, $E[W_{i,j}^2] = 1$, and $E[W_{i,j}^4] < \infty$. Let $y = \lim_{n \to \infty} p/n$. Then $\lim_{n \to \infty} \sigma_{\max}(n^{-1/2}W) = 1 + \sqrt{y}$ and $\lim_{n \to \infty} \sigma_{\min}(n^{-1/2}W) = 1 - \sqrt{y}$ almost-surely.

The following proposition is copied from Vershynin (2010, Theorem 5.39).

Proposition 14. Let $W$ be a $n \times p$, $n > p$, matrix with i.i.d entries $W_{i,j}$ such that $E[W_{i,j}] = 0$, $E[W_{i,j}^2] = 1$ and there exists $\nu > 0$ such that $\log E[e^{\lambda W_{i,j}}] \leq \frac{\lambda^2}{2}$ for all $\lambda \in \mathbb{R}$. Then there are constants $C, c > 0$ depending only on $\nu$ such that with probability at least $1 - 2\exp(-ct^2)$ one has
\[ \sqrt{n} - C \sqrt{p} - t \leq \sigma_{\min}(W) \leq \sigma_{\max}(W) \leq \sqrt{n} + C \sqrt{p} + t. \]