PC ADJUSTED TESTING FOR LOW DIMENSIONAL PARAMETERS

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ABSTRACT. In this paper we consider the effect of high dimensional Principal Component (PC) adjustments while inferring the effects of variables on outcomes. This problem is particularly motivated by applications in genetic association studies where one performs PC adjustment to account for population stratification. We consider simple statistical models to obtain asymptotically precise understanding of when such PC adjustments are supposed to work in terms of providing valid tests with controlled Type I errors. We also verify these results through a class of numerical experiments.

1. INTRODUCTION

Testing statistical hypotheses, where one needs to take special care of complications of high dimensional data structures is a staple in modern data science. Indeed, a quintessential example of this type problems arise naturally in the context of genetic association studies. Although such questions are not specific to the domain of genetic associate studies, the seminal paper of Price et al. [2006] has put forward a Principal Component (PC) adjustment based procedure to adjust for population stratification type confounding and has been applied across a vast canvas of omics type applications beyond Genome Wide Association Studies (GWAS). As another specific example, Barfield et al. [2014] explores the applicability of the same principle in epigenome wide association studies. A major appeal of this method, that we will try lend a theoretical lens to in this paper, is availability of the EIGENSTRAT package of Price et al. [2006] that allows fast implementation of this principle and has therefore been immensely popular as a standard adjustment procedure to account for confounding bias in such studies.

In spite of the immense practical popularity of PC adjustment for high dimensional nuisance parameters, the most basic theoretical questions remain unanswered for this high popular and regularly used principle. For example, the most traditional statistical questions that arise as a part of planning a real data analysis pertains to sample size and power calculations. Interestingly, the answers to even such simple questions remain unexplored. Indeed, the two stage method involving a principal component adjustment before testing for genetic association, implies interesting statistical phenomenon in high dimensional problems where the number of genetic variants under study is large [Patterson et al., 2006]. In contrast to such implied caveats and potential pathologies of inconsistencies in high dimensional PCA [Johnstone and Lu, 2009], empirical success of the procedure in practical problems in turn go far towards making a strong case for the PC based adjustments in these applications [Yang et al., 2014a]. This paper is aimed at providing first steps towards a theoretical formalism and reconciling these issues and thereby potentially resolve questions regarding when and why such PC-based adjustments are reliable and mathematically valid.

2. SETUP

We consider data on \((Y_i, X_i)_{i=1}^n \sim \mathcal{P}\) where where \(Y_i \in \mathbb{R}\) denotes an outcome of interest and \(X_i \in \mathbb{R}^p\) collects predictor variables under study. In many case, it is of interest to test the effect of specific variables/components in \(X\) on \(Y\) while conditioning on other variables in \(X\). More precisely, we will partition \(X\) as \(X = [A, W]^T\) where \(A \in \mathbb{R}\) is the variable whose effect on \(Y\) is of interest and \(W\) collects confounders one wishes to adjust while decoding this relationship. Our main question
of interest concerns a specific way of inferring the effect of $A$ on $Y$ – namely principal component adjustment for the confounding variables in $X$. We will study the precise asymptotic properties of this specific method through the lens of a hypothesis testing problem for the effect of $A$ on $Y$. To obtain sharp asymptotics and precise answers, for our theoretical developments we will focus on the Gaussian linear regression set-up where

$$Y_i = A_i \delta + W_i^T \beta + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma_y^2), \quad (2.1)$$

and thereby consider the hypothesis testing problem for $\delta$ defined as

$$H_0: \delta = 0 \quad \text{vs} \quad H_1(h): \delta = \frac{h}{\sqrt{n}}. \quad (2.2)$$

The choice of the alternative converging to 0 at $1/\sqrt{n}$ rate is driven by the fact that the detection threshold for testing $\delta$ scales accordingly in the asymptotic regimes we will work with in this paper. Subsequently, with an abuse of notation that suppresses dependence on other parameters, we will denote the distribution $P$ of $Y|A, W$ corresponding to model (2.1) as $P_{\delta}$ to underscore the main object of the hypothesis test i.e. $\delta$. Finally, throughout we assume that $||\beta||$ is bounded away from 0 to reflect a scenario where the effect of $A$ on $Y$ experiences non-trivial confounding through $W$.

The standard test for (2.2) is the Generalized Likelihood Ratio Test (GLRT) – which for known $\sigma_y^2$ reduces to the chi-square test with 1-degree of freedom. Although the same test has non-trivial local power for testing (2.2) even for growing dimension $p$: (1) it is often believed that suitable dimension reduction techniques on the regression of $X$ on $Y$ by relying on the intuition that dimension reduction techniques capture underlying structures of the problem (e.g. sparsity, low rank etc) and thereby yields more power for the testing problem compared to vanilla GLRT; and (2) performing GLRT at the scale of modern high dimensional problems such as GWAS is computationally expensive ($O(\min\{p^3, np^2, n^2p\})$) and performing dimension reduction on $X$ substantially reduces this burden. To account for these concerns, one method that has gained popularity is that of performing Principal Component Analysis (PCA) based dimension reduction on $X$ which amounts to including “a few top principal components” in the regression (and can be computed through Fast-PCA type algorithms [Galinsky et al., 2016]) of $Y$ on $X$ [Barfield et al., 2014, Patterson et al., 2006, Price et al., 2006]. In this regard, for testing effect of $A$ on $Y$, it is natural to consider PC adjustment on $W$ only. However, one attractive piece of the EIGENSTRAT method introduced in Price et al. [2006] is the fact that it allows the investigator to only run PCA on the whole of $X$ data matrix only once and including them in the regression analysis of $Y$ on any $X_j$ (and not a specific component $A$ as considered here) which is a component of $X$. More specifically, we shall study the statistical properties (Type I and Type II error of testing for $\delta$ in the model (2.1)) of testing for a specific component $A$ of $X$, our set up is in parallel to traditional GWAS analysis where is a standard practice to run PCA on the whole data matrix of $X$ (instead on the matrix obtained by removing $A$-observations from it) and include them in the analyses – instead of running a new PCA every time for testing for a new variable in $X$. Here we will explore both the cases when the PC is run on the whole of $X$ (a case more relevant for GWAS type analyses [Price et al., 2006]) and for the case when PC adjustments are performed on $W$ (a case relevant in certain epigenetic studies where $A$ contains DNA methylation levels of a particular cytosine-phosphate-guanine (CpG) site of interest and one performs PCA on genetic variants $W$ to account for population stratification Barfield et al. [2014].)

To initiate a theoretical study of this method, we begin by with setting up the necessary mathematical notation to describe the procedure. As discussed above, one standard approach in practice is to perform Principal Component (PC) analysis on the data matrix of $X$ and only use the top

\footnote{We will throughout assume this and show through numerical experiments that the results for unknown $\sigma_y^2$ should be qualitatively similar.}
principal component directions while adjusting for confounders in the regression of $Y$ on $A$. Mathematically, such a formalism can be written as follows through the data vectors $Y = (Y_1, \ldots, Y_n)^T$, $A = (A_1, \ldots, A_n)^T$ and the data matrix of covariates $X = [X_1: \cdots: X_n]^T$:

(i) Given $k \in \mathbb{N}$, let $\tilde{V}_{k,\text{in}}$ denote the matrix composed of the first $k$ right singular vectors of $X$.

(ii) Perform a linear regression of $Y$ on $(A, X\tilde{V}_{k,\text{in}})$ to get a score or level of significance for $\delta$.

Here the subscript in refers to the fact that a $A$ is a part of the variables in $X$ on which the PC was performed. Mathematically, for any cut-off $t$ we consider the test that rejects for value of the likelihood ratio larger than $t$ as follows

$$\varphi_{k,\text{in}}(t) = 1 \left( \text{LR}_{k,\text{in}} > t \right),$$

where

$$\text{LR}_{k,\text{in}} = Y^T P_{C(A_{k,\text{in}})} Y, \quad A_{k,\text{in}} = (I - P_{C(X\tilde{V}_{k,\text{in}})}) A$$

Here for any matrix $M$ we use $C(M)$ to denote its column space and $P_{C(M)}$ to denote the projection matrix onto $C(M)$. An analogous can be constructed where the PC adjustment was performed only on $\tilde{W} = [\tilde{W}_1: \cdots: \tilde{W}_n]^T$ – which we shall refer to as

$$\varphi_{k,\text{out}}(t) = 1 \left( \text{LR}_{k,\text{out}} > t \right)$$

with

$$\text{LR}_{k,\text{out}} = Y^T P_{C(A_{k,\text{out}})} Y, \quad A_{k,\text{out}} = (I - P_{C(\tilde{W}\tilde{V}_{k,\text{out}})}) A$$

and $\tilde{V}_{k,\text{out}}$ now collects the top right singular vectors of $\tilde{W}$.

This approach, similar in essence to Principal Component Regression (to be denoted by PCR hereafter) raises a few immediate questions:

(i) What is the behavior of $\varphi_{k,\text{ind}}(t)$, $\text{ind} \in \{\text{in, out}\}$ under $H_0$ and does there exist a distributional cut-off $t_\alpha$ such that the Type I error of $\varphi_{k,\text{ind}}(t_\alpha)$ converges to $\alpha$?

(ii) How to characterize the power function of $\varphi_{k,\text{ind}}(t)$, $\text{ind} \in \{\text{in, out}\}$ for any given $(k, t)$?

To understand these questions, we operate in a regime which allows $p$ to be larger than sample size but to scale proportionally with $n$. In this asymptotic regime, the main results and contributions of this paper in view of the above questions are as follows:

(i) Under a generalized spiked model for $W$ (see Definition 2.2) we provide exact asymptotic results for testing (2.2) after PC adjustments. The precise description of the testing errors can be elaborated as follows.

(a) Our results show an interesting distinction between a fixed effects and random effects on $\beta$.

In particular, we show that when $\beta$ in (2.2) is considered fixed and unknown the Type I error of the test for (2.2) after PC adjustments converges to 1 exponentially in sample size $n$ – even after including “enough” principal component direction in the regression. In contrast, when $\beta$ has a mean zero random effect distribution the Type I error of the test is bounded away from both 1 and the nominal desired level. (See Theorem 3.1i.-ii.).

(b) For random effects on $\beta$, we derive the precise power function of the test for (2.2) after PC adjustments and show that without further assumptions it might not be possible to estimate the power function exactly to either correct for the Type I error inflation or perform sample size/power calculations (See Theorem 3.1ii.).

(ii) We show that, when $W$ is derived from a mixture of mean-shift type distributions, a similar phenomenon persists in terms of the behavior of the test for (2.2) after PC adjustments. We further verify similar behavior through extensive simulations even when the distribution of $X$ arises from mixture of discrete distributions. These simulations provide interesting insights into the subtleties and success of the highly popular EIGENSTRAT method of Price et al. [2006] (See Theorem 3.3).
The probability measure \( \delta \) where \( \text{Empirical Spectral Distribution (ESD)} \) \( H \) follows. In Section 3.1 we present asymptotic results on the power function of our results in Section 2.1. We divide the main theoretical results in Section 3 into three parts as

We first introduce the notation, definitions, and assumptions to set up the main building blocks of our results in Section 2.1. We divide the main theoretical results in Section 3 into three parts as follows. In Section 3.1 we present asymptotic results on the power function of \( \varphi_{k, \text{ind}} \) noted in points (i) and (ii) above to disappear. (See Theorem 3.4-3.7).

The rest of the paper, organized as follows, makes the above claims precise, rigorous, and elaborate. We first introduce the notation, definitions, and assumptions to set up the main building blocks of our results in Section 2.1. We divide the main theoretical results in Section 3 into three parts as follows. In Section 3.1 we present asymptotic results on the power function of \( \varphi_{k, \text{ind}} \) noted in points (i) and (ii) above to disappear. (See Theorem 3.4-3.7).

2.1. Technical Preparations. In this subsection we present definitions, assumptions and related discussions, and notation that will be used throughout the rest of the paper.

2.1.1. Definitions. To present our main results of this section we first need a few definitions to set up the notion of generalized spiked models. We start with the definition of empirical spectral measure of a Hermitian matrix.

**Definition 2.1.** For a \( p \)-dimensional Hermitian matrix \( \Sigma_p \) with eigenvalues \( \lambda_{1,p}, \lambda_{2,p}, \ldots, \lambda_{p,p} \), the **Empirical Spectral Distribution (ESD)** \( H_p \) is defined as the distribution function corresponding to the probability measure

\[
H_p(x) = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_{i,p}}(x),
\]

where \( \delta_{\lambda_{i,p}}(x) = 1 \) when \( x = \lambda_{i,p} \), otherwise 0. For a sequence \( \{\Sigma_p\}_{p \geq 1} \) of deterministic Hermitian matrices, if the corresponding sequence \( \{H_p\}_{p \geq 1} \) of ESDs converges weakly to a non-random probability distribution \( H \) as \( p \to \infty \), then \( H \) is defined as the **Limiting Spectral Distribution (LSD)** of the sequence \( \{\Sigma_p\}_{p \geq 1} \).

With this definition in hand we are ready to present the definition of generalized spiked models as proposed by Bai and Yao [2012].

**Definition 2.2.** A sequence \( \{\Sigma_p\}_{p \geq 1} \) of deterministic Hermitian matrices is called a sequence of **generalized spiked population matrices** if the following hold.

(i) \( \Sigma_p \) can be written as,

\[
\Sigma_p = \begin{bmatrix}
\Sigma_m^{(A)} & 0 \\
0 & \Sigma_{p-m}^{(B)}
\end{bmatrix},
\]

where \( \Sigma_m^{(A)} \) and \( \Sigma_{p-m}^{(B)} \) are non-negative and non-random Hermitian matrices of dimensions \( m \times m \) (\( m \) is finite and fixed) and \( (p-m) \times (p-m) \), respectively.

(ii) The sequence \( \{H_p\}_{p \geq 1} \) of ESDs corresponding to \( \{\Sigma_p\}_{p \geq 1} \) converges weakly to a non-random probability distribution \( H \).

(iii) Let \( \Gamma_H \) be the support of \( H \), and let the sets of eigenvalues of the submatrices \( \Sigma_m^{(A)} \) and \( \Sigma_{p-m}^{(B)} \) be \( \{\alpha_1 \geq \ldots \geq \alpha_m\} \) and \( \{\beta_1 \geq \ldots \geq \beta_{p-m}\} \), respectively. Then, \( \alpha_i \notin \Gamma_H \) for \( i = 1, \ldots, m \), and \( \max_{1 \leq i \leq p-m} d(\beta_i, \Gamma_H) \to 0 \) as \( p \to \infty \), where \( d(x, S_A) = \inf_{y \in S_A} |x - y| \) is a distance metric from a point \( x \) to a set \( S_A \).
In this case, the eigenvalues of $\Sigma_m^{(A)}$ are called the generalized spikes, and the eigenvalues of $\Sigma_{p-m}^{(B)}$ are called the non-spikes. The distribution $H$ is same as the LSD of the sequence $\{\Sigma_{p-m}\}$.

We note that the traditional spiked model [Johnstone, 2001] is a special case of the generalized spiked model where $H$ is the degenerate distribution at unity. Next, we will introduce the phase transition boundaries for the generalized spikes analogous to the phase transition boundary [Baik et al., 2005] established in the spiked model.

**Definition 2.3.** For $\alpha \notin \Gamma_H$, $\alpha \neq 0$, we define the following function:

$$\psi(\alpha) = \alpha + \gamma \alpha \int \frac{\lambda dH(\lambda)}{\alpha - \lambda},$$

Then, a generalized spike $\alpha_i$ is called a “distant spike” if $\psi'(\alpha_i) > 0$, and “close spike” if $\psi'(\alpha_i) \leq 0$, where $\psi'$ is the first derivative of $\psi$.

Depending on whether a generalized spike is a distant or a close spike, the asymptotic convergence of the corresponding sample eigenvalues differ according to Theorem 4.1 and Theorem 4.2 of [Bai and Yao, 2012]. Therefore, the sample eigenvalues corresponding to the generalized spikes go through a phase transition at the boundaries where $\psi'(\alpha) = 0$. Unlike in the spiked model where the phase transition happens only at the two boundaries ($1 \pm \sqrt{\gamma}$), the generalized spiked model can have more than two phase transition boundaries. The next assumption is intended to simplify our mathematical derivations by only allowing one phase transition boundary $\alpha^* > \sup \Gamma_H$, and by assuming that all the generalized spikes have multiplicity one and are above that boundary (i.e., all distant spikes). The extension of our derivations to allow close spikes, and generalized spikes around multiple phase transition boundaries are similar but tedious, and hence omitted in this paper. Finally we define covariate data distributions we will working with throughout.

**Definition 2.4.** We say that a data matrix $\tilde{X}_{n \times d}$ follows a generalized spiked distribution with $k^*$ spike eigenvalue-eigenvector pairs $\{(\lambda_j, v_j)\}_{j=1}^{k^*}$ if $\tilde{X} = Z \Lambda_d^{1/2} V_d$, where $Z$ is an $n \times d$ random matrix with i.i.d. sub-gaussian elements such that $E(Z_{ij}) = 0, E(|Z_{ij}|^2) = 1$, and $\Lambda_d^{1/2}$ is the positive definite Hermitian square root of $\Lambda_d$ such that

(a) $\{\Sigma_d\}_{d \geq 1}$ is a sequence of real symmetric positive definite matrices with spectral decomposition $\Sigma_d = V_d \Lambda_d V_d^*$, and $\Lambda_d$ satisfies the generalized spiked assumptions as outlined above (Definition 2.2) with $k^*$ (finite) generalized spikes. The eigenvalues and eigenvectors of $\Sigma_d$ are given by $\lambda_1, \ldots, \lambda_d$ and $v_1, \ldots, v_d$, respectively.

(b) The sequence $\{||\Sigma_d||\}$ of spectral norms is bounded.

(c) $\lambda_1 > \lambda_2 > \ldots > \lambda_{k^*} > \sup \Gamma_H$ denote the generalized spikes of $\Sigma_d$, and $\psi'(\lambda_i) > 0$ for $i = 1, \ldots, k^*$.

In this case we denote $\tilde{X} \sim \text{GSp}((\lambda_j, v_j))_{j=1}^{k^*}; \Gamma_H; n, d$.

Some of our results are derived under the classical spiked model [Johnstone, 2001]. To that end we will use the following definition.

**Definition 2.5.** We say that a data matrix $\tilde{X}_{n \times d}$ follows a spiked distribution with $k^*$ spike eigenvalue-eigenvector pairs $\{(\lambda_j, v_j)\}_{j=1}^{k^*}$ if $\tilde{X} = Z \Sigma_{1/2}^{1/2}$, where $Z$ is an $n \times d$ random matrix with i.i.d. sub-gaussian elements such that $E(Z_{ij}) = 0, E(|Z_{ij}|^2) = 1$, and $\Sigma_{1/2}^{1/2} = I + \sum_{j=1}^{k^*} \lambda_j v_j v_j^T$ with $\lambda_1 \geq \ldots \lambda_{k^*} > \sqrt{\gamma}$ where $\gamma = \lim p/n$ and $v_1, \ldots, v_{k^*}$ are orthonormal vectors. In this case we denote $\tilde{X} \sim \text{Sp}((\lambda_j, v_j))_{j=1}^{k^*}; n, d$.

2.1.2. Assumptions. Using the above definitions, we can now state our assumptions various subsets of which will be useful for our theoretical results.
Assumption 2.6. (a) $p \to \infty, n \to \infty, p/n \to \gamma \in (0, \infty)$.
(b) $\mathbb{W} \sim \text{GSp}((\lambda_j, v_j))_{j=1}^{K^*} ; \Gamma_H; n, p$.
(c) $X := [A, \mathbb{W}] \sim \text{GSp}((\lambda_j, v_j))_{j=1}^{K^*} ; \Gamma_H; n, p + 1$.
(c)' $X := [A, \mathbb{W}] \sim \text{Sp}((\lambda_j, v_j))_{j=1}^{K^*} ; p + 1$.

We will mostly assume the following dependence between $A$ and $\mathbb{W}$.

Assumption 2.7. Let $A = \mathbb{W}\theta + \eta$ with $\eta \sim N(0, \sigma^2 \mathbb{I})$.

Although assumption 2.7 seems restrictive, we keep it here for keeping our arguments short and only for the precise analysis of the test $\varphi_{k,\text{out}}$ – this assumption is often not needed either for analysis of $\varphi_{k,\text{in}}$ or while demonstrating a lower bound on the Type I error of $\varphi_{k,\text{out}}$ instead of deriving a precise limit. Indeed, this result is easy to extend to sub-Gaussian $A$'s and we additionally verify through extensive simulations (see Section 4) that the intuitions from our main theorems continue to be valid even without assuming the above specific conditional distribution of $A|X$. Finally we note that for the analysis in epigenetic studies [Barfield et al., 2014], where $A$ contains DNA methylation levels of a particular CpG site of interest and one performs PCA on genetic variants $\mathbb{W}$ to account for population stratification, assumption 2.7 is often reasonable. Our last assumption removes this restrictions in some of our results at the cost of obtaining bounds instead of precise limiting objects.

Assumption 2.8. Let $A_1$’s be centered and sub-Gaussian with parameter $\sigma^2_a$.

Assumption 2.8 will be used for deriving lower bounds on Type I error for tests based on $\text{LR}_{k,\text{out}}$ and obtain partial sharp limiting Type I error for tests based on $\text{LR}_{k,\text{in}}$ (see e.g. Theorem 3.2).

2.1.3. Notation. The results in this paper are mostly asymptotic (in $n$) in nature and thus requires some standard asymptotic notations. If $a_n$ and $b_n$ are two sequences of real numbers then $a_n \gg b_n$ (and $a_n \ll b_n$) implies that $a_n/b_n \to \infty$ (and $a_n/b_n \to 0$) as $n \to \infty$, respectively. Similarly $a_n \gtrless b_n$ (and $a_n \lesssim b_n$) implies that $\liminf_{n \to \infty} a_n/b_n = C$ for some $C \in (0, \infty]$ (and $\limsup_{n \to \infty} a_n/b_n = C$ for some $C \in [0, \infty)$). Alternatively, $a_n = o(b_n)$ will also imply $a_n \ll b_n$ and $a_n = O(b_n)$ will imply that $\limsup_{n \to \infty} a_n/b_n = C$ for some $C \in [0, \infty)$). If $C > 0$ then we write $a_n = \Theta(b_n)$. If $a_n/b_n \to 1$, then we say $a_n \sim b_n$. A sequence of random variable $X_n$ is called $\Omega_\mathbb{P}$, a.s. $\mathbb{P}$ if $\exists C > 0$ such that $\mathbb{P}(X_n > C) \to 1$.

3. Main Results

The behavior of the tests $\varphi_{k,\text{ind}}(t), \text{ind} \in \{\text{in, out}\}$, crucially depends on the “strength” of principal components in the population model which in turn is reflective of the strength of population stratification under consideration for the GWAS studies. To capture this, we first present results for fixed “strength” of principal components in Section 3.1. Subsequently, in Section 3.3 we also present a sharp phase transition depending on spike strength in diverging spike strength of population principal components while considering the traditional spiked model [Johnstone, 2001]. The implications of these results to GWAS type problems is discussed in Section 3.2. Finally, 3.2 also presents results when the studies come from a mixture of populations and thereby directly addressing population stratification type issues in GWAS.

3.1. Fixed Strength of Population PCs. We begin by stating and discussing the results for $\text{LR}_{k,\text{ind}}$ fixed stratification strength, i.e., $\lambda_1 = O(1)$ whenever $X$ or $\mathbb{W}$ follow a generalized spiked distribution with top spiked eigenvalue $\lambda_1$. 
**Theorem 3.1.** Consider testing (2.2) under (2.1) using $\varphi_{k,\text{ind}}(t)$. Then the following hold with any fixed $k \geq k^*$ under Assumptions 2.6 (a), (b), and 2.7 for ind = out and 2.6 (a) and (c) for ind = in.

i. Suppose that $\beta, \theta$ are fixed effects. Then for any fixed cut-off $t \in \mathbb{R}$ and fixed $M > 0$ one has

$$
\lim_{n \to \infty} \sup_{p/n \to 0} \mathbb{P}_{\delta=0} \left( LR_{k,\text{out}} > t \right) = 1,
$$

and

$$
\lim_{n \to \infty} \sup_{p/n \to 0} \mathbb{P}_{\delta=0} \left( LR_{k,\text{in}} > t \right) = 1.
$$

ii. Assume that $\beta \sim N(0, \sigma_{\beta}^2 I/p)$. Then $\exists$ function $v_{\text{out}}(\cdot, \cdot) : \mathbb{R}^2 \to \mathbb{R}_+$ such that for any $h, t \in \mathbb{R}$ and $\delta = h_1/\sqrt{n}$ and fixed $h_2$ one has

$$
\lim \mathbb{P}_{\delta=h/\sqrt{n}}(LR_{k,\text{out}} > t) = v_{\text{out}}(t, h) \quad \forall \theta \quad \text{s.t.} \quad \|\theta\| \geq h_2;
$$

and

$$
\lim \mathbb{P}_{\delta=h/\sqrt{n}}(LR_{k,\text{in}} > t) = v_{\text{in}}(t, h).
$$

The function $v_{\text{out}}$ depends on $\{\gamma, \sigma_{y}^2, \sigma_{\beta}^2, k^*, k, \Gamma_H, \{(\psi_{j}, \theta)\}_{j=1}^{k^*}\}$ and the function $v_{\text{in}}$ depends on $\{\gamma, \sigma_{y}^2, \sigma_{\beta}^2, k^*, k, \Gamma_H, \{(\lambda_j)_{j=1}^{k^*}\}$. 2 and is larger than $\alpha$ at $h = 0, t = \chi_1^2(\alpha)$ (the $\alpha$-quantile of $\chi_1^2$). A qualitatively similar result holds for either $\beta$ non-random and $\theta$ random or both $\beta, \theta$ random effects 3

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**Remark 1.** Although some levels of Type I error is expected for fixed and low spike strength [Patterson et al., 2006], Theorem 3.1 implies that the Type I error can be arbitrarily close to 1 for using any fixed cut-off – which automatically covers any distribution based cut-off. Indeed, $LR_{k,\text{ind}}$ diverges in this set-up and as our proof will suggest that this is not an artifact of specific adversarial choices of $\beta, \theta$ but actually holds for uncountably many choices of $\beta, \theta$. Our proof also suggests that the Type I error is somewhat less pathological when $\beta$ is orthogonal to the leading population eigenvectors – and thereby providing intuitive justification of the results in the random effects parts of Theorem 3.1 since mean 0 random $\beta$ is “on average orthogonal” to any fixed directions.

**Remark 2.** In the notation $\mathbb{P}_{\delta}$ we have suppressed the dependence of $\mathbb{P}$ on $\beta, \theta$ to not only maintain succinct notation but also to avoid confusion when one of $\beta$ and $\theta$ is random. Consequently, in statements of the theorem whenever a supremum over $\beta$ or $\theta$ appears, it implicitly acknowledges the dependence of $\mathbb{P}_{\delta}$ on the respective parameters.

**Remark 3.** We note that the results for $LR_{k,\text{ind}}$ does not involve a supremum over $\theta$. This is because assuming a spiked model on $X$ does not allow a free choice of $\theta$ since by representing $\theta$ as the population least squares coefficients implies that $\theta$ is a function of $\Sigma$. Also, we assume $\|\theta\| \geq h_2 > 0$ is bounded away from 0 to reflect a scenario where the effect of $A$ on $Y$ experiences non-trivial confounding through $W$.

**Remark 4.** The results above do not change if one changes the distribution random effects from Gaussian to other suitable sub-Gaussian distributions as long as the leading population eigenvectors $v_1, \ldots, v_{k^*}$ are delocalized. However, the results can be quite specific to various possibilities of localizations and distributions of the random effects otherwise. We do not explore this aspect here in detail.

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2 the precise forms of the $v_{\text{ind}}$ can be found in the proof where its dependence on the sequence of tuples $\{\langle \psi_{j}, \theta \rangle, \{(\lambda_j)_{j=1}^{k^*}\}\}$ is suitably defined in a limiting sense. Throughout we shall implicitly assume that suitable quadratic forms of the type $\sum_{j=1}^{p} \psi(\lambda_j)\zeta^T v_j^T \zeta$ for certain deterministic functions $\psi$ and sequence of vectors $\zeta$ of bounded norm, that arise in the proof of the theorem, exists. Otherwise, our results can be written more tediously in terms of upper and lower bounds on the power function involving liminf’s and limsup’s of similar quadratic forms.

3 with analogous but different limiting functions.
Remark 5. We consider a simple application of Theorem 3.1. Consider the population covariance matrix be the classical spike model [Johnstone, 2001] i.e. $\Sigma = I + \lambda_1 e_1 e_1^T$, where $\lambda_1 > 1 + \sqrt{\tau}$. By Lemma 7.1 one has

$$LR_{k, \text{out}} | A, \mathbb{W} \sim \chi^2_1(\kappa_{k, \text{out}}^2), \quad \kappa_{k, \text{out}}^2 = \frac{((\beta^T \mathbb{W}^T + A^T \delta) (I - P_C(\mathbb{W} \sim \mathbb{W}_{k, \text{out}})) A)^2}{A^T (I - P_C(\mathbb{W} \sim \mathbb{W}_{k, \text{out}})) A}.$$ 

Note that,

$$\mathbb{P}_\delta(LR_{k, \text{out}} > t_\alpha) = \mathbb{E} \left( \Phi(t_\alpha - \kappa_{k, \text{out}}^2) - \Phi(-t_\alpha - \kappa_{k, \text{out}}^2) \right)^2,$$

where $\Phi$ is the standard normal cdf and $\Phi = 1 - \Phi$. Hence, it will be sufficient to derive asymptotic distribution of $\kappa_{k, \text{out}}^2$ followed by an application of uniform integrability principle to derive the asymptotic behavior of the likelihood ratio test.

Let $\beta \sim N \left( 0, \frac{1}{p} \sigma_\beta^2 \right)$ and $\theta := e_1$. We have shown, in (6.13),

$$\kappa_{k, \text{out}}^2 \Rightarrow \frac{\sigma_\beta^2 (\sigma_g^2 m_1 + c_4)}{c_0 + \sigma_g^2} \chi^2(h^2(c_0 + \sigma_g^2)^2) = \mathcal{L},$$

where $c_0 = \lim_n \sum_{j=k+1}^{n/p} \lambda_j \theta^T v_j v_j^T \theta$, $c_4 = \lim_n \frac{1}{p} \sum_{j=k+1}^{n/p} d_j \theta^T v_j v_j^T \theta$, and $m_1 = \lim_n \frac{1}{p} \sum_{j=k+1}^{n/p} \lambda_j$. Now, $m_1 = m_1, \gamma$ is the mean of Marchenko-Pastur distribution. To compute the precise values of $c_0, c_4$, note that the limiting spectral distribution of $\Sigma$ is $\delta_1$, the non-random distribution which is degenerate at 1. Now we invoke Lemma 7.2 to obtain that $c_0 = \sum_{j=1}^{n/p} \phi_{1j} \theta^T v_j v_j^T \theta$ and $c_4 = \frac{1}{p} \sum_{j=1}^{n/p} \phi_{2j} \theta^T v_j v_j^T \theta$, where

$$\phi_{1j} = \begin{cases} \frac{\gamma + 1}{\lambda}, & j = 1 \\ 1, & j > 1, \end{cases}$$

$$\phi_{2j} = \begin{cases} \frac{\gamma + 1}{\lambda} + \frac{\gamma^2 (\lambda + 1)^2}{\lambda^2}, & j = 1 \\ 1 + \gamma, & j > 1. \end{cases}$$

Note that, $\Sigma = (1 + \lambda_1) e_1 e_1^T + \sum_{j=2}^{n/p} e_j e_j^T$. So, $v_j = e_j$, $c_0 = \frac{\lambda_1 + 1}{\lambda}$, and $c_4 = \frac{\lambda_1 + 1}{\lambda} + \frac{\gamma^2 (\lambda + 1)^2}{\lambda^2}$. Hence,

$$\mathbb{P}_\delta(LR_{k, \text{out}} > t_\alpha) \Rightarrow \mathbb{E} \left( \Phi(t_\alpha - \mathcal{L}) - \Phi(-t_\alpha - \mathcal{L}) \right)^2.$$

A few further remarks are in order regarding the assumptions and implications of Theorem 3.1 regarding the behavior of $\varphi_{k, \text{ind}}(t)$ for ind $\in \{\text{in, out}\}$. First, Theorem 3.1 (i) implies that under fixed effects model on the regression of $Y \mid A, X$ and $A \mid X$ one has pathological behavior of PC adjustment based tests in the sense that for any fixed cut-off $t$, the LRT following PC adjustments has size converging to 1. In Section 4 we further present simulation results towards universality of this phenomenon by verifying that this is indeed not an artifact of the particular choice of regression of $A \mid X$ in our analytical explorations. Similarly, Theorem 3.1 (ii) demonstrates that although the pathology of the size is somewhat diluted for random effects in the regressions of $Y \mid A, X$ and $A \mid X$, the resulting size is still strictly above the desired level $\alpha$ while using the standard $\chi^2(\alpha)$ type cutoffs. Indeed, in view of the proportional asymptotic regime (i.e. $p/n \to \gamma \in (0, \infty)$) and associated inconsistency of PCA [Johnstone and Lu, 2009], one might expect some level of discrepancy in the size and power of the PC adjustment based test $\varphi_{k, \text{ind}}$ considered – and Theorem 3.1 provides precise nature of this discrepancy. Subsequently, it is natural to ask whether one can recover the desired $\alpha$-level by suitably inverting the asymptotic power function of the test $\varphi_{k, \text{ind}}(t)$. In this regard, we first focus on the case of random $\beta$ and a close look at the formulae obtained for the power functions $v_{\text{ind}}$ in Theorem 3.1 reveals their intricate dependence on $\{(v_j, \theta), \lambda_j \}_{j=1}^{k^*}$ –
Consider testing Theorem 3.2. In some cases, when $v_{\text{ind}}$ does not depend on the projection of $\theta$ in the directions of population eigenvectors (see e.g. Remark 5 for the very special case of classical spiked model [Johnstone, 2001] and specific assumption on $\theta$) estimation of the power function is possible – however in general this seems to be impossible without assuming further structure on $\theta$ and population $v_j$'s. In contrast when $\theta$ is random, one has irrespective of $\beta$ that the power function only depends on the $\Gamma_M$ (the population spectral distribution for the distribution of $X$ or $W$) and hence can be potentially estimated. To keep our discussions focused we do not further pursue this avenue here.

To further argue that the pathologies notes above are not an artifact of Assumption 2.7, we now present analogues of the results (in somewhat less precise form) from Theorem 3.1 for the case when $A|W$ is not a linear regression. Indeed this is the case when $A$ is discrete (as is the situation for GWAS) and as a result Theorem 3.1 does not apply immediately. However as we will see that the qualitative nature of the problem conveyed by Theorem 3.1 continues to hold – with the difference being in the nature of preciseness at which we are able to pinpoint the accurate limit of the Type I error (as in Theorem 3.1ii.) in the sense that we are only able to provide a lower bound instead of a precise limit.

**Theorem 3.2.** Consider testing (2.2) under (2.1) using $\varphi_{k,\text{ind}}(t)$. Also assume that $k \geq k^*$ is fixed and Assumptions 2.6 (a) and 2.8 hold.

i. The following holds under Assumption 2.6 (b) for any $M > 0$.

$$\lim_{n \to \infty} \sup_{p/n, \gamma > 0} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{out}} > \chi^2_1(\alpha)) > \alpha.$$ 

ii. Suppose $\beta \sim N(0, \sigma_2^2 I/p)$ and that Assumption 2.6(b) holds. Then

$$\lim_{p/n \to \infty} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{out}} > \chi^2_1(\alpha)) > \alpha.$$ 

iii. Suppose that Assumption 2.6 (c) holds. Let $\beta_0 = I_{-1} \beta$ with $I_{-1} = [e_2; \ldots; e_{p+1}]$ and $c^*_p(\beta_0) = \sum_{j=1}^p \phi_{1j}^0 \beta_0^\top v_j v_j^\top e_1$ with $\phi_{1j}$ defined in Lemma 7.2 and $e_j, j \geq 1$ canonical basis $\mathbb{R}^{p+1}$.

(a) If $\beta$ is such that $\liminf_{n \to \infty} |c^*_p(\beta_0)| > 0$ then for any $t \in \mathbb{R}$

$$\lim_{p/n \to \infty} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{in}} > t) = 1.$$ 

(b) If $\beta$ is such that $\limsup_{n \to \infty} |c^*_p(\beta_0)| = 0$ and $\liminf_{n \to \infty} |\sqrt{p}c^*_p(\beta)| > 0$ then

$$\lim_{p/n \to \infty} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{in}} > \chi^2_1(\alpha)) > \alpha.$$ 

(c) If $\beta$ is such that $\limsup_{n \to \infty} |\sqrt{p}c^*_p(\beta_0)| = 0$ then the following holds if $\liminf_{n \to \infty} \lambda^*_p > 0$.

$$\lim_{p/n \to \infty} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{in}} > \chi^2_1(\alpha)) = \alpha.$$ 

iv. Suppose $\beta \sim N(0, \sigma_2^2 I/p)$ and that Assumption 2.6(b) holds. Then

$$\lim_{p/n \to \infty} \mathbb{P}_{\delta=0} (\text{LR}_{k,\text{in}} > \chi^2_1(\alpha)) > \alpha.$$ 

A few remarks are in order regarding the nature of the results above. First, the result shows the necessity to at least modify the currently used cut-offs for testing using LR$_{k,\text{out}}$. Although we believe and demonstrate in the simulation section that a result similar to Theorem 3.1 (i.e. Type
I error converging to 1 for any fixed cut-off) our proofs techniques do not naturally extend to the case of arbitrary $A$. The reason we can still demonstrate an inflated Type I error while using classical cut-offs is because our proof essentially relies on the case where $A \perp W$ and thereby is analogous to the case of $\beta = 0$ in the context of Theorem 3.1 – implying no confounding through of $A$ and $W$. However, the result for $LR_{k,in}$ can remain pathological owing to the fact of double use of $A$ both as a regressor for $Y$ as well as the in the PC’s used in the same regression. In order to provide insight about the nature of the quantity driving the behavior of $LR_{k,in}$, we elaborate using the special case classical spiked model with $\Sigma = I + \lambda vv^T$. In this case the result depends on the localization structure of $v$. First if $v \perp e_1$ then $c^*_{p}(\beta_0) = 0$ for any $\beta_0$ and hence a $\chi^2_1$ cut-off is valid for $LR_{k,in}$. This is indeed expected since $v \perp e_1$ implies no confounding between $Y$ and $A$ through $W$. Suppose now $\lim \inf \|\langle v, e_1 \rangle\| > 0$ and $\lim \inf \|\langle v, \beta \rangle\| > 0$ then we land in the situation of part (a) of Theorem 3.2iii. (a) since using the fact that $\beta^T_0 e_1 = 0$ in this case we have $\lim \inf \|c^*_{p}(\beta_0)\| = \lim \inf \|\varphi_{11} - \varphi_{12}\| \beta^T_0 vv^T e_1 + \beta^T_0 e_1 = \lim \inf \|\varphi_{11} - \varphi_{12}\| \beta^T_0 vv^T e_1 > 0$. Finally if $\|\langle v, e_1 \rangle\| = \Theta(1/\sqrt{p})$ we can appeal to 3.2iii. (b) and a Type error inflation occurs while using traditional $\chi^2_1$ cut-off.

3.2. Implications for GWAS type Analyses. As mentioned in the introduction, the method analyzed above has especially gathered immense popularity in GWAS type analysis where adjusting for variables in $X$ crucially adjusts for population stratification and unmeasured confounding [Price et al., 2006]. In particular, a classical problem of modern GWAS is that of testing for individual genetic variants while adjusting for other variants and environmental factors [Visscher et al., 2017]. In this regard, the issue of population stratification is one of the main challenges in modern genetic association studies. In particular, the presence of population sub-structure, (i.e. when data set consists of several sub-populations, different phenotypic means across strata in combination with varying allele frequencies across populations) can lead to confounding of the disease-gene relationship. Consequently, many commonly used association tests may be severely biased. Indeed, several methods exist to account for such population structure. The most commonly used ones among them can be organized around three broad themes – (a) the method of genomic control [Devlin and Roeder, 1999] (this addresses the effects that unknown population-admixture might have on the variance of commonly used test test statistics); (b) methods that rely on a model and data on the additional genetic markers [Pritchard et al., 2000] to infer the latent population structure and subsequently incorporates this model into down stream analysis; and (c) methods that use linear combinations of other genetic markers (which capture population sub-structure in their distribution) as covariates in the analysis using linear or logistic regression (these markers serve as surrogates for the underlying strata Chen et al. [2003], Price et al. [2006], Zhang et al. [2003], Zhu et al. [2002]). Owing to the seminal paper of Price et al. [2006], this third approach which we analyze here, have emerged as the most popular of these available methods.

The implications of Theorem 3.4 can be best understood through its intuitive connection to a simple population admixture model described as follows. Suppose that $X_i = (X_{i1}, \ldots, X_{ip})$ is such that there exists $S \subset \{1, \ldots, p\}$ coordinates where the distributions of $X_{ij}, j \in S$ are a mixture between two population and for $j \in S^c$ the $X_{ij}$’s are same among the two populations. For studying GWAS type problems, under LD pruning [Hartl et al., 1997, Laird and Lange, 2011] of the genotypes, one such situation can be idealized through independently having $X_{ij} \sim \frac{1}{2}\text{Bin}(2, q_{ij}) + \frac{1}{2}\text{Bin}(2, q_{ij})$ with $q_{ij} = q_{ij} = q$ for $j \in S$ and $q_{ij} = q_{ij} = q_2$ for $j \in S^c$. It is easy to check that in this case, $\text{Var}(X) = \sigma^2 I + (q_1 - q_2)^2 S |vv^T|$ for some $\sigma^2 > 0$ and unit vector $v$. Consequently, in the language of spiked model formulation, the variance covariance matrix of $X$ indeed follows a spiked model with spike strength proportional to $|S|$. Theorem 3.4 pertains to the traditional spiked model as an intuitive simplification from the motivating mixture model described above and establishes precise phase transition for the performance of EIGENSTRAT type procedures based on population stratification strength – as captured by the leading spike strength. Indeed, this
provides an useful benchmark to check the validity of using PC adjustment based testing for low dimensional parameters.

Our next result is targeted towards showing that we can translate the results from the generalized spike model set up to a more relevant case of mixture models on the rows of $X$. In particular, it is natural to assume such a mixture distribution for the genotypes in genetic association studies while considering population admixture models [Price et al., 2006].

**Theorem 3.3.** Consider testing (2.2) under (2.1) using $\varphi_{k,\text{ind}}(t)$. Then the same conclusion as of Theorem 3.1 holds with any fixed $k \geq 1$ under Assumptions 2.6 (a), and 2.7 for ind = out when $W \sim \sum_{i=1}^{L} w_i F(\mu_i, \Sigma)$ for any fixed $L$ with $w_i \geq 0$, with $\sum_{i=1}^{L} w_i = 1$, $\sup_i \|\mu_i\| \leq 1$, $\|\Sigma\| = O(1)$ where $F(\mu, \Sigma)$ is the distribution of a random vector $\Sigma^{1/2}Z + \mu$ where $Z$ is a random vector with mean zero i.i.d. sub-Gaussian coordinates. When ind = in, the same conclusion holds under Assumption 2.6 (a) when $X \sim \sum_{i=1}^{L} w_i F(\mu_i, \Sigma)$.

It is worth noting that mixture models on $X$ implies spiked models on the variance covariance matrix of $X$ and thereby the above result is somewhat intuitive given the validity of Theorem 3.1. Moreover, in our numerical experiments we shall additionally verify the universality of the results for non-mean-shift type mixture models on $X$ (e.g. mixtures of binomial distributions on the coordinates of $X$ as more natural candidates for modeling genotypes under admixture of populations under Hardy-Weinberg equilibrium).

### 3.3. Diverging Strength of Population PCs

Section 3.1 explored the necessity of potential caution while using EIGENSTRAT type procedure for PC adjustment testing of low-dimensional components. However, these results are not able to reconcile the empirical success and popularity of this procedure. Moreover, to an expert in the results of random matrix theory, the above results might suggest the main issue being the bias in the eigenvectors as for fixed spike strengths. Indeed, the fact that PC based analysis of genetic variations have been able to reveal known population structures [Novembre et al., 2008], prompts one to believe that a diverging spike strength might be the main underlying recipe behind the success of the PC adjustment based testing procedures. However, as we shall see below, that simply diverging spike strength is not sufficient to explain away the pathologies noted above – and rather a specific signal strength can indeed be calibrated to pin point the regimes of success of EIGENSTRAT type procedures.

In this regard, we now present first results in this direction to derive necessary and sufficient conditions on the success of this procedure under the classical spiked model [Johnstone, 2001] with diverging spike strengths. In the regime of diverging signal strength, it turns out that we can additionally take into account the effect of the distances between $\beta, \theta$ and the population spike eigenvectors. This seems to be a reasonable consideration to explore since using the sample PC directions as the regressors finds its natural analogue in the population when

$$V = \text{close to} \text{ the linear span of the population spiked eigenvectors}. $$

Therefore to introduce the results we will require the following natural notion of distance between vectors and sub-spaces. In particular, given a set $V$ and a fixed vector $\beta$ we define $d(\beta, V) = 1 - \frac{\|P_V(\beta)\|^2}{\|\beta\|^2}$ (with $P_V$ denoting th orthogonal projection operator onto $V$) and $C_\tau(V) = \{\beta; \|\beta\| \leq 1, d(\beta, V) \leq \rho^{-\tau}\}$. Note that, if $\tau_1 > \tau_2$, $C_{\tau_1}(V) \subseteq C_{\tau_2}(V)$ and larger $\tau$ implies lesser angle of the vector $\beta$ with elements of $V$. Moreover, the results in this case for LR$_{k,\text{ind}}$ additionally depend on the nature of localization of the coordinates of the spikes. This is intuitively understandable since certain nature of localized coordinates implies a highly strong effect of coordinates of $W$ on $A$ whereas delocalized eigenvectors imply otherwise. To avoid confusion, we therefore first present the results for LR$_{k,\text{out}}$.

**Theorem 3.4.** Consider testing (2.2) under (2.1) using $\varphi_{k,\text{out}}(t)$ and suppose that Assumptions 2.6 (a), (b)', and 2.7 hold. Further assume that $\lambda_1, \lambda_k = \Theta(p^{\tau_0})$ with $\tau_0 > 0$. Then the following hold for any $\tau > 0$.
i. Suppose that $\beta, \theta$ are not random.
   (a) If $\min\{\tau_0, \tau\} < 1/2$, then for any fixed cut-off $t \in \mathbb{R}$ and $\gamma < 1$,
   $$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > t) = 1.$$ 
   (b) If $\min\{\tau_0, \tau\} > 1/2$, then for any $k \geq k^*$
   $$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{out}} > \chi_1^2(\alpha)) = \alpha.$$ 

ii. Suppose $\beta \sim N(0, \frac{1}{p} \sigma_\beta^2 I_p)$. Then for any $\tau_0 \geq 0$ and $\gamma < 1$ one has
   $$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > \chi_1^2(\alpha)) > \alpha.$$ 

   Further, if $\theta \sim N(0, \frac{1}{p} \sigma_\theta^2 I_p)$,
   $$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > \chi_1^2(\alpha)) > \alpha.$$ 

iii. Assume $\theta \sim N(0, \frac{1}{p} \sigma_\theta^2 I_p)$ but $\beta$ is not random. If $\tau_0 > 0$, then
   $$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{out}} > \chi_1^2(\alpha)) = \alpha.$$ 

Above $S_{V_{k^*}}$ refers to the subspace spanned by $v_1, \ldots, v_{k^*}$.

A few remarks are in order regarding the phase transitions implied by Theorem 3.4. First, it is worth noting that the phase transitions for the Type I error of $\varphi_{k,\text{out}}$ depends not only whether $\theta, \beta$ are random effects but also on the angle between $\theta, \beta$ (whichever is fixed effects) and $v_1$. As for the range of $\tau$ (the parameter deciding the angle with $v_1$), Theorem 3.4 only records the results for $\tau > 0$. Indeed, for $\tau = 0$, the spaces for $\beta, \theta$ are rendered unrestricted. In this case, our next result demonstrates the lack of phase transition compared to the results in Theorem 3.4.

**Proposition 3.5.** Consider testing (2.2) under (2.1) using $\varphi_{k,\text{out}}(t)$. Further assume that $\lambda_1 = \Theta(p^{\gamma_0}), \tau_0 > 0$ and $\gamma < 1$. Then the following hold under Assumptions 2.6 (a), (b):

$$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > \chi_1^2(\alpha)) > \alpha.$$ 

Further, when $\beta \sim N(0, \frac{1}{p} \sigma_\beta^2 I_p)$, the following holds under Assumptions 2.6 (a), (b):

$$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > \chi_1^2(\alpha)) > \alpha.$$ 

If $\beta \sim N(0, \frac{1}{p} \sigma_\beta^2 I_p)$ and $\theta \sim N(0, \frac{1}{p} \sigma_\theta^2 I_p)$, then

$$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k^*,\text{out}} > \chi_1^2(\alpha)) > \alpha.$$ 

However, if $\theta \sim N(0, \frac{1}{p} \sigma_\theta^2 I_p)$, for any $\gamma > 0$,

$$\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{out}} > \chi_1^2(\alpha)) = \alpha.$$ 

Before proceeding to the analysis of $LR_{k,\text{in}}$ we present a partial result on the behavior of $LR_{k,\text{out}}$ under a regime which avoids the reliance on Assumption 2.7.
Proposition 3.6. Consider testing (2.2) under (2.1) using \( \varphi_{k,\text{out}}(t) \). Further assume that \( \lambda_1 = \Theta(p^{\tau_0}) \) and \( \tau, \tau_0 > 0 \) and \( \gamma < 1 \). Then the following hold under Assumptions 2.6 (a), (b)', and 2.8 whenever \( \min\{\tau, \tau_0\} < \frac{1}{2} \).

\[
\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{out}} > \chi_1^2(\alpha)) > \alpha.
\]

If \( \beta \sim N(0, \frac{1}{p} \sigma^2 \beta I_p) \). Then one has

\[
\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{out}} > \chi_1^2(\alpha)) > \alpha.
\]

Our final result pertains to the behavior of LR\(_{k,\text{in}}\) in the regime of divergence spikes. As noted above, this behavior is subtle and depends on the nature of localization of the coordinates of the leading eigenvectors of \( \Sigma \). Since the complete characterization of all the possible cases that can arise is beyond the scope of the paper, we focus on a simple special case of single spiked model below with completely delocalized spiked eigenvector.

Theorem 3.7. Consider testing (2.2) under (2.1) using \( \varphi_{k,\text{in}}(t) \) and suppose that Assumptions 2.6 (a), (c)', and 2.7 hold.

i. Assume that \( k^* = 1 \), \( \lambda_1 = \Theta(p^{\tau_0}) \) with \( \tau_0 > 0 \) and that \( \inf_j |v_1(j)|, \sup_j |v_1(j)| = \Theta(1/\sqrt{p}) \). Then the following hold with any fixed \( k \geq 1 \) and fixed \( M > 0 \)

\[
\liminf_{n \to \infty} \sup_{p/n \to \gamma > 0} \mathbb{P}_{\delta=0}(LR_{k,\text{in}} > \chi_1^2(\alpha)) = \alpha.
\]

ii. If \( \beta \sim N(0, \frac{\sigma^2}{p} I_p) \),

\[
\liminf_{n \to \infty} \mathbb{P}_{\delta=0}(LR_{1,\text{in}} > \chi_1^2(\alpha)) > \alpha.
\]

Indeed, for diverging spikes using \( A \) twice, once in regression of \( Y \) on \( A \) and also while adjusting for confounding through PCA, is more beneficial compared to LR\(_{k,\text{out}}\). This is in contrast to existing intuition which only considers power of the procedures and ignores the Type I error considerations [Listgarten et al., 2012, Mai and Alquier, 2021, Yang et al., 2014b].

4. Numerical Experiments

In this section, we present detailed numerical experiments to not only verify our theoretical results but also to provide additional evidence on the potential universality of the main narrative behind our results that persists beyond the working assumptions of our theoretical results.

We first present results on tests based on LR\(_{k,\text{out}}\). Our simulations are set up to explore the following features of PC adjustment based procedure for testing (2.2) under true underlying model (2.1) by varying the following features: (i) marginal distribution of \( W \) and associated strength of confounding as captured by the spiked strength in case of the generalized spiked model or a suitable notion of mixing strength for mixture models on \( W \); (ii) conditional distribution of \( A|W \); (iii) aspect ratio between the sample size and the number of confounding variables; (iv) the nature of the regression of \( Y|A, W \) (i.e. fixed or random effects as driven by the nature of \( \beta \) in model (2.1)); and (v) the nature of the regression of \( A|W \) (i.e. once again fixed or random effects as driven by the nature of \( \theta \) in model (2.7)). Below we first provide a description of the variations that different types of cases we will consider in this regard.

- **Distribution of \( W \):** We shall consider two broad sub-cases in this regard with further variations as follows.
(1) **Spiked Model:** In this case we will consider \( W_i \sim N(0, \Sigma) \) with \( \Sigma = I + \sum_{j=1}^{k^*} \lambda_j v_j v_j^T \) with \( \lambda_1 \geq \ldots, \lambda_{k^*} > 0 \). We shall consider \( k^* = 1 \), and \( \lambda_1 = p^{\tau_0} \) to regulate the spike strength, where \( \tau_0 \in \{0, 0.05, 0.10, \ldots, 1\} \).

(2) **Mixture Model:** We shall consider two types of mixture models: (i) **Gaussian Mixture Model** \( W_i \sim \frac{1}{2} N(\mu_1, I) + \frac{1}{2} N(\mu_2, I) \) with \( \mu_i = (\mu_{i1}, \ldots, \mu_{ip}) \) for \( i = 1, 2 \), and \( \mu_{ij} = \mu_{2j} = 1 \) for \( j = 1, \ldots, m \) and \( \mu_{ij} = 0 \) for \( j \geq m + 1 \); and (ii) **Binomial Mixture Model** \( W_i = (W_{i1}, \ldots, W_{ip}) \) with \( W_{ij} \) following a Binomial distribution with parameters \( q_{ij} = 0.3, q_{2j} = 0.7 \) for \( j = 1, \ldots, m \) and \( q_{ij} = q_{2j} = 0.5 \) for \( j \geq m + 1 \). For this model, we vary \( m = \lceil p^{\tau_0} \rceil \) to regulate the strength of the population stratification, where \( \tau_0 \in \{0, 0.05, 0.10, \ldots, 1\} \), and \( \lceil \cdot \rceil \) denotes the ceiling function.

- **Regression of \( A|W \):** We shall consider two cases: (i) **Continuous Exposure** \( A_i \in \mathbb{R} \) with \( A_i = W_i^T \theta + \eta_i \) where \( \eta_i \sim N(0, \sigma_{\eta}^2) \); and (ii) **Binomial Exposure** \( A_i \sim \text{Bin}(2, p_i) \) with \( p_i = \frac{\exp(\theta^T W_i)}{1 + \exp(\theta^T W_i)} \). We take \( \sigma_{\eta}^2 = 1 \) for our simulations.

- **Aspect Ratio:** We shall consider two different aspect ratios \( \gamma \in \{0.5, 2\} \) between the sample size and the number of confounding variables in our simulations. In all our simulations, we shall let \( p = 1000 \) (and thus the sample size \( n \in \{500, 2000\} \)).

- **Regression Coefficients for \( Y|A, W \):** We shall consider both fixed and random effects for \( \beta \) in the model (2.1). When \( \beta \) is a fixed effect, we shall vary the angle/distance metric \( d(\beta, S_{v_1}) \) by setting \( \beta = av_1 + \sqrt{1-a^2}v_2 \), where \( v_1 \) and \( v_2 \) are the eigenvectors corresponding to the largest and second largest eigenvalues of \( \mathbb{E}(W^T W/n) \), and \( a = 1 - p^{\tau_0} \). The specification of \( \tau_0 \) remains the same as described in the context of varying spike strength. When \( \beta \) is a random effect, \( \beta \) is drawn randomly from \( N_p(0, 1/pI) \).

- **Regression Coefficients for \( A, W \):** We shall consider both fixed and random effects for \( \theta \) in the model (2.7). The specifications of \( \theta \) as fixed and random effects are exactly the same as described above for \( \beta \).

We are now ready to present our numerical experiments which delves into combinations of the setups presented above. In particular, we shall consider three different combinations of the distributional assumptions of \( W \) and \( A|W \), namely, (1) Spiked Model on \( W \) and continuous exposure \( A \); (2) Gaussian mixture model on \( W \) and continuous exposure \( A \); and (3) Binomial mixture model on \( W \) and continuous exposure \( A \). In each of these cases and for all combinations of different aspect ratios \( \gamma \) and different specifications of \( \beta \) and \( \theta \), we simulate the outcomes under the null model (i.e. \( \delta = 0 \) in (2.1)) by taking \( \sigma_{\eta}^2 = 1 \). We performed 2000 replications of the dataset and tested \( \varphi_{k,\text{out}}(\chi^2_1(\alpha)) \) on each dataset by taking \( k = 1 \) and \( \alpha = 0.05 \). Finally, we plot the empirical type I error rate of the test across varying \( \tau_0 \) in Figure 1.

In Figure 1, the left and the right columns present the results based on the two different aspect ratios, \( \gamma = 2 \) and 0.5, respectively. From top to bottom, the three rows represent simulation setups (1), (2), and (3) as described above. In each of the plots, the black line corresponds to both \( \beta \) and \( \theta \) being fixed effects, the blue line corresponds to \( \beta \) being a fixed effect and \( \theta \) being a random effect, the red line corresponds to \( \beta \) being a random effect and \( \theta \) being a fixed effect, and the pink line corresponds to both \( \beta \) and \( \theta \) being random effects. The results verify the claims made in Theorem 3.4, as well as Theorems 3.1.3.3 when \( \tau_0 = 0 \).

Next, we present results on tests based on \( LR_{k,\text{in}} \). Below we provide a description of different aspects of the simulation procedure that we will consider.

- **Distribution of \( X \):** We shall consider a spiked model for \( X \). In particular, we shall consider \( X_i \sim N(0, \Sigma) \) with \( \Sigma = I + \sum_{j=1}^{k^*} \lambda_j v_j v_j^T \) with \( \lambda_1 \geq \ldots, \lambda_{k^*} > 0 \). We shall set \( k^* = 1 \), and \( \lambda_1 = p^{\tau_0} \) to regulate the spike strength, where \( \tau_0 \in \{0, 0.05, 0.10, \ldots, 1\} \). We shall further generate \( v_1 \) by drawing randomly from \( N_p(0, 1/pI) \) and normalizing afterwards. Next, we shall partition \( X = [A; W] \), i.e., take the first column of \( X \) as \( A \) and the rest as \( W \).
Figure 1. Simulation results in out-regression for different marginal distributions of $W$, conditional distributions of $A|W$, aspect ratios, regression coefficients, and strength of the spike (or population stratification).
Figure 2. Simulation results in in-regression for different marginal distributions of $X$, aspect ratios, regression coefficients, and spike strengths

- **Aspect Ratio**: We shall consider two different aspect ratios $\gamma \in \{0.5, 2\}$ between the sample size and the number of confounding variables in our simulations. In all our simulations, we shall let $p = 1000$ (and thus the sample size $n \in \{500, 2000\}$).
- **Regression Coefficients for $Y|A, W$**: We shall consider both fixed and random effects for $\beta$ in the model (2.1). When $\beta$ is a fixed effect, we shall set $\beta = \Sigma_{(22)}^{-1}\Sigma_{(21)}$, where $\Sigma_{(21)}, \Sigma_{(22)}$ are defined based on the partition of $\Sigma$,

$$
\Sigma = \begin{pmatrix}
\Sigma_{(11)} & \Sigma_{(12)} \\
\Sigma_{(21)} & \Sigma_{(22)}
\end{pmatrix}.
$$

Here $\Sigma_{(11)}$ is a scalar. When $\beta$ is a random effect, $\beta$ is drawn randomly from $N_p(0, \frac{1}{p}I)$.

For all combinations of different aspect ratios and different specifications of $\beta$, we simulate the outcomes under the null model (i.e. $\delta = 0$ in (2.1)) by taking $\sigma^2_y = 1$. We performed 2000 replications of the dataset and tested $\phi_{k,in}(\chi^2_{1}(\alpha))$ on each dataset by taking $k = 1$ and $\alpha = 0.05$. Finally, we plot the empirical type I error rate of the test across varying $\tau_0$ in Figure 2.

Figures 2a and 2b present the results based on the two different aspect ratios, $\gamma = 2$ and 0.5, respectively. In each of the plots, the black line corresponds to $\beta$ being fixed effects, and the red line corresponds to $\beta$ being random effects. The results verify the claims made in Theorem 3.7.

5. DISCUSSIONS

In this paper we consider hypothesis testing of individual parameters in high dimensional linear regression set up under proportional asymptotics while adjusting for additional confounding through principal component analysis. This method is regularly employed in large-scale genetic and epigenetic association studies and in this paper, we take some initial steps to shed light on necessary and sufficient conditions for the validity of this procedure. Indeed, several interesting directions remain to be explored. A non-exhaustive list of such avenues is as follows: (i) What is a complete picture of phase transitions for $LR_{k,in}$ in diverging spiked models? (ii) How to analyze $LR_{k,ind}$ for more realistic genetic admixture models [Price et al., 2006]? (iii) How to capture
similar results when $A|W$ follows a multiple logistic regression with Hardy-Weinberg equilibrium proportions depending through the logistic link on $W$? (iv) How to perform analogous analysis for case-control studies? and (v) How to construct corrections to the cut-offs for LR$_{k,in}$ in regimes where the Type-I error of the tests is inflated? We keep these and other important directions for future research endeavors.

6. Proofs of Main Results

Throughout our proofs whenever the context is clear, with an abuse of notation, we shall write both $W$ and $X$ as $\sum_{j=1}^{n/p} \tilde{d}_j \tilde{u}_j \tilde{v}_j^T$ and denote $\tilde{X}_j = \tilde{d}_j / \sqrt{n}$ – and use them accordingly in the context of LR$_{k,out}$ and LR$_{k,in}$ respectively.

6.1. Proof of Theorem 3.1. We only prove the result for LR$_{k,out}$ and note that the proof for LR$_{k,in}$ follows by similar arguments by simply replacing $\beta, \theta$ by $\tilde{\beta} = \tilde{I}_1 \beta$ and $\tilde{\theta} = \tilde{I}_1 \theta$ respectively with $\tilde{I}_1 := [e_2: \cdots : e_p]$ and $e_j$ denotes the $j^{th}$ canonical basis of $\mathbb{R}^{p+1}$.

We begin by noting that by Lemma 7.1 one has

$$\text{LR}_{k,out} | A, W \sim \chi^2_{\kappa^2_{k,out}}(\kappa^2_{k,out}), \quad \tilde{\kappa}^2_{k,out} = \frac{\left( (\beta^T W^T + A^T \delta) \left( I - P_{C(W \tilde{\nu}_{k,out})} A \right) \right)^2}{A^T \left( I - P_{C(W \tilde{\nu}_{k,out})} A \right)}. $$

Since

$$\mathbb{P}_{\delta=0}(LR_{k,out} > t_\alpha) = \mathbb{E} \left( \Phi(t_\alpha - \tilde{\kappa}^2_{k,out}) - \Phi(-t_\alpha - \tilde{\kappa}^2_{k,out}) \right)^2,$$

where $\Phi$ is the standard normal cdf and $\tilde{\Phi} = 1 - \Phi$, it will be sufficient to derive asymptotic distribution of $\tilde{\kappa}^2_{k,out}$ followed by an application of uniform integrability principle to derive the asymptotic behavior of the likelihood ratio test.

Proof of Theorem 3.1i. The non-centrality parameter $\kappa^2_{k,out}$ under $H_0$ is given by

$$\kappa^2_{k,out} = (W\beta)^T P_{C(A_k)} (W\beta) = \frac{\left( \beta^T W^T \left( I - P_{C(W \tilde{\nu}_{k,out})} A \right) \right)^2}{A^T \left( I - P_{C(W \tilde{\nu}_{k,out})} A \right)} := \frac{T_2^2}{T_1^2}. \quad (6.1)$$

First note that the coordinates of $A_j$ are i.i.d with finite $\psi_2$-norm (this follows from Assumption 2.7 and (2.1)). Therefore by Bernstein’s inequality, $\exists C_2, C'_2 > 0$ such that $\|A\|_2 \leq C_2 n$ w.p. $\geq 1 - e^{-C_2^2 n}$. Hence,

$$\frac{T_2^2}{n} \leq \frac{\|A\|^2_2}{n} \leq C_2,$$

w.p. $\geq 1 - e^{-C_2^2 n}$. Next we show that there exists a constant $C_1$ and a pair $\beta, \theta$ such that with probability converging to 1 one has $T_1^2 \geq C_2 n^2$. To this end note that for any $\beta, \theta$,

$$T_1 = \beta^T W^T \left( I - P_{C(W \tilde{\nu}_{k,out})} \right) W \theta + \beta^T W^T \left( I - P_{C(W \tilde{\nu}_{k,out})} \right) \eta_1 = T_{11} + T_{12}. \quad (6.2)$$

Therefore it is enough to find $\beta, \theta, C_1$ such that Now, we will show that with high probability both of the following hold: (a) $|T_{11}| \geq 2C_1 n$ and (b) $|T_{12}| \leq C_1 n$ Combining we will have the desired result.

To show (a) note that for $\beta = \theta$ one has

$$T_{11}^2 = \left( \frac{1}{n} \theta^T W^T \left( I - P_{C(W \tilde{\nu}_{k,out})} \right) W \theta \right)^2 = \left( \sum_{j=1}^{n/p} d_j \theta^T \tilde{u}_j \tilde{v}_j^T \theta \right)^2 = \left( \sum_{j=1}^{n/p} \hat{\lambda}_j \theta^T \tilde{v}_j \tilde{v}_j^T \theta \right)^2.$$
Now using Lemma 7.2, there exists $\|\theta\|_2^2 \leq M$ such that there exists $C_1 > 0$ with $\sum_{j=k+1}^{n \wedge p} \hat{\lambda}_j \theta^T \hat{v}_j \hat{v}_j^T \theta \to 2C_1 > 0$ a.s.. Hence, with probability converging to 1 one has for $\beta = \theta$ of unit norm $T_{11}^2 \geq 4C_1^2 n^2$ with probability converging to 1.

Next to show (b) note that $\mathbb{E}(T_{12}^2|\mathbb{W}) = 0$, and for this choice of $\beta = \theta$ one has

$$\text{Var}\left(\frac{1}{n} T_{12}|\mathbb{W}\right) = \frac{1}{n^2} \mathbb{E}\left[\theta^T \mathbb{W}^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) \mathbb{W}\theta\right] \leq \hat{\lambda}_{k+1}^2 / n,$$

yielding $\frac{1}{n} T_{12} = o_p(1)$ since $\hat{\lambda}_{k+1} = O_p(1)$. This completes the proof of Theorem 3.1i.

**Proof of Theorem 3.1ii.** Let $\beta \sim \mathcal{N}(0, \frac{\sigma_\theta^2}{n} I_p)$ and $\theta \in \mathbb{R}^p$ be a fixed vector with $\|\theta\| \leq M$ for some fixed $M > 0$. For some $h \neq 0$, let $\delta = \frac{h}{\sqrt{n}}$. Recall that, the non-centrality parameter of the likelihood ratio test under alternative $\delta$ is $\hat{\kappa}_{k,\text{out}}^2$ given by,

$$\hat{\kappa}_{k,\text{out}}^2 = \left( (\beta^T \mathbb{W}^T + A^T \delta) \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) A \right)^2 / \left( I - P_{C(\mathbb{W}v_{k,\text{out}})} \right) A.$$

Using SVD of $\mathbb{W}$,

$$\frac{1}{n} \mathbb{W}^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) \mathbb{W} \theta = \frac{1}{n} \sum_{j=k+1}^{n \wedge p} \hat{d}_j^2 \theta^T \hat{v}_j \hat{v}_j^T \theta = \sum_{j=k+1}^{n \wedge p} \hat{\lambda}_j \theta^T \hat{v}_j \hat{v}_j^T \theta \overset{a.s.}{\to} c_0,$$

where the specific form of $c_0$ is provided in Lemma 7.2. Hence, $\mathbb{E}\left(\frac{T_{12}}{n}\right) \overset{a.s.}{\to} c_0 + \sigma_g^2$. Further,

$$\text{Var}\left(\frac{T_{12}}{n}|\mathbb{W}\right) = \frac{2\sigma_\theta^4}{n^2} \text{Tr} \left( I - P_{C(\mathbb{W}v_{k,\text{out}})} \right) + \frac{4\sigma_\theta^2}{n^2} \theta^T \mathbb{W}^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) \mathbb{W} \theta.$$

The second quantity of RHS converges to 0 a.s. under $\mathbb{P}$ by (6.5) and the first quantity is deterministic and $O\left(\frac{2\sigma_\theta^4}{n}\right) = o(1)$. So,

$$\frac{T_{12}}{n} \overset{p}{\to} c_0 + \sigma_g^2,$$

unconditionally on $\mathbb{W}$ using Dominated Convergence Theorem.

Next, we derive asymptotic behavior of $T_1/\sqrt{n}$. Recall that, $A = \mathbb{W} \theta + \eta$ and

$$T_1 = \beta^T \mathbb{W}^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) A + \delta A^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) A.$$

Since $\delta = h/\sqrt{n},$

$$\frac{\delta}{\sqrt{n}} A^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) A = \frac{h}{n} A^T \left(I - P_{C(\mathbb{W}v_{k,\text{out}})}\right) A \overset{p}{\to} h(c_0 + \sigma_g^2),$$
using (6.6). Next, define

$$T_3 := A^T \left( I - P_{C(\mathcal{W}_k)} \right) \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) A. \quad (6.7)$$

Conditioned on \(\mathcal{W}, A\),

$$\beta^T \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) A / \sqrt{n} \sim N(0, \sigma_\beta^2). \quad (6.8)$$

We will show \(T_3 / np\) converges, in probability, to a positive constant. To this end note that,

$$\mathbb{E} \left( \frac{T_3}{np} | \mathcal{W} \right) = \frac{\sigma_\beta^2}{np} \text{Tr} \left( \left( I - P_{C(\mathcal{W}_k)} \right) \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) \right)$$

$$+ \frac{1}{np} \theta^T \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) \mathbb{W} \theta. \quad (6.9)$$

The first quantity of RHS equals

$$\frac{\sigma_\beta^2}{np} \text{Tr} \left( \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) \mathbb{W} \right) = \frac{\sigma_\beta^2}{np} \text{Tr} \left( \sum_{j=k+1}^{np} \hat{d}_j^2 \hat{v}_j \hat{v}_j^\top \right) = \frac{\sigma_\beta^2}{np} \sum_{j=k+1}^{np} \hat{\lambda}_j \overset{\text{a.s.}}{\rightarrow} \sigma_\theta^2 \chi^2_1 \quad (6.10)$$

using Lemma 7.5. The second term equals

$$\frac{1}{np} \sum_{j=k+1}^{np} \hat{d}_j^4 \theta^T \hat{v}_j \hat{v}_j^\top \theta \overset{\text{a.s.}}{\rightarrow} c_4 > 0, \quad (6.11)$$

using Lemma 7.2. Finally,

$$\text{Var} \left( \frac{T_3}{np} | \mathcal{W} \right)$$

$$= \frac{2\sigma_\beta^4}{np^2} \text{tr} \left( \left( \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) \mathbb{W} \right)^2 \right) + \frac{4\sigma_\beta^4}{np^2} \theta^T \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) \theta$$

$$\leq \frac{2\sigma_\beta^4}{np^2} \sum_{j=k+1}^{np} \hat{\lambda}_j^2 + \frac{4\sigma_\beta^4}{np^2} \sum_{j=k+1}^{np} \hat{\lambda}_j^3 \theta^T \hat{v}_j \hat{v}_j^\top \theta \overset{\text{a.s.}}{\rightarrow} 0. \quad (6.12)$$

using Lemma 7.5 and the fact \(\hat{\lambda}_{k+1} = O_\beta(1)\). Hence, \(T_3 / np \overset{\text{P}}{\rightarrow} \sigma_\theta^2 \chi^2_1 + c_4\), using Dominated Convergence Theorem. By Slutsky’s theorem

$$\frac{T_1}{\sqrt{n}} \Rightarrow N(h(c_0 + \sigma_\theta^2), \sigma_\theta^2(\sigma_\theta^2 m_1 + c_4)).$$

Using (6.6), this implies

$$\hat{\kappa}_{k,\text{out}}^2 \Rightarrow \frac{\sigma_\theta^2 (\sigma_\theta^2 m_1 + c_4)}{c_0 + \sigma_\theta^2} \chi^2(h^2(c_0 + \sigma_\theta^2)^2). \quad (6.13)$$

Next consider \(\theta \sim N(0, \sigma_\theta^2 / p I_p)\) and \(\beta \in \mathbb{R}^p\) be fixed. Recall that the denominator of \(\hat{\kappa}_{k,\text{out}}^2\) is

$$T_2 = A^T \left( I - P_{C(\mathcal{W}_k)} \right) A$$

where \(A | \mathcal{W} \sim N(0, \sigma_\theta^2 / p \mathbb{W} \mathbb{W}^\top + \sigma_\theta^2 I_p)\). Hence

$$\mathbb{E} \left( \frac{T_2}{n} | \mathcal{W} \right) = \frac{1}{n} \text{tr} \left( \frac{\sigma_\theta^2}{p} \mathbb{W} \mathbb{W}^\top \left( I - P_{C(\mathcal{W}_k)} \right) + \sigma_\theta^2 \left( I - P_{C(\mathcal{W}_k)} \right) \right)$$
hence by the previous case, we immediately obtain

\[ T \]

using (6.12). Hence,

\[ \text{RHS} \]

by (6.12). Hence, \( T \)

\[ \text{RHS} \]

The first term in the RHS converges a.s. to \( \sigma \) positive constant, where \( \sigma \) is defined in (6.7). Note that,

\[ \text{Var}\left( \begin{array}{c} \hat{\kappa}_{k,\text{out}}^2 \\ \beta^T \mathbb{W}^T \end{array} \right) \]

\[ = \sqrt{T_3} \]

where

\[ T_3 := \beta^T \mathbb{W}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \left( \frac{\sigma_2}{p} \mathbb{W} \mathbb{W}^T + \sigma_g \mathbb{I}_p \right)^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \beta. \]

Now, observe that, \( T_3 \xrightarrow{p} C_1 \), for some \( C_1 \geq 0 \) by calculation similar to (6.4) and (6.9). Finally

\[ \frac{\delta}{\sqrt{n}} \mathbb{A}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{A} = \frac{h}{n} \mathbb{A}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{A} \xrightarrow{p} h(\sigma_g^2 m_2 + \sigma_g^2). \]

Hence, \( T_3 \xrightarrow{\text{as}} N(h(\sigma_g^2 m_2 + \sigma_g^2), C_1) \) yielding

\[ \hat{\kappa}_{k,\text{out}}^2 \xrightarrow{\text{as}} \frac{C_1}{\sigma_g^2 m_2 + \sigma_g^2} \chi^2(h^2(\sigma_g^2 m_2 + \sigma_g^2)^2). \]  

Finally consider \( \beta \sim N\left(0, \frac{\sigma_2^2}{p} \mathbb{I}_p \right) \) and \( \theta \sim N\left(0, \frac{\sigma_2^2}{p} \mathbb{I}_p \right) \). Once again we want to find the asymptotic distribution of \( \hat{\kappa}_{k,\text{out}}^2 \), where \( \hat{\kappa}_{k,\text{out}}^2 \) was defined as (6.3). To this end, observe that, \( T_2 \) is free of \( \beta \) hence by the previous case, we immediately obtain \( T_2 \xrightarrow{p} \sigma_g^2 m_2 + \sigma_g^2 \).

To derive the asymptotic distribution of \( T_1 \), we will show \( T_4 \xrightarrow{\text{as}} \) converges, in probability, to a positive constant, where \( T_3 \) is defined in (6.7). Note that,

\[ \mathbb{E}\left( \frac{T_3}{np} \right) \]

\[ = \frac{\sigma_2^2}{np} \text{Tr} \left( \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \mathbb{W}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \right) \]

\[ + \frac{1}{np} \mathbb{D} \left( \mathbb{W} \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \right)^2 \]

The first term in the RHS converges a.s. to \( \sigma_g^2 m_1 \) using (6.10). Denoting the second term on the RHS by \( T_4 \), note

\[ \mathbb{E}(T_4|\mathbb{W}) = \frac{\sigma_2^2}{np^2} \text{Tr} \left( \left( \mathbb{W}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \right)^2 \right) = \frac{\sigma_2^2}{p} \sum_{j=k+1}^{n^\wedge p} \hat{\lambda}_j^2 \xrightarrow{\text{as}} \sigma_g^2 m_2, \]

using Lemma 7.5 and

\[ \text{Var}(T_4|\mathbb{W}) = \frac{2\sigma_2^4}{np^4} \text{Tr} \left( \left( \mathbb{W}^T \left( I - P_{C(W\mathbb{V}_{k,\text{out}})} \right) \mathbb{W} \right)^4 \right) = \frac{1}{np^4} \sum_{j=k+1}^{n^\wedge p} \hat{d}_j^4 \xrightarrow{\text{as}} 0. \]

Therefore,

\[ \frac{T_1}{\sqrt{n}} \xrightarrow{\text{as}} N(h(\sigma_g^2 m_1 + \sigma_g^2), \sigma_g^2(\sigma_g^2 m_1 + \sigma_g^2 m_2)). \]
Hence, using Slutsky’s theorem,

\[ \hat{\kappa}_{k,\text{out}}^2 = \frac{\sigma^2(\sigma^2 m_1 + \sigma^2 m_2)}{\sigma^2 m_1 + \sigma^2 g} \lambda^2 \left( \kappa^2 (\sigma^2 m_1 + \sigma^2 g)^2 \right), \]  

(6.15)

concluding the proof of the theorem for LR_{k,\text{out}}.

6.2. Proof of Theorem 3.2. We divide the proof according to the parts of the theorem.

Proof of Theorem 3.2i. We once again begin by noting that by Lemma 7.1 one has

\[ \text{LR}_{k,\text{out}}|A, \mathbb{W} \sim \chi^2(\hat{\kappa}_{k,\text{out}}^2), \quad \hat{\kappa}_{k,\text{out}}^2 = \frac{\left( (\beta^T \mathbb{W}^T \mathbb{A}^T + \mathbb{A}^T \delta) \left( I - P_{C(\mathbb{W}^k,\text{out})} \right) \mathbb{A} \right)^2}{\mathbb{A}^T \left( I - P_{C(\mathbb{W}^k,\text{out})} \right) \mathbb{A}}. \]

Since projection contracts norm and \( A \) is sub-Gaussian we immediately have

\[ \mathbb{A}^T \left( I - P_{C(\mathbb{W}^k,\text{out})} \right) \mathbb{A} \leq \|A\|_2^2 \leq cn \]

with high probability for some constant \( c > 0 \). To lower bound the numerator of \( \hat{\kappa}_{k,\text{out}}^2 \) we consider a specific instance where \( A \perp \mathbb{W} \) which implies that

\[ T_1 := \mathbb{A}^T \left( I - P_{C(\mathbb{W}^k,\text{out})} \right) \mathbb{W} \beta \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{A} \]

has mean

\[ \mathbb{E}(T_1|\mathbb{W}) = \text{Tr} \left( (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \right) = \beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta. \]

Also, since coordinates of \( A \) are sub-Gaussian we have by Sub-Gaussian moment bounds that for some constant \( C > 0 \)

\[ \text{Var} \left( T_1 | \mathbb{W} \right) \leq C \left( \beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta \right)^2. \]

Therefore by Paley-Zygmund Inequality one has for some \( 0 < \zeta < 1 \)

\[ \mathbb{P}(T_1 \geq \zeta \mathbb{E}(T_1|\mathbb{W})|\mathbb{W}) \geq \zeta. \]

Now note that \( \beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta = n \sum_{j=k+1}^{n/p} \hat{\lambda}_j \langle \beta, \hat{v}_j \rangle^2 \) and that by Lemma 7.2 we have \( \sum_{j=k+1}^{n/p} \hat{\lambda}_j \langle \beta, \hat{v}_j \rangle^2 \xrightarrow{P} e^* > 0 \) for some \( e^* > 0 \). This completes the proof of the desired result.

3.2 ii. We invoke the same proof as part i. By the Paley-Zygmund Inequality, it is again enough to that there exists \( c_0 > 0 \) such that \( \frac{1}{n} \mathbb{E}(\beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta) \xrightarrow{P} c_0 \). To this end note that,

\[ \frac{1}{n} \mathbb{E}(\beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta) = \frac{\sigma^2}{p} \sum_{j=k+1}^{n/p} \hat{\lambda}_j \rightarrow \frac{m_1 \sigma^2}{\gamma} > 0, \]

by Lemma 7.5. Also,

\[ \text{Var} \left( \frac{1}{n} \beta^T \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \beta \right) = \frac{\sigma^4}{n^2p} \text{Tr} \left( \mathbb{W}^T (I - P_{C(\mathbb{W}^k,\text{out})}) \mathbb{W} \right)^2 \rightarrow 0. \]

This yields the desired conclusion.
Proof of Theorem 3.2iv. Recall that, \( I_{-1} = [e_2: \cdots : e_p] \) and \( W = X I_{-1} \) and \( A = X e_1 \). By Lemma 7.1,
\[
\hat{\kappa}_{k, \text{in}}^2 = \frac{\beta^\top I_{-1} X^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X e_1}{e_1^\top X^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X e_1} \tag{6.16}
\]

By Lemma 7.2,
\[
\hat{\kappa}_{k, \text{in}}^2 = (1 + o(1)) n^{-1} \left( \sum_{j=1}^{n} \phi_j \beta_0^\top v_j v_j^\top e_1 \right)^2 = (1 + o_p(1)) \frac{1}{\gamma} \left( \sum_{j=1}^{n} \phi_j e_1^\top v_j v_j^\top e_1 \right)
\]

Note that, \( \exists C_1, C_2 > 0 \) such that \( C_1 \leq \phi_i \leq C_2 \) for all \( j \). Hence, \( C_1 \leq \sum_{j=1}^{n} \phi_j e_1^\top v_j v_j^\top e_1 \leq C_2 \).

Hence if \( |c_p^*(\beta_0)| > 0 \), \( \hat{\kappa}_{k, \text{in}}^2 \) a.s. \( \rightarrow \infty \), proving (a). If \( \lim \inf \sqrt{p} c_p^*(\beta_0) \leq 1 \), then \( \exists C_3 > 0 \) such that \( \hat{\kappa}_{k, \text{in}}^2 \geq C_4 > 0 \) with high probability, proving (b). Finally, if \( \lim \sup \sqrt{p} c_p^*(\beta_0) = 0 \), \( \hat{\kappa}_{k, \text{in}}^2 = o_p(1) \), proving (c).

Proof of Theorem 3.2iv. We want to analyse the behavior of \( \hat{\kappa}_{k, \text{in}}^2 \) given by (6.16). By Lemma 7.2, the denominator is \( O_p(n) \). Since \( \beta \sim N(0, \frac{1}{p} \sigma^2 I_p) \), it is enough to show \( \frac{T_3}{n^2} = \Omega_p(1) \), where
\[
T_3 = e_1^\top X^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X I_{-1} I_{-1}^\top X^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X e_1. \tag{6.17}
\]

Note that, \( I_{-1} I_{-1}^\top = I - e_1 e_1^\top \). Hence,
\[
\frac{T_3}{n^2} = \frac{1}{n^2} \left( e_1^\top \left( X^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X \right)^2 e_1 - \left( e_1^\top \left( I - P_{C(XV_{k, \text{in}})} \right) X e_1 \right)^2 \right)
\]
\[
= \sum_{j=2}^{n} \lambda_j^2 (e_1, \tilde{v}_j)^2 - \left( \sum_{j=2}^{n} \lambda_j (e_1, \tilde{v}_j)^2 \right)^2
\]
\[
\geq \left( \sum_{j=2}^{n} \lambda_j^2 (e_1, \tilde{v}_j)^2 \right) \left( 1 - \sum_{j=2}^{n} (e_1, \tilde{v}_j)^2 \right) = \Omega_p(1),
\]

where the first term is \( \Omega_p(1) \) using 7.2. This completes the proof of the Theorem.

6.3. Proof of Theorem 3.3. We begin by stating couple of Lemmas with would be useful for the proof of the Theorem.

The first lemma establishes a desired moment bounds on \( W \) for \( \text{ind} = \text{out} \) and on \( X \) for \( \text{ind} = \text{in} \).

Lemma 6.1. Let \( D \sim \sum_{i=1}^{L} w_i F(\mu_i, \Sigma) \) for any fixed \( L \) with \( w_i \geq 0 \), with \( \sum_{i=1}^{L} w_i = 1 \), sup \( \| \mu_i \| \leq 1 \), \( \| \Sigma \| = O(1) \) where \( F(\mu, \Sigma) \) is the distribution of a random vector \( \Sigma^{1/2} Z + \mu \) where \( Z \) is a random vector with mean zero i.i.d. sub-Gaussian coordinates. Let \( C \) be a deterministic \( p \times p \) matrix. Define
\( T_3 = \mathbb{E}(DD^\top) \). Define \( \bar{C} = \Sigma^{1/2} C \Sigma^{1/2} \). Then for any \( q \in \mathbb{N} \),
\[
\mathbb{E}[|D^\top CD - tr(C)C^\top|^q] \leq K_q \left( (tr(\bar{C}C^\top))^q + tr((\bar{C}C^\top))^q + (tr(C))^q \right). \tag{6.18}
\]

Proof. Note that, \( D = \Sigma^{1/2} Z + \sum_{i=1}^{L} \mu_i \xi_i \), where \( \xi = (\xi_1, \ldots, \xi_L) \sim \text{Mult}(1; (w_1, \ldots, w_L)) \). Define \( R = \sum_{i=1}^{L} \mu_i \xi_i \). Notice that, \( D^\top CD = Z^\top \bar{C} Z + R^\top (C + C^\top) \Sigma^{1/2} Z + R^\top CR \). Also,
Using [Mestre, 2006, Lemma 3], the first summand is upper bounded by
\[
\mathbb{E}[\|D^\top CD - \text{tr}(CT)\|^q] \leq \bar{K}_q \left(\mathbb{E}[\|Z^\top CZ - \text{tr}(C\Sigma)\|^q] + \mathbb{E}[\|R^\top(C + C^\top)\Sigma^{1/2}Z\|^q]
+ \mathbb{E}[\|R^\top CR - \text{tr}(C\Sigma RR^\top)\|^q]\right).
\]
Using [Mestre, 2006, Lemma 6.1. Hence, the empirical spectral distribution of \( \hat{q} \) is bounded by a constant only depending on \( \beta \) and bound its moments using Lemma 6.1. The remaining proof follows once we observe
\[
\text{Finally } \mathbb{R}^\top \mathbb{C}R = \sum_{i=1}^L \xi_i \mu_i^\top C \mu_i.
\]
Hence,
\[
\mathbb{E}[\|R^\top CR - \text{tr}(C\Sigma RR^\top)\|^q] \leq C(q) \sum_{i=1}^L \left(\mu_i^\top C \mu_i\right)^q \leq C(q)L(\text{tr} C)^q
\]
This completes the proof. \( \blacksquare \)

Now, we prove analogue of [Mestre, 2006, Theorem 5] for mixture models which yields the limit of bilinear forms.

**Lemma 6.2.** Define \( \hat{R} = \frac{1}{n}DD^\top \) and \( T = EDD^\top \), where \( D \) is defined as in Lemma 6.1. Then [Mestre, 2006, Thm 5] holds if one replaces the eigenvalues and eigenvectors of \( R \) by \( T \).

**Proof.** Note that, the assumptions of [Bai and Zhou, 2008, Theorem 1.1] are satisfied by \( \hat{R} \) with \( T = EDD^\top \) since \( ||T|| \leq ||E|| + ||ERR^\top|| = O(1) \) as we are working under fixed spike strength assumption and using Lemma 6.1. Hence, the empirical spectral distribution of \( \hat{R} \) converges with the limit given by [Bai and Zhou, 2008, (1.1)]. Define \( \hat{R}_{(n)} = \hat{R} - \frac{1}{n}d_n d_n^\top \). Then, it is enough to show [Mestre, 2006, Eq 17,18] with \( R \) replaced by \( T \). To this end, note that [Mestre, 2006, Eq 17] follows immediately from [Mestre, 2006, Lemma 6] and convergence of ESD of \( \hat{R} \). The proof of [Mestre, 2006, Eq 25] follows the same way once we define
\[
\theta_n = b^\top d_n d_n^\top (\hat{R}_{(n)} - zI)^{-1} - b^\top T (\hat{R}_{(n)} - zI)^{-1} a,
\]
and bound its moments using Lemma 6.1. The remaining proof follows once we observe \( \frac{1}{n^{\gamma/2}} \mathbb{E}(||T_n||^{4q}) \) is bounded by a constant only depending on \( q \) since \( ||\mu|| = 1 \). \( \blacksquare \)

Now, Lemma 6.2 and Lemma 7.2 yields the limits of bilinear forms of sample eigenvectors. The rest of the proof can now be done in the exact same way as Theorem 3.1.

### 6.4. Proof of Theorem 3.4

We divide the proof according to the parts of the theorem.

**Proof of Theorem 3.4i.** Similar to the proof of Theorem 3.1 we will only need to analyse the behavior of the non-centrality parameter \( \hat{k}_{k,\text{out}}^2 \) defined by (6.1). Recall that, \( \lambda_1, \lambda_k^\ast = \Theta(p_{\gamma_0}) \), \( \tau_0 > 0 \).

Let \( \beta, \theta \) be fixed vectors with \( ||\beta||, ||\theta|| \leq 1 \). The denominator of \( \hat{k}_{k,\text{out}}^2 \) is \( T_2 = A^\top \left(I - P_{C(W\tilde{V}_{k,\text{out}})}\right) A \) which does not depend on \( \beta \). Since \( A = \mathbb{W}\theta + \eta \), write \( T_2 = D_1 + D_2 + D_3 \), where \( D_1 = \theta^\top \mathbb{W}^\top \left(I - P_{C(W\tilde{V}_{k,\text{out}})}\right) \mathbb{W}\theta, D_2 = 2\eta^\top \left(I - P_{C(W\tilde{V}_{k,\text{out}})}\right) \mathbb{W}\theta, D_3 = \eta^\top \left(I - P_{C(W\tilde{V}_{k,\text{out}})}\right) \eta \). Note, \( D_3/n \overset{p}{\to} \sigma^2_g, \mathbb{E}(D_2|\mathbb{W}) = 0 \),
\[
\text{Var} \left(\frac{D_2}{n}\right) = \frac{4}{n} \sum_{j=k^\ast+1}^n \frac{d_j^2}{n} \langle \hat{v}_j, \theta \rangle^2 \leq \frac{4}{n} \lambda_{k^\ast+1} ||\theta||^2 = o_p(1),
\]
(6.19)
since [Cai et al., 2020, Theorem 2.5] implies $\hat{\lambda}_{k^*+1} = O_p(1)$ and $\|\theta\| \leq 1$. By similar argument $0 \leq \frac{1}{n}D_1 = O_p(1)$. Therefore, $\frac{1}{n}T_2 = O_p(1)$ and $P(T_2 \geq \sigma_g^2) \rightarrow 1$, yielding both upper and lower bounds on $T_2$.

For the numerator, note that

$$
\frac{T_1}{\sqrt{n}}W \sim N\left(\frac{1}{\sqrt{n}}\beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \theta, \frac{\sigma_g^2}{n} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \beta\right).
$$

Note that for any $k \geq k^*$, the conditional variance equals

$$
\frac{\sigma_g^2}{n} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \beta \leq \sigma_g^2 \sum_{j=k^*+1}^{n \wedge p} \frac{1}{n} (\hat{\nu}_j, \beta)^2 \leq \sigma_g^2 \hat{\lambda}_{k^*+1} \sum_{j=k^*+1}^{n \wedge p} (\hat{\nu}_j, \beta)^2.
$$

By [Cai et al., 2020, Theorem 2.5], $\hat{\lambda}_{k^*+1} = O_p(1)$. Further, [Bao et al., 2020, (2.13)] implies, for $j \leq k^*$,

$$
(\hat{\nu}_j, \beta)^2 = \langle v_j, \beta \rangle^2 \frac{\lambda_j^2 - \gamma}{\lambda_j (\lambda_j + \gamma)} + O_P \left(\frac{1}{\sqrt{n \lambda_j^2}}\right) = \langle v_j, \beta \rangle^2 + o_P \left(\frac{1}{\lambda_j}\right).
$$

Since $\beta \in C_\tau(S_{V_{k^*}})$, $\tau > 0$, and $\lambda_{k^*} \rightarrow \infty$,

$$
\sum_{j=k^*+1}^{n \wedge p} (\hat{v}_j, \beta)^2 \leq \|\beta\|^2 d(\beta, S_{V_{k^*}}) + o_P \left(\frac{1}{\lambda_{k^*}}\right) \leq o_P(p^{-\tau}) + o_P \left(\frac{1}{\lambda_{k^*}}\right) \overset{a.s.}{\longrightarrow} 0.
$$

For the conditional mean, consider the case $\min\{\tau_0, \tau\} < 1/2$ and $k = k^*$. Since $\gamma < 1$, assume $p \leq n$. When $\tau_0 < 1/2$,

$$
\sup_{\beta, \theta \in C_\tau(S_{V_{k^*}})} \frac{1}{\sqrt{n}} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \theta \geq \sqrt{n} \lambda_{\beta}^2 \sum_{j=k^*+1}^{p} \langle \hat{v}_j, v_1 \rangle^2 \overset{a.s.}{\longrightarrow} \infty,
$$

by choosing $\beta = \theta = v_1$ since $1 - \langle \hat{v}_1, v_1 \rangle^2 = \Omega_P \left(\frac{1}{\lambda_{k^*}}\right)$ and $\langle \hat{v}_1, v_1 \rangle^2 = \Omega_P \left(\frac{1}{\lambda_{k^*}}\right)$. Now, if $\tau_0 > 1/2$ but $\tau < 1/2$, fix a vector $\xi$ such that $\xi \in C_\tau(S_{V_{k^*}})$ and $d(\xi, S_{V_{k^*}}) = \Omega(p^{-\tau})$. Hence,

$$
\sup_{\beta, \theta \in C_\tau(S_{V_{k^*}})} \frac{1}{\sqrt{n}} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \theta \geq \sqrt{n} \lambda_{\beta}^2 \sum_{j=k^*+1}^{p} \langle \hat{v}_j, \xi \rangle^2
$$

$$
= \sqrt{n} \lambda_{\beta}^2 \left(\Omega(p^{-\tau}) + o(p^{-\tau})\right) \overset{a.s.}{\longrightarrow} \infty.
$$

Finally, when $\min\{\tau_0, \tau\} > 1/2$ and $k \geq k^*$,

$$
\frac{1}{\sqrt{n}} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \theta \leq \left(\frac{1}{\sqrt{n}} \beta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \beta\right)^\frac{1}{2} \left(\frac{1}{\sqrt{n}} \theta^T \bar{W}^T \left(I - P_{C(\bar{W}_{k,\text{out}})}\right) \bar{W} \theta\right)^\frac{1}{2}.
$$

Each term of RHS can be upper bounded, as above, by

$$
\sqrt{n} \lambda_{\beta, k^*+1}^2 \left(o_P(p^{-\tau}) + o_P \left(\frac{1}{\lambda_{k^*}}\right)\right) \overset{a.s.}{\longrightarrow} 0.
$$

Hence, if $\min\{\tau_0, \tau\} < 1/2$, $\hat{\lambda}_{k,\text{out}}^2 \overset{a.s.}{\longrightarrow} \infty$, and if $\min\{\tau_0, \tau\} > 1/2$, $\hat{\lambda}_{k,\text{out}}^2 \overset{a.s.}{\longrightarrow} 0$. This completes the proof for fixed $\beta, \theta$. 


Proof of Theorem 3.4ii. When $\tau_0 = 0$, the proof follows from 3.1. So, set $\tau_0 > 0$. Let $\theta$ be a vector with $||\theta|| \leq 1$ and $\beta \sim N(0, \frac{\sigma_g^2}{p} I_p)$. As shown in the proof of Theorem 3.4, $\frac{1}{n} T_2 = O_P(1)$ and $\mathbb{P}(T_2 \geq \sigma_g^2) \to 1$. By (6.8), it is enough to show $\frac{1}{np} T_3$ is stochastically bounded away from 0, where $T_3$ is defined by,

$$T_3 := A^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \mathbb{W} \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) A.$$

We can upper bound the conditional variance of $T_3$ using (6.12) as,

$$\text{Var} \left( \frac{T_3}{np} \mathbb{W} \right) \leq \frac{2\sigma_g^4}{p^2} \sum_{j=k^*+1}^{n/p} \hat{\lambda}_j^2 + \frac{4\sigma_g^2 n}{p^2} \sum_{j=k^*+1}^{n/p} \hat{\lambda}_j^2 \theta^T \tilde{v}_j \tilde{v}_j^T \theta.$$

Using $\hat{\lambda}_{k^*+1} = O_P(1)$ by [Cai et al., 2020, Theorem 2.5] and noting that $\theta \in C_\tau(S_{V_k})$ with $\tau > 0$, we obtain $\text{Var} \left( \frac{T_3}{np} \mathbb{W} \right) \rightarrow 0$. For the conditional mean, we invoke (6.9) and (6.10) to obtain $\mathbb{E}(\frac{T_3}{np} \mathbb{W}) \geq (1 - o_P(1)) \sigma_g^2 \hat{\lambda}_{n,p}$, which is stochastically bounded away from 0 by Baik and Silverstein [2006], yielding our claim.

If $\theta \sim N(0, \frac{\sigma_g^2}{p} I_p)$, it is enough to analyze $T_3$ defined by (6.7) where $A \mathbb{W} \sim N(0, \frac{\sigma_g^2}{p} \mathbb{W} \mathbb{W}^T + \sigma_g^2 I_p)$.

To this end, note that,

$$\mathbb{E} \left( \frac{T_3}{np} \mathbb{W} \right) = \frac{1}{np} \text{tr} \left[ \left( \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \mathbb{W} \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \right) \left( \frac{\sigma_g^2}{p} \mathbb{W} \mathbb{W}^T + \sigma_g^2 I_p \right) \right]$$

$$= \frac{\sigma_g^2}{np} \sum_{j=k^*+1}^{n/p} d_j^4 + \frac{\sigma_g^2}{np} \sum_{j=k^*+1}^{n/p} d_j^2 = O_P(1).$$

The conditional variance is,

$$\text{Var} \left( \frac{T_3}{np} \mathbb{W} \right) = \frac{1}{n^2 p^2} \text{tr} \left[ \left( \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \mathbb{W} \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \right) \left( \frac{\sigma_g^2}{p} \mathbb{W} \mathbb{W}^T + \sigma_g^2 I_p \right) \right]^2$$

$$\text{a.s.} \rightarrow 0,$$

since $\sum_{j=k^*+1}^{n/p} \hat{\lambda}_j^2 = o_P(n^2 p^4)$ by Lemma 7.4, concluding the proof.

Proof of Theorem 3.4iii. We analyze $\hat{k}_{k,out}^2$ under $\theta \sim N(0, \frac{\sigma_g^2}{p} I_p)$. For the denominator of $\hat{k}_{k,out}^2$, using (6.19), $\text{Var}(\frac{1}{n} D_2 \mathbb{W}) = o_P(1)$ since $||\theta||^2 = O_P(1)$ by law of large numbers. Similar bounds hold for $D_1$ yielding $T_2$ has similar behavior as the case of fixed $\theta$. Here, first consider $\beta$ be a fixed vector with $||\beta|| \leq 1$. We have shown before, $\beta^T \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \eta / \sqrt{n} \overset{P}{\to} 0$, so it enough to analyze $T_{11} = \beta^T \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \mathbb{W} \theta$. Defining $T_4 := \beta^T \left( \mathbb{W}^T \left( I - P_{C(W\tilde{\nu}_{k,out})} \right) \mathbb{W} \right)^2 \beta$, we have

$$\frac{T_{11}/\sqrt{n}}{\sqrt{T_4/np}} \Rightarrow N(0, \sigma_g^2).$$

Now,

$$\frac{T_4}{np} \leq (1 + o_P(1)) \frac{1}{\gamma} \hat{\lambda}_{k^*+1} \sum_{j=k^*+1}^{n/p} (\tilde{v}_j, \beta)^2 \overset{\text{a.s.}}{\rightarrow} 0,$$

using (6.23) for any $\tau_0 > 0$. This completes the proof of the Theorem.
6.5. Proof of Proposition 3.5. Recall that, if \( \tau_1 > \tau_2 \), \( C_{\tau_1}(SV_{k^*}) \subseteq C_{\tau_2}(SV_{k^*}) \). Hence,

\[
\sup_{\beta \in C_{0.25}(SV_{k^*})} \hat{\kappa}_{k,\text{out}}^2 \leq \sup_{\beta \in C_{0}(SV_{k^*})} \hat{\kappa}_{k,\text{out}}^2.
\]

Since the asymptotic distribution of LR_{k,\text{out}} is stochastically increasing function in \( \hat{\kappa}_{k,\text{out}}^2 \), it is enough to show \( C_{0.25}(SV_{k^*}) \) is stochastically bounded away from 0 as \( n \to \infty \). To this end, note that the conclusion is immediate via Theorem 3.4 for all the cases except when \( \theta \sim N(0, \frac{\sigma^2}{p} I_p) \) and \( \beta \) is a fixed vector. So, we will only consider that scenario. Here, \( A|W \sim N(0, \frac{\sigma^2}{p} WW^T + \sigma^2 I_p) \).

Since \( \gamma < 1 \), assume \( p < n \). As before, the denominator is \( O_p(n) \). For the numerator, it is enough to analyze the quantity \( T_3/n \) where

\[
T_3 = \beta^T WW^T \left( I - P_{C(WV_{k^*,\text{out}})} \right) \left( \frac{\sigma^2}{p} WW^T + \sigma^2 I_p \right) \left( I - P_{C(WV_{k^*,\text{out}})} \right) W/\beta.
\]

Note that,

\[
\frac{T_3}{n} = \frac{p \sigma^2}{n} \sum_{j=k^*+1}^p \hat{\lambda}_j^2 (\hat{v}_j, \beta)^2 + \sigma^2 \sum_{j=k^*+1}^p \lambda_j (\hat{v}_j, \beta)^2
\geq \left( \frac{p \sigma^2}{n} \hat{\lambda}_p^2 + \sigma^2 \hat{\lambda}_p \right) (||\beta||^2 - \sum_{j=1}^{k^*} (\beta, v_j)^2 + O_p(1/\lambda_1)).
\]

By Baik and Silverstein [2006], \( \hat{\lambda}_p^2 \) is stochastically bounded away from 0. Pick \( \beta \) such that \( ||\beta||^2 = 1 \) and \( P_{SV_{k^*}}(\beta) = 0 \), implying \( T_3/n \overset{a.s.}{\to} C_1 > 0 \), for some \( C_1 > 0 \), yielding the conclusion.

6.6. Proof of Proposition 3.6. Since \( \gamma < 1 \) we have that \( p < n \). Note that the size of the test LR_{k^*,\text{out}} can be lower bounded through the specific instance where \( A \perp W \) and has mean 0. We now analyze \( \hat{\kappa}_{k^*,\text{out}} \) in this regime. As noted in the proof of Theorem 3.2, the denominator of \( \hat{\kappa}_{k^*,\text{out}} \) satisfies \( A^T (I - P_{C(WV_{k^*,\text{out}})}) A \leq c n \) with high probability for some constant \( c > 0 \). We have the numerator of \( \hat{\kappa}_{k^*,\text{out}} \) as

\[
T_1 = A^T (I - P_{C(WV_{k^*,\text{out}})}) W/\beta A^T WW^T (I - P_{C(WV_{k^*,\text{out}})}) A
\]

The mean and variance of \( T_1 \) can bounded as in the proof of Theorem 3.2, and by Paley-Zygmund Inequality one has,

\[
P(T_1 \geq \zeta E(T_1|W)|W) \geq \zeta
\]

Recall that, \( \beta^T WW^T (I - P_{C(WV_{k^*,\text{out}})}) W/\beta = n \sum_{j=k^*+1}^p \hat{\lambda}_j^2 (\beta, \hat{v}_j)^2 \). Also, if \( \min\{\tau_0, \tau\} < 1/2 \), using (6.21) and (6.22), \( \sup_{\beta \in C_{\tau}(SV_{k^*})} n \hat{\lambda}_p (||\beta||^2 - \sum_{j=1}^{k^*} (\beta, v_j)^2) \overset{a.s.}{\to} \infty \). This proves the desired result.

Finally, when \( \beta \) is random effects, the proof of Theorem 3.2 ii follows noting

\[
\frac{1}{n} E\left( \beta^T WW^T (I - P_{C(WV_{k^*,\text{out}})}) W/\beta \right) = \frac{\sigma^2}{p} \sum_{j=k^*+1}^{n/p} \hat{\lambda}_j \geq \frac{\sigma^2}{p} \hat{\lambda}_p = \Omega_p(1),
\]

yielding the desired conclusion.

6.7. Proof of Theorem 3.7.
Proof of 3.7i. Recall that, $X_i = [A_i, W_i] \sim N(0, I + \lambda vv^\top)$. Writing $A_i = W_i^T \theta + \eta$, we obtain that $\theta = (I + \lambda v_{-1}v_{-1}^\top)^{-1} \lambda_1 v(1)v_{-1}$, where $v = (v(1), v_{-1})$. By the Sherman-Morrison formula, we obtain

$$\theta = \frac{\lambda v(1)}{1 + \lambda \|v_{-1}\|^2} v_{-1}. \quad (6.25)$$

So, $\|\theta\| = \Theta(\frac{1}{\sqrt{n}})$ by our assumption of delocalization. Thereafter, with $k = 1$, as before we consider the asymptotic behavior of $\hat{k}_{1, in}^2 = \frac{T_2}{T_2} n$ with $T_1 = A^T(I - P_{C(WV_{1, i})})W^\top \beta$ and $T_2 = A^T(I - P_{C(WV_{1, i})})A$. Then we claim that $T_2 = \Omega_F(n)$. To see this, we write $T_2 = \theta_0^T X^T(I - P_{C(WV_{1, i})})X \beta_0 + 2 \eta^T(I - P_{C(WV_{1, i})})X \beta_0 + \eta^T(I - P_{C(WV_{1, i})})\eta$ where $\theta_0 = I_1 \theta$ with $I_1 = [e_2; \ldots; e_{p+1}]$. It is easy to see that the first term in the expansion is non-negative and the last term is $\Omega_F(n)$. Therefore, it is enough to show that the second summand is $o_F(1)$. To that end note that this term divided by $n$ has mean 0 conditional on $X$ and has conditional variance $\frac{1}{n^2} \times n \times \lambda_2^2 \|\theta_0\|^2 = o_F(1)$ by Cai et al. [2020]. Therefore the $o_F(n)$ nature of the second term follows by Dominated Convergence Theorem. Thereafter, to conclude to the proof of this part of the theorem we claim that $T_1/\sqrt{n} = o_F(1)$. To that end note that $T_1 = \theta_0^T X^T(I - P_{C(WV_{1, i})})X \beta_0 + \eta^T(I - P_{C(WV_{1, i})})\eta$ where $\theta_0 = I_1 \theta$ and $\beta_0 = I_1 \beta$ with $I_1 = [e_2; \ldots; e_{p+1}]$. The second term in the expression for $T_1$ divided by $\sqrt{n}$ has mean 0 conditional on $X$ and has conditional variance $\sum_{j=2}^{n} \lambda_j^2 \|\beta_j\|^2 \leq \lambda_2^2 \|\beta\|^2 o_F(p^{-\tau_0}) = o_F(1)$ by Cai et al. [2020]. Hence this term is $o_F(1)$ by Dominated Convergence Theorem. Focusing on the first summand of $T_1$, we have by writing $\beta = c^* v$ for $|c^*| \leq M$ we note that this term divided by $\sqrt{n}$ can be bounded by $\sqrt{n} \lambda_2^2 C^* O(\|\theta_0\|) O_F(p^{-\tau_0}) = o_F(p^{-\tau_0}) = o_F(1)$ since $\|\theta_0\| = \|\theta\| = O(1/\sqrt{p}) = O(1/\sqrt{n})$. The proof follows.

Proof of 3.7ii. Let $\beta \sim (0, \frac{\sigma_2^2}{p} I_p)$. Recall that, by (6.25), $\theta = \frac{\lambda v(1)}{1 + \lambda \|v_{-1}\|^2} v_{-1}$. We again consider the asymptotic behavior of $\hat{k}_{1, in}^2 = \frac{T_2}{T_2} n$. Note that,

$$\frac{T_2}{n} = \frac{1}{n} e^T X^T(I - P_{C(WV_{1, i})})X e_1 \leq \hat{\lambda}_2 = O_F(1),$$

by Cai et al. [2020]. To understand the behavior of the numerator, note that, $T_1 = \theta_0^T X^T(I - P_{C(WV_{1, i})})X \beta_0 + \eta^T(I - P_{C(WV_{1, i})})X \beta_0$. Now, conditional on $X$,

$$\frac{1}{\sqrt{n}} \theta_0^T X^T(I - P_{C(WV_{1, i})})X \beta_0 \sim N\left(0, \frac{1}{np} \theta_0^T X^T(I - P_{C(WV_{1, i})})X (I - e_1 e_1^T) X^T(I - P_{C(WV_{1, i})})X \theta_0 \right)$$

The variance above can be upper bounded by $\frac{1}{np} \theta_0^T X^T(I - P_{C(WV_{1, i})})X)^2 \theta_0 \leq \hat{\lambda}_2^2 \|\theta_0\|^2 = o_F(1)$. Moreover, conditional on $X, \beta$,

$$\frac{1}{\sqrt{n}} \eta^T(I - P_{C(WV_{1, i})})X \beta_0 \sim N\left(0, \frac{1}{n} \beta_0^T X^T(I - P_{C(WV_{1, i})})X \beta_0 \right).$$

Denoting the variance above by $T_4$, note that $\mathbb{E}(T_4 | X) = \frac{1}{np} \text{Tr}(X^T(I - P_{C(WV_{1, i})})X) \geq C_1$ a.s., for some $C_1 > 0$. Now $\text{Var}(T_4 | X) = \frac{1}{np^2} \sum_{j=2}^{np} \beta_j^2 = o_F(1)$. Hence, $\frac{T_4}{\sqrt{n}} = o_F(1)$, yielding the conclusion.
7. Technical Lemmas:

**Lemma 7.1.** Under Model 2.1 one has that

\[
\text{LR}_{k,\text{out}} | \mathbf{A}, \mathcal{W} \sim \chi^2(k_{k,\text{out}}^2), \quad \hat{k}_{k,\text{out}}^2 = \frac{\left( (\beta^T \mathcal{W}^T + \mathbf{A}^T \mathbf{A} \delta) \left( I - P_{C(\mathcal{W} \text{out})} \right) \mathbf{A} \right)^2}{\mathbf{A}^T \left( I - P_{C(\mathcal{W} \text{out})} \right) \mathbf{A}}.
\]

Similarly,

\[
\text{LR}_{k,\text{in}} | \mathcal{X} \sim \chi^2(k_{k,\text{in}}^2), \quad \hat{k}_{k,\text{in}}^2 = \frac{\left( (\beta^T \mathcal{W}^T + \mathbf{A}^T \mathbf{A} \delta) \left( I - P_{C(\mathcal{X} \text{in})} \right) \mathbf{A} \right)^2}{\mathbf{A}^T \left( I - P_{C(\mathcal{X} \text{in})} \right) \mathbf{A}}.
\]

**Proof.** The proof follows by standard calculations and Fisher-Cochran Theorems and hence is omitted.

**Lemma 7.2.** Let \( s_1 \) and \( s_2 \) be (a sequence of) \( p \times 1 \) non-random vectors with uniformly bounded norms. \( \tilde{\mathcal{X}} \sim \text{GSp} \left( \{ (\lambda_j, v_j) \}^k_1 ; \Gamma_H ; n, d \right) \). Suppose \( \hat{\Sigma} = \frac{1}{n} \tilde{\mathcal{X}} \tilde{\mathcal{X}} \) has spectral decomposition \( \hat{\Sigma} = \sum_{j=1}^{n/p} \hat{\lambda}_j \hat{v}_j \hat{v}_j^T \). For \( \alpha \notin \Gamma_H, \alpha \neq 0 \), let us define the function,

\[
\psi(\alpha) = \alpha \left( 1 + \gamma \int_{\Gamma_H} \frac{\lambda d\mathcal{H}(\lambda)}{\alpha - \lambda} \right),
\]

and the first derivative is denoted by \( \psi'(\alpha) \). Then the following hold under Assumption 2.6(a).

(i) [For Generalized Spikes]

\[
\left| \hat{\lambda}_j s_1^T \hat{v}_j \hat{v}_j^T s_2 - \xi_{rj} s_1^T v_j v_j^T s_2 \right| \overset{a.s.}{\longrightarrow} 0, \quad r = 1, 2, \text{ and } j = 1, \ldots, k^*,
\]

where,

\[
\xi_{rj} = \lambda_j \psi(\lambda_j) r^{-1} \psi'(\lambda_j).
\]

(ii) [For Non-Spikes]

\[
\left| \sum_{j=k^*+1}^{p} \hat{\lambda}_j s_1^T \hat{v}_j \hat{v}_j^T s_2 - \sum_{j=1}^{p} \phi_{rj} s_1^T v_j v_j^T s_2 \right| \overset{a.s.}{\longrightarrow} 0, \quad r = 1, 2,
\]

where,

\[
\phi_{1j} = \begin{cases} 
\lambda_j [1 - \psi'(\lambda_j)], & j = 1, \ldots, k^* \\
\lambda_j, & j = k^* + 1, \ldots, p,
\end{cases}
\]

\[
\phi_{2j} = \begin{cases} 
\gamma \lambda_j \int_{\Gamma_H} \frac{\lambda d\mathcal{H}(\lambda)}{(\lambda_j - \lambda)^2} + [\psi(\lambda_j) - \lambda_j] [1 - \psi'(\lambda_j)], & j = 1, \ldots, k^* \\
\lambda_j^2 + \gamma \lambda_j \int_{\Gamma_H} \lambda d\mathcal{H}(\lambda), & j = k^* + 1, \ldots, p.
\end{cases}
\]

**Proof.** To derive the results, we analyze the following bi-linear forms,

\[
\hat{m}_{\mathcal{P}}(z) = s_1^T \left( \hat{\Sigma} - z I \right)^{-1} s_2 = \sum_{j=1}^{p} s_1^T \hat{v}_j \hat{v}_j^T s_2, \quad \forall z \in \mathbb{C}^+.
\]

Throughout the proof of Lemma 7.2 and 7.4, let us further denote the unique eigenvalues and corresponding eigenspaces of \( \Sigma_p \) by \( \lambda_1 > \lambda_2 > \ldots > \lambda_p \) and \( \hat{V}_1, \ldots, \hat{V}_p \). Assume \( M_j \) to be the multiplicity of \( \lambda_j \), \( M_j = 1 \) for \( j = 1, \ldots, k^* \), and thus the dimension of the eigenspace matrix (vector) \( \hat{V}_j \) is given by \( p \times M_j \). This change of notation was done to accommodate non-spikes having multiplicities more than one. Then, Mestre [2006] provides the following result,
Lemma 7.3. Suppose $\hat{X} \sim \text{GSp}(\{(\lambda_j, v_j)\}_{j=1}^{k^*}; \Gamma_H; n, d)$ and $\hat{\Sigma} = \frac{1}{n} \hat{X}^\top \hat{X}$ has spectral decomposition $\hat{\Sigma} = \sum_{j=1}^{n\wedge p} \hat{\lambda}_j \hat{v}_j \hat{v}_j^\top$. The following holds under Assumption 2.6(a),

$$|\hat{m}_p(z) - m_p(z)| \xrightarrow{a.s.} 0; \quad \forall z \in \mathbb{C}^+,$$

(7.1)

where,

$$\hat{m}_p(z) = s_1^\top \left(\hat{\Sigma} - z I\right)^{-1} s_2 = \sum_{j=1}^{p} \frac{s_1^\top \hat{v}_j \hat{v}_j^\top s_2}{\hat{\lambda}_j - z}; \quad \forall z \in \mathbb{C}^+,$$

and

$$m_p(z) = s_1^\top (w(z)\Sigma - z I)^{-1} s_2 = \sum_{j=1}^{p} \frac{s_1^\top \bar{V}_j \bar{V}_j^\top s_2}{\lambda_j w(z) - z}; \quad \forall z \in \mathbb{C}^+.$$

The function $w(z) = 1 - \gamma - \gamma z b_F(z)$, where for all $z \in \mathbb{C}^+$, $b_F(z) = b$ is the unique solution to the equation,

$$b = \frac{1}{p} \sum_{j=1}^{p} \frac{M_j}{\lambda_j (1 - \gamma - \gamma z b) - z}$$

in the set $\{b \in \mathbb{C} : \gamma b - (1 - \gamma)/z \in \mathbb{C}^+\}$.

The domain for $z \in \mathbb{C}^+$ can be extended to $\mathbb{C}^-$ for the functions $\hat{m}_p, m_p, b_F$ by defining $\hat{m}_p(z) = \hat{m}_p^*(z^*)$, $m_p(z) = m_p^*(z^*)$, $b_F(z) = b_F^*(z^*)$ for $z \in \mathbb{C}^-$. Here, $(\cdot)^*$ represents the complex-conjugate. It is easy to see that Result 7.3 is also satisfied when $z \in \mathbb{C}^-$. Let us further define $f(z) = z/w(z)$ for $z \in \mathbb{C} \setminus \mathbb{R}$. Then, using Result 7.3, we can derive the following fixed point equation,

$$z = f(z) \left(1 - \gamma \sum_{j=1}^{p} \frac{M_j \bar{\lambda}_j}{\lambda_j - f(z)}\right).$$

We can further extend this definition to the entire $\mathbb{C}$ by allowing $b(z) = \lim_{y \to 0} z + iy$ for $z \in \mathbb{R} \setminus \{0\}$ (the existence of such limits is shown in Silverstein and Choi [1995]), and defining $f(0) = 0$ for $\gamma \leq 1$ and $f(0) = f_0$ for $\gamma > 1$, where $f_0$ is the unique negative solution to the equation

$$1 + \gamma \sum_{j=1}^{p} \frac{M_j \bar{\lambda}_j}{f_0 - \lambda_j} = 0.$$

The following lemma then provides the convergence of integrals of $\hat{m}_p$ over different contours.

Lemma 7.4. Suppose $\hat{X} \sim \text{GSp}(\{(\lambda_j, v_j)\}_{j=1}^{k^*}; \Gamma_H; n, d)$ and $\hat{\Sigma} = \frac{1}{n} \hat{X}^\top \hat{X}$ has spectral decomposition $\hat{\Sigma} = \sum_{j=1}^{n\wedge p} \hat{\lambda}_j \hat{v}_j \hat{v}_j^\top$. The following holds under Assumption 2.6(a),

$$\left|\frac{1}{2\pi i} \oint_{\partial \hat{S}_y(\hat{\mathcal{L}}_j)} z^r \hat{m}_p(z) dz - \frac{1}{2\pi i} \oint_{\partial S_y(L_j)} z^r m_p(z) dz\right| \xrightarrow{a.s.} 0,$$

(7.2)

for $r = 0, 1, 2$, and $j = 1, \ldots, k^*, \tilde{p}$. The contours $\partial \hat{S}_y(\hat{\mathcal{L}}_j)$ and $\partial S_y(L_j)$ are negatively oriented boundaries of the rectangles $\hat{S}_y(\hat{\mathcal{L}}_j)$ and $S_y(L_j)$ of width $y > 0$ (across imaginary axis) defined by,

$$\hat{S}_y(\hat{\mathcal{L}}_j) = \{z \in \mathbb{C} : \hat{a}_1(j) \leq \text{Re}(z) \leq \hat{a}_2(j), |\text{Im}(z)| \leq y\}, \quad \hat{\mathcal{L}}_j = \left\{\{\hat{\lambda}_j\}, \quad j = 1, \ldots, k^* \right\}$$

$$\{\hat{\lambda}_{k^*+1}, \ldots, \hat{\lambda}_{p}\}, \quad j = \tilde{p}$$

$$S_y(L_j) = \{z \in \mathbb{C} : a_1(j) \leq \text{Re}(z) \leq a_2(j), |\text{Im}(z)| \leq y\}, \quad \mathcal{L}_j = \left\{\{\psi(\bar{\lambda}_j)\}, \quad j = 1, \ldots, k^* \right\},$$

$$\{\Gamma_F, \quad j = \tilde{p} \right\}.$$
where $\Gamma_F$ is the support of the LSD $F$ of the sample eigenvalues $\hat{\lambda}_1, \ldots, \hat{\lambda}_p$. The interval $[\hat{a}_1(j), \hat{a}_2(j)]$ is chosen such that $\hat{L}_j \subset [\hat{a}_1(j), \hat{a}_2(j)]$ and $\hat{L}_j' \cap [\hat{a}_1(j), \hat{a}_2(j)] = \emptyset$ for $j' \in \{1, \ldots, k^*, \bar{p}\}, j' \neq j$. Similarly, the interval $[a_1(j), a_2(j)]$ is chosen such that $L_j \subset [a_1(j), a_2(j)]$ and $L_j' \cap [a_1(j), a_2(j)] = \emptyset$ for $j' \in \{1, \ldots, k^*, \bar{p}\}, j' \neq j$.

**Remark 6.** The ESD of the sample covariance matrix converges weakly to the Marčenko-Pastur distribution [Bai and Yao, 2012, Marčenko and Pastur, 1967], and therefore $F$ can be considered as the Marčenko-Pastur distribution as well. Since traditionally, Marčenko-Pastur distribution is defined for the traditional spiked model where $\lambda_{k^*-1} = \ldots = \lambda_p = 1$, for the generalized spiked model, we can call this distribution the “Generalized Marčenko-Pastur” distribution.

**Remark 7.** The choices for intervals $[a_1(j), a_2(j)]$ exist due to the exact separation of eigenvalue clusters as described in Propositions 3.1 and 3.2 in Bai and Yao [2012].

**Remark 8.** We have only derived results in this paper based on the assumption that all the generalized spikes are distant spikes, and larger than $\text{sup} \Gamma_H$. However, other scenarios such as the existence of close spikes, or spikes smaller than $\text{sup} \Gamma_H$ can also be accommodated by manipulating the definitions of the sets $\hat{L}_j$ and $L_j$. For example, if $\lambda_j$-s are distant spikes for $j = 1, \ldots, k_1$ and close spikes for $j = k_1 + 1, \ldots, k_2$, then the definitions of $L_j$ and $\hat{L}_j$ will remain the same as defined in Lemma 7.4 with $k^* = k_1$, which is equivalent to treating the close spikes as non-spikes.

Thereafter, we note that,

$$
\frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} z^r \hat{m}_p(z) dz = \begin{cases}
\hat{\lambda}_1^ts_1^\top \hat{v}_t \hat{v}_t^\top s_2, & t = 1, \ldots, k^*
\sum_{j=k^*+1}^{\bar{p}} \hat{\lambda}_j^ts_1^\top \hat{v}_j \hat{v}_j^\top s_2, & t = \bar{p}.
\end{cases}
$$

Therefore, in order to complete the proof of the lemma, we need to find

$$
\frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} z^r m_p(z) dz = \frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} \sum_{j=1}^{\bar{p}} z^r s_1^\top \hat{V}_j \hat{V}_j^\top s_2 dz
\begin{align*}
= & \sum_{j=1}^{\bar{p}} g(\bar{\lambda}_j, \partial S_y^-(L_t), r) s_1^\top \hat{V}_j \hat{V}_j^\top s_2,
\end{align*}
$$

where,

$$
g(\bar{\lambda}_j, \partial S_y^-(L_t), r) = \frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} \frac{z^r}{\bar{\lambda}_j w(z) - z} dz,
\begin{align*}
= & \frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} \frac{f(z)z^{r-1}}{\bar{\lambda}_j - f(z)} dz, & \text{(by replacing } w(z) = z/f(z)),
\end{align*}
\begin{align*}
= & \frac{1}{2\pi i} \oint_{\partial S_y^-(L_t)} \frac{f(z)}{\bar{\lambda}_j - f(z)} \left\{ f(z) \left( 1 - \frac{\sum_{q=1}^{\bar{p}} M_q \bar{\lambda}_q}{\bar{\lambda}_q - f(z)} \right) \right\}^{r-1} \frac{1}{\bar{\lambda}_j - f(z)} dz
\begin{align*}
= & \frac{1}{2\pi i} \oint_{f(\partial S_y^-(L_t))} f \left\{ f \left( 1 - \frac{\sum_{q=1}^{\bar{p}} M_q \bar{\lambda}_q}{\bar{\lambda}_q - f} \right) \right\}^{r-1} \left\{ 1 - \frac{\sum_{q=1}^{\bar{p}} M_q \left( \bar{\lambda}_q - \frac{1}{\bar{\lambda}_q - f} \right)^2 }{\bar{\lambda}_j - f} \right\} df.
\end{align*}
$$

To compute the integral, we have employed a change of variable from $z$ to $f$, and the contour on which the integration is to be performed has been changed from $\partial S_y^-(L_t)$ to $f(\partial S_y^-(L_t))$. The justification behind using the $f(\partial S_y^-(L_t))$ as an integration contour is given in Mestre [2008] Appendix III.

For the rest of the proof, we refrain from mentioning $L_t$ in $S_y(L_t)$ where it is obvious for brevity of notations. We compute this integral using residue theorem case by case.
Case 1: \( r = 1 \): 

\[
g(\lambda_j, \partial S_y^-, 1) = \frac{1}{2\pi i} \oint_{f(\partial S_y^-)} \frac{f}{\lambda_j - f} \left\{ 1 - \frac{\gamma}{p} \sum_{q=1}^{\bar{p}} M_q \left( \frac{\lambda_q}{\lambda_j - \lambda_q} \right)^2 \right\} df.
\]

The integrand here has poles at each \( \lambda_q \) for \( q = 1, \ldots, \bar{p} \). The multiplicity of each pole is two if \( q \neq j \), and three if \( q = j \). Therefore, the complex residues at these poles are,

\[
\text{Res} \left( g(\lambda_j, \partial S_y^-, 1), \lambda_q \right) = \begin{cases} 
\frac{\gamma \lambda_j M_q}{p} \left( \frac{\lambda_q}{\lambda_j - \lambda_q} \right)^2, & q \neq j, \\
\lambda_j \left[ 1 - \frac{2}{p} \sum_{l \neq j} M_l \left( \frac{\lambda_l}{\lambda_j - \lambda_l} \right)^2 \right], & q = j.
\end{cases}
\]

Case 1a: For \( t = 1, \ldots, k^* \): the contour \( f(\partial S_y^-) \) only surrounds the eigenvalue \( \lambda_t \) and no other eigenvalue. Therefore, using the residue theorem,

\[
g(\lambda_j, \partial S_y^-, 1) = \begin{cases} 
\frac{\gamma \lambda_j M_t}{p} \left( \frac{\lambda_t}{\lambda_j - \lambda_t} \right)^2, & t \neq j, \\
\lambda_j \left[ 1 - \frac{2}{p} \sum_{l \neq j} M_l \left( \frac{\lambda_l}{\lambda_j - \lambda_l} \right)^2 \right], & t = j.
\end{cases}
\]

The limit of the integral when \( p \to \infty \),

\[
\lim_{p \to \infty} g(\lambda_j, \partial S_y^-, 1) = \begin{cases} 
0, & t \neq j \\
\lambda_j \psi'(\lambda_j), & t = j.
\end{cases}
\]

Case 1b: For \( t = \bar{p} \): the contour \( f(\partial S_y^-) \) surrounds all the non-spikes \( \lambda_{k^*+1}, \ldots, \lambda_{\bar{p}} \). Therefore, using the residue theorem,

\[
g(\lambda_j, \partial S_y^-, 1) = \begin{cases} 
\frac{\gamma \lambda_j M_t}{p} \left( \frac{\lambda_t}{\lambda_j - \lambda_t} \right)^2, & j = 1, \ldots, k^* \\
\lambda_j \left[ 1 - \frac{2}{p} \sum_{q=1}^{k^*} M_q \left( \frac{\lambda_q}{\lambda_j - \lambda_q} \right)^2 \right], & j = k^* + 1, \ldots, \bar{p}.
\end{cases}
\]

The limit of the integral when \( p \to \infty \),

\[
\lim_{p \to \infty} g(\lambda_j, \partial S_y^-, 1) = \begin{cases} 
\gamma \lambda_j \int_{\Gamma_h} \left( \frac{\lambda}{\lambda_j - \lambda} \right)^2 dH(\lambda), & j = 1, \ldots, k^* \\
\lambda_j, & j = k^* + 1, \ldots, \bar{p}.
\end{cases}
\]

Case 2: \( r = 2 \):

\[
g(\lambda_j, \partial S_y^-, 2) = \frac{1}{2\pi i} \oint_{f(\partial S_y^-)} \frac{f^2}{\lambda_j - f} \left\{ 1 - \frac{\gamma}{p} \sum_{q=1}^{\bar{p}} M_q \lambda_q \right\} \left\{ 1 - \frac{\gamma}{p} \sum_{q=1}^{\bar{p}} M_q \left( \frac{\lambda_q}{\lambda_j - \lambda_q} \right)^2 \right\} df.
\]

The integrand has poles at each \( \lambda_q \) for \( q = 1, \ldots, \bar{p} \). The multiplicity of each pole is three if \( q \neq j \), and four if \( q = j \). Therefore, the complex residues at these poles are,

\[
\text{Res} \left( g(\lambda_j, \partial S_y^-, 2), \lambda_q \right) = \begin{cases} 
\frac{\gamma}{p} \frac{\lambda_j M_q \lambda_q^2}{(\lambda_j - \lambda_q)^2} \left[ 1 + \frac{\gamma}{p} \sum_{l=1}^{\bar{p}} M_l \lambda_l \lambda_q (\lambda_l - \lambda_q) \right], & q \neq j, \\
\lambda_j^2 \left[ 1 + \frac{\gamma}{p} \sum_{l=1}^{\bar{p}} M_l \lambda_l^2 (\lambda_l - \lambda_j)^2 \right] + \left( 1 + \frac{2}{p} \sum_{l \neq j} M_l \lambda_l \lambda_j (\lambda_j - \lambda_l)^2 \right) \left( 1 - \frac{2}{p} \sum_{l \neq j} M_l \lambda_l^2 \lambda_j (\lambda_j - \lambda_l)^2 \right), & q = j.
\end{cases}
\]
Case 2a: For \( t = 1, \ldots, k^* \): the contour \( f(\partial S_y^-) \) only surrounds the eigenvalue \( \lambda_t \) and no other eigenvalue. Therefore, using the residue theorem,

\[
g(\lambda_j, \partial S_y^-, 2) = \begin{cases} \frac{\gamma \bar{\lambda}_j M_q \lambda_j^3}{p(\lambda_j - \lambda_q)^2} \left[ 1 + \frac{\gamma \bar{\lambda}_j M_q \lambda_j^3}{p(\lambda_j - \lambda_q)^2} \right] & t \neq j, \\ \frac{\gamma M_j^3}{p} \left( 1 + \frac{\gamma M_j^3}{p} \sum_{q=1}^{p} \frac{M_j \lambda_j}{(\lambda_j - \lambda_q)^2} \right) \left( 1 - \frac{\gamma M_j^3}{p} \sum_{q=1}^{p} \frac{M_j \lambda_j}{(\lambda_j - \lambda_q)^2} \right) & t = j. \end{cases}
\]

The limit of the integral when \( p \to \infty \),

\[
\lim_{p \to \infty} g(\lambda_j, \partial S_y^-, 2) = \begin{cases} 0, & t \neq j \\ \lambda_j \psi(\lambda_j) \psi'(\lambda_j), & t = j. \end{cases}
\]

Case 2b: For \( t = \tilde{p} \): the contour \( f(\partial S_y^-) \) surrounds all the non-spikes \( \lambda_{k^*+1}, \ldots, \lambda_{\tilde{p}} \). Therefore, we first calculate the function \( g(\lambda_j, \partial S_y^-, 2) \) for \( j = 1, \ldots, k^* \) using the residue theorem,

\[
g(\lambda_j, \partial S_y^-, 2) = \sum_{q=k^*+1}^{p} \frac{\gamma \bar{\lambda}_j M_q \lambda_j^3}{p(\lambda_j - \lambda_q)^2} \left[ 1 + \frac{\gamma \bar{\lambda}_j M_q \lambda_j^3}{p(\lambda_j - \lambda_q)^2} \right] + \frac{\gamma M_j^3}{p} \sum_{q=1}^{p} \frac{M_j \lambda_j}{(\lambda_j - \lambda_q)^2} \sum_{q=1}^{p} \frac{M_j \lambda_j}{(\lambda_j - \lambda_q)^2}.
\]

Now, for any pair of indices \( q \) and \( l \) such that \( l \neq q \), one can show through some algebraic manipulation,

\[
\frac{M_q \lambda_q^3 M_l \lambda_l}{(\lambda_j - \lambda_q)^2(\lambda_q - \lambda_l)} + \frac{M_l \lambda_l^3 M_q \lambda_q}{(\lambda_j - \lambda_l)^2(\lambda_l - \lambda_q)} = \frac{\bar{\lambda}_j M_q \lambda_q^3 M_l \lambda_l}{(\lambda_j - \lambda_q)^2(\lambda_q - \lambda_l)} + \frac{\bar{\lambda}_j M_l \lambda_l^3 M_q \lambda_q}{(\lambda_j - \lambda_l)^2(\lambda_l - \lambda_q)}.
\]

Therefore,

\[
g(\lambda_j, \partial S_y^-, 2) = \frac{\gamma \bar{\lambda}_j}{p} \sum_{q=k^*+1}^{p} \frac{M_q \lambda_q^3}{(\lambda_j - \lambda_q)^2} + \frac{\gamma^2 \lambda_j^2}{p^2} \sum_{q=k^*+1}^{p} \frac{M_q \lambda_q^3}{(\lambda_j - \lambda_q)^2} + \frac{\gamma^2 \lambda_j^2}{p^2} \sum_{q=1}^{p} \frac{M_q \lambda_q^3}{(\lambda_j - \lambda_q)^2} \sum_{q=1}^{p} \frac{M_q \lambda_q^3}{(\lambda_j - \lambda_q)^2}.
\]
The limit of the integral when $p \to \infty$,

$$
\lim_{p \to \infty} g(\lambda_j, \partial S_y^-, 2) = \gamma \lambda_j \int_{\Gamma_H} \frac{\lambda^3}{(\lambda_j - \lambda)^2} dH(\lambda) + \gamma^2 \lambda_j^2 \left[ \int_{\Gamma_H} \frac{\lambda}{\lambda_j - \lambda} dH(\lambda) \right] \left[ \int_{\Gamma_H} \left( \frac{\lambda}{\lambda_j - \lambda} \right)^2 dH(\lambda) \right].
$$

Next, we calculate the function $g(\lambda_j, \partial S_y^-, 2)$ for $j = k^* + 1, \ldots, p$ using the residue theorem,

$$
g(\lambda_j, \partial S_y^-, 2) = \sum_{q=k^*+1}^{p} \frac{\gamma \lambda_j M_q \lambda_q^3}{p(\lambda_j - \lambda_q)^2} \left[ \frac{1}{p} + \frac{\gamma \lambda_j M_q}{p(\lambda_j - \lambda_q)} + \frac{\gamma}{p} \sum_{l=q}^{p} \frac{M_l \lambda_l}{\lambda_q - \lambda_l} \right]
+ \lambda_j^2 \left[ \frac{\gamma M_j}{p} \left( 1 + \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q^3}{(\lambda_j - \lambda_q)^3} \right) + \left( 1 + \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q}{\lambda_j - \lambda_q} \right) \left( 1 - \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q^2}{(\lambda_j - \lambda_q)^2} \right) \right]
= \sum_{q=k^*+1}^{p} \frac{\gamma \lambda_j M_q \lambda_q^3}{p(\lambda_j - \lambda_q)^2} \sum_{q=1}^{p} \frac{M_q \lambda_q}{(\lambda_j - \lambda_q)^3} + \frac{\gamma^2 \lambda_j^2}{p} \sum_{q=k^*+1}^{p} \frac{M_q \lambda_q^2}{(\lambda_j - \lambda_q)^3} + \lambda_j^2 \left[ \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q}{\lambda_j - \lambda_q} - \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q^2}{(\lambda_j - \lambda_q)^2} \right]
- \lambda_j^2 \left( \frac{\gamma}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q}{(\lambda_j - \lambda_q)^2} \right)
$$

Terms 1, 7, 8 yield,

$$
\sum_{q=k^*+1}^{p} \frac{\gamma \lambda_j M_q \lambda_q^3}{p(\lambda_j - \lambda_q)^2} + \frac{\gamma \lambda_j^2}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q}{\lambda_j - \lambda_q} - \frac{\gamma \lambda_j^2}{p} \sum_{q=1}^{p} \frac{M_q \lambda_q^2}{(\lambda_j - \lambda_q)^2} = \frac{\gamma \lambda_j}{p} \sum_{q=1}^{p} M_q \lambda_q + O(1/p).
$$
Terms 2 and 3 yield,
\[
\sum_{q=k^*+1}^{p} \frac{\gamma^2 \lambda_j^2}{p^2} M_j^2 \lambda_q^3 + \frac{\gamma^2 \lambda_j}{p^2} \sum_{q=k^*+1}^{p} \sum_{l=q+1}^{p} \frac{M_q \lambda_j^3 M_l \lambda_l}{(\lambda_j - \lambda_q)^3} \lambda_l = \sum_{q=1}^{p} \frac{\gamma^2 \lambda_j^2}{p^2} M_j^2 \lambda_q^3 + \frac{\gamma^2 \lambda_j}{p^2} \sum_{q=k^*+1}^{p} \sum_{l=q+1}^{p} \frac{M_q \lambda_j^3 M_l \lambda_l}{(\lambda_j - \lambda_q)^3} \lambda_l + O(1/p)
\]

using similar algebraic manipulations as in Case 1. Therefore,
\[
g(\tilde{\lambda}_j, \partial S_y, 2) = \frac{\gamma^2 \lambda_j^2}{p} \left( 1 + \frac{\gamma \lambda_j}{p} \right) + \frac{\gamma \lambda_j}{p} \sum_{q=1}^{p} M_q \tilde{\lambda}_q + O(1/p)
\]

\[
= \frac{\gamma \lambda_j}{p} \sum_{q=1}^{p} M_q \tilde{\lambda}_q + O(1/p).
\]

The limit of the integral when \( p \to \infty \),
\[
\lim_{p \to \infty} g(\tilde{\lambda}_j, \partial S_y, 2) = \frac{\gamma \lambda_j}{p} \int_{\Gamma_H} \lambda dH(\lambda).
\]

And hence we have derived all the asymptotic quantities mentioned in Lemma 7.2. The final step of replacing the quantities \( g(\tilde{\lambda}_j, \partial S_y, r) \) with their corresponding limits follows from the dominated convergence theorem by noting that \( s_1, s_2 \) have uniformly bounded norms, and thus \( \sum_{j=1}^{p} \tilde{V}_j V_j^\top s_2 \) is bounded.

**Proof of Lemma 7.4.** First, we show that \( \tilde{a}_1(j), \tilde{a}_2(j), a_1(j), a_2(j) \) can be chosen to satisfy \( \tilde{a}_1(j) \to a_1(j) \) and \( \tilde{a}_2(j) \to a_2(j) \) for \( j = 1, \ldots, k^* \).

For \( j = 1, \ldots, k^* \), the eigenvalues \( \tilde{\lambda}_j \) are distant spikes. Thus, according to Theorem 4.1 of Bai and Yao [2012], \( \tilde{\lambda}_j \xrightarrow{a.s.} \psi(\lambda_j) \). Further, \( \psi(\lambda_j) \) is bounded away from \( \Gamma_F \), the support of the sample LSD, as well as from any other \( \psi(\lambda_{j'}) \) for \( j \in \{1, \ldots, k^*\}, j \neq j' \). Therefore, there exists an interval \( I \) such that for large enough \( p \) and \( n \), \( \{\tilde{\lambda}_j, \psi(\lambda_j)\} \subset I \) and \( I \cap L_{j'} = \emptyset \), \( I \cap L_{j'} = \emptyset \) for \( j' \in \{1, \ldots, k^* \}, j' \neq j \), with probability 1. We can then choose the intervals \( [\tilde{a}_1(j), \tilde{a}_2(j)], [a_1(j), a_2(j)] \subset I \) to satisfy the claim above. Further, we can choose the interval boundaries to also be bounded away from \( \Gamma_F = \Gamma_F \cup \{\psi(\lambda_1), \ldots, \psi(\lambda_{k^*})\} \).

For \( j = \tilde{p} \), the ESD of the sample eigenvalues corresponding to non-spikes converge to the sample LSD (or the generalized Marčenko-Pastur distribution) \( F \). Thus, there exists an interval \( I \) such that for large enough \( p \) and \( n \), \( \Gamma_H \subset I \), \( \{\tilde{\lambda}_{k^*+1}, \ldots, \tilde{\lambda}_{\tilde{p}}\} \subset I \) and \( I \cap L_j = \emptyset \), \( I \cap L_j = \emptyset \) for \( j \in \{1, \ldots, k^*\} \), with probability 1. We can then choose the intervals \( [\tilde{a}_1(j), \tilde{a}_2(j)], [a_1(j), a_2(j)] \subset I \) to satisfy the claim above. Further, we can choose the interval boundaries to also be bounded away from \( \Gamma_F \).
Then,
\[
\left| \frac{1}{2\pi i} \oint_{\partial S^+ L_j} z^r \hat{m}_p(z) \, dz - \frac{1}{2\pi i} \oint_{\partial S^- L_j} z^r m_p(z) \, dz \right| \\
\leq \frac{1}{2\pi} \left\{ \sup_{z \in \partial S^- L_j \cup \partial S^+ L_j} |z^r \hat{m}_p(z)| \right\} \left( |\hat{a}_1(j) - a_1(j)| + |\hat{a}_2(j) - a_2(j)| \right) \\
+ \frac{1}{2\pi} \oint_{\partial S^- L_j} |z^r||\hat{m}_p(z) - m_p(z)||\,dz.
\]

For the first term, using Cauchy-Schwarz inequality, we have,
\[
|z^r \hat{m}_p(z)| \leq \frac{\|z^r\|\|s_1\|\|s_2\|}{d(z, \Gamma_F)},
\]
where \( d(z, S) = \inf_{y \in S} |z - y| \) for \( S \subset \mathbb{C} \). Since \( a_1(z), a_2(z) \) are chosen such that \( d\left( a_1(z), \widetilde{\Gamma}_F \right) > 0, d\left( a_1(z), \Gamma_F \right) > 0, \exists M, P \) large enough such that for \( p > P \), with probability one,
\[
\sup_{z \in \partial S^- L_j \cup \partial S^+ L_j} |z^r \hat{m}_p(z)| < M.
\]

Therefore, the convergence of the first term on the right-hand side above to zero is complete as \( \hat{a}_1(z) \to a_1(z) \) and \( \hat{a}_2(z) \to a_2(z) \).

For the second term, as \( \hat{m}_p(z) \) and \( m_p(z) \) are holomorphic on the compact set \( \partial S^- L_j \), we have \( \sup_{z \in \partial S^- L_j} |z^r| \) bounded above and \( \sup_{z \in \partial S^- L_j} |\hat{m}_p(z) - m_p(z)| \) bounded above with probability one. Moreover, from Result 7.3, \( |\hat{m}_p(z) - m_p(z)| \overset{a.s.}{\to} 0 \) point-wise for \( z \in \mathbb{C} \setminus \mathbb{R} \). Therefore, using Lebesgue’s dominated convergence theorem, the second term on the right-hand side above converges to zero almost surely, and that completes the proof.

\[\square\]

**Lemma 7.5.** Suppose \( \widetilde{X} \sim \mathbb{G} \mathbb{S}(\{\{\lambda_j, v_j\}\}_{j=1}^{k^*}; \Gamma_H; n, p) \) and \( \hat{\Sigma} = \frac{1}{n} \widetilde{X}^\top \widetilde{X} \) has spectral decomposition \( \hat{\Sigma} = \sum_{j=1}^{n\wedge p} \hat{\lambda}_j \hat{v}_j \hat{v}_j^\top \). Under Assumption 2.6(a), there exists \( m_1, m_2 > 0 \) depending on \( \Gamma_H \) such that,
\[
\frac{1}{p} \sum_{j=k+1}^{n\wedge p} \hat{\lambda}_j \to m_1,
\]
\[
\frac{1}{p} \sum_{j=k+1}^{n\wedge p} \hat{\lambda}_j^2 \to m_2.
\]

**Proof.** See e.g. Couillet and Debhab [2011], Bai and Silverstein [2010]. \[\square\]

**REFERENCES**

Zhidong Bai and Jack W Silverstein. *Spectral analysis of large dimensional random matrices*, volume 20. Springer, 2010.

Zhidong Bai and Jianfeng Yao. On sample eigenvalues in a generalized spiked population model. *Journal of Multivariate Analysis*, 106:167 – 177, 2012. ISSN 0047-259X. doi: https://doi.org/10.1016/j.jmva.2011.10.009. URL http://www.sciencedirect.com/science/article/pii/S0047259X11002041.
Zhiding Bai and Wang Zhou. Large sample covariance matrices without independence structures in columns. *Statistica Sinica*, pages 425–442, 2008.

Jinho Baik and Jack W Silverstein. Eigenvalues of large sample covariance matrices of spiked population models. *Journal of multivariate analysis*, 97(6):1382–1408, 2006.

Jinho Baik, Gérard Ben Arous, Sandrine Péché, et al. Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *The Annals of Probability*, 33(5):1643–1697, 2005.

Zhigang Bao, Xiucai Ding, Jingming Wang, and Ke Wang. Statistical inference for principal components of spiked covariance matrices. *arXiv preprint arXiv:2008.11903*, 2020.

Richard T Barfield, Lynn M Almli, Varun Kilaru, Alicia K Smith, Kristina B Mercer, Richard Duncan, Torsten Klengel, Divya Mehta, Elisabeth B Binder, Michael P Epstein, et al. Accounting for population stratification in dna methylation studies. *Genetic epidemiology*, 38(3):231–241, 2014.

T Tony Cai and Anru Zhang. Rate-optimal perturbation bounds for singular subspaces with applications to high-dimensional statistics. *The Annals of Statistics*, 46(1):60–89, 2018.

T Tony Cai, Xiao Han, and Guangming Pan. Limiting laws for divergent spiked eigenvalues and largest nonspiked eigenvalue of sample covariance matrices. *The Annals of Statistics*, 48(3):1255–1280, 2020.

H-S Chen, X Zhu, H Zhao, and S Zhang. Qualitative semi-parametric test for genetic associations in case-control designs under structured populations. *Annals of human genetics*, 67(3):250–264, 2003.

Romain Couillet and Merouane Debbah. *Random matrix methods for wireless communications*. Cambridge University Press, 2011.

Bernie Devlin and Kathryn Roeder. Genomic control for association studies. *Biometrics*, 55(4):997–1004, 1999.

Kevin J Galinsky, Gaurav Bhatia, Po-Ru Loh, Stoyan Georgiev, Sayan Mukherjee, Nick J Patterson, and Alkes L Price. Fast principal-component analysis reveals convergent evolution of adh1b in europe and east asia. *The American Journal of Human Genetics*, 98(3):456–472, 2016.

Daniel L Hartl, Andrew G Clark, and Andrew G Clark. *Principles of population genetics*, volume 116. Sinauer associates Sunderland, 1997.

Iain M Johnstone. On the distribution of the largest eigenvalue in principal components analysis. *Annals of statistics*, pages 295–327, 2001.

Iain M Johnstone and Arthur Yu Lu. On consistency and sparsity for principal components analysis in high dimensions. *Journal of the American Statistical Association*, 104(486):682–693, 2009.

Nan M Laird and Christoph Lange. *The fundamentals of modern statistical genetics*. Springer, 2011.

Jennifer Listgarten, Christoph Lippert, Carl M Kadie, Robert I Davidson, Eleazar Eskin, and David Heckerman. Improved linear mixed models for genome-wide association studies. *Nature methods*, 9(6):525–526, 2012.

The Tien Mai and Pierre Alquier. Understanding the population structure correction regression. *arXiv preprint arXiv:2108.05655*, 2021.

V A Marčenko and L A Pastur. Distribution of eigenvalues for some sets of random matrices. *Mathematics of the USSR. Sbornik*, 1(4):457–483, 1967. ISSN 0025-5734.

Xavier Mestre. On the asymptotic behavior of quadratic forms of the resolvent of certain covariance-type matrices. Technical report, Tech. Rep. CTTC/RC/2006-01, Centre Tecnologic de Telecomunicacions de Catalunya, 2006.

Xavier Mestre. On the asymptotic behavior of the sample estimates of eigenvalues and eigenvectors of covariance matrices. *IEEE Transactions on Signal Processing*, 56(11):5353–5368, 2008.

John Novembre, Toby Johnson, Katarzyna Bryc, Zoltán Kutalik, Adam R Boyko, Adam Auton, Amit Indap, Karen S King, Sven Bergmann, Matthew R Nelson, et al. Genes mirror geography within europe. *Nature*, 456(7218):98–101, 2008.
Nick Patterson, Alkes L Price, and David Reich. Population structure and eigenanalysis. *PLoS genetics*, 2(12):e190, 2006.

Amelia Perry, Alexander S Wein, Afonso S Bandeira, and Ankur Moitra. Optimality and sub-optimality of pca i: Spiked random matrix models. *The Annals of Statistics*, 46(5):2416–2451, 2018.

Alkes L Price, Nick J Patterson, Robert M Plenge, Michael E Weinblatt, Nancy A Shadick, and David Reich. Principal components analysis corrects for stratification in genome-wide association studies. *Nature genetics*, 38(8):904, 2006.

Jonathan K Pritchard, Matthew Stephens, and Peter Donnelly. Inference of population structure using multilocus genotype data. *Genetics*, 155(2):945–959, 2000.

J.W Silverstein and S.I Choi. Analysis of the limiting spectral distribution of large dimensional random matrices. *Journal of multivariate analysis*, 54(2):295–309, 1995. ISSN 0047-259X.

Peter M Visscher, Naomi R Wray, Qian Zhang, Pamela Sklar, Mark I McCarthy, Matthew A Brown, and Jian Yang. 10 years of gwas discovery: biology, function, and translation. *The American Journal of Human Genetics*, 101(1):5–22, 2017.

Fan Yang, Kjell Doksum, and Kam-Wah Tsui. Principal component analysis (pca) for high-dimensional data. pca is dead. long live pca. *Perspectives on Big Data Analysis: Methodologies and Applications*, 622:1–22, 2014a.

Jian Yang, Noah A Zaitlen, Michael E Goddard, Peter M Visscher, and Alkes L Price. Advantages and pitfalls in the application of mixed-model association methods. *Nature genetics*, 46(2):100–106, 2014b.

Shuanglin Zhang, Xiaofeng Zhu, and Hongyu Zhao. On a semiparametric test to detect associations between quantitative traits and candidate genes using unrelated individuals. *Genetic Epidemiology: The Official Publication of the International Genetic Epidemiology Society*, 24(1):44–56, 2003.

Xiaofeng Zhu, ShuangLin Zhang, Hongyu Zhao, and Richard S Cooper. Association mapping, using a mixture model for complex traits. *Genetic Epidemiology: The Official Publication of the International Genetic Epidemiology Society*, 23(2):181–196, 2002.

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