

RATE-OPTIMAL POSTERIOR CONTRACTION FOR SPARSE PCA

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Principal component analysis (PCA) is possibly one of the most widely used statistical tools to recover a low-rank structure of the data. In the high-dimensional settings, the leading eigenvector of the sample covariance can be nearly orthogonal to the true eigenvector. A sparse structure is then commonly assumed along with a low rank structure. Recently, minimax estimation rates of sparse PCA were established under various interesting settings. On the other side, Bayesian methods are becoming more and more popular in high-dimensional estimation, but there is little work to connect frequentist properties and Bayesian methodologies for high-dimensional data analysis. In this paper, we propose a prior for the sparse PCA problem and analyze its theoretical properties. The prior adapts to both sparsity and rank. The posterior distribution is shown to contract to the truth at optimal minimax rates. In addition, a computationally efficient strategy for the rank-one case is discussed.

1. Introduction. Principal component analysis is a classical statistical tool used to project data into a lower dimensional space while maximizing the variance [Jolliffe (1986)]. When the sample size n is small compared to the number of variables p , Johnstone and Lu (2009) show that the standard PCA may fail in the sense that the leading eigenvector of the sample covariance can be nearly orthogonal to the true eigenvector. Therefore, the recovery of principal components in the high-dimensional setting requires extra structural assumptions. The sparse PCA, assuming that the leading eigenvectors or eigen-subspace only depend on a relatively small number of variables, is applied in a wide range of applications. Estimation methods for sparse PCA problems are proposed in Zou, Hastie and Tibshirani (2006) and d'Aspremont et al. (2007). Amini and Wainwright (2009) and Ma (2013) obtain rates of convergence of sparse PCA methods under the spiked covariance model proposed in Johnstone and Lu (2009). Minimax rates of sparse PCA problems are established by Birnbaum et al. (2013), Cai, Ma and Wu (2014, 2013) and Vu and Lei (2013) under various interesting settings.

Bayesian methods have been very popular in high-dimensional estimation, but there is little work to connect frequentist properties and Bayesian methodologies for high-dimensional models. This paper serves as a bridge between the frequentist

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and Bayesian worlds by addressing the following question for high-dimensional PCA: Is it possible for a Bayes procedure to optimally recover the leading principal components in the sense that the posterior distribution contracts to the truth with a minimax rate? The optimal posterior contraction rate immediately implies that the posterior mean attains the optimal convergence rate as a point estimator.

In this paper we consider a spiked covariance model with an unknown growing rank. We propose a sparse prior on the covariance matrix with a spiked structure and show that the induced posterior distribution contracts to the truth with an optimal minimax rate. The assumptions are nearly identical to those in [Vu and Lei \(2013\)](#), where the rank of the principal space $r = O(\log p)$ and the number of nonzero entries of each spike s is allowed to be at the order of p^{1-c} for any $c \in (0, 1)$, as long as the minimax rate $\frac{rs \log p}{n} \rightarrow 0$. In addition, we prove that the posterior distribution consistently estimates the rank. To the best of our knowledge, this is the first work where a Bayes procedure is able to adapt to both the sparsity and the rank.

There are two key ingredients in our approach. The first ingredient is in the design of the prior. We propose a prior that imposes a spiked structure on a random covariance matrix, under which each spike is sparse and orthogonal to each other. This leads to sufficient prior concentration together with the sparse property. In addition, each spike has a bounded l^2 norm under the prior distribution such that there is a fixed eigen-gap between the spikes and the noise, which eventually leads to consistent rank estimation. The second ingredient is in constructing appropriate tests in the proof of posterior contraction under spectral and Frobenius norms. We first construct a test with the alternative hypothesis outside of the neighborhood of the true covariance under the spectral norm. For the covariance matrices inside the neighborhood of the truth under the spectral norm, we propose a delicate way to divide the region into many small pieces, where the likelihood ratio test is applicable in each small region. A final test is then constructed by combining these small tests. The errors are controlled by correctly calculating the covering number under the metric for measuring the distance of subspaces.

The theoretical tools we use for this problem follow the recent line of developments in Bayesian nonparametrics pioneered by [Barron \(1988\)](#) and [Barron, Schervish and Wasserman \(1999\)](#), which generalize the testing theory of [Le Cam \(1973\)](#) and [Schwartz \(1965\)](#) to construct an exponentially consistent test on the essential support of a prior to prove posterior consistency. The idea was later extended by [Ghosal, Ghosh and van der Vaart \(2000\)](#) and [Shen and Wasserman \(2001\)](#) to prove rates of convergence of posterior distribution. Compared to Bayesian nonparametrics, little work has been done for Bayesian high-dimensional estimation, especially in the sparse setting. [Castillo and van der Vaart \(2012\)](#) is the first work in this area. They prove rates of convergence in sparse vector estimation for a large class of priors.

The works closely related to this paper are [Banerjee and Ghosal \(2014\)](#) and [Pati et al. \(2014\)](#). [Banerjee and Ghosal \(2014\)](#) study rates of convergence for Bayesian

precision matrix estimation by considering a conjugate prior. But as discussed in [Birnbaum et al. \(2013\)](#), estimation of sparse or bandable covariance/precision matrix is different from that of sparse principal subspace. The optimal rates of convergence can be different. [Pati et al. \(2014\)](#) study Bayesian covariance matrix estimation for a sparse factor model, which is similar to the spiked covariance model in the PCA problem. Instead of estimating the principal subspace as in the PCA problem, they consider estimating the whole covariance matrix. The posterior rate of convergence they obtain is not optimal, especially when the rank r is allowed to grow with the sample size n .

The paper is organized as follows. In Section 2, we introduce the sparse PCA problem and define the parameter space. In Section 3, we propose a prior and state the main result of the posterior convergence. Section 4 introduces an algorithm to compute the posterior mean in the rank-one case along with other discussions. All the proofs are presented in Section 5, with some technical results given in the supplementary material [[Gao and Zhou \(2015\)](#)].

2. The sparse PCA. Let X_1, \dots, X_n be i.i.d. observations from $P_\Sigma = N(0, \Sigma)$, with Σ being a $p \times p$ covariance matrix with a spiked structure

$$\Sigma = \sum_{l=1}^r \theta_l \theta_l^T + I_{p \times p},$$

where $\theta_l^T \theta_k = 0$ for any $l \neq k$. It is easy to see that $(\|\theta_1\|^{-1}\theta_1, \dots, \|\theta_r\|^{-1}\theta_r)$ are the first r eigenvectors of Σ , with the corresponding eigenvalues $(\|\theta_1\|^2 + 1, \dots, \|\theta_r\|^2 + 1)$. The rest $p - r$ eigenvalues are all 1. The spiked covariance is proposed by [Johnstone and Lu \(2009\)](#) to model data with a sparse and low-rank structure. An equivalent representation of the data is

$$(2.1) \quad X_i = V_0 \Lambda_0^{1/2} W_i + Z_i \quad \text{for } i = 1, 2, \dots, n,$$

where $W_i \sim N(0, I_{r \times r})$ and $Z_i \sim N(0, I_{p \times p})$ are independent. The matrix V_0 is defined as $V_0 = [\|\theta_1\|^{-1}\theta_1, \dots, \|\theta_r\|^{-1}\theta_r]$ and $\Lambda_0 = \text{diag}(\|\theta_1\|^2, \dots, \|\theta_r\|^2)$. In such latent variable representation, $V_0 \Lambda_0^{1/2} W_i$ models the signal part, which lives in an r -dimensional subspace, and Z_i is the noise part, which has the same variance on every direction. Since the r -dimensional subspace is determined by its projection matrix $V_0 V_0^T$, the goal here is to recover the principal subspace by estimating its projection matrix in the Frobenius loss,

$$\|\hat{V} \hat{V}^T - V_0 V_0^T\|_F.$$

In a high-dimensional setting, extra structural assumptions are needed for consistent estimation. We assume that the first r eigenvectors are sparse, in the sense that each of them only depends on a few coordinates among the total number p . Define $S_{0,l} = \text{supp}(\theta_l)$ for $l = 1, 2, \dots, r$, the support of the l th eigenvector. We

assume l^0 sparsity on each spike by $\max_{1 \leq l \leq r} |S_{0,l}| \leq s$. The parameter space for the covariance matrix is

$$\mathcal{G}(p, s, r) = \left\{ \begin{array}{l} \Sigma = \sum_{l=1}^r \theta_l \theta_l^T + I : \max_{1 \leq l \leq r} |S_{0,l}| \leq s, \theta_l \in \mathbb{R}^p, \\ \theta_l^T \theta_k = 0 \text{ for } k \neq l, \|\theta_l\|^2 \in (K^{-1}, K) \end{array} \right\},$$

where $K > 0$ is a constant, which we treat as being known in this paper. The sparsity we consider matches the column sparsity in [Vu and Lei \(2013\)](#) in the l^0 case. We require both upper and lower bounds for $\|\theta_l\|^2$. The lower bound implies an eigengap, which leads to rank adaptation and subspace estimation, while the upper bound controls the spectral norm of Σ , which leads to estimation of the whole covariance matrix. [Vu and Lei \(2013\)](#) prove that under the assumptions

$$r \leq m \log p \quad \text{and} \quad s \leq p^{1-c} \quad \text{for some constants } c \in (0, 1) \text{ and } m > 0,$$

the minimax rate¹ of principal subspace estimation is

$$\inf_{\hat{V}} \sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \|\hat{V} \hat{V}^T - V_0 V_0^T\|_F^2 \asymp \frac{rs \log p}{n}.$$

The goal of this paper is to prove an alternative result, adaptive Bayesian estimation, by designing an appropriate prior Π , such that

$$(2.2) \quad \sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \Pi(\|VV^T - V_0 V_0^T\|_F^2 > M \varepsilon^2 | X^n) \leq \delta \quad \text{for some } M > 0,$$

where $\varepsilon^2 = \frac{rs \log p}{n}$ is the minimax rate and $X^n \sim P_{\Sigma}^n$. The number $\delta > 0$ satisfies $\lim_{(n,s,p,r) \rightarrow \infty} \delta = 0$. The posterior contraction (2.2) leads to a risk bound of a point estimator. Let \mathbb{E}_{Π} be the expectation under the prior distribution Π . Consider the posterior mean of the subspace projection matrix $\mathbb{E}_{\Pi}(VV^T | X^n)$. Its risk upper bound is given in the following proposition. We prove the proposition in the supplementary material [[Gao and Zhou \(2015\)](#)].

PROPOSITION 2.1. *Equation (2.2) implies*

$$\sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \|\mathbb{E}_{\Pi}(VV^T | X^n) - V_0 V_0^T\|_F^2 \leq M \varepsilon^2 + 2(p+r)\delta.$$

REMARK 2.1. In this paper, the number δ in (2.2) is at an order of $\exp(-C'n\varepsilon^2)$ for some $C' > 0$. Thus the dominating term in $M\varepsilon^2 + 2(p+r)\delta$ is $M\varepsilon^2$. The posterior mean is a rate-optimal point estimator.

¹The minimax rate is obtained by combining Theorem 3.5 and Corollary 3.2 in [Vu and Lei \(2013\)](#). The upper bound is a special case of their Corollary 3.2 because our parameter space is a subset of theirs. The lower bound holds by observing that the least favorable class in the proof of their Theorem 3.5 is a subset of our parameter space.

REMARK 2.2. The matrix $\mathbb{E}_\Pi(VV^T|X^n)$ may not be a projection matrix. However, it is still a valid estimator of the true projection matrix $V_0V_0^T$. A projection matrix estimator can be obtained by projecting the posterior mean $\mathbb{E}_\Pi(VV^T|X^n)$ to the space of projection matrices under the Frobenius norm. Denote the projection by $\hat{V}\hat{V}^T$. It can be shown that $\|\hat{V}\hat{V}^T - V_0V_0^T\|_F \leq 2\|\mathbb{E}_\Pi(VV^T|X^n) - V_0V_0^T\|_F$.

2.1. *Notation.* In this paper, we use Γ to denote a $p \times p$ spiked covariance matrix with structure $\Gamma = AA^T + I$, where $A = [\eta_1, \eta_2, \dots, \eta_\xi]$ is a $p \times \xi$ matrix with orthogonal columns. We use S_l to denote the support of η_l for each $l = 1, 2, \dots, \xi$. Define

$$V = [\|\eta_1\|^{-1}\eta_1, \|\eta_2\|^{-1}\eta_2, \dots, \|\eta_\xi\|^{-1}\eta_\xi],$$

$$\Lambda = \text{diag}(\|\eta_1\|^2, \|\eta_2\|^2, \dots, \|\eta_\xi\|^2).$$

Then V is a $p \times \xi$ unitary matrix, and Γ has an alternative representation $\Gamma = V\Lambda V^T + I$. We use P_Γ to denote the probability or the expectation under the multivariate normal distribution $N(0, \Gamma)$ and P_Γ^n to denote the product measure. The symbol \mathbb{P} stands for a generic probability whose distribution will be made clear through the context. Correspondingly, we use $(\Sigma, A_0, r, \theta_l, S_{0l}, V_0, \Lambda_0)$ to denote the true version of $(\Gamma, A, \xi, \eta_l, S_l, V, \Lambda)$.

For a matrix A , we use $\|A\|$ to denote its spectral norm and $\|A\|_F$ for the Frobenius norm. We define $\mathcal{U}(d, r)$ to be the space of all $d \times r$ unitary matrices for $d \geq r$ such that for any $U \in \mathcal{U}(d, r)$, $U^T U = I_{r \times r}$. For any $U, V \in \mathcal{U}(d, r)$, define the distance $d_\Lambda(\cdot, \cdot)$ by $d_\Lambda(\cdot, \cdot) = \|U\Lambda U^T - V\Lambda V^T\|_F$ for some diagonal matrix Λ . We omit the subscript Λ and write $d(\cdot, \cdot) = d_\Lambda(\cdot, \cdot)$ whenever $\Lambda = I$. The number ε^2 stands for the minimax rate $\frac{rs \log p}{n}$ throughout the paper.

3. The prior and the main results. We propose a prior Π from which we can sample a random covariance matrix with structure $\Gamma = AA^T + I = \sum_{i=1}^\xi \eta_i \eta_i^T + I$, where A is a $p \times \xi$ matrix. The prior Π is described as follows:

- (1) for each $l \in \{1, \dots, \lfloor p^{\gamma/2} \rfloor\}$, we randomly choose $S_l \subset \{1, \dots, p\}$ by letting the indicator $\mathbb{1}\{i \in S_l\}$ for each $i = 1, \dots, p$ follow a Bernoulli distribution with parameter $p^{-(1+\gamma)}$;
- (2) given $(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor})$, we sample a $p \times \lfloor p^{\gamma/2} \rfloor$ matrix $\bar{A} = [\eta_1, \dots, \eta_{\lfloor p^{\gamma/2} \rfloor}]$ from $G_{(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor})}$ to be specified below, and then let $\Gamma = \bar{A}\bar{A}^T + I$.

The $p \times \lfloor p^{\gamma/2} \rfloor$ matrix \bar{A} (Figure 1) may contain some zero columns under the above sampling procedure. With slight abuse of notation, we gather those nonzero columns to form the matrix $A = [\eta_1, \dots, \eta_\xi]$, with S_l being the support of the column η_l . Note that $\Gamma = \bar{A}\bar{A}^T + I = AA^T + I$, where A is a $p \times \xi$ matrix. After specifying the distribution $G_{(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor})}$, the number of nonzero columns ξ is also the rank of A .

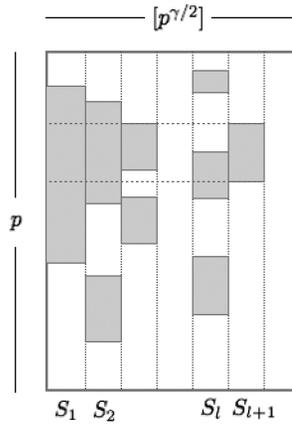


FIG. 1. An illustration of the prior. The shaded areas are $\{S_l\}_{l=1}^{\lfloor p^{\gamma/2} \rfloor}$. The parts inside the dashed lines correspond to u_1, \dots, u_l defined in (3.2).

REMARK 3.1. The number $\gamma > 0$ is a fixed constant in the prior. With $p^{-(1+\gamma)}$ as the mean for $\mathbb{I}\{i \in S_l\}$, the cardinality $|S_l|$ is small with high probability under the prior distribution.

REMARK 3.2. The number $\lfloor p^{\gamma/2} \rfloor$ is an upper bound of the rank ξ . In this paper, we assume that the true rank r is at the order of $O(\log p)$. Since $\log p \ll p^{\lfloor \gamma/2 \rfloor}$, the range of ξ covers the range of r .

We need to define a distribution G_d^* on \mathbb{R}^d to help introduce $G_{(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor})}$. Let $Z = (Z_1, \dots, Z_d)$ follow $N(0, I_{d \times d})$ and U follow the uniform distribution on the interval $[(2K)^{-1/2}, (2K)^{1/2}]$. Then G_d^* is defined to be the distribution of

$$(3.1) \quad \left(\frac{UZ_1}{\|Z\|}, \dots, \frac{UZ_d}{\|Z\|} \right).$$

Now we are ready to specify the random matrix prior $G_{(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor})}$, which induces a distribution over the matrix $\bar{A} = [\eta_1, \eta_2, \dots, \eta_{\lfloor p^{\gamma/2} \rfloor}]$. For any vector v and any subset S , we use the notation $v^T = (v_S^T, v_{S^c}^T)$. We describe the prior through a sequential sampling procedure. If $|S_1| = 0$, we set $\eta_1 = 0$. Otherwise, we sample $\eta_{1, S_1} \sim G_{|S_1|}^*$ and let

$$\eta_1 = \begin{pmatrix} \eta_{1, S_1} \\ 0 \end{pmatrix}.$$

Suppose we have already obtained (η_1, \dots, η_l) and then sample η_{l+1} , conditioning on (η_1, \dots, η_l) . We set $\eta_{l+1, S_{l+1}^c} = 0$. The prior distribution of $\eta_{l+1, S_{l+1}}$ depends on η_i , $1 \leq i \leq l$, through values of η_i 's on the index set S_{l+1} . For simplicity, denote

$$(3.2) \quad (u_1, \dots, u_l) = (\eta_{1, S_{l+1}}, \dots, \eta_{l, S_{l+1}}).$$

Define $l^* = \dim(\text{span}\{u_1, \dots, u_l\})$. If $|S_{l+1}| - l^* \leq 0$, we set $\eta_{l+1, S_{l+1}} = 0$. Otherwise, let H_l be the projection matrix from $\mathbb{R}^{S_{l+1}}$ to the subspace spanned by $\{u_1, \dots, u_l\}$. There is a bijective linear isometry T_l induced by H_l such that

$$T_l : (I - H_l)\mathbb{R}^{S_{l+1}} \rightarrow \mathbb{R}^{|S_{l+1}| - l^*}, \quad T_l^{-1} : \mathbb{R}^{|S_{l+1}| - l^*} \rightarrow (I - H_l)\mathbb{R}^{S_{l+1}}.$$

Remember that a linear isometry preserves the norms in the sense that $\|T_l v\| = \|v\|$. We sample \bar{u}_{l+1} from $G_{|S_{l+1}| - l^*}^*$ and let $u_{l+1} = T_l^{-1} \bar{u}_{l+1}$. Set $\eta_{l+1, S_{l+1}} = u_{l+1}$. Then we have specified η_{l+1}^T , which is $(\eta_{l+1, S_{l+1}}^T, 0^T)$. Repeating this step, we obtain $A = [\eta_1, \dots, \eta_{\lfloor p/2 \rfloor}]$. The prior Π on the random covariance matrix Γ is now fully specified.

After collecting the nonzero η_l 's, we observe that the prior Π explicitly samples a spiked covariance matrix $\Gamma = \bar{A}\bar{A}^T + I = AA^T + I = \sum_{l=1}^\xi \eta_l \eta_l^T + I$ with the number of spikes being ξ . The prior Π imposes orthogonality on the spikes, since η_{l+1} is sampled on the orthogonal complement of the space $\text{span}\{\eta_1, \eta_2, \dots, \eta_l\}$. Therefore, $\eta_k^T \eta_l = 0$ for each $k \neq l$, and $\{\|\eta_l\|^{-1} \eta_l\}_{l=1}^\xi$ are the eigenvectors. For each eigenvector $\|\eta_l\|^{-1} \eta_l$, its support is in S_l , whose cardinality is small under the prior distribution. Moreover, the first ξ eigenvalues are all bounded from 1 and ∞ because $\|\eta_l\|^2 \in [(2K)^{-1}, (2K)]$.

Given the data $X^n = (X_1, \dots, X_n) \sim P_\Sigma^n$, the posterior distribution is defined as

$$(3.3) \quad \Pi(B|X^n) = \int_B \frac{dP_\Gamma^n}{dP_\Sigma^n}(X^n) d\Pi(\Gamma) / \left(\int \frac{dP_\Gamma^n}{dP_\Sigma^n}(X^n) d\Pi(\Gamma) \right),$$

for any measurable set B . The following theorem is the main result of this paper. The posterior distribution contracts to the truth with an optimal minimax rate.

THEOREM 3.1. *Assume $\varepsilon \rightarrow 0$, $r \leq m(s \wedge \log p)$ and $n \leq p^m$ for some constant $m > 0$. Then there exists $M'_{\gamma, K, m} > 0$, such that for any $M' > M'_{\gamma, K, m}$, we have*

$$\sup_{\Sigma \in \mathcal{G}(p, s, r)} P_\Sigma^n \Pi(\|V V^T - V_0 V_0^T\|_F > M' \varepsilon | X^n) \leq \exp(-C_{(\gamma, K, m, M')} n \varepsilon^2),$$

for some constant $C_{(\gamma, K, m, M')} > 0$ only depending on (γ, K, m, M') .

Note that we have obtained the optimal posterior contraction rate under a ‘‘mildly growing rank’’ regime $r \leq m \log p$, which is also assumed in [Vu and Lei \(2013\)](#), for them to match the upper and lower bounds for minimax estimation. The assumption $n \leq p^m$ is a convenient but mild condition in high-dimensional statistics to prove rates of convergence in expectation rather than with high probability; see [Cai, Liu and Luo \(2011\)](#), [Paul and Johnstone \(2012\)](#), etc. The posterior contraction result implies the same rate of convergence in expectation of a point estimator ([Corollary 3.1](#)), and thus we need such an assumption to hold. Additionally, we assume $r \leq ms$, which means that the level of the rank is not above the

level of sparsity. This assumption is due to the fact that V_0 can be only identified up to a unitary transformation, that is, $V_0 V_0^T = (V_0 Q)(V_0 Q)^T$ for any $Q \in \mathcal{U}(r, r)$, and for some Q such that each row of $V_0 Q$ may have at least r nonzero entries.

As shown in Proposition 2.1, we can use the posterior mean as a point estimator to achieve the minimax optimal rate of convergence.

COROLLARY 3.1. *Under the setting of Theorem 3.1, we have*

$$\sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \|\mathbb{E}_{\Pi}(V V^T | X^n) - V_0 V_0^T\|_F^2 \leq 2M'^2 \varepsilon^2,$$

for sufficiently large (n, p, s, r) .

The result follows from the fact that the $2(p + r)\delta$ part of Proposition 2.1 is exponentially small; hence, it is dominated by $M'^2 \varepsilon^2$.

4. Discussion. In Section 4.1, we state a result on posterior contraction rate under the spectral norm. A computationally efficient algorithm is developed in Section 4.2 for the rank-one case. In Section 4.3, we discuss the possibility of using a simpler prior for sparse PCA.

4.1. Posterior convergence under spectral norm. In proving Theorem 3.1, there are some by-products serving as intermediate steps. The following theorem says that the posterior distribution concentrates on the true covariance matrix under the spectral norm, and the subspace projection matrix concentrates on the true subspace projection matrix under the spectral norm. In addition, the posterior distribution consistently estimates the rank of the true subspace. The theorem holds under a slightly weaker assumption without assuming $r \leq ms$.

THEOREM 4.1. *Consider the same prior Π and rate ε as in Theorem 3.1. Assume $\varepsilon \rightarrow 0$, $r \leq m \log p$ and $n \leq p^m$ for some constant $m > 0$. Then there exists $M_{\gamma,K,m} > 0$, such that for any $M > M_{\gamma,K,m}$, we have*

$$(4.1) \quad \sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon | X^n) \leq \exp(-C_{(\gamma,K,m,M)} n \varepsilon^2),$$

$$\sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \Pi(\|V V^T - V_0 V_0^T\| > M\varepsilon | X^n) \leq \exp(-C_{(\gamma,K,m,M)} n \varepsilon^2),$$

$$(4.2) \quad \sup_{\Sigma \in \mathcal{G}(p,s,r)} P_{\Sigma}^n \Pi(\xi \neq r | X^n) \leq \exp(-C_{(\gamma,K,m,M)} n \varepsilon^2),$$

for some constant $C_{(\gamma,K,m,M)}$ only depending on (γ, K, m, M) .

REMARK 4.1. It is not practical to assume that K is known in Theorems 3.1 and 4.1. To weaken the assumption, we can replace the prior in (3.1) by sampling $U \sim \text{Unif}[L_n^{-1}, L_n]$, for some sequence L_n slowly grows to infinity as $n \rightarrow \infty$. Then the conclusions of the two theorems still hold without knowing K .

REMARK 4.2. The posterior rate of convergence (4.1) for estimating the whole covariance matrix under the spectral norm does not require the assumption $\|\theta_l\|^2 > K^{-1}$ in the definition of $\mathcal{G}(p, s, r)$. To remove this assumption, we need a slightly different prior with (3.1) modified by sampling $U \sim \text{Unif}[0, (2K)^{1/2}]$. However, such modification may not lead to rank adaptation (4.2) due to lack of eigengap, which is critical for establishing the result in Theorem 3.1.

REMARK 4.3. Results (4.1) and (4.2) together imply posterior convergence of the whole covariance matrix under the Frobenius norm. This is because when $\xi = r$, we have $\|\Gamma - \Sigma\|_F = \|V \Lambda V^T - V_0 \Lambda_0 V_0^T\|_F \leq \sqrt{2r} \|V \Lambda V^T - V_0 \Lambda_0 V_0^T\| = \sqrt{2r} \|\Gamma - \Sigma\|$. Hence the convergence rate for the loss $\|\Gamma - \Sigma\|_F$ is $\sqrt{r} \varepsilon = \sqrt{\frac{r^2 s \log p}{n}}$.

Pati et al. (2014) consider estimating the whole covariance matrix under spectral norm in a sparse factor model. Under their assumption $rs \gtrsim \log p$, they obtain a posterior convergence rate of $\sqrt{\frac{r^3 s \log p}{n}} \sqrt{\log n}$ under the loss function $\|\Gamma - \Sigma\|$, compared with our rate $\sqrt{\frac{rs \log p}{n}}$.

Though an improvement over the result of Pati et al. (2014), whether $\sqrt{\frac{rs \log p}{n}}$ is the optimal rate of convergence for the loss functions $\|\Gamma - \Sigma\|$ and $\|V V^T - V_0 V_0^T\|$ is still an open problem. To the best of our knowledge, the only minimax result addressing these two loss functions for sparse PCA problem is in Cai, Ma and Wu (2014). However, they consider a different sparsity class, defined as

$$\mathcal{G}_1(p, s, r) = \left\{ \begin{array}{l} \Sigma = \sum_{l=1}^r \theta_l \theta_l^T + I : \left| \bigcup_{1 \leq l \leq r} S_{0l} \right| \leq s, \theta_l \in \mathbb{R}^p, \\ \theta_l^T \theta_k = 0 \text{ for } k \neq l, \|\theta_l\|^2 \in (K^{-1}, K) \end{array} \right\}.$$

Under the current setting, the results of Cai, Ma and Wu (2014) can be written as

$$\inf_{\hat{\Sigma}} \sup_{\Sigma \in \mathcal{G}_1(p, s, r)} P_{\Sigma}^n \|\hat{\Sigma} - \Sigma\|^2 \asymp \frac{s \log p}{n} + \frac{r}{n},$$

$$\inf_{\hat{V}} \sup_{\Sigma \in \mathcal{G}_1(p, s, r)} P_{\Sigma}^n \|\hat{V} \hat{V}^T - V V^T\|^2 \asymp \frac{s \log p}{n}.$$

Observe the relation that

$$\mathcal{G}_1(p, s, r) \subset \mathcal{G}(p, s, r) \subset \mathcal{G}_1(p, rs, r).$$

Hence when $r \leq O(\log p)$, the minimax rates for the class $\mathcal{G}(p, s, r)$ under both loss functions lie between $\frac{s \log p}{n}$ and $\frac{rs \log p}{n}$. We claim that the posterior convergence rate obtained in Theorem 4.1 is optimal when $r \leq O(1)$. For a growing r , it at most misses a factor of r .

4.2. *A computational strategy of the rank-one case.* Bayesian procedures using sparse priors are usually harder to compute because the sampling procedure needs to mix all possible subsets. Castillo and van der Vaart (2012) develop an efficient algorithm for computing exact posterior mean in the setting of Bayesian sparse vector estimation. They explore the combinatorial nature of the posterior mean formula and show that it is sufficient to compute the coefficients of some p th order polynomials. In this section, we use their idea to develop an algorithm for computing approximate posterior mean for the single spike model. In this rank-one case, there is no need for the prior to adapt to the rank. We do not need the prior to put constraint on the l^2 norm of the eigenvector as in (3.1). Thus we use the following simple prior on the single spiked covariance:

- (1) sample a cardinality q according to the distribution π supported on $\{1, 2, \dots, p\}$;
- (2) given q , sample a support $S \subset \{1, 2, \dots, p\}$ with cardinality $|S| = q$ uniformly from all $\binom{p}{q}$ subsets;
- (3) given S , sample $\eta_S \sim N(0, I_{|S| \times |S|})$, let $\eta^T = (\eta_S^T, \eta_{S^c}^T) = (\eta_S^T, 0^T)$ and the covariance matrix is $\Gamma = \eta\eta^T + I$.

We choose π to be $\pi(q) \propto \exp(-\kappa q \log p)$ for some constant $\kappa > 0$. We let $\varepsilon^2 = \frac{s \log p}{n}$ be the minimax rate when $r = 1$. The posterior distribution induced by the above prior has the following desired property:

THEOREM 4.2. *Assume $\varepsilon \rightarrow 0$ and $n \leq p^m$ for some constant $m > 0$. Then there exists $M_{\gamma, K, m} > 0$, such that for any $M > M_{\kappa, K, m}$, we have*

$$\sup_{\Sigma \in \mathcal{G}(p, s, 1)} P_{\Sigma}^n \Pi(\min\{\|\eta - \theta\|, \|\eta + \theta\|\} > M\varepsilon | X^n) \leq \exp(-C_{(\kappa, K, m, M)} n \varepsilon^2),$$

for some constant $C_{(\kappa, K, m, M)} > 0$ only depending on (κ, K, m, M) .

Note that the loss function is the l^2 norm, which is stronger than the loss function used in Theorem 3.1. The theorem above is proved in the supplementary material [Gao and Zhou (2015)]. We use the posterior mean $\mathbb{E}_{\Pi}(\eta | X^n)$ to estimate the spike θ .

We present a way for computing $\mathbb{E}_{\Pi}(\eta | X^n)$. Under the rank-one situation, representation (2.1) can be written as

$$(4.3) \quad X_{ij} = W_i \theta_j + Z_{ij}, \quad i = 1, \dots, n, j = 1, \dots, p,$$

with Z_{ij} and W_i following i.i.d. $N(0, 1)$ for all i and j . Representation (4.3) resembles the Gaussian sequence model considered in Castillo and van der Vaart (2012). Following their idea, the j th coordinate of $\mathbb{E}_{\Pi}(\eta | X^n)$ can be written as

$$\mathbb{E}_{\Pi}(\eta_j | X^n) = \frac{\int \eta_j \int \prod_{i=1}^n \prod_{j=1}^p \phi(X_{ij} - W_i \eta_j) \phi(W^n) dW^n d\Pi(\eta)}{\int \int \prod_{i=1}^n \prod_{j=1}^p \phi(X_{ij} - W_i \eta_j) \phi(W^n) dW^n d\Pi(\eta)},$$

where $\phi(W^n) dW^n = \prod_{i=1}^n \phi(W_i) dW_1 \cdots dW_n$ and ϕ is the density function of $N(0, 1)$. By Fubini's theorem, we have

$$\mathbb{E}_\Pi(\eta_j | X^n) = \frac{\int N_{n,j}(W^n) \phi(W^n) dW^n}{\int D_n(W^n) \phi(W^n) dW^n},$$

where for each W^n ,

$$\begin{aligned} D_n(W^n) &= \int \prod_{i=1}^n \prod_{j=1}^p \phi(X_{ij} - W_i \eta_j) d\Pi(\eta) \\ &= \sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} \sum_{|S|=q} \prod_{j \notin S} \left\{ \prod_{i=1}^n \phi(X_{ij}) \right\} \prod_{j \in S} \left\{ \int \prod_{i=1}^n \phi(X_{ij} - W_i \eta_j) \phi(\eta_j) d\eta_j \right\}, \end{aligned}$$

by the definition of the prior. In the same way,

$$\begin{aligned} N_{n,j}(W^n) &= \int \eta_j \prod_{i=1}^n \prod_{k=1}^p \phi(X_{ik} - W_i \eta_k) d\Pi(\eta) \\ &= \sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} \sum_{|S|=q} \prod_{k \notin S} \left\{ \prod_{i=1}^n \phi(X_{ik}) \right\} \\ &\quad \times \prod_{k \in S, k \neq j} \left\{ \int \prod_{i=1}^n \phi(X_{ik} - W_i \eta_k) \phi(\eta_k) d\eta_k \right\} \\ &\quad \times \mathbb{I}\{j \in S\} \int \eta_j \prod_{i=1}^n \phi(X_{ij} - W_i \eta_j) \phi(\eta_j) d\eta_j. \end{aligned}$$

Define

$$\begin{aligned} f(X_{\cdot j}) &= \prod_{i=1}^n \phi(X_{ij}), \\ h(X_{\cdot j}, W^n) &= \int \prod_{i=1}^n \phi(X_{ij} - W_i \eta_j) \phi(\eta_j) d\eta_j, \\ \xi(X_{\cdot j}, W^n) &= \int \eta_j \prod_{i=1}^n \phi(X_{ij} - W_i \eta_j) \phi(\eta_j) d\eta_j. \end{aligned}$$

Then we may rewrite $D_n(W^n)$ and $N_{n,j}(W^n)$ as

$$D_n(W^n) = \sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} C(q, W^n), \quad N_{n,j}(W^n) = \sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} C_j(q, W^n).$$

The critical fact observed by Castillo and van der Vaart (2012) is that $C(q, W^n)$ is the coefficient of Z^q of the polynomial

$$Z \mapsto \prod_{j=1}^p (f(X_{\cdot j}) + h(X_{\cdot j}, W^n)Z),$$

and $C_j(q, W^n)$ is the coefficient of Z^q of the polynomial

$$Z \mapsto \xi(X_{\cdot j}, W^n)Z \prod_{k \in \{1, \dots, p\} \setminus \{j\}} (f(X_{\cdot k}) + h(X_{\cdot k}, W^n)Z).$$

For a given W^n , the coefficients $\{C(q, W^n)\}_q$ and $\{C_j(q, W^n)\}_{(j,q)}$ can be computed efficiently. In the Gaussian sequence model, there is no randomness by W^n , and the posterior mean can be computed exactly by finding the coefficients of the above polynomials. In the PCA case, we propose an approximation by first drawing $W_1^n, W_2^n, \dots, W_T^n$ i.i.d. from $N(0, I_{n \times n})$ and then computing

$$\hat{\theta}_j = \frac{1}{T} \sum_{t=1}^T \left(\sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} C(q, W_t^n) \right) / \left(\frac{1}{T} \sum_{t=1}^T \left(\sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} C_j(q, W_t^n) \right) \right) \tag{4.4}$$

for $j = 1, 2, \dots, p$.

One set of coefficients takes at most $O(p^2)$ steps to compute. Thus the total computational complexity is $O(Tp^3 + Tnp)$ for computing coefficients of $O(Tp)$ polynomials and computing all the values of $f(X_{\cdot j}), h(X_{\cdot j}, W^n)$ and $\xi(X_{\cdot j}, W^n)$.

The above strategy can be directly generalized to the multiple rank case. However, it only works for the following prior without the ability for rank adaptation. To be specific, we assume the rank r is known. Then, the third step of the prior is modified as follows:

(3) Given S , sample an $|S| \times r$ matrix A_S , with each entry i.i.d. $N(0, 1)$. Let the matrix A be defined as

$$A = \begin{pmatrix} A_S \\ 0 \end{pmatrix}.$$

The covariance matrix is $\Gamma = AA^T + I$.

Note that instead of sampling an individual support S_l for each column of A , we sample a common support S for all columns. When $r \leq O(1)$, this will not be a problem because of the simple observation $rs \asymp s$. The theoretical justification of the prior is stated in Theorem 4.3. Denote the j th row of A by A_j^T . Then the posterior mean has formula

$$\mathbb{E}_\Pi(A_j | X^n) = \frac{\int N_{n,j}(W^n) \phi(W^n) dW^n}{\int D_n(W^n) \phi(W^n) dW^n},$$

where for each W^n , we have

$$D_n(W^n) = \sum_{q=1}^p \frac{\pi(q)}{\binom{p}{q}} \sum_{|S|=q} \prod_{j \notin S} \left\{ \prod_{i=1}^n \phi(X_{ij}) \right\} \\ \times \prod_{j \in S} \left\{ \int \prod_{i=1}^n \phi(X_{ij} - W_i^T A_j) \phi(A_j) dA_j \right\},$$

and a similar formula for $N_{n,j}(W^n)$. Note that the only difference from the rank-one case is the inner product $W_i^T A_j$. The notation W^n stands for (W_1, \dots, W_n) , where each W_i is an r -dimensional standard Gaussian vector. A similar formula holds for $N_{n,j}(W^n)$. Thus we can apply the same Monte Carlo approximation (4.4) for $\mathbb{E}_\Pi(A_j | X^n)$ as is done in the rank-one case.

In addition to our method, there are other methods proposed in the literature. A Gaussian shrinkage prior for Bayesian PCA have been developed by [Bishop \(1999a, 1999b\)](#) in the classical setting, but it is not appropriate for sparse PCA. More general shrinkage priors have been discussed in [Polson and Scott \(2011\)](#) and [Bhattacharya et al. \(2012\)](#) for high-dimensional mean vector estimation. One can extend the framework to sparse PCA and develop Gibbs sampling by taking advantage of the latent representation (2.1). We refer to [Pati et al. \(2014\)](#) and [van der Pas, Kleijn and van der Vaart \(2014\)](#) for some theoretical justifications of shrinkage priors.

4.3. Further remarks on the prior. The prior we proposed in Section 3 on the random covariance matrix $\Gamma = AA^T + I$ imposes orthogonality on the columns of A . The orthogonality constraint is convenient for creating an eigengap between the spikes and the noise. This leads to the rank adaptation (4.2). One may wonder if a simpler prior such as the one proposed in Section 4.2 without orthogonality constraint would also lead to a desired eigengap.

The answer is negative in the current proof technique. Let us consider the simplest case where the supports $S_{01}, S_{02}, \dots, S_{0r}$ are known and $S_{01} = S_{02} = \dots = S_{0r} = S_0$. When the rank r is not known, it is necessary to sample ξ according to some prior distribution. Then, after sampling the rank ξ , we only need to sample a $|S_0| \times \xi$ submatrix of A , with rows in S_0 . Let us denote the submatrix by A_{S_0} . Consider the prior distribution of A_{S_0} where each element follows i.i.d. $N(0, 1)$. Assume $r \leq s$ so that we can also restrict $\xi < s$. It is easy to see that the ξ th eigenvalue of the matrix $\Gamma = AA^T + I$ is $\lambda_{\min}(A_{S_0} A_{S_0}^T) + 1$. Hence the eigengap is $\lambda_{\min}(A_{S_0} A_{S_0}^T)$. For rank adaptation (4.2), we need a positive eigengap $\lambda_{\min}(A_{S_0} A_{S_0}^T) > 0$. By nonasymptotic random matrix theory [[Vershynin \(2010\)](#)],

$$(4.5) \quad \Pi(\lambda_{\min}(A_{S_0} A_{S_0}^T) > \sqrt{s} - \sqrt{\xi} - t|\xi) \geq 1 - 2e^{-t^2/2},$$

for any $t > 0$. For $\sqrt{s} - \sqrt{\xi} - t > 0$, t cannot be larger than \sqrt{s} , leading to a tail not smaller than $2 \exp(-s/2)$. In order that there is an eigengap under the posterior distribution, the desired tail needed in the classical Bayes nonparametric theory [see Barron (1999) and Castillo (2008)] is $\exp(-Cn\varepsilon^2) = \exp(-Crs \log p)$ for some $C > 0$. Hence the random matrix theory tail in (4.5) is not enough for our purpose, and the current proof technique does not lead to the desired posterior convergence for this simpler prior. One may consider a larger support S with $|S| \asymp rs \log p$ in the prior distribution, such that the tail probability in (4.5) is $\exp(-Crs \log p)$ for some $C > 0$. However, it can be shown that the prior does not have sufficient mass around the truth.

Nonetheless, if we assume the rank is known and $r \leq O(1)$, then rank adaptation is not needed. In this case, the prior in Section 4.2 leads to the desired posterior rate of convergence. Remember $\varepsilon^2 = \frac{s \log p}{n}$.

THEOREM 4.3. *Assume $\varepsilon \rightarrow 0$, $n \leq p^m$ and $r \leq m$ for some constant $m > 0$. Then there exists $M_{\gamma, K, m} > 0$, such that for any $M > M_{\kappa, K, m}$, we have*

$$\sup_{\Sigma \in \mathcal{G}(p, s, r)} P_{\Sigma}^n \Pi(\|V V^T - V_0 V_0^T\|_F > M\varepsilon | X^n) \leq \exp(-C_{(\kappa, K, m, M)} n \varepsilon^2),$$

for some constant $C_{(\kappa, K, m, M)} > 0$ only depending on (κ, K, m, M) .

It would be an interesting problem to consider whether new techniques can be developed to prove optimal posterior rate of convergence for a simpler prior when the rank r is not known.

5. Proofs. The results of Theorems 3.1 and 4.1 are special cases for bounding

$$(5.1) \quad P_{\Sigma}^n \Pi(B | X^n) = P_{\Sigma}^n \frac{N_n(B)}{D_n},$$

where $D_n = \int \frac{dP_{\Sigma}^n}{dP_{\Sigma}^n}(X^n) d\Pi(\Gamma)$ and $N_n(B) = \int_B \frac{dP_{\Sigma}^n}{dP_{\Sigma}^n}(X^n) d\Pi(\Gamma)$ for different B . To bound (5.1), it is sufficient to upper bound the numerator $N_n(B)$ and lower bound the denominator D_n . Following Barron, Schervish and Wasserman (1999) and Ghosal, Ghosh and van der Vaart (2000), this involves three steps:

(1) Show the prior Π puts sufficient mass near the truth; that is, we need

$$\Pi(K_n) \geq \exp(-Cn\varepsilon^2),$$

where $K_n = \{\Gamma : \frac{\|\Gamma - \Sigma\|_F}{\lambda_{\min}(\Gamma)} \leq \varepsilon\}$.

(2) Choose an appropriate subset \mathcal{F} , and show the prior is essentially supported on \mathcal{F} in the sense that

$$\Pi(\mathcal{F}^c) \leq \exp(-Cn\varepsilon^2).$$

This controls the complexity of the prior. Note that it is sufficient to have $\Pi(\mathcal{F}^c | X^n) \leq \exp(-Cn\varepsilon^2)$.

(3) Construct a testing function ϕ for the following testing problem:

$$H_0 : \Gamma = \Sigma, \quad H_1 : \Gamma \in B \cap \mathcal{F}.$$

We need to control the testing error in the sense that

$$P_\Sigma^n \phi \vee \sup_{\Gamma \in B \cap \mathcal{F}} P_\Gamma^n (1 - \phi) \leq \exp(-Cn\varepsilon^2).$$

Notice the constants C 's are different in the above three steps, and should satisfy some constraints in the proof. Step 1 lower bounds the prior concentration near the truth, which leads to a lower bound for D_n . In its original form [Schwartz (1965)], K_n is taken to be a fixed neighborhood of the truth defined through Kullback–Leibler divergence. Step 2 and step 3 are mainly for upper bounding $N_n(B)$. The testing idea in step 3 is initialized by Le Cam (1973) and Schwartz (1965). Step 2 goes back to Barron (1988), who proposes the idea to choose an appropriate \mathcal{F} to regularize the alternative hypothesis in the test; otherwise the testing function for step 3 may never exist; see Le Cam (1973) and Barron (1989).

We list key technical lemmas needed in the proof for all three steps as follows. From now on, all capital letters C with or without subscripts are absolute constants. They do not depend on other quantities unless otherwise mentioned.

LEMMA 5.1. *Assume $\varepsilon \rightarrow 0$. Then for any $b > 0$, we have*

$$P_\Sigma^n (D_n \leq \Pi(K_n) \exp(-(b + 1)n\varepsilon^2)) \leq \exp(-4C_2 b^2 K^{-1} n\varepsilon^2),$$

where $C_2 > 0$ is an absolute constant.

LEMMA 5.2. *Assume $\varepsilon \rightarrow 0$ and $r \vee \log n \leq m \log p$ for some $m > 0$. Then we have*

$$\Pi(K_n) \geq \exp(-(\gamma + 2 + mC_1 \log K + mC_1)n\varepsilon^2),$$

with some absolute constant $C_1 > 0$.

Lemma 5.1 lower bounds the denominator D_n . It is a general result for all Gaussian covariance matrix estimation problems. Lemma 5.2 lower bounds $\Pi(K_n)$ in step 1.

LEMMA 5.3. *Let $S = S_1 \cup \dots \cup S_\xi$. Assume $\varepsilon \rightarrow 0$. When $r \vee \log n \leq m \log p$ for some $m > 0$, we have*

$$P_\Sigma^n \Pi(|S| > \text{Ars} | X^n) \leq \exp\left(-\frac{\gamma A}{8} n\varepsilon^2\right) + \exp(-4C_2 K^{-1} n\varepsilon^2),$$

for any $A > 8\gamma^{-1}(\gamma + 4 + mC_1 \log K + mC_1)$.

Lemma 5.3 establishes the sparse property of the prior Π . It corresponds to step 2, where \mathcal{F} is the sparse subset $\{\Gamma : |S| \leq \text{Ars}\}$. Note that the parameter space we consider requires $\max_{1 \leq l \leq r} |S_{0l}| \leq s$. The sparsity constraint in \mathcal{F} is much weaker, which means \mathcal{F} is larger than the parameter space we consider. Since we only need \mathcal{F} to control the regularity of the parameters in the alternative for hypothesis testing in step 3, the oversized \mathcal{F} here does not cause a problem. In many Bayes nonparametric problems, the parameter space can be negligible compared with the set \mathcal{F} . Zhao (2000) provides an example where the parameter space receives no prior probability, while the set \mathcal{F} receives prior probability close to one; see also van der Vaart and van Zanten (2008).

LEMMA 5.4. *Assume $\varepsilon \rightarrow 0$. There exists some constant $M_{A,K,m}$ depending only on (A, K, m) , such that for any $M > M_{A,K,m}$, we have a testing function ϕ satisfying*

$$P_{\Sigma}^n \phi \leq 3 \exp\left(-\frac{C_3 M^2}{8K^2} n\varepsilon^2\right)$$

and

$$\sup_{\Gamma \in \{\Gamma : \|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars}\}} P_{\Gamma}^n (1 - \phi) \leq \exp\left(-\frac{C_3 M}{8} n\varepsilon^2\right).$$

The existence of a test and its error rates in step 3 are established in Lemma 5.4. These lemmas prove Theorem 4.1.

In order to prove Theorem 3.1, we need to establish a stronger testing procedure. Since we have the conclusion of Theorem 4.1, it is sufficient to consider the subset $\{\Gamma : \|\Sigma - \Gamma\| \leq M\varepsilon\}$. More specifically, we are going to test $\Sigma = V_0 \Lambda_0 V_0^T + I$ against the following alternative:

$$\mathcal{H}_1 = \{\Gamma = V \Lambda V^T + I : \|V V^T - V_0 V_0^T\|_F > M'\varepsilon, \xi = r, |S| \leq \text{Ars}\}.$$

Note that $S = S_1 \cup \dots \cup S_{\xi}$ is the joint support. The existence of the test is established by the following lemma.

LEMMA 5.5. *Assume $\varepsilon \rightarrow 0$, $r \vee \log n \leq m \log p$ and $r \leq ms$ for some absolute constant $m > 0$. There exists some constant $M'_{A,K,m}$ only depending on (A, K, m) , and for any $M' > M'_{A,K,m}$, we have a testing function ϕ such that*

$$P_{\Sigma}^n \phi \leq 3 \exp\left(-\frac{1}{8} C_5 \delta'_K \bar{M}^2 n\varepsilon^2\right)$$

and

$$\sup_{\Gamma \in \mathcal{H}_1} P_{\Gamma}^n (1 - \phi) \leq 2 \exp(-C_5 \delta'_K \bar{M}^2 n\varepsilon^2),$$

where $\bar{M} = 2^{-3/2} K^{-1} M'$, δ'_K only depending on K , and C_5 is an absolute constant.

We are going to develop the proofs in several parts. In Section 5.1, we establish the main results based on the key lemmas above. All key lemmas are proved in the later sections. In Section 5.2, we prove Lemma 5.2, which is for the prior concentration (step 1). In Section 5.3, we prove Lemma 5.3 by showing that the prior puts most mass on a sparse set (step 2). Sections 5.4 and 5.5 are devoted in proving Lemmas 5.4 and 5.5, respectively (step 3). The proof of Lemma 5.1 is stated in supplementary material [Gao and Zhou (2015)].

5.1. *Proofs of the main results.* In this section we prove Theorems 3.1 and 4.1. Since the proof of Theorem 3.1 depends on the conclusion of Theorem 4.1, we prove the latter one first.

5.1.1. *Proof of Theorem 4.1.* We decompose the posterior by

$\Pi(\|\Gamma - \Sigma\| > M\varepsilon | X^n) \leq \Pi(\|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars} | X^n) + \Pi(|S| > \text{Ars} | X^n)$,
 where $S = S_1 \cup \dots \cup S_\xi$. By Lemma 5.3, we have

$$P_\Sigma^n \Pi(|S| > \text{Ars} | X^n) \leq \exp(-\gamma A n \varepsilon^2 / 8) + \exp(-4C_2 K^{-1} n \varepsilon^2),$$

for any $A > 8\gamma^{-1}(\gamma + 4 + mC_1 \log K + mC_1)$. From now on, we fix A to be $A = 9\gamma^{-1}(\gamma + 4 + mC_1 \log K + mC_1)$. Then it is sufficient to bound

$$P_\Sigma^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars} | X^n).$$

Let ϕ be the testing function in Lemma 5.4, and we have

$$\begin{aligned} & P_\Sigma^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars} | X^n) \\ & \leq P_\Sigma^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars} | X^n) \{D_n > \Pi(K_n) \exp(-2n\varepsilon^2)\} (1 - \phi) \\ & \quad + P_\Sigma^n \phi + P_\Sigma^n (D_n < \Pi(K_n) \exp(-2n\varepsilon^2)). \end{aligned}$$

There are three terms on the right-hand side above. By Lemma 5.4, $P_\Sigma^n \phi \leq 3 \exp(-\frac{C_3 M^2}{8K^2} n \varepsilon^2)$ for sufficiently large M . By Lemma 5.1, we have $P_\Sigma^n (D_n < \Pi(K_n) \exp(-2n\varepsilon^2)) \leq \exp(-4C_2 K^{-1} n \varepsilon^2)$. Now it remains to bound the first term. Let $H_1 = \{\Gamma : \|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars}\}$. We have

$$\begin{aligned} & P_\Sigma^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon, |S| \leq \text{Ars} | X^n) \{D_n > \Pi(K_n) \exp(-2n\varepsilon^2)\} (1 - \phi) \\ & = P_\Sigma^n \left(\left(\int_{H_1} \frac{dP_\Gamma^n}{dP_\Sigma^n} d\Pi(\Gamma) / D_n \right) \{D_n > \Pi(K_n) \exp(-2n\varepsilon^2)\} (1 - \phi) \right) \\ & \leq \frac{\exp(2n\varepsilon^2)}{\Pi(K_n)} P_\Sigma^n \int_{H_1} \frac{dP_\Gamma^n}{dP_\Sigma^n} (1 - \phi) d\Pi(\Gamma) \\ & = \frac{\exp(2n\varepsilon^2)}{\Pi(K_n)} \int_{H_1} P_\Gamma^n (1 - \phi) d\Pi(\Gamma) \\ & \leq \frac{\exp(2n\varepsilon^2)}{\Pi(K_n)} \sup_{\Gamma \in H_1} P_\Gamma^n (1 - \phi), \end{aligned}$$

which is bounded by $\exp(-\frac{C_3 M}{16} n \varepsilon^2)$ because $\sup_{\Gamma \in H_1} P_\Gamma^n (1 - \phi)$ is upper bounded by Lemma 5.4, and $\Pi(K_n)$ is lower bounded by Lemma 5.2 for sufficiently large M . By summing up the error probability, we have

$$P_\Sigma^n \Pi(\|\Gamma - \Sigma\| > M\varepsilon | X^n) \leq \exp(-C_{(\gamma, K, m, M)} n \varepsilon^2),$$

for some constant $C_{(\gamma, K, m, M)}$ only depending on (γ, K, m, M) .

To obtain the rest of the results, it is sufficient to prove

$$(5.2) \quad \{\|\Gamma - \Sigma\| \leq M\varepsilon\} \subset \{\xi = r\}$$

and

$$(5.3) \quad \{\|\Gamma - \Sigma\| \leq M\varepsilon\} \subset \{\|VV^T - V_0V_0^T\| \leq KM\varepsilon\}.$$

Note that

$$\Gamma = \sum_{l=1}^{\xi} \eta_l \eta_l^T + I,$$

and the eigenvalues of the covariance Γ are $(\|\eta_1\|^2 + 1, \dots, \|\eta_\xi\|^2 + 1, 1, \dots, 1)$, where the first ξ eigenvalues are in the range $[(2K)^{-1} + 1, (2K) + 1]$ as specified by the prior. Similarly, the eigenvalues of the covariance Σ are $(\|\theta_1\|^2 + 1, \dots, \|\theta_r\|^2 + 1, 1, \dots, 1)$, and the first r eigenvalues are in the range $[K^{-1} + 1, K + 1]$. Suppose $r < \xi$, let $v \in \text{span}(V) \cap \text{span}(V_0)^\perp$ and $\|v\| = 1$. Then $v^T \Sigma v = 1$ and $v^T \Gamma v \geq \lambda_\xi(\Gamma) \geq 1 + (2K)^{-1}$, which contradicts $\|\Gamma - \Sigma\| \leq M\varepsilon$. The same argument leads to contradiction when $r > \xi$. Thus we must have $\xi = r$ when $\|\Gamma - \Sigma\| \leq M\varepsilon$.

Finally, (5.3) is an immediate consequence of the Davis–Kahan sin-theta theorem (Lemma 5.11). It is easy to check that the eigengap δ in Lemma 5.11 is K^{-1} .

5.1.2. *Proof of Theorem 3.1.* With the results from Lemma 5.3 and Theorem 4.1, we decompose the posterior distribution as follows:

$$\begin{aligned} & \Pi(\|VV^T - V_0V_0\|_F > M'\varepsilon | X^n) \\ & \leq \Pi(\|VV^T - V_0V_0\|_F > M'\varepsilon, \|\Gamma - \Sigma\| \leq M\varepsilon, |S| \leq \text{Ars} | X^n) \\ & \quad + \Pi(\|\Gamma - \Sigma\| > M\varepsilon | X^n) + \Pi(|S| > \text{Ars} | X^n) \\ & \leq \Pi(\|VV^T - V_0V_0\|_F > M'\varepsilon, \xi = r, |S| \leq \text{Ars} | X^n) \\ & \quad + \Pi(\|\Gamma - \Sigma\| > M\varepsilon | X^n) + \Pi(|S| > \text{Ars} | X^n), \end{aligned}$$

where the last inequality is due to (5.2). Note that the later two terms converge to zero, as shown in Lemma 5.3 and Theorem 4.1. Therefore, we only need to bound

$$P_\Sigma^n \Pi(\|VV^T - V_0V_0\|_F > M'\varepsilon, \xi = r, |S| \leq \text{Ars} | X^n).$$

Remembering the definition of \mathcal{H}_1 , then, by Lemma 5.5, there exists a testing function ϕ for \mathcal{H}_1 with the desired error bound. Using a similar argument as in the proof of Theorem 4.1, we have established Theorem 3.1.

5.2. *The prior concentration of Π .* We prove Lemma 5.2 in this section. The main strategy for proving Lemma 5.2 is to explore the structure of the prior. Specifically, since the prior Π is defined by a sampling procedure for η_{l+1} conditioning on $\text{span}\{\eta_1, \dots, \eta_l\}$, we need to take advantage of this feature by using the chain rule and conditional independence.

PROOF OF LEMMA 5.2. Since $\lambda_{\min}(\Gamma) \geq 1$, we have

$$\frac{\|\Gamma - \Sigma\|_F}{\lambda_{\min}(\Gamma)} \leq \|\Gamma - \Sigma\|_F.$$

Write

$$\begin{aligned} &\Pi(\|\Gamma - \Sigma\|_F \leq \varepsilon) \\ &\geq \Pi(\|\Gamma - \Sigma\|_F \leq \varepsilon | (S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)) \\ &\quad \times \Pi((S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)). \end{aligned}$$

The second term in the above product is

$$\begin{aligned} &\Pi((S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)) \\ &\geq \prod_{l=1}^r \Pi(S_l = S_{0l}) \prod_{l=r+1}^{\lfloor p^{\gamma/2} \rfloor} \left(1 - \frac{1}{p^{\gamma+1}}\right)^p \\ &\geq \left(1 - \frac{1}{p^{\gamma+1}}\right)^{p^{1+\gamma/2}} \prod_{l=1}^r \left(\frac{1}{p^{\gamma+1}}\right)^{|S_{0l}|} \\ &\geq \exp(-2p^{-\gamma/2}) p^{-rs(\gamma+1)} \\ &\geq \exp(-(\gamma + 2)rs \log p) \end{aligned}$$

because $p^{-\gamma/2}$ is at a smaller order of $rs \log p$. Then we lower bound

$$\Pi(\|\Gamma - \Sigma\|_F \leq \varepsilon | (S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)).$$

When $(S_1, \dots, S_{\lfloor p^{\gamma/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)$, we have

$$\begin{aligned} \|\Gamma - \Sigma\|_F &= \left\| \sum_{l=1}^r \eta_l \eta_l^T - \sum_{l=1}^r \theta_l \theta_l^T \right\|_F \leq \sum_{l=1}^r \|\eta_l \eta_l^T - \theta_l \theta_l^T\|_F \\ &= \sum_{l=1}^r \|\eta_{l, S_{0l}} \eta_{l, S_{0l}}^T - \theta_{l, S_{0l}} \theta_{l, S_{0l}}^T\|_F \\ &\leq \sum_{l=1}^r \|\eta_{l, S_{0l}} - \theta_{l, S_{0l}}\| (\|\theta_{l, S_{0l}}\|_\infty + \|\eta_{l, S_{0l}}\|_\infty) \\ &\leq (\sqrt{2} + 1) K^{1/2} \sum_{l=1}^r \|\eta_{l, S_{0l}} - \theta_{l, S_{0l}}\|. \end{aligned}$$

We use the notation G to represent the probability $G_{(S_1, \dots, S_r)}$ defined in Section 3. By conditional independence, we have

$$\begin{aligned} \Pi(\|\Gamma - \Sigma\|_F \leq \varepsilon | (S_1, \dots, S_{\lfloor p^{r/2} \rfloor}) = (S_{01}, \dots, S_{0r}, \emptyset, \dots, \emptyset)) \\ = G\left(\left\|\sum_{l=1}^r \eta \eta^T - \sum_{l=1}^r \theta \theta^T\right\|_F \leq \varepsilon\right) \\ \geq G\left((\sqrt{2} + 1)K^{1/2} \sum_{l=1}^r \|\eta_{l, S_{0l}} - \theta_{l, S_{0l}}\| \leq \varepsilon\right) \\ \geq G((\sqrt{2} + 1)K^{1/2} \|\eta_{l, S_{0l}} - \theta_{l, S_{0l}}\| \leq \varepsilon_l, l = 1, \dots, r), \end{aligned}$$

where $\sum_{l=1}^r \varepsilon_l \leq \varepsilon$. In particular, we choose

$$\varepsilon_i = c(r, \varepsilon)(3\sqrt{2}K)^i, \quad i = 1, \dots, r,$$

with $c(r, \varepsilon) = \frac{2}{3}\varepsilon(3\sqrt{2}K)^{-r}$. Then as long as $K \geq 1$, we have

$$K \sum_{i=1}^l \varepsilon_i \leq \frac{1}{2}\varepsilon_{l+1}$$

and

$$\sum_{i=1}^r \varepsilon_i \leq \varepsilon.$$

Define $\mathcal{T}_l = \bigcap_{i=1}^l \mathcal{U}_i$ with

$$\mathcal{U}_i = \{(\sqrt{2} + 1)K^{1/2} \|\eta_{i, S_{0i}} - \theta_{i, S_{0i}}\| \leq \varepsilon_i\} \quad \text{for } i = 1, \dots, r.$$

Using the chain rule, we have

$$G(\mathcal{T}_r) = G(\mathcal{U}_1) \prod_{l=1}^{r-1} G(\mathcal{T}_{l+1} | \mathcal{T}_l).$$

For each $G(\mathcal{T}_l | \mathcal{T}_{l-1})$, we present a lower bound and prove it in the supplementary material [Gao and Zhou (2015)].

PROPOSITION 5.1. *For each $l = 1, 2, \dots, r - 1$, we have*

$$\begin{aligned} G(\mathcal{T}_{l+1} | \mathcal{T}_l) &\geq \frac{c(r, \varepsilon)}{2(2 + \sqrt{2})e^{K/2}} (3\sqrt{2}K)^{l+1} \\ &\quad \times \exp\left(-s \log \frac{(4\sqrt{2} + 1)K^{1/2}}{c(r, \varepsilon)} - s \log(2\sqrt{s}/3)\right). \end{aligned}$$

Moreover, $G(\mathcal{U}_1)$ can be lower bounded by the above formula with $l = 0$.

Using this result, we have

$$\begin{aligned}
 G(\mathcal{U}_1) \prod_{l=1}^{r-1} G(\mathcal{T}_{l+1}|\mathcal{T}_l) &\geq \left(\frac{c(r, \varepsilon)}{2(2 + \sqrt{2})e^{K/2}} \right)^r (3\sqrt{2}K)^{r(r+1)/2} \\
 &\quad \times \exp\left(-rs \log \frac{(4\sqrt{2} + 1)K^{1/2}}{c(r, \varepsilon)} - C_1rs \log s \right) \\
 &\geq \exp\left(-C_1r^2s \log K - C_1rs \log \frac{1}{\varepsilon} - C_1rs \log s \right),
 \end{aligned}$$

for some absolute constant $C_1 > 0$ when $\frac{K}{\log K} \leq rs$. Therefore, we have

$$\begin{aligned}
 \Pi\left(\frac{\|\Gamma - \Sigma\|_F}{\lambda_{\min}(\Gamma)} \leq \varepsilon \right) \\
 \geq \exp\left(-(\gamma + 2)rs \log p - C_1r^2s \log K - C_1rs \log \frac{1}{\varepsilon} - C_1rs \log s \right).
 \end{aligned}$$

Since

$$\varepsilon^2 = \frac{rs \log p}{n},$$

we have

$$\Pi\left(\frac{\|\Gamma - \Sigma\|_F}{\lambda_{\min}(\Gamma)} \leq \varepsilon \right) \geq \exp(-(\gamma + 2 + mC_1 \log K + mC_1)n\varepsilon^2),$$

under the assumption $r \vee \log n \leq m \log p$ for some constant $m > 0$. \square

5.3. *The sparsity of Π .* We prove Lemma 5.3 in this section. The result is implied by the prior sparsity stated in the following lemma.

LEMMA 5.6. *For the sparsity prior specified above, we have for any $A > 0$,*

$$\Pi(|S_1 \cup \dots \cup S_\xi| \geq Ars) \leq \exp\left(-\frac{A\gamma}{4}rs \log p \right).$$

PROOF OF LEMMA 5.6. First, we have

$$\Pi(|S_1 \cup \dots \cup S_\xi| > Ars) \leq \Pi(|S_1 \cup \dots \cup S_{\lfloor p^{\gamma/2} \rfloor}| > Ars).$$

Note that there is a slight abuse of notation above. The $\{S_l\}_{l=1}^\xi$ on the left-hand side are from $\{S_l\}_{l=1}^{\lfloor p^{\gamma/2} \rfloor}$ on the right-hand side by excluding those S_l with $\eta_l = 0$. Let $B = |S_1 \cup \dots \cup S_{\lfloor p^{\gamma/2} \rfloor}|$. Note that B is a Binomial random variable with parameter

α satisfying $\alpha \leq p^{-1-\gamma/2}$. Therefore,

$$\begin{aligned} \Pi(B > \text{Ars}) &\leq \sum_{k=[\text{Ars}]}^p \binom{p}{k} \alpha^k (1-\alpha)^{p-k} \leq \sum_{k=[\text{Ars}]}^p \binom{p}{k} \alpha^k \\ &\leq \sum_{k=[\text{Ars}]}^p \exp(k \log p) (p^{-1-\gamma/2})^k \\ &\leq \sum_{k=[\text{Ars}]}^p \exp\left(-k \frac{\gamma}{2} \log p\right) \leq \exp\left(-\frac{A\gamma}{4} r s \log p\right). \end{aligned}$$

Thus the proof is complete. \square

Now we are ready to prove Lemma 5.3 by upper bounding the numerator and lower bounding the denominator of $\Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars} | X)$. This can be done by combining the results of Lemmas 5.6, 5.1 and 5.2.

PROOF OF LEMMA 5.3. Since $D_n = \int \frac{dP_\Gamma^n}{dP_\Sigma^n}(X) d\Pi(\Gamma)$ and $K_n = \{\frac{\|\Gamma - \Sigma\|_F}{\lambda_{\min}(\Gamma)} \leq \varepsilon\}$, we have

$$\begin{aligned} &P_\Sigma^n \Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars} | X) \\ &\leq P_\Sigma^n \Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars} | X) \{D_n \geq \Pi(K_n) \exp(-(b+1)n\varepsilon^2)\} \\ &\quad + P_\Sigma^n \{D_n \leq \Pi(K_n) \exp(-(b+1)n\varepsilon^2)\} \\ &\leq \frac{\exp((b+1)n\varepsilon^2)}{\Pi(K_n)} P_\Sigma^n \int_{|S_1 \cup \dots \cup S_\xi| > \text{Ars}} \frac{dP_\Gamma^n}{dP_\Sigma^n}(X) d\Pi(\Gamma) \\ &\quad + \exp(-4C_2 K^{-1} b^2 n\varepsilon^2) \\ &\leq \exp((b+1)n\varepsilon^2) \frac{\Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars})}{\Pi(K_n)} + \exp(-4C_2 K^{-1} b^2 n\varepsilon^2), \end{aligned}$$

where we have used Lemma 5.1. Using Lemmas 5.6 and Lemma 5.2, we have

$$\frac{\Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars})}{\Pi(K_n)} \leq \exp\left(-\left(\frac{A\gamma}{4} - (\gamma + 2 + mC_1 \log K + mC_1)\right)n\varepsilon^2\right).$$

Hence by choosing $b = 1$, we have

$$\begin{aligned} &P_\Sigma^n \Pi(|S_1 \cup \dots \cup S_\xi| > \text{Ars} | X) \\ &\leq \exp\left(-\left(\frac{A\gamma}{4} - (\gamma + 4 + mC_1 \log K + mC_1)\right)n\varepsilon^2\right) \\ &\quad + \exp(-4C_2 K^{-1} n\varepsilon^2). \end{aligned}$$

The conclusion then follows by letting $A > 8\gamma^{-1}(\gamma + 4 + mC_1 \log K + mC_1)$. \square

5.4. *Testing in spectral norm.* We prove Lemma 5.4 in this section. Because of the constraint $|S_1 \cup \dots \cup S_\xi| \leq \text{Ars}$, we can break the testing problem into many low-dimensional testing problems. Then a final test can be constructed by combining the small tests. The following lemma establishes the existence of such a low-dimensional test and bounds its error probability.

LEMMA 5.7. *For the random variable $Y^n = (Y_1, \dots, Y_n)$ in \mathbb{R}^d and any $M > 0$, there exists a testing function ϕ , such that*

$$\begin{aligned}
 P_{\bar{\Sigma}}^n \phi(Y^n) &\leq \exp\left(C_3 d - \frac{C_3 M^2}{4 \|\bar{\Sigma}\|^2} n \varepsilon^2\right) + 2 \exp(C_3 d - C_3 M^{1/2} n), \\
 \sup_{\{\bar{\Gamma} : \|\bar{\Gamma} - \bar{\Sigma}\| > M \varepsilon\}} P_{\bar{\Gamma}}^n(1 - \phi(Y^n)) &\leq \exp\left(C_3 d - \frac{C_3 M n \varepsilon^2}{4} \max\left\{1, \frac{M}{(M^{1/2} + 2)^2 \|\bar{\Sigma}\|^2}\right\}\right),
 \end{aligned}$$

with some absolute constant $C_3 > 0$.

Notice $\bar{\Sigma}$ is a general $d \times d$ covariance matrix for some d . It will be specified in the proof of Lemma 5.4. To prove Lemma 5.7, we need the following random matrix inequality. Its proof is given in the supplementary material [Gao and Zhou (2015)].

LEMMA 5.8. *Let Y_1, \dots, Y_n be i.i.d. from $N(0, \bar{\Sigma})$, where $\bar{\Sigma}$ is a $d \times d$ covariance matrix. Let $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T$ be the sample covariance matrix, and then there is an absolute constant $C_3 > 0$, such that for any $t > 0$,*

$$P_{\bar{\Sigma}}^n(\|\hat{\Sigma} - \bar{\Sigma}\| > t \|\bar{\Sigma}\|) \leq \exp(-C_3(-d + n(t \wedge t^2))).$$

PROOF OF LEMMA 5.7. Denote the alternative set by $H_1 = \{\bar{\Gamma} : \|\bar{\Gamma} - \bar{\Sigma}\| > M \varepsilon\}$, and then it will have following decomposition:

$$H_1 \subset \bigcup_{j=0}^{\infty} H_{1j},$$

where

$$H_{10} = \{\|\bar{\Gamma} - \bar{\Sigma}\| > M \varepsilon, \|\bar{\Gamma}\| \leq (M^{1/2} + 2) \|\bar{\Sigma}\|\},$$

and for $j \geq 1$,

$$H_{1j} = \{(M^{1/2} + 2)(M \varepsilon^2)^{-(j-1)/2} \|\bar{\Sigma}\| < \|\bar{\Gamma}\| \leq (M^{1/2} + 2)(M \varepsilon^2)^{-j/2} \|\bar{\Sigma}\|\}.$$

We divide the alternative set into pieces so that the spectral norm of $\bar{\Gamma}$ is bounded in each piece. For the prior in Section 3, this is not needed because the prior only samples a random covariance matrix with bounded spectrum. However, the prior in Section 4.2 does not impose a bounded spectrum constraint. The strategy for dividing the alternative set is general for both cases.

We test each alternative hypothesis separately and then combine the test and use the union bound to control the error. To test against H_{10} , we use

$$\phi_0 = \mathbb{I} \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Sigma} \right\| > M\varepsilon/2 \right\}.$$

To test against H_{1j} , we use

$$\phi_j = \mathbb{I} \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T \right\| > \frac{M^{1/2} + 2}{2} \|\bar{\Sigma}\| (M\varepsilon^2)^{-(j-1)/2} \right\}.$$

From Lemma 5.8, we have

$$P_{\bar{\Sigma}}^n \phi_0 \leq \exp \left(C_3 d - \frac{C_3 M^2}{4 \|\bar{\Sigma}\|^2} n \varepsilon^2 \right)$$

and

$$\begin{aligned} P_{\bar{\Sigma}}^n \phi_j &\leq P_{\bar{\Sigma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Sigma} \right\| + \|\bar{\Sigma}\| > \frac{M^{1/2} + 2}{2} \|\bar{\Sigma}\| (M\varepsilon^2)^{-(j-1)/2} \right\} \\ &\leq P_{\bar{\Sigma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Sigma} \right\| > \frac{M^{1/2}}{2} \|\bar{\Sigma}\| (M\varepsilon^2)^{-(j-1)/2} \right\} \\ &\leq \exp(C_3 d - C_3 M^{1-j/2} n \varepsilon^{-(j-1)}). \end{aligned}$$

Next, we control the type II error. For any $\bar{\Gamma} \in H_{10}$, we have

$$\begin{aligned} P_{\bar{\Gamma}}^n (1 - \phi_0) &\leq P_{\bar{\Gamma}}^n \left\{ \|\bar{\Gamma} - \bar{\Sigma}\| - \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| < M\varepsilon/2 \right\} \\ &\leq P_{\bar{\Gamma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| > M\varepsilon/2 \right\} \\ &\leq P_{\bar{\Gamma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| > \|\bar{\Gamma}\| \frac{M\varepsilon}{2(M^{1/2} + 2)\|\bar{\Sigma}\|} \right\} \\ &\leq \exp \left(C_3 d - \frac{C_3 M^2}{4(M^{1/2} + 2)^2 \|\bar{\Sigma}\|^2} n \varepsilon^2 \right). \end{aligned}$$

For any H_{1j} , we have

$$\begin{aligned} P_{\bar{\Gamma}}^n(1 - \phi_j) &\leq P_{\bar{\Gamma}}^n \left\{ \|\bar{\Gamma}\| - \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| < \frac{M^{1/2} + 2}{2} \|\bar{\Sigma}\| (M\varepsilon^2)^{-(j-1)/2} \right\} \\ &\leq P_{\bar{\Gamma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| > \frac{M^{1/2} + 2}{2} \|\bar{\Sigma}\| (M\varepsilon^2)^{-(j-1)/2} \right\} \\ &\leq P_{\bar{\Gamma}}^n \left\{ \left\| \frac{1}{n} \sum_{i=1}^n Y_i Y_i^T - \bar{\Gamma} \right\| > \|\bar{\Gamma}\| M^{1/2} \varepsilon / 2 \right\} \\ &\leq \exp\left(C_3 d - \frac{C_3 M}{4} n \varepsilon^2\right). \end{aligned}$$

Now we combine the test by $\phi = \max_{0 \leq j \leq \infty} \phi_j$. The error of the combined test can be bounded by

$$\begin{aligned} P_{\bar{\Sigma}}^n \phi &\leq \sum_{j=0}^{\infty} P_{\bar{\Sigma}}^n \phi_j \\ &\leq \exp\left(C_3 d - \frac{C_3 M^2}{4 \|\bar{\Sigma}\|^2} n \varepsilon^2\right) + \exp(C_3 d) \sum_{j=1}^{\infty} \exp\left(-C_3 M n \varepsilon \left(\frac{1}{M^{1/2} \varepsilon}\right)^j\right) \\ &\leq \exp\left(C_3 d - \frac{C_3 M^2}{4 \|\bar{\Sigma}\|^2} n \varepsilon^2\right) + \exp(C_3 d) \sum_{j=1}^{\infty} \exp\left(-j C_3 M n \varepsilon \left(\frac{1}{M^{1/2} \varepsilon}\right)\right) \\ &\leq \exp\left(C_3 d - \frac{C_3 M^2}{4 \|\bar{\Sigma}\|^2} n \varepsilon^2\right) + 2 \exp(C_3 d - C_3 M^{1/2} n) \end{aligned}$$

and

$$\begin{aligned} P_{\bar{\Gamma}}^n(1 - \phi) &\leq P_{\bar{\Gamma}}^n \min_j (1 - \phi_j) \\ &\leq \exp\left(C_3 d - \frac{C_3 M n \varepsilon^2}{4} \max\left\{1, \frac{M}{(M^{1/2} + 2)^2 \|\bar{\Sigma}\|^2}\right\}\right). \end{aligned}$$

Thus the proof is complete. \square

To prove Lemma 5.4, we combine the small tests and control the error by union bound.

PROOF OF LEMMA 5.4. We denote the alternative set by

$$H_1 = \{\Gamma : \|\Gamma - \Sigma\| > M\varepsilon, |S_1 \cup \dots \cup S_{\xi}| < \text{Ars}\}.$$

Define $S = S_1 \cup \dots \cup S_\xi$ and $S_0 = S_{01} \cup \dots \cup S_{0r}$. We decompose H_1 by

$$H_1 \subset \bigcup_{B: |B| < \text{Ars}} H_{1,B},$$

where $H_{1,B} = \{\Gamma: \|\Gamma - \Sigma\| > M\varepsilon, S = B\}$. Define $\bar{B} = S \cup S_0$, and it is easy to see that

$$\|\Gamma - \Sigma\| = \|\bar{\Gamma} - \bar{\Sigma}\|,$$

where

$$\bar{\Gamma} = \sum_{l=1}^{\xi} \eta_{l,\bar{B}} \eta_{l,\bar{B}}^T + I, \quad \bar{\Sigma} = \sum_{l=1}^r \theta_{l,\bar{B}} \theta_{l,\bar{B}}^T + I.$$

Thus it is sufficient to test the following sub-problem in $\mathbb{R}^{\bar{B}}$ for each B :

$$H'_0: \bar{\Gamma} = \bar{\Sigma}, \quad H'_{1,B}: \|\bar{\Gamma} - \bar{\Sigma}\| > M\varepsilon.$$

By Lemma 5.7, there exists ϕ_B depending on the observations $(Y_1, \dots, Y_n) = (X_{1,\bar{B}}, \dots, X_{n,\bar{B}})$, such that

$$\begin{aligned} P_{\Sigma}^n \phi_B &\leq \exp\left(C_3(A+1)rs - \frac{C_3 M^2}{4K^2} n\varepsilon^2\right) \\ &\quad + 2 \exp(C_3(A+1)rs - C_3 M^{1/2} n) \\ &\leq 3 \exp\left(-C_3\left(\frac{M^2}{4K^2} - (A+1)\right) n\varepsilon^2\right), \end{aligned}$$

$$\begin{aligned} \sup_{\Gamma \in H_{1,B}} P_{\Gamma}^n (1 - \phi_B) &\leq \exp\left(C_3(A+1)rs - \frac{C_3 M n \varepsilon^2}{4} \max\left\{1, \frac{M}{(M^{1/2} + 2)^2 K^2}\right\}\right) \\ &\leq \exp\left(-C_3\left(\frac{M}{4} - (A+1)\right) n\varepsilon^2\right). \end{aligned}$$

Then we combine the tests by $\phi = \max_B \phi_B$. By the union bound, we have

$$\begin{aligned} P_{\Sigma}^n \phi &\leq \left(\sum_{q=1}^{[\text{Ars}]} \binom{p}{q}\right) 3 \exp\left(-C_3\left(\frac{M^2}{4K^2} - (A+1)\right) n\varepsilon^2\right) \\ &\leq 3 \text{Ars} \exp\left(\text{Ars} \log \frac{ep}{\text{Ars}}\right) \exp\left(-C_3\left(\frac{M^2}{4K^2} - (A+1)\right) n\varepsilon^2\right) \\ &\leq 3 \exp(2 \text{Ars} \log p) \exp\left(-C_3\left(\frac{M^2}{4K^2} - (A+1)\right) n\varepsilon^2\right) \\ &\leq 3 \exp\left(-\left(\frac{C_3 M^2}{4K^2} - C_3(A+1) - 2A\right) n\varepsilon^2\right) \end{aligned}$$

and

$$\sup_{\Gamma \in H_1} P_\Gamma^n(1 - \phi) \leq \exp\left(-C_3\left(\frac{M}{4} - (A + 1)\right)n\epsilon^2\right).$$

Hence the proof is complete by choosing sufficiently large M . \square

5.5. *Testing in subspace distance $d(\cdot, \cdot)$.* We prove Lemma 5.5 in this section. At first thought, there seems to be no obvious test for testing the subspace projection matrix under the distance $d(\cdot, \cdot)$ due to the complicated sparse and low-rank structure. Our strategy is to break the alternative set into many levels and pieces. The goal is that for each piece, it is a low-dimensional small testing problem in the following form:

$$H_0: \bar{\Gamma} = \bar{\Sigma}, \quad H_1: \|\bar{\Gamma} - \bar{\Gamma}'\|_F \leq \delta_K \|\bar{\Sigma} - \bar{\Gamma}'\|_F.$$

The small testing problem can be solved by considering the likelihood ratio test. The error bound is stated in the following lemma. Its proof is given in the supplementary material [Gao and Zhou (2015)].

LEMMA 5.9. *Consider observations $Y^n = (Y_1, \dots, Y_n)$ in \mathbb{R}^d . There exist constants δ_K and δ'_K only depending on K , and a testing function ϕ such that*

$$P_{\bar{\Sigma}}^n \phi(Y^n) \leq 2 \exp(-C_5 \delta'_K n \|\bar{\Sigma} - \bar{\Gamma}'\|_F^2),$$

$$\sup_{\{\bar{\Gamma}: \|\bar{\Gamma} - \bar{\Gamma}'\|_F \leq \delta_K \|\bar{\Sigma} - \bar{\Gamma}'\|_F\}} P_{\bar{\Gamma}}^n(1 - \phi(Y^n)) \leq 2 \exp(-C_5 \delta'_K n \|\bar{\Sigma} - \bar{\Gamma}'\|_F^2),$$

where $C_5 > 0$ is an absolute constant.

We need a lemma to bound the covering number under different subspace distances. We use $N(\delta, \mathcal{H}, \rho)$ to denote the δ -covering number of \mathcal{H} under the distance ρ . The proof of Lemma 5.10 is given in the supplementary material [Gao and Zhou (2015)].

LEMMA 5.10. *For any $U \in \mathcal{U}(d, r)$, $R_1, R_2 > 0$ and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_r)$ with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r$, we have*

$$\log N(R_1 \epsilon, \{V \in \mathcal{U}(d, r) : d(U, V) \leq R_2 \epsilon\}, d_\Lambda)$$

$$\leq dr \log\left(\frac{12\lambda_1(R_2 + 1)}{R_1}\right) + r^2 \log \frac{6\sqrt{r}}{\epsilon}.$$

Last but not least, we need the following sin-theta theorem to bound the difference of subspaces by the difference of matrices.

LEMMA 5.11 [Davis and Kahan (1970)]. Consider symmetric matrices F and \hat{F} , with eigenvalue decomposition

$$F = U_1 D_1 U_1^T + U_2 D_2 U_2^T, \quad \hat{F} = \hat{U}_1 \hat{D}_1 \hat{U}_1^T + \hat{U}_2 \hat{D}_2 \hat{U}_2^T.$$

If the eigenvalues D_1 are contained in an interval (a, b) , and the eigenvalues \hat{D}_2 are excluded from the interval $(a - \delta, b + \delta)$ for some $\delta > 0$, then

$$\|U_1 U_1^T - \hat{U}_1 \hat{U}_1^T\|_F \leq \sqrt{2} \delta^{-1} \|F - \hat{F}\|_F$$

and

$$\|U_1 U_1^T - \hat{U}_1 \hat{U}_1^T\| \leq \delta^{-1} \|F - \hat{F}\|.$$

PROOF OF LEMMA 5.5. The proof has two major steps.

Step 1: Decompose the alternative set into many levels and pieces. We first decompose \mathcal{H}_1 by $\mathcal{H}_1 \subset \bigcup_{B: |F| \leq A r s} H_{1,B}$, where

$$H_{1,B} = \{\Gamma = V \Lambda V^T + I : \|V V^T - V_0 V_0^T\|_F > M' \varepsilon, \xi = r, S = B\}.$$

Define $\bar{B} = B \cup S_0$ with $S_0 = S_{01} \cup \dots \cup S_{0r}$, and

$$V_{\bar{B}} = [\|\eta_{1,\bar{B}}\|^{-1} \eta_{1,\bar{B}}, \dots, \|\eta_{r,\bar{B}}\|^{-1} \eta_{r,\bar{B}}],$$

$$V_{0,\bar{B}} = [\|\theta_{1,\bar{B}}\|^{-1} \theta_{1,\bar{B}}, \dots, \|\theta_{r,\bar{B}}\|^{-1} \theta_{r,\bar{B}}].$$

Note that both $V_{\bar{B}}$ and $V_{0,\bar{B}}$ are $|\bar{B}| \times r$ matrices with $|\bar{B}| \leq (A + 1) r s$, and $\|V V^T - V_0 V_0^T\|_F = \|V_{\bar{B}} V_{\bar{B}}^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F$. Then we can rewrite $H_{1,B}$ as

$$H_{1,B} = \{\Gamma = V \Lambda V^T + I : \|V_{\bar{B}} V_{\bar{B}}^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F > M' \varepsilon\},$$

where we omit $\xi = r$ for simplicity of notation, and we consider both Λ and Λ_0 $r \times r$ diagonal matrices from now on.

Note that $\|\Lambda^{-1}\|_\infty \vee \|\Lambda\|_\infty \leq 2K$ for any $\Gamma \in \text{supp}(\Pi)$. We can show there exists diagonal matrices $\{\Lambda_1, \dots, \Lambda_T\} \subset \{\Lambda : \|\Lambda^{-1}\|_\infty \vee \|\Lambda\|_\infty \leq 2K\}$ such that

$$\{\Lambda : \|\Lambda^{-1}\|_\infty \vee \|\Lambda\|_\infty \leq 2K\} \subset \bigcup_{t=1}^T \{\Lambda : \|\Lambda - \Lambda_t\|_F \leq \varepsilon\},$$

where $\log T \leq r \log(12K \sqrt{r} \varepsilon^{-1})$, because we regard $\{\Lambda : \|\Lambda^{-1}\|_\infty \vee \|\Lambda\|_\infty \leq 2K\}$ as a subset of $\{\Lambda : \|\Lambda\|_F \leq 2K \sqrt{r}\}$ so that it is essentially a covering number calculation in \mathbb{R}^r as in Pollard (1990). We further decompose $H_{1,B}$ by $H_{1,B} \subset \bigcup_{t=1}^T H_{1,B,t}$, where

$$H_{1,B,t} = \{\Gamma = V \Lambda V^T + I : \|V_{\bar{B}} V_{\bar{B}}^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F > M' \varepsilon, \|\Lambda - \Lambda_t\|_F \leq \varepsilon\},$$

and decompose $H_{1,B,t}$ by $H_{1,B,t} \subset \bigcup_{j=1}^{\infty} H_{1,B,t,j}$, where

$$H_{1,B,t,j} = \{\Gamma = V \Lambda V^T + I : jM'\varepsilon < \|V_{\bar{B}} V_{\bar{B}}^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F \leq (j+1)M'\varepsilon, \\ \|\Lambda - \Lambda_t\|_F \leq \varepsilon\}.$$

According to Lemma 5.10, there exists

$$\{U_1, \dots, U_{N_j}\} \subset \mathcal{U}(|\bar{B}|, r) \cap \{U : jM'\varepsilon < \|UU^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F \leq (j+1)M'\varepsilon\},$$

such that for some constant δ_K only depending on K ,

$$\{jM'\varepsilon < \|V_{\bar{B}} V_{\bar{B}}^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\|_F \leq (j+1)M'\varepsilon\} \\ \subset \bigcup_{i=1}^{N_j} \{\|V_{\bar{B}} \Lambda_t V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq (\delta_K j \bar{M} - 1)\varepsilon\},$$

where $\bar{M} = 2^{-1/2} K^{-1} M'$, and we may bound N_j by

$$\log N_j \leq |\bar{B}|r \log\left(\frac{12\lambda_1((j+1)M' + 1)}{j\delta_K \bar{M} - 1}\right) + r^2 \log \frac{6\sqrt{r}}{\varepsilon} \\ \leq (A+1)r^2 s \log(48\sqrt{2}\delta_K^{-1} K) + r^2 \log(6\sqrt{r}) + \frac{1}{2}r^2 \log n,$$

when we choose $M' > \max\{2\sqrt{2}\delta_K^{-1} K, \frac{1}{2}\}$. Using the triangle inequality, we have

$$\|V_{\bar{B}} \Lambda V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq \|V_{\bar{B}} \Lambda_t V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F + \|\Lambda - \Lambda_t\|_F.$$

Therefore,

$$\{\|V_{\bar{B}} \Lambda_t V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq (\delta_K j \bar{M} - 1)\varepsilon, \|\Lambda - \Lambda_t\|_F \leq \varepsilon\} \\ \subset \{\|V_{\bar{B}} \Lambda V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq (\delta_K j \bar{M})\varepsilon\}.$$

By the sin-theta theorem (Lemma 5.11), we have

$$\|U_i \Lambda_t U_i^T - V_{0,\bar{B}} \Lambda_0 V_{0,\bar{B}}^T\|_F \geq 2^{-1/2} K^{-1} \|U_i U_i^T - V_{0,\bar{B}} V_{0,\bar{B}}^T\| \\ \geq 2^{-1/2} K^{-1} jM'\varepsilon \geq j\bar{M}\varepsilon.$$

Hence

$$\{\|V_{\bar{B}} \Lambda_t V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq (\delta_K j \bar{M} - 1)\varepsilon, \|\Lambda - \Lambda_t\|_F \leq \varepsilon\} \\ \subset \{\|V_{\bar{B}} \Lambda V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \leq \delta_K \|U_i \Lambda_t U_i^T - V_{0,\bar{B}} \Lambda_0 V_{0,\bar{B}}^T\|_F\}.$$

Our final decomposition is $H_{1,B,t,j} \subset \bigcup_{i=1}^{N_j} H_{1,B,t,j,i}$, where

$$H_{1,B,t,j,i} = \{\Gamma = V \Lambda V^T + I : \|V_{\bar{B}} \Lambda V_{\bar{B}}^T - U_i \Lambda_t U_i^T\|_F \\ \leq \delta_K \|U_i \Lambda_t U_i^T - V_{0,\bar{B}} \Lambda_0 V_{0,\bar{B}}^T\|_F\}.$$

Step 2: Combine tests from all levels and pieces. We have reduced the original testing problem to the above small pieces for each (B, t, j, i) . For each small piece, it is equivalent to the testing problem in Lemma 5.9. Since we already know the coordinates \bar{B} , the testing problem is on $\mathbb{R}^{\bar{B}}$. The observations in Lemma 5.9 is $(Y_1, \dots, Y_n) = (X_{1, \bar{B}}, \dots, X_{n, \bar{B}})$. The triple $(\bar{\Sigma}, \bar{\Gamma}', \bar{\Gamma})$ in Lemma 5.9 corresponds to $(V_{0, \bar{B}} \Lambda_0 V_{0, \bar{B}}^T + I, U_i \Lambda_t U_i^T + I, V_{\bar{B}} \Lambda V_{\bar{B}}^T + I)$ for every (B, t, j, i) . Then by the conclusion of Lemma 5.9, there exists a testing function $\phi_{B,t,j,i}$ with error bounded by

$$P_{\Sigma}^n \phi_{B,t,j,i} \leq 2 \exp(-C_5 \delta'_K n \|U_i \Lambda_t U_i^T - V_{0, \bar{B}} \Lambda_0 V_{0, \bar{B}}^T\|_F^2),$$

$$\sup_{\Gamma \in H_{B,t,j,i}} P_{\Gamma}^n (1 - \phi_{B,t,j,i}) \leq 2 \exp(-C_5 \delta'_K n \|U_i \Lambda_t U_i^T - V_{0, \bar{B}} \Lambda_0 V_{0, \bar{B}}^T\|_F^2),$$

for some δ'_K only depending on K and some absolute constant C_5 . Since $\|U_i \Lambda_t U_i^T - V_{0, \bar{B}} \Lambda_0 V_{0, \bar{B}}^T\|_F \geq j \bar{M} \varepsilon$, we have

$$P_{\Sigma}^n \phi_{B,t,j,i} \leq 2 \exp(-C_5 \delta'_K n j^2 \bar{M}^2 \varepsilon^2),$$

$$\sup_{\Gamma \in H_{B,t,j,i}} P_{\Gamma}^n (1 - \phi_{B,t,j,i}) \leq 2 \exp(-C_5 \delta'_K n j^2 \bar{M}^2 \varepsilon^2).$$

Now we are ready to integrate these little tests step by step for each index. For each (B, t, j) , define

$$\phi_{B,t,j} = \max_{1 \leq i \leq N_j} \phi_{B,t,j,i},$$

and we have

$$P_{\Sigma}^n \phi_{B,t,j} \leq \sum_{i=1}^{N_j} P_{\Sigma}^n \phi_{B,t,j,i}$$

$$\leq 2N_j \exp(-C_5 \delta'_K n j^2 \bar{M}^2 \varepsilon^2)$$

$$\leq 2 \exp\left(-C_5 \delta'_K j^2 \bar{M}^2 n \varepsilon^2 + (A + 1)r^2 s \log(48\sqrt{2}\delta_K^{-1} K) + r^2 \log(6\sqrt{r}) + \frac{1}{2}r^2 \log n\right).$$

Since we assume $r \vee \log n \leq m \log p$ and $r \leq ms$, we have $r^2 s \leq mn \varepsilon^2$, $r^2 \log(6\sqrt{r}) \leq mn \varepsilon^2$ and $r^2 \log n \leq m^2 n \varepsilon^2$. Hence

$$P_{\Sigma}^n \phi_{B,t,j} \leq 2 \exp(-C_5 \delta'_K j^2 \bar{M}^2 - (A + 1)m \log(48\sqrt{2}\delta_K^{-1} K) - m - m^2/2)n \varepsilon^2)$$

$$\leq 2 \exp(-\frac{1}{2}C_5 \delta'_K j^2 \bar{M}^2 n \varepsilon^2),$$

as long as we pick

$$\bar{M}^2 \geq 2C_5^{-1} \delta'_K^{-1} (A + 1)m \log(48\sqrt{2}\delta_K^{-1} K) + 2C_5^{-1} \delta'_K^{-1} m + C_5^{-1} \delta'_K^{-1} m^2.$$

In addition, for each (B, t, j) ,

$$\sup_{\Gamma \in H_{1,B,t,j}} P_{\Gamma}^n(1 - \phi_{B,t,j}) \leq 2 \exp(-C_5 \delta'_K j^2 \bar{M}^2 n \varepsilon^2).$$

For each (B, t) , we define

$$\phi_{B,t} = \max_j \phi_{B,t,j},$$

whose errors are bounded as follows:

$$\begin{aligned} P_{\Sigma}^n \phi_{B,t} &\leq \sum_j P_{\Sigma}^n \phi_{B,t,j} \\ &\leq 2 \sum_j \exp\left(-\frac{1}{2} C_5 \delta'_K j^2 \bar{M}^2 n \varepsilon^2\right) \\ &\leq 3 \exp\left(-\frac{1}{2} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right) \end{aligned}$$

and

$$\sup_{\Gamma \in H_{B,t}} P_{\Gamma}^n(1 - \phi_{B,t}) \leq 2 \exp(-C_5 \delta'_K \bar{M}^2 n \varepsilon^2).$$

For each B , we define

$$\phi_B = \max_{1 \leq t \leq T} \phi_{B,t},$$

and we have the errors bounded by

$$\begin{aligned} P_{\Sigma}^n \phi_B &\leq \sum_{t=1}^T P_{\Sigma}^n \phi_{B,t} \\ &\leq 3 \exp\left(-\frac{1}{2} C_5 \delta'_K \bar{M}^2 n \varepsilon^2 + \log T\right) \\ &\leq 3 \exp\left(-\frac{1}{2} C_5 \delta'_K \bar{M}^2 n \varepsilon^2 + r \log(12K \sqrt{r} \varepsilon^{-1})\right) \\ &\leq 3 \exp\left(-\frac{1}{4} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right) \end{aligned}$$

and

$$\sup_{\Gamma \in H_B} P_{\Gamma}^n(1 - \phi_B) \leq 2 \exp(-C_5 \delta'_K \bar{M}^2 n \varepsilon^2).$$

Finally, the ultimate test is defined as

$$\phi = \max_B \phi_B,$$

with type I error $P_{\Sigma}^n \phi$ bounded by

$$\begin{aligned} \sum_B P_{\Sigma}^n \phi_B &\leq \left(\sum_{q=1}^{[Ars]} \binom{p}{q} \right) 3 \exp\left(-\frac{1}{4} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right) \\ &\leq 3 \text{Ars} \exp(\text{Ars} \log p) \exp\left(-\frac{1}{4} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right) \\ &\leq 3 \exp(2 \text{Ars} \log p) \exp\left(-\frac{1}{4} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right) \\ &\leq 3 \exp\left(-\left(\frac{1}{4} C_5 \delta'_K \bar{M}^2 - 2A\right) n \varepsilon^2\right) \\ &\leq 3 \exp\left(-\frac{1}{8} C_5 \delta'_K \bar{M}^2 n \varepsilon^2\right), \end{aligned}$$

as long as we choose $\bar{M}^2 \geq 16 \delta'_K{}^{-1} C_5^{-1} A$, and for type II error we have

$$\sup_{\Gamma \in \mathcal{H}_1} P_{\Gamma}^n(1 - \phi) \leq 2 \exp(-C_5 \delta'_K \bar{M}^2 n \varepsilon^2).$$

Thus the proof is complete. \square

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SUPPLEMENTARY MATERIAL

Supplement to “Rate-optimal posterior contraction for sparse PCA” (DOI: 10.1214/14-AOS1268SUPP; .pdf). In the supplementary text [Gao and Zhou (2015)], we present proofs of Proposition 2.1, Lemmas 5.1, 5.8, 5.10, Theorem 4.2, Proposition 5.1 and Lemma 5.9.

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