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On the sample covariance matrix estimator of reduced effective rank population matrices, with applications to fPCA

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This work provides a unified analysis of the properties of the sample covariance matrix Σ_n over the class of $p \times p$ population covariance matrices Σ of reduced effective rank $r_e(\Sigma)$. This class includes scaled factor models and covariance matrices with decaying spectrum. We consider $r_e(\Sigma)$ as a measure of matrix complexity, and obtain sharp minimax rates on the operator and Frobenius norm of $\Sigma_n - \Sigma$, as a function of $r_e(\Sigma)$ and $\|\Sigma\|_2$, the operator norm of Σ. With guidelines offered by the optimal rates, we define classes of matrices of reduced effective rank over which Σ_n is an accurate estimator. Within the framework of these classes, we perform a detailed finite sample theoretical analysis of the merits and limitations of the empirical scree plot procedure routinely used in PCA. We show that identifying jumps in the empirical spectrum that consistently estimate jumps in the spectrum of Σ is not necessarily informative for other goals, for instance for the selection of those sample eigenvalues and eigenvectors that are consistent estimates of their population counterparts. The scree plot method can still be used for selecting consistent eigenvalues, for appropriate threshold levels. We provide a threshold construction and also give a rule for checking the consistency of the corresponding sample eigenvectors. We specialize these results and analysis to population covariance matrices with polynomially decaying spectra, and extend it to covariance operators with polynomially decaying spectra. An application to fPCA illustrates how our results can be used in functional data analysis.

Keywords: covariance matrix; eigenvalue; eigenvector; fPCA; high dimensions; minimax rate; optimal rate of convergence; PCA; scree plot; sparsity

1. Introduction

High dimensional covariance matrix estimation has received a high amount of attention over the last few years. This was largely motivated by the fact that the sample covariance matrix Σ_n, based on a sample of size n, is not necessarily a consistent estimator of the covariance matrix Σ of a random vector $X \in \mathbb{R}^p$, if $p > n$. In this regime, the shortcomings of Σ_n have been well understood for over a decade, whenever we estimate a *spiked* covariance matrix; see, for instance, the seminal works of Baik and Silverstein [3] and Johnstone [17]. By definition, spiked models have a fixed number of large eigenvalues and the rest equal to one. Therefore, the effective number of parameters in such models is of order p^2, and there is no hope to estimate them accurately from a small sample. To address this issue, classes of *sparse* covariance matrices have been introduced in recent years. Depending on the type of sparsity (entry-wise, row-wise, off-diagonal

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decay), appropriate estimators have been introduced and shown to adapt to the unknown sparsity structures, see, for instance, [5,6,9,10], among many others. It is important to note that although sparse matrices, by definition, have a reduced number of parameters, they can still be spiked. Therefore, the usage of the sample covariance matrix Σ_n in this context would still be questionable, in addition to not rendering the appropriate sparse structure. It is also of importance to observe that all sparse covariance matrix models carry with them implicit modeling assumptions. For instance, they are appropriate whenever many of the components of X are weakly correlated. They are also powerful for modeling temporally or spatially ordered variables, in cases where it is reasonable to assume that variables apart in time or space have very little association.

However, there are many instances where these assumptions are not satisfied, for example when the observed variables are known to have strong associations with each other. If the association is approximately linear, Σ will be close to being a degenerate, rank $r < p$ matrix, with possibly much fewer parameters than p^2, if r is small. To treat general, positive definite covariance matrices, which have *effectively* reduced rank, we make use of the notion of *effective rank*, first suggested by Vershynin [25] and given by

$$r_e(\Sigma) = \frac{\operatorname{trace}(\Sigma)}{\|\Sigma\|_2}. \tag{1.1}$$

Here $\|\Sigma\|_2$ denotes the operator norm, or the largest singular value, of Σ. Clearly, $r_e(\Sigma)$ is smaller than the rank for degenerate matrices and, in general, it can be significantly smaller than p if a large number of eigenvalues of Σ are relatively small.

Perhaps surprisingly, the finite sample properties of the sample covariance matrix as an estimator of population matrices of reduced effective rank are largely unstudied. For classes of matrices Σ for which $r_e(\Sigma)$ and $\|\Sigma\|_2$ are appropriately bounded, but allowed to vary with n and p, we study the following problems:

(1) Rate optimal estimation of Σ via Σ_n, with respect to the Frobenius and operator norms, in finite samples.
(2) Finite sample estimation of the location of a jump in the spectrum of Σ, via Σ_n.
(3) Finite sample determination of the number of eigenvalues and eigenvectors of Σ_n that are accurate estimates, respectively, of the eigenvalues and eigenvectors of Σ.
(4) Extensions of (2) and (3) to covariance operators, for functional data.

We study problem (1) in Section 2. For data generated from a class of sub-Gaussian distributions defined in Section 2.1, we establish upper bounds on the Frobenius norm $\|\Sigma_n - \Sigma\|_F$ and operator norm $\|\Sigma_n - \Sigma\|_2$ that hold, with high probability, and are near minimax optimal. We summarize these results in Table 1, which reveals that even if $p > n$, as long as $r_e(\Sigma)$ and $\|\Sigma\|_2$ are appropriately small, Σ_n continues to be an accurate estimator of Σ. The derivation of these bounds is presented in Section 2.2, where we also study $\mathbb{E}\|\Sigma_n - \Sigma\|_F$ and $\mathbb{E}\|\Sigma_n - \Sigma\|_2$, which have similar bounds, but sharper by $\ln n$ factors. Guided by these results, we introduce and discuss classes of covariance matrices of reduced effective rank, also in Section 2.2.

For problems (2) and (3), and their extension to (4), we investigate in detail estimation performed by the ubiquitous scree plot method, described below. Let $\{\lambda_k, 1 \le k \le p\}$, arranged in descending order, denote the eigenvalues of Σ. Similarly, let $\{\widehat{\lambda}_k, 1 \le k \le p\}$, arranged in descending order, denote the eigenvalues of the sample covariance matrix Σ_n, henceforth called

Table 1. Optimal rates for the Frobenius and operator norm of $\Sigma_n - \Sigma$: orders of magnitude depending on the regime of p. Within each regime, the sizes of $r_e(\Sigma)$ and $\|\Sigma\|_2$ govern the rate

Norm/values of p	$p = \mathrm{O}(n^\gamma), \gamma \geq 0$	$p = \mathrm{O}\{\exp(n)\}$
Frobenius: $\|\Sigma_n - \Sigma\|_F$	$\|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \sqrt{\frac{\ln n}{n}}$	$\|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \sqrt{\frac{\ln n}{n}}$
Operator: $\|\Sigma_n - \Sigma\|_2$	$\|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \frac{\ln pn}{n}$, if $r_e(\Sigma) \geq \frac{n}{\ln pn}$	$\|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \sqrt{\frac{\ln n}{n}}$
	$\|\Sigma\|_2 \cdot \sqrt{r_e(\Sigma)} \cdot \sqrt{\frac{\ln pn}{n}}$, if $r_e(\Sigma) \leq \frac{n}{\ln pn}$	

the sample eigenvalues. For a given number τ, called the threshold level, the scree plot method consists in calculating the number $K =: \max\{k : \widehat{\lambda}_k \geq \tau\}$ and retaining the K largest sample eigenvalues. Typically, one also retains the corresponding sample eigenvectors $\widehat{\boldsymbol{\psi}}_k$, $k \leq K$, for further analysis. In Sections 3 and 4, we study when this practice can be justified and for which threshold levels. To the best of our knowledge, no theoretical study of the thresholding method applied to Σ_n, of this nature, exists in the literature.

We study problem (2) in Section 3, where we give a data-dependent construction of τ for detecting minimal jumps in the spectrum of Σ. We say that a minimal spectral jump occurs when there exists an index s such that λ_s is a constant multiple of the noise level, and there is a gap of at least the size of the noise level between λ_s and λ_{s+1}. The appropriate noise level for this class of problems is proportional to $\mathbb{E}\|\Sigma_n - \Sigma\|_2$. The precise definition and result are given in Theorem 3.2. We apply this result to consistent estimation of the number of factors in factor models in Example 3.1, complementing existing methods, for example the AIC-type criterion in [2].

For population matrices with special structures, a spectral jump at the minimal noise level may not exist. This is, for example, the case of population matrices whose spectra exhibit a polynomial decay, which we study in Section 3.1. In this case, spectral jumps can still be detected, but they have to be larger than the noise level, with order of magnitude depending on the rate of decay. We treat this in Theorem 3.3, where we offer guidance on a data-dependent choice of τ for consistent jump detection under this scenario.

We study problem (3) in Section 4. Finite sample bounds on the difference between sample eigenvalues and eigenvectors and their population counterparts have been much less studied when $p > n$, and no unifying analysis over the class of covariance matrices of reduced effective rank exists. The study of consistent estimation of the eigenvalues and eigenvectors of Σ via Σ_n, in the classical asymptotic framework where p is fixed and $n \to \infty$, dates back half a century, with notable works including those of Anderson [1] and Muirhead [22]. Asymptotic analyses that allow p to grow with n have been chiefly conducted in spike models, when p/n converges to a constant, and mostly concern the behavior of the largest sample eigenvalue and corresponding eigenvector, see, for instance, [17] and [23]. None of these analyses can be directly used or extended for studying problem (3). The most closely related results to ours are those of Kneip and Sarda [19], who studied the finite sample convergence rates of the sample eigenvalues and eigenvectors of Σ_n/p in factor models, where $r_e(\Sigma/p)$ is finite and independent of n and p. We show in Section 4 that their results are particular cases of ours on studying problem (3) over classes of population matrices of reduced effective rank. We show in Theorem 4.1 that, for a given desired precision level α, we can construct a data-dependent threshold level, which is a function of an estimate of the minimum noise level and α, such that all sample eigenvalues above this threshold are close to the theoretical values at this precision level, with high probability. A known result by Kneip and Utikal [20] can be used to show that, in general, it would be misleading to conclude that the sample eigenvectors corresponding to the sample eigenvalues thus selected are also close to their population counterparts. Our Theorem 4.2 shows how to complement the scree plot method by another simple strategy, in order to further determine which sample eigenvectors are accurate estimates. Interestingly, when the spectrum of Σ decays polynomially, the scree plot method once again suffices for accurate estimation of both eigenvalues and eigenvectors and we make this precise in Theorem 4.3.

In Section 5, we treat problem (4), by showing how the results of the previous sections can be employed in fPCA. The data consists in a sample of n independent trajectories $X_i(t)$, of a background stochastic process $X(t)$ with covariance operator $\mathcal{K}$. Each trajectory is observed at the same m discrete data points $t_1 < t_2 < \cdots < t_m$, and is corrupted by noise. Problem (2) has not been studied in this context, but aspects of problem (3) have been thoroughly studied, however only in asymptotic contexts. For perfectly observed trajectories, at all time points t and without additive noise, Hall and Hosseini-Nassb [14] use a result by Dauxois *et al.* [12] to develop a bootstrap based approach for selecting the sample eigenvalues and eigenfunctions that estimate the population counterparts at the parametric rate. For discretely observed trajectories, the theoretical properties of the estimated eigenvalues and eigenvectors have been established by, for instance, Yao *et al.* [27], Hall *et al.* [15] and Benko *et al.* [4]. However, all these results are relative to the first few fixed eigenvalues and eigenfunctions of $\mathcal{K}$, are of asymptotic nature, and the selection of the appropriate number of features, in finite samples, is left open. We bridge this gap here.

We study the class of covariance operators $\mathcal{K}$ with spectra having polynomial decay, of which the Brownian motion is a chief example. For this class, we show how the sample covariance matrix, in connection with the scree plot method, can be employed to detect jumps in the spectrum of the covariance operator, and to determine the number of sample eigenvalues and eigenvectors that are accurate estimates of the population eigenvalues and eigenfunctions, the latter evaluated at the discrete observation points. Instrumental in this analysis, and new relative to what we already developed in Sections 3 and 4, are the results of Section 5.1.

We denote by π_m the projection mapping $X(t)$ into an m-dimensional space $\mathbb{R}^m$, defined by $\pi_m(X) = (X(t_1), \ldots, X(t_m))$. We refer to the distributions on $\mathbb{R}^m$ induced by π_m as the finite-dimensional distributions of X. Let $\mathbf{K} = m^{-1}\{\mathcal{K}(t_{j_1}, t_{j_2})\}_{1\le j_1, j_2\le m}$ be the scaled covariance matrix corresponding to the m-dimensional distribution of X. In Section 5.1, we establish finite sample approximations of the eigenvalues and eigenfunctions of the operator $\mathcal{K}$ by the eigenvalues and eigenvectors of $\mathbf{K}$. This allows us to transfer the assumptions on the operator $\mathcal{K}$ to the matrix $\mathbf{K}$, which in turn allows us to apply the theory developed in Sections 2–4 to functional data. Jump detection is presented in Section 5.2 and the selection of the accurate sample eigenvalues and eigenvectors is treated in Section 5.3.

The proofs of all our theoretical results are given in the Appendix and in the supplemental material. We shall use the following notation throughout our paper: $\|\cdot\|_F$, the Frobenius norm; $\|\cdot\|_2$, the spectral/operator norm; $\|\cdot\|_1$, the nuclear norm; $\|\cdot\|$, the Euclidean norm of a vector; $\operatorname{tr}(\cdot)$, the trace of a square matrix; I_p, an identity matrix of dimension p. We will also use the notation $\lesssim$ for inequalities that hold up to multiplicative constants independent of n and p (or m). Throughout this paper, we regard a sample eigenvector $\widehat{\boldsymbol{\psi}}$ as an estimate of its population counterpart $\boldsymbol{\psi}$ and assume the sign of $\widehat{\boldsymbol{\psi}}$ is selected so that $\widehat{\boldsymbol{\psi}}'\boldsymbol{\psi} \geq 0$.

2. Some inequalities for the sample covariance matrix

2.1. Sub-Gaussian distributions

All the results of this paper are proved for a certain class of sub-Gaussian distributions. In particular they all hold for Gaussian vectors or processes. We recall that a zero-mean random variable $X \in \mathbb{R}$ is *sub-Gaussian* if there exists a constant $\sigma > 0$ such that $\mathbb{E}\exp(tX) \leq \exp(t^2\sigma^2/2)$, for all $t \in \mathbb{R}$. Then it can be shown that $\sup_{k\geq 1} k^{-1/2}(\mathbb{E}|X|^k)^{1/k} < \infty$ and the sub-Gaussian norm of X is defined to be $\|X\|_{\psi_2} = \sup_{k\geq 1} k^{-1/2}(\mathbb{E}|X|^k)^{1/k}$. A zero-mean random vector $X \in \mathbb{R}^p$ is *sub-Gaussian* if for any non-random $u \in \mathbb{R}^p$, $u'X$ is sub-Gaussian. The sub-Gaussian norm of X is defined as $\|X\|_{\psi_2} = \sup_{u\in\mathbb{R}^p\setminus\{0\}} \|u'X\|_{\psi_2}/\|u\|$. We will impose an additional assumption on a sub-Gaussian random vector:

Assumption 1. *For a zero-mean sub-Gaussian random vector $X \in \mathbb{R}^p$, we assume that there exists a constant $c_0 > 0$ such that $\mathbb{E}(u'X)^2 \geq c_0\|u'X\|_{\psi_2}^2$ for all $u \in \mathbb{R}^p$.*

Assumption 1 effectively bounds the higher moments of X as polynomial functions of the second moments of X. Let Σ be the covariance matrix of X, then $u'\Sigma u \geq c_0\|u'X\|_{\psi_2}^2$, for all $u \in \mathbb{R}^p$, under Assumption 1. We will provide a number of distributions of interest that meet this assumption below. Note first that if $X \in \mathbb{R}^p$ is sub-Gaussian and satisfies Assumption 1 and $O \in \mathbb{R}^{p\times p}$ is an orthonormal matrix, then OX is also sub-Gaussian and satisfies Assumption 1 with the same c_0.

Example 2.1. Let $X \in \mathbb{R}^p$ be a random vector from a zero-mean multivariate normal distribution. Then X satisfies Assumption 1 with $c_0 = \pi/2$ ([26]).

Example 2.2. Let $X = (X_1, \dots, X_p)'$ and the components X_j are independent and have a zero-mean sub-Gaussian distribution. Suppose there is a common constant $\sigma > 0$ such that $\mathbb{E}\exp(tX_j/\sqrt{\Sigma_{jj}}) \leq \exp(t^2\sigma^2/2)$ for all j, where Σ_{jj} is the variance of X_j. Then X is sub-Gaussian and satisfies Assumption 1. Moreover, if $\widetilde{X} = OX$ where $O \in \mathbb{R}^{p\times p}$ is an orthonormal matrix, then $\widetilde{X}$ is sub-Gaussian and satisfies Assumption 1.

A proof of the statements in Example 2.2 is provided in Appendix A.1.2.

2.2. Accuracy of the sample covariance matrix over classes of population matrices of reduced effective rank

Let $X_1, \dots, X_n$ be i.i.d. observations of a random vector $X \in \mathbb{R}^p$. Without loss of generality, we assume that $\mathbb{E}(X) = 0$. Let $\bar{X} = n^{-1}\sum_{i=1}^n X_i$ and $\Sigma_n = n^{-1}\sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})'$ be the sample covariance matrix. We establish below sharp probability upper bounds on $\Sigma_n - \Sigma$, in terms of both the Frobenius and the operator norms, as well as sharp bounds on the expectation of either norm. The bounds stated below hold up to multiplicative constants defined precisely in Appendix A.1.3. Specifically, c_1, c_2 and c_3 are defined in Propositions A.2, A.3 and A.4, respectively. The constants are independent of n and p and depend only on c_0 in Assumption 1. As announced in the Introduction, we show that the effective rank defined in (1.1) governs the size of these bounds. As a consequence, we introduce classes of population matrices over which Σ_n can be employed accurately even if $p > n$. In some cases, we offer high-level practical guidance on assessing whether, for a given data set, it is reasonable to assume the covariance matrix of a generating distribution belongs to these classes.

Theorem 2.1. *Suppose X is a random vector that satisfies Assumption 1. With probability at least* $1 - 5n^{-1}$,

$$\|\Sigma_n - \Sigma\|_F \leq 2c_1 \cdot \|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \sqrt{\frac{\ln n}{n}}.$$

Furthermore,

$$\mathbb{E}\big(\|\Sigma_n - \Sigma\|_F^2\big) \leq 2 \cdot \|\Sigma\|_2^2 \cdot \frac{r_e(\Sigma)^2}{n^2} \cdot \big\{16c_1^2 c_2 + 1 + 2\big(c_1^2 + c_1\big)\exp(1)\big\}.$$

Theorem 2.2. *Suppose X is a random vector that satisfies Assumption 1. With probability at least* $1 - 4n^{-1}$,

$$\|\Sigma_n - \Sigma\|_2 \leq (1 + c_1 + c_3) \cdot \|\Sigma\|_2 \cdot \max\left\{\sqrt{\frac{r_e(\Sigma) \cdot \ln pn}{n}}, \frac{r_e(\Sigma) \cdot \ln pn}{n}\right\}.$$

Furthermore, with $C =: 2\{5c_3^2 + 1 + 2(c_1^2 + c_1)\exp(1)\}$,

$$\mathbb{E}\big(\|\Sigma_n - \Sigma\|_2^2\big) \leq C \cdot \|\Sigma\|_2^2 \cdot \max\left\{\frac{r_e(\Sigma) \cdot \ln p}{n}, \left(\frac{r_e(\Sigma) \cdot \ln p}{n}\right)^2\right\}.$$

Remark 2.1.

(i) As it can be seen from the proofs in Appendix A.1.3, all our results continue to hold if Σ is singular.

(ii) Probability bounds on $\|\Sigma_n - \Sigma\|_2$, similar to those in Table 1, have been first derived for distributions with bounded support in [25], Section 5.4.3.

(iii) A probability bound on $\|\Sigma_n - \Sigma\|_2$, of the same order of magnitude as the one given by Theorem 2.2, has been established independently by Lounici [21], as this work developed. However, our proof is based on a version of Berstein's inequality for unbounded matrices, whereas Lounici [21] employs a version of this inequality developed for bounded matrices, and therefore uses a different argument to complete his proof. The rest of the results presented in Theorems 2.1 and 2.2, including the bounds on expected values in both cases are, to the best of our knowledge, new. The rates given by Theorems 2.1 and 2.2 above are minimax optimal over the class of matrices with effective rank bounded by $\min(\sqrt{n}, p)$, up to logarithmic terms. We refer to Theorem 2 of [21] for the lower bound derivations with respect to the operator norm. The lower bound with respect to the squared Frobenius norm derived in Theorem 2 of [21] is of the order of $\|\Sigma\|_2^2 \cdot r_e(\Sigma) \cdot p/n$ and is larger than the rate we derived in Theorem 2.1. However, the proof of Theorem 2 in [21] can be tightened, by keeping only the first line of his inequality (5.27), to show that the minimax lower bound is in fact $\|\Sigma\|_2^2 \cdot r_e^2(\Sigma)/n$. Therefore, our rate is near minimax optimal, over the class of matrices of effective ranks bounded by $\min(\sqrt{n}, p)$.

(iv) It is noteworthy that the sample estimator Σ_n is already minimax rate optimal, in both Frobenius and operator norm, over the class of matrices of effective ranks bounded by $\min(\sqrt{n}, p)$. This suggests that, over this class, very little can be gained from further thresholding or shrinking operations. For instance, the nuclear norm penalized estimator, that would have appeared to be a more appropriate estimator over this class, has the same and optimal bound in operator norm ([21]), and very similar performance to Σ_n in the simulations we have conducted.

In most situations, a scale-independent accuracy measure for Σ_n is desired. One such measure is provided by the ratio between $\|\Sigma_n - \Sigma\|_F$ or $\|\Sigma_n - \Sigma\|_2$ and $\|\Sigma\|_2$. Then, recalling that $\lesssim$ denotes inequalities that hold up to multiplicative constants, Theorems 2.1 and 2.2 show that, with high probability,

$$\frac{\|\Sigma_n - \Sigma\|_F}{\|\Sigma\|_2} \lesssim r_e(\Sigma)\sqrt{\frac{\ln n}{n}}, \tag{2.1}$$

and

$$\frac{\|\Sigma_n - \Sigma\|_2}{\|\Sigma\|_2} \lesssim \max\left\{\sqrt{\frac{r_e(\Sigma) \cdot \ln pn}{n}}, \frac{r_e(\Sigma) \cdot \ln pn}{n}\right\}. \tag{2.2}$$

The above relative measures are informative even if $\|\Sigma\|_2$ increases with p and they motivate the introduction of the following classes of population matrices. Let $\varepsilon \in (0, 1)$ be a complexity index that may decrease to zero with n and p. Let $\gamma \geq 0$ be a given number. Define

$$\mathcal{P}_1(\varepsilon) := \left\{\Sigma : r_e(\Sigma) \lesssim \varepsilon \frac{n}{\ln pn}; p = \mathrm{O}(n^\gamma)\right\},$$

and

$$\mathcal{P}_2(\varepsilon) := \left\{\Sigma : r_e(\Sigma) \lesssim \varepsilon \sqrt{\frac{n}{\ln n}}\right\}.$$

The definition of these classes resembles sparsity definitions in sparse covariance matrix models, where a certain sparsity measure is controlled. The introduction of $\mathcal{P}_1(\varepsilon)$ or $\mathcal{P}_2(\varepsilon)$ complements therefore the literature on sparse models, by advocating the study of low complexity models, where $r_e(\Sigma)$ is used as a complexity measure. Then, similar to existing results which show that accurate estimation over classes of population covariance matrices of a certain low complexity level is possible even if $p > n$, Theorems 2.1 and 2.2 show that estimation of covariance matrices with reduced effective ranks can also be performed accurately even if $p > n$, as long as the complexity index ε is appropriately small. And this can be achieved, in terms of rate optimality, by the ubiquitously used sample covariance matrix. Specifically:

(i) *For any n and p*, if $\Sigma \in \mathcal{P}_2(\varepsilon)$, then Theorems 2.1 and 2.2 yield:

$$\frac{\|\Sigma_n - \Sigma\|_2}{\|\Sigma\|_2} \leq \frac{\|\Sigma_n - \Sigma\|_F}{\|\Sigma\|_2} \lesssim \varepsilon,$$

since $\|M\|_2 \leq \|M\|_F$ for any matrix M. Thus, if $\varepsilon = \mathrm{o}(1)$, the scaled operator and Frobenius norms will be small. Note that this size of ε implies that $r_e(\Sigma) = \mathrm{o}(\sqrt{n/\ln n})$.

(ii) If $p = \mathrm{O}(n^\gamma)$, $\gamma \geq 0$, then Theorem 2.2 guarantees the accuracy of Σ_n with respect to the operator norm over a larger class of population matrices, with a less restrictive size of $r_e(\Sigma)$. Specifically, if $\Sigma \in \mathcal{P}_1(\varepsilon)$, then

$$\frac{\|\Sigma_n - \Sigma\|_2}{\|\Sigma\|_2} \lesssim \varepsilon,$$

which is small as long as $\varepsilon = \mathrm{o}(1)$, implying that $r_e(\Sigma) = \mathrm{o}(n/\ln pn)$. We note that the restriction on the growth of p is induced by the explicit dependency on p in the logarithmic term of the bound (2.2), which makes this bound non-informative if $p = \mathrm{O}\{\exp(n)\}$, or if $p \to \infty$ independently of n. If this is the case, we can use the results from (i) above, which are valid for any n and p, albeit over a smaller class of population matrices.

In general, it is challenging to determine whether the population covariance matrix is in $\mathcal{P}_1(\varepsilon)$ or $\mathcal{P}_2(\varepsilon)$, for some ε. Whereas a full solution to this problem is beyond the scope of this paper, we offer guidance for a particular case below. It is based on the following result, also independently derived by Lounici [21].

Theorem 2.3. *For any random vector X satisfying Assumption 1,*

$$\left|\mathrm{tr}(\Sigma_n) - \mathrm{tr}(\Sigma)\right| \leq 4c_1\sqrt{\frac{\ln n}{n}} \cdot \mathrm{tr}(\Sigma),$$

with probability at least $1 - 5n^{-1}$.

Remark 2.2. By Theorems 2.2 and 2.3 we have, for any p and n large enough and with high probability that

$$\|\Sigma_n - \Sigma\|_2 \leq \|\Sigma_n - \Sigma\|_F \lesssim \mathrm{tr}(\Sigma)\sqrt{\frac{\ln n}{n}} \leq 2\,\mathrm{tr}(\Sigma_n)\sqrt{\frac{\ln n}{n}},$$

or

$$\mathbb{E}\|\Sigma_n - \Sigma\|_2 \leq \mathbb{E}\|\Sigma_n - \Sigma\|_F \lesssim \frac{\mathrm{tr}(\Sigma)}{\sqrt{n}} \leq \frac{2\,\mathrm{tr}(\Sigma_n)}{\sqrt{n}}.$$

Theorem 2.3 provides direct practical guidance on the accuracy of the un-scaled Frobenius and operator norm, irrespective of the size of $\|\Sigma\|_2$. It shows that, as a first simple check, one should compare $\mathrm{tr}(\Sigma_n)$ to $\sqrt{n}$ in order to decide whether Σ_n suffices as an estimator of Σ. This is particularly useful when we have reasons to believe that the population covariance matrix has a large number of very small eigenvalues.

Remark 2.3. By Theorems 2.2 and 2.3, we can derive an upper bound for $r_e(\Sigma_n)$ as an estimator of $r_e(\Sigma)$; see Theorem A.4 in Appendix A.1.7.

3. Detectable spectral jumps for population covariance matrices of reduced effective rank

In this section, we discuss consistent estimation of an index s of a population eigenvalue that is sufficiently separated from the next one, and therefore sufficiently large itself. We will refer to such an index as a jump. In what follows, sufficiently large and sufficiently separated will be defined relative to the bounds on $\mathbb{E}\|\Sigma_n - \Sigma\|_2$ given by Theorems 2.1 and 2.2 in Section 2.2. We will use a slightly enlarged, by a $\sqrt{\ln n}$ multiplicative factor, version of these bounds, which yields the appropriate noise levels for index consistency analysis, as illustrated in Theorem 3.1 below. Specifically, if $p = \mathrm{O}(n^\gamma)$, for some $\gamma \geq 0$, the noise level is

$$\eta_1 := C\|\Sigma\|_2 \cdot \sqrt{r_e(\Sigma)} \cdot \sqrt{\ln pn/n}, \tag{3.1}$$

and, if $p = \mathrm{O}\{\exp(n)\}$, the noise level is

$$\eta_2 := C\|\Sigma\|_2 \cdot r_e(\Sigma) \cdot \sqrt{\ln n/n}. \tag{3.2}$$

To avoid notational clutter, we introduced above a constant $C > 0$ to bound all other constants appearing in the bounds of Theorems 2.1 and 2.2. Note that C does not depend on n or p. For a data-dependent threshold $\widetilde{\tau}$, define

$$\widehat{s}(\widetilde{\tau}) := \max\{k : \widehat{\lambda}_k \geq \widetilde{\tau}\}, \tag{3.3}$$

where we recall that $\widehat{\lambda}_k$, $1 \leq k \leq p$, in decreasing order, are the sample eigenvalues. The following general theorem shows the interplay between the quantities needed to define an index s of the spectrum of Σ that can be regarded as a jump and consistently estimated and the conditions required of a data-dependent thresholding level $\widetilde{\tau}$ that makes $\widehat{s}(\widetilde{\tau})$ a consistent estimate of s. Recall that λ_k, $1 \leq k \leq p$, in decreasing order, are the population eigenvalues.

Theorem 3.1. *Let $j \in \{1, 2\}$ be fixed. Suppose $\Sigma \in \mathcal{P}_j(\varepsilon)$, for some $\varepsilon \in (0, 1)$ and that Assumption 1 holds. If there exist an index s and positive quantities τ_1 and τ_2 such that*

$$\lambda_s \geq \tau_1 + \eta_j \quad \text{and} \quad \lambda_{s+1} \leq \tau_2 - \eta_j, \tag{3.4}$$

and a data-dependent threshold $\widetilde{\tau}$ that satisfies

$$\mathbb{P}(\tau_2 \leq \widetilde{\tau} \leq \tau_1) \geq 1 - \delta \tag{3.5}$$

for some $\delta \in (0, 1)$, *then*

$$\mathbb{P}\big(\widehat{s}(\widetilde{\tau}) = s\big) \geq 1 - 5n^{-1} - \delta.$$

Remark 3.1.

(i) Note that if (3.4) holds, with either $j = 1$ or $j = 2$, then implicitly

$$\tau_1 \geq \tau_2 > \eta_j \quad \text{and} \quad \lambda_s - \lambda_{s+1} > 2\eta_j + (\tau_1 - \tau_2).$$

Thus, condition (3.4) re-states the well understood fact that in order to estimate with high probability the index s of what we declare a large enough eigenvalue, at least larger than the noise level, there must also be a gap larger than the noise level between this eigenvalue and the one following it.

(ii) If an index s satisfying (3.4) exists, we will call it a jump in the spectrum of Σ relative to the triplet (τ_1, τ_2, η).

Theorem 3.1 makes it clear that, for each $j \in \{1, 2\}$, the minimal allowable values for τ_1 and τ_2 are of the order of η_j, and are larger than η_j. The following result specializes Theorem 3.1 to this situation and offers a concrete construction of data-dependent thresholds that satisfy (3.5) with $\delta = \mathrm{O}(n^{-1})$. We begin by defining two data-dependent levels:

$$\widetilde{\eta}_1 = C\|\Sigma_n\|_2 \cdot \sqrt{\frac{r_e(\Sigma_n) \cdot \ln pn}{n}}, \tag{3.6}$$

and

$$\widetilde{\eta}_2 = C\|\Sigma_n\|_2 \cdot r_e(\Sigma_n) \cdot \sqrt{\frac{\ln n}{n}}, \tag{3.7}$$

where the constant C is the same as in the definitions of η_1 and η_2. We will also use the following notation throughout this section: we let c_1, c_2 and c_3 be the constants defined in Section 2, and we let

$$\varepsilon_1 = 4c_1\sqrt{\ln n/n}, \qquad C_1 = 0.9, \qquad C_2 = 1. \tag{3.8}$$

Theorem 3.2. *Let* $j \in \{1, 2\}$ *be fixed. Suppose* $\Sigma \in \mathcal{P}_j(\varepsilon)$, *for some* $\varepsilon \in (0, 1)$ *and that Assumption 1 holds. Let* η_j *be defined by either* (3.1) *or* (3.2) *above. Assume that there exists an index* s_j *such that*

$$\lambda_{s_j} \geq \frac{2(1+\varepsilon_1)}{C_j}\eta_j + \eta_j, \qquad \lambda_{s_j+1} < 2C_j(1-\varepsilon_1)\eta_j - \eta_j.$$

Then, if $j = 1$ *and* $(1 + c_1 + c_3)\sqrt{\varepsilon} < 0.19$,

$$\mathbb{P}\big\{\widehat{s}(2\widetilde{\eta}_1) = s_1\big\} \geq 1 - 11n^{-1}.$$

If $j = 2$,

$$\mathbb{P}\big\{\widehat{s}(2\widetilde{\eta}_2) = s_2\big\} \geq 1 - 11n^{-1}.$$

Remark 3.2. Theorem 3.2 shows that it is possible to detect, with high probability, fine jumps, at the minimal level of the noise levels quantified by (3.1) or (3.2), respectively, via data-dependent thresholds. However, the expressions given for $\widetilde{\eta}_1$ and $\widetilde{\eta}_2$ above depend on unknown constants, that in turn depend on the unknown distribution of the data. For practical use, we suggest cross validation.

Example 3.1 (Estimating the number of factors in a factor model). Let Σ be a covariance matrix arising from a finite factor model (see, for example, [11,13]), with the decomposition

$$\frac{\Sigma}{p} = \sum_{r=1}^{R} \lambda_r \boldsymbol{\xi}_r \boldsymbol{\xi}_r' + \frac{\sigma^2}{p} I_p, \tag{3.9}$$

where R is a fixed number, $\lambda_1 > \cdots > \lambda_R > 0$ can be upper bounded independently of p, and $\boldsymbol{\Xi} = [\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_R]$ satisfies $\boldsymbol{\Xi}'\boldsymbol{\Xi} = I_R$. Then Σ/p has finite effective rank, $\eta_2 = C \cdot \operatorname{tr}(\Sigma/p)\sqrt{\ln n/n} = \mathrm{O}(\sqrt{\ln n/n})$. Assume further that $n = \mathrm{o}(p^2)$. Then, when n is sufficiently large, both $\sigma^2/p < 2(1-\varepsilon_1)\eta_2 - \eta_2$ and $\lambda_R + \sigma^2/p \geq 2(1+\varepsilon_1)\eta_2 + \eta_2$ hold. By Theorem 3.2, $\widehat{s}(2\widetilde{\eta}_2/p)$ estimates R, the number of factors, accurately, with high probability.

3.1. Population covariance matrices with polynomially decaying spectrum: Jump detection

In this section, the analysis presented in Theorem 3.1 is specialized to particular modeling assumptions on Σ. With a view towards Section 5, in which we discuss functional data, we treat here in more detail the class of population covariance matrices whose spectrum exhibits a polynomial decay. Specifically, we consider matrices satisfying the conditions below. Let $EG(\Sigma) := \{\lambda_1, \ldots, \lambda_p\}$.

Assumption 2. *There exist absolute constants $C_{1\lambda}$, $C_{2\lambda}$ and $\beta_2 \geq \beta_1 > 1$ such that $C_{2\lambda} k^{-\beta_2} \leq \lambda_k \leq C_{1\lambda} k^{-\beta_1}$, for all k. Moreover, there exist absolute constants $C_{3\lambda}$ and $\beta_3 > \beta_2$ such that $\min_{\lambda \in EG(\Sigma), \lambda \neq \lambda_k} |\lambda - \lambda_k| \geq C_{3\lambda} k^{-\beta_3}$, for all k.*

We will show in Section 5 that these conditions appear naturally in the study of data generated from the Brownian motion, and in that case we give specific values for β_1, β_2 and β_3. Note that the largest eigenvalue of any population matrix Σ satisfying Assumption 2 is a constant independent of p. Moreover, since $\beta_1 > 1$, the effective rank $r_e(\Sigma)$ of such matrices will also have a constant value. Therefore, Assumption 2 ensures that Σ belongs to $\mathcal{P}_2(\varepsilon)$ with $\varepsilon \lesssim \sqrt{\ln n/n}$, irrespective of the value of p. If $p = \mathrm{O}(n^\gamma)$, then $\Sigma \in \mathcal{P}_2(\varepsilon)$, with $\varepsilon \lesssim \ln pn/n$. Note further that the order of the noise levels η_1 and η_2 given by (3.1) and (3.2), respectively, are, under Assumption 2, $\sqrt{\ln pn/n}$ and $\sqrt{\ln n/n}$, and therefore only differ by a $\sqrt{\ln p}$ factor when $r_e(\Sigma)$ is a constant.

In the analysis below we will consider only $\eta_2 = \mathrm{O}(\sqrt{\ln n/n})$, to allow for the possibility of p growing independently of n. We will specialize Theorem 3.1 by determining the minimal values of τ_1 and τ_2 that define a detectable jump. We note that they will differ from the values given by

Theorem 3.2, which is not applicable to the class of models satisfying Assumption 2. To see why, first notice that Theorem 3.2 presupposes the existence of an index s such that λ_s (or λ_{s+1}) and $\lambda_s - \lambda_{s+1}$ are constant multiples of the noise level η_2. An index with these properties does not exist under Assumption 2. It is immediate to see why: assuming that such an s exists would imply that $\frac{1}{s^{\beta_1}} < \frac{1}{s^{\beta_3}}$, which cannot hold for $\beta_3 > \beta_1$. However, if the jump in the theoretical spectrum occurs at a level that is larger, in order, than the noise level, then it can be again detected, with high probability, as illustrated by the following theorem.

Theorem 3.3. *Suppose Σ satisfies Assumptions 1 and 2. Assume n is sufficiently large such that the following mild technical condition holds,*

$$(1+\varepsilon_1)^{\beta_1/\beta_3} - (1-\varepsilon_1)^{\beta_1/\beta_3} < C_{1\lambda}^{-1}\big(3C_{3\lambda}^{-1}\big)^{-\beta_1/\beta_3}\eta_2^{1-\beta_1/\beta_3}.$$

If there exists an index s such that

$$\lambda_s \geq \big\{C_{4\lambda}(1+\varepsilon_1)\eta_2\big\}^{\beta_1/\beta_3} + \eta_2, \qquad \lambda_{s+1} < \big\{C_{4\lambda}(1-\varepsilon_1)\eta_2\big\}^{\beta_1/\beta_3} - \eta_2$$

with $C_{4\lambda} = 3C_{2\lambda}^{-1}C_{1\lambda}^{\beta_3/\beta_1}$, then

$$\mathbb{P}\big\{\widehat{s}\big((C_{4\lambda}\widetilde{\eta}_2)^{\beta_1/\beta_3}\big) = s\big\} \geq 1 - 11n^{-1}.$$

Remark 3.3.

(i) The technical condition holds for sufficiently large n because $(1+\varepsilon_1)^{\beta_1/\beta_3} - (1-\varepsilon_1)^{\beta_1/\beta_3} = \mathrm{O}(\varepsilon_1) = \mathrm{O}(\eta_2) = \mathrm{o}(\eta_2^{1-\beta_1/\beta_3})$.

(ii) The discussion prior to Theorem 3.3 above illustrates that attempting to determine spectral jumps in the population matrix that occur at the minimal noise level may be an ill posed problem for certain classes of covariance matrices. Theorem 3.3 offers a solution when Assumption 2 is met.

(iii) Under Assumption 2, Theorem 3.3 shows that by setting $\widetilde{\tau} = (C_{4\lambda}\widetilde{\eta}_2)^{\beta_1/\beta_3} = \mathrm{O}_P\{(\ln n/n)^{\beta_1/(2\beta_3)}\}$ in (3.3) we can estimate the jump with high probability.

4. Accuracy of the sample eigenvalues and eigenvectors selected via scree plot methods

In this section, we investigate whether the eigenvalues and the corresponding eigenvectors, obtained via the simple thresholding method, for appropriate data-dependent thresholds, are accurate estimates of their population counterparts. We begin by discussing eigenvalue estimation. By Weyl's theorem, we always have $|\widehat{\lambda}_k - \lambda_k| \leq \|\Sigma_n - \Sigma\|_2$, for all k. However, this inequality is not particularly informative when λ_k is small, and the relative difference $\widehat{\lambda}_k/\lambda_k - 1$ may be more appropriate and is used here. By combining Weyl's theorem and the results in Section 2.2, we obtain the following corollary.

Corollary 4.1. *Suppose that Assumption 1 holds. Let $\eta_{\min}$ be either η_1 or η_2, defined in (3.1) and (3.2).*

(i) *Then*

$$\left|\frac{\widehat{\lambda}_k}{\lambda_k} - 1\right| \le \frac{\eta_{\min}}{\lambda_k}, \tag{4.1}$$

holds simultaneously for all k, with probability larger than $1 - 5n^{-1}$.

(ii) *For any n and p, and for all k, we have*

$$\frac{|\widehat{\lambda}_k - \lambda_k|}{p} \lesssim \frac{\operatorname{tr}(\Sigma)}{p}\sqrt{\frac{\ln n}{n}}, \tag{4.2}$$

with probability larger than $1 - 5n^{-1}$.

Example 4.1 (Estimation of eigenvalues in a factor model). For the factor model (3.9) defined above, Kneip and Sarda [19], in their Theorem 2, bound the left-hand side in (4.2), for all $k \le R$, by a term of order $1/p + (\log p/n)^{1/2}$, when $p > \sqrt{n}$. Under this scenario both their bound and ours have the same order of magnitude, $\mathrm{O}(\sqrt{\ln n/n})$. Corollary 4.1 above shows that, moreover, the $\mathrm{O}(\sqrt{\ln n/n})$ rate of convergence is still valid when (i) $p < \sqrt{n}$; (ii) p grows independently of n or $p = \mathrm{O}\{\exp(n)\}$, since (4.2) does not contain a $\log p$ factor.

Inequality (4.1) of Corollary 4.1 shows that, in order to have $|\widehat{\lambda}_k/\lambda_k - 1| \le \alpha$, where α is a small number in (0, 1), for all $k \le K$, the index K has to satisfy $\lambda_K \ge \eta_{\min}/\alpha$. Note further that the last population eigenvalue that can be accurately estimated only needs to be larger than this threshold, and there are no further requirements on the relative size of the following eigenvalue or on the size of their gap. Therefore, taking K equal to one of the estimators of the detectable jumps derived in the previous section is unnecessary and would be misleading, as in this way we would identify only the consistent estimates of those population eigenvalues up to where jumps occur. The following theorem shows how to identify the data-dependent number of sample eigenvalues close to their population counterparts, under very mild assumptions.

Theorem 4.1. *Let $j \in \{1, 2\}$ be fixed. Suppose $\Sigma \in \mathcal{P}_j(\varepsilon)$, for some $\varepsilon \in (0, 1)$ and that Assumption 1 holds. For ε_1 and C_j defined in (3.8) above, and for some given $\alpha \in (0, 1)$, let*

$$\widetilde{K}_j = \max\left\{k : \widehat{\lambda}_k \ge \frac{\widetilde{\eta}_j}{C_j(1-\varepsilon_1)}\left(1 + \alpha^{-1}\right)\right\} \tag{4.3}$$

for the data dependent $\widetilde{\eta}_j$ given by (3.6) or (3.7) above. Then, $|\widehat{\lambda}_k/\lambda_k - 1| \le \alpha$, for all $k \le \widetilde{K}_j$, with probability larger than $1 - 11n^{-1}$.

The study of the accuracy of the sample eigenvectors is more complex and Proposition 4.1 below shows that the accuracy of sample eigenvectors depends on both $\eta_{\min}$ and the gaps between successive eigenvalues. Recall that $\boldsymbol{\psi}_k$ is the eigenvector of Σ associated with λ_k and denote by $\widehat{\boldsymbol{\psi}}_k$ the counterpart from the sample covariance matrix. The sign of $\widehat{\boldsymbol{\psi}}_k$ is selected so that $\widehat{\boldsymbol{\psi}}_k'\boldsymbol{\psi}_k \geq 0$.

Proposition 4.1. *Let Assumption 1 hold. Let $\eta_{\min}$ be given by either (3.1) or (3.2). Assume that $\lambda_1 > \lambda_2 > \cdots > \lambda_p > 0$. Then, with probability $1 - 5n^{-1}$,*

$$\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\psi}_k\| \leq \frac{\eta_{\min}}{\min_{\lambda \in EG(\Sigma), \lambda \neq \lambda_k} |\lambda - \lambda_k|} + \frac{6(\eta_{\min})^2}{\min_{\lambda \in EG(\Sigma), \lambda \neq \lambda_k} |\lambda - \lambda_k|^2} \tag{4.4}$$

for each $k = 1, \dots, n \wedge p$.

The above proposition follows by combining Lemma A.1 in [20] with the results of Section 2.2. Furthermore, by taking $\eta_{\min} = \eta_2$ and using the same reasoning as the one following Corollary 4.1, we can derive sharper bounds on the left-hand side of (4.4) than those derived, for factor models, in Theorem 2 of [19]. These bounds will hold for all n and p, and are valid for more general matrices Σ.

Proposition 4.1 makes it clear that, without further information on the degree of separation of the spectrum of Σ, the scree plot method applied to the spectrum of Σ_n, for any data-adaptive threshold, cannot guarantee that the retained sample eigenvectors are close to their population counterparts. The theorem below provides a simple way for evaluating accuracy of estimated eigenvectors, based on the gaps between consecutive sample eigenvalues.

Theorem 4.2. *Let $0 < \alpha < 1$ be given and define $\widehat{\lambda}_0 = +\infty$, and $\widehat{\lambda}_{p+1} = 0$. Let $j \in \{1, 2\}$ be fixed. Suppose $\Sigma \in \mathcal{P}_j(\varepsilon)$, for some $\varepsilon \in (0, 1)$ and that Assumption 1 holds. Let ε_1 and C_j as defined in (3.8) above, and let $\widetilde{\eta}_j$ be given by (3.6) or (3.7). Then for all $k \geq 1$ such that*

$$\min(\widehat{\lambda}_{k-1} - \widehat{\lambda}_k, \widehat{\lambda}_k - \widehat{\lambda}_{k+1}) \geq \frac{\widetilde{\eta}_j}{C_j(1 - \varepsilon_1)}\big(2 + 3\alpha^{-1}\big), \tag{4.5}$$

we have $\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\psi}_k\| \leq \alpha$, with probability larger than $1 - 11n^{-1}$.

Remark 4.1. The theorem shows that, in order to establish accuracy of a certain sample eigenvector, one just needs to check whether (4.5) holds. The procedure is general, but $\widetilde{\eta}_j$ still depends on unknown constants that in turn depend on the distribution of the data. We suggest the usage of a cross-validation type criterion for practical use. Also, note that if both consistent eigenvalue *and* eigenvector estimation is of interest, then one can use the scree plot method outlined in Theorem 4.1 to determine the maximum number of consistent eigenvalues, then use the procedure described in Theorem 4.2 to evaluate which of the retained eigenvectors are also consistent.

4.1. Population covariance matrices with polynomially decaying spectrum: Accurate feature estimation

If Assumption 2 holds, we have knowledge of the degree of separation of the population spectrum. In this case, Theorem 4.2 suggests that we just need to find the largest k such that (4.5) holds, since (4.5) will hold for all smaller k. Furthermore, under Assumption 2, the two inequalities in (4.3) and (4.5) will be equivalent. This means that we can use again the scree plot method and develop a data-dependent threshold $\widetilde{\eta}_{\text{ev}}$ that guarantees both eigenvalue and eigenvector consistency. We formalize this below, again using η_2 as the benchmark noise level. Results in terms of η_1 can be derived in a similar manner.

Theorem 4.3. *Let $0 < \alpha < 1$ be given. Suppose that Assumption 1 holds and let ε_1 be given by (3.8) above. Under Assumption 2, define*

$$\widetilde{\eta}_{\text{ev}} = C_{1\lambda}\left[\frac{3\widetilde{\eta}_2}{(1-\varepsilon_1)C_{3\lambda}\alpha}\right]^{\beta_1/\beta_3} + \frac{\widetilde{\eta}_2}{1-\varepsilon_1} \tag{4.6}$$

for $\widetilde{\eta}_2$ given in (3.7). Let

$$\widetilde{K}_{\text{ev}} = \max\{k : \widehat{\lambda}_k \geq \widetilde{\eta}_{\text{ev}}\}.$$

Then $\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\psi}_k\| \leq \alpha$ and $|\widehat{\lambda}_k/\lambda_k - 1| \leq \alpha/3$, for all $k \leq \widetilde{K}_{\text{ev}}$, with probability larger than $1 - 11n^{-1}$.

5. An application to fPCA

In this section, we specialize our results to the analysis of sample covariance matrices constructed from functional data. Let $X_i(s)$, $i = 1, \dots, n$, denote an i.i.d. sample of trajectories from a Gaussian process $\{X(t) : 0 \leq t \leq 1\}$, with covariance function $\mathcal{K}(s,t) = \text{cov}\{X(s), X(t)\}$. Assume that we observe discretized versions of these trajectories, possibly corrupted by noise

$$Y_i(t_j) = \mu(t_j) + X_i(t_j) + E_{ij}, \tag{5.1}$$

where $\mu(\cdot)$ is the mean function and E_{ij} are mean zero measurement errors that are independent of $X_i(\cdot)$. Assume $\text{var}(E_{ij}) = \sigma^2$ is finite. We assume that all trajectories are observed at the same set of m points $\{0 < t_1 < t_2 < \cdots < t_{m-1} < t_m < 1\}$ in $[0, 1]$.

We consider classes of covariance operators satisfying the following assumptions.

Assumption A. *$\mathcal{K}(s,t)$ is continuous and a positive semi-definite kernel.*

Under Assumption A, Mercer's theorem guarantees that $\mathcal{K}(s,t)$ admits the representation $\sum_{k=1}^{\infty} \rho_k \phi_k(s)\phi_k(t)$, where $\{\rho_1 \geq \rho_2 \geq \cdots \geq 0\}$ are non-decreasing eigenvalues and $\{\phi_k(\cdot), k = 1, \dots\}$ are eigenfunctions that are orthonormal in $L_2[0,1]$. Moreover, $\sum_k \rho_k =: \rho_0 < \infty$.

Assumption B. $\sup_k \sup_{s\in[0,1]} |\phi_k(s)|$ *is bounded by a constant $C_{5\lambda}$.*

Assumption C. $\frac{\partial \mathcal{K}(t,t)}{\partial t}$ *is continuous in $(0,1)$, right continuous at 0 and left continuous at 1. Moreover, $\int |\frac{\partial K(t,t)}{\partial t}| \,\mathrm{d}t$ is finite.*

Assumption D. $\sup_{s\in[0,1]} |\phi_k^{(1)}(s)| \le C_{6\lambda} k^{\gamma_1}$ *for all* k *where* $\phi_k^{(1)}(s)$ *is the derivative of* ϕ_k *and* C_1, γ_1 *are positive constants. Here* $\phi_k^{(1)}(0)$ *is the right derivative of* ϕ_k *at* 0 *and* $\phi_k^{(1)}(1)$ *is the left derivative of* ϕ_k *at* 1.

Note that the trigonometric basis satisfies Assumptions B–D.

Assumption E. *Assumption 2 of Section 3.1 holds for the eigenvalues of* $\mathcal{K}$, *and moreover,* $\beta_1 > \gamma_1$.

Remark 5.1. All these assumptions hold for the Brownian motion and the Brownian bridge on $[0,1]$, with $\beta_1 = \beta_2 = 2$, $\beta_3 = 3$, and $\gamma_1 = 1$.

We denote by π_m the projection mapping $X(t)$ into an m-dimensional space $\mathbb{R}^m$, defined by $\pi_m(X) = (X(t_1), \dots, X(t_m))$. We refer to the distributions on $\mathbb{R}^m$ induced by π_m as the finite-dimensional distributions of X. Let $\mathbf{K} = m^{-1}\{\mathcal{K}(t_{j_1}, t_{j_2})\}_{1\le j_1, j_2 \le m}$ be the scaled covariance matrix for the m-dimensional distribution of X. Let $Y_i = \{Y_i(t_1), \dots, Y_i(t_m)\}'$, $\bar{Y}(t) = n^{-1}\sum_{i=1}^n Y_i(t)$ and $\bar{Y} = \{\bar{Y}(t_1), \dots, \bar{Y}(t_m)\}'$. To facilitate the application of the results derived in the previous sections to functional data we denote

$$\Sigma = \mathbf{K} + m^{-1}\sigma^2 I_m. \tag{5.2}$$

An estimate of Σ is the scaled sample covariance matrix, corresponding to discretely observed trajectories:

$$\Sigma_n = m^{-1} n^{-1} \sum_i (Y_i - \bar{Y})(Y_i - \bar{Y})'.$$

To keep our presentation focused, we have employed the sample mean $\bar{Y}$ as an estimator of the mean function of the process. For the scenario we study below, of densely sampled trajectories, $\bar{Y}$ suffices. One may also use a smooth estimator, but then an appropriate equivalent of Proposition A.2 will be needed and it is deferred to future work.

We shall discuss in detail the usage of the scree plot method based on the sample covariance matrix Σ_n for estimating: (i) the location of jumps in the spectrum of the covariance operator $\mathcal{K}$; (ii) the number of sample eigenvalues and eigenvectors that are accurate estimates of their population counterparts. The diagram below illustrates the connections needed for this analysis.

$$\big\{\mathcal{K}(s,t)\big\}_{s,t\in[0,1]} \longleftrightarrow_1 \mathbf{K} =: m^{-1}\big\{\mathcal{K}(t_{j_1}, t_{j_2})\big\}_{1\le j_1, j_2\le m} \longleftrightarrow_2 \Sigma =: \mathbf{K} + m^{-1}\sigma^2 I_m \longleftrightarrow_3 \Sigma_n.$$

First, recall that we assumed (Assumption E) that the spectrum of the covariance *operator* $\mathcal{K}$ has polynomial decay, and that in Sections 3.1 and 4.1 we addressed in detail (i) and (ii) for covariance *matrices* whose spectra have polynomial decay such that the largest eigenvalue and the effective rank are both finite. In order to employ these results here, we need to identify a matrix that can be formed from $\mathcal{K}$ by evaluating it at a discrete set of points and whose spectrum has essentially the same properties as that of $\mathcal{K}$. For us, this matrix is $\mathbf{K}$ defined above: without scaling it by m their respective spectra cannot be close, as they are not of the same order. We show this in Proposition 5.1 below and, moreover, we show that the eigenvectors of $\mathbf{K}$ are close to the vectors formed by evaluating the eigenfunctions of $\mathcal{K}$ at the time points $(t_1, \dots, t_m)$. Assumptions B–D above are crucial for establishing these connections. To account for error terms in model (5.1), we will consider a slight modification of $\mathbf{K}$, namely Σ defined above in (5.2), which has features similar to $\mathbf{K}$. We therefore expect that the scree plot method applied to Σ_n will lead to consistent estimates of (i) and (ii) above, and we show that this is indeed the case in Sections 5.2 and 5.3.

5.1. Finite approximations of eigenfunctions and eigenvalues

Here we provide a deterministic analysis of the quality of $\mathbf{K}$ as an approximation to $\mathcal{K}$. With slight abuse of notation, we denote the eigenvalues of $\mathbf{K}$ by $\{\lambda_1, \lambda_2, \dots\}$ and the associated eigenvectors by $\{\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \dots\}$. The eigenvalues and eigenvectors of Σ are then $\{\lambda_k + m^{-1}\sigma^2, \boldsymbol{\psi}_k\}$. We let $\boldsymbol{\phi}_k = m^{-1/2}(\phi_k(t_1), \dots, \phi_k(t_m))'$. Note that we intend to compare $\boldsymbol{\psi}_k$, which is an eigenvector and therefore has Euclidean norm equal to one, with $\boldsymbol{\phi}_k$, hence the need for scaling in its definition. We also denote by $EG(\mathcal{K})$ the spectrum of $\mathcal{K}$. The following assumption is also needed.

Assumption F. *For the fixed design points $\{t_j : 1 \le j \le m\}$, there exists a constant $M > 0$ such that $M^{-1}m^{-1} \le \min_{0 \le j \le m} |t_{j+1} - t_j| \le \max_{0 \le j \le m} |t_{j+1} - t_j| \le Mm^{-1}$. Here $t_0 = 0, t_{m+1} = 1$.*

Proposition 5.1. *If Assumptions A–F hold and if m is sufficiently large so that $m^{(1-\beta_1)/(\beta_1+\gamma_1)} \le 1/12C_{7\lambda}$, for $C_{7\lambda}$ given in (A.6), then we have*

$$\sup_{k \ge 1} |\lambda_k - \rho_k| \le C_{8\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)}, \tag{5.3}$$

where $C_{8\lambda} = C_{5\lambda}^2 C_{1\lambda}/(\beta_1 - 1) + C_{1\lambda} + 13C_{7\lambda}\lambda_0$ and also

$$\left|\operatorname{tr}(\mathbf{K}) - \rho_0\right| \le C_{9\lambda} m^{-1} \tag{5.4}$$

for some fixed positive constant $C_{9\lambda}$, independent of m. Moreover, we have

$$\begin{aligned} \|\boldsymbol{\psi}_k - \boldsymbol{\phi}_k\| \le{}& \frac{C_{8\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)}}{\min_{\rho \in EG(\mathcal{K}), \rho \ne \rho_k} |\rho - \rho_k|} \\ &+ 6\left\{\frac{C_{8\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)}}{\min_{\rho \in EG(\mathcal{K}), \rho \ne \lambda_k} |\rho - \rho_k|}\right\}^2 + 7C_{7\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)} \end{aligned} \tag{5.5}$$

for all $k \le m^{1/(\beta_1+\gamma_1)}$.

To the best of our knowledge, the result in Proposition 5.1 is new. The proof is given in Appendix A.4.1. Whereas the global result (5.4) is an immediate consequence of approximating integrals by finite sums, the derivation of (5.3) and (5.5) is much more involved, and depends crucially on the behavior of the spectrum and eigenfunctions of the covariance operator $\mathcal{K}$. The combination of (5.3) and (5.4) immediately yields the result below.

Corollary 5.1. *Under the assumptions of Proposition 5.1*, $r_e(\mathbf{K}) = \mathrm{O}(1)$ *and, moreover*, $r_e(\Sigma) = \mathrm{O}(1)$.

This result shows that the finite dimensional distributions of processes with eigenvalues decaying as in Assumption E automatically have scaled covariance matrices $\mathbf{K}$ of finite effective rank.

5.2. Detectable jumps in the spectrum of a covariance operator

The results derived in Theorem 3.3 can be easily extended to the consistent estimation of an index of the spectrum of the covariance operator where a jump occurs. The following theorem shows that we can detect spectral jumps of an appropriate size via a data driven thresholding of the spectrum of Σ_n. Since Proposition 5.1 guarantees that the spectra of $\mathcal{K}$ and $\mathbf{K}$ are close, the construction of these thresholds follows from Theorem 3.3.

Theorem 5.1. *Suppose that* $X(t)$ *is a Gaussian process with a covariance function that satisfies Assumptions A–F. The assumption on* m *is the same as in Proposition 5.1. Let* η_2 *be given by* (3.7). *Assume* n *is sufficiently large such that the following mild technical condition holds*,

$$(1+\varepsilon_1)^{\beta_1/\beta_3} - (1-\varepsilon_1)^{\beta_1/\beta_3} < C_{1\lambda}^{-1}\big(3C_{3\lambda}^{-1}\big)^{-\beta_1/\beta_3}\eta_2^{1-\beta_1/\beta_3}.$$

If there exists an index s *such that*

$$\rho_s \geq \big\{C_{4\lambda}(1+\varepsilon_1)\eta_2\big\}^{\beta_1/\beta_3} + C_{8\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)} + m^{-1}\sigma^2 + \eta_2,$$
$$\rho_{s+1} < \big\{C_{4\lambda}(1-\varepsilon_1)\eta_2\big\}^{\beta_1/\beta_3} - C_{8\lambda} m^{(1-\beta_1)/(\beta_1+\gamma_1)} - m^{-1}\sigma^2 - \eta_2$$

with $C_{4\lambda} = 3C_{3\lambda}^{-1}C_{1\lambda}^{\beta_3/\beta_1}$, *then*

$$\mathbb{P}\big\{\widehat{s}\big((C_{4\lambda}\widetilde{\eta}_2)^{\beta_1/\beta_3}\big) = s\big\} \geq 1 - 11n^{-1}$$

for $\widetilde{\eta}_2$ *given by* (3.7) *above.*

Remark 5.2. We have stated Theorem 5.1 in terms of η_2 given by (3.2) of Section 3 above. Since $r_e(\Sigma)$ and $\|\Sigma\|_2$ are finite in the context of Section 4, then $\eta_2 = \mathrm{O}(\sqrt{\ln n/n})$. From the results of Section 2.2, summarized in Table 1, we recall that this is the optimal bound on $\|\Sigma_n - \Sigma\|_2$, in the regime $m = \mathrm{O}\{\exp(n)\}$, as η_2 is independent of m, and can therefore be employed even if $m \to \infty$. This facilitates the direct translation of our results to the ideal case of perfectly sampled trajectories, when $m = \infty$. For each fixed m, the noise level η_1 given by (3.1), of order $\mathrm{O}(\sqrt{\ln nm/n})$ can also be employed, and in this case the data adaptive threshold will be a function of $\widetilde{\eta}_1$.

Remark 5.3. Recall that for the Brownian motion $\beta_1 = \beta_2 = 2$, $\beta_3 = 3$ and $\gamma_1 = 1$. In this case, Theorem 5.1 shows that by thresholding the sample covariance matrix at a level of

$O_P\{(\ln n/n)^{1/3} + m^{-1/3}\}$ we can identify the location of the population eigenvalue larger than the minimal level $O\{(\ln n/n)^{1/3} + m^{-1/3}\}$, as long as the following eigenvalue is also $O\{(\ln n/n)^{1/3} + m^{-1/3}\}$ apart. This is similar to the results of Section 3.1. The difference resides in the existence of the extra additive term $m^{-1/3}$, which quantifies the approximation error.

5.3. On the accuracy of the sample eigenvalues and eigenvectors selected via thresholding methods for functional data

We specialize the results of Section 4 for data generated as in (5.1), and when Assumptions A–F hold. For this, we first establish finite sample upper bounds for the sample eigenvalues and eigenvectors.

Proposition 5.2. *Suppose that $X(t)$ is a Gaussian process with a covariance function that satisfies Assumptions A–F. The assumption on m is the same as in Proposition 5.1. Let $C_{10\lambda} = \max(m^{-1}\sigma^2 + c_2\rho_0, C_{8\lambda})$ where c_2 is as in Theorem 2.1 and $C_{8\lambda}$ is as in Proposition 5.1. Define*

$$\eta_f =: C_{10\lambda}\big(\eta_2 + m^{(1-\beta_1)/(\beta_1+\gamma_1)}\big). \tag{5.6}$$

Then with probability at least $1 - 5n^{-1}$, the following holds for each k:

$$|\widehat{\lambda}_k - \rho_k| \leq \eta_f.$$

Furthermore, with probability at least $1 - 5n^{-1}$, for each $1 \leq k \leq m^{1/(\beta_1+\gamma_1)}$,

$$\begin{aligned}\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\phi}_k\| \leq & \frac{\eta_f}{\min_{\rho\in EG(\mathcal{K}),\lambda\neq\rho_k}|\rho-\rho_k|} + \frac{6\eta_f^2}{\min_{\rho\in EG(\mathcal{K}),\rho\neq\rho_k}|\rho-\rho_k|^2} \\ & + 7C_{8\lambda}m^{(1-\beta_1)/(\beta_1+\gamma_1)}.\end{aligned} \tag{5.7}$$

The proof of Proposition 5.2 follows directly from Proposition 5.1, Corollary 4.1, and Proposition 4.1, hence the details are omitted.

Remark 5.4. Proposition 5.2 evaluates the accuracy of sample eigenvalues and eigenvectors as a function of both the sample size and the number of observations per subject. In particular, for the Brownian motion, we recall that $\eta_2 = O\{(\ln n/n)^{1/2}\}$ and thus

$$|\widehat{\lambda}_k - \rho_k| \lesssim (\ln n/n)^{1/2} + m^{-1/3} \qquad \text{for each } k$$

with high probability. Reasoning as in Theorem 4.1 of Section 4, it also follows that the ratio between all sample eigenvalues above η_f, or above an estimate of it, and the corresponding theoretical values, will also be close to one, with high probability.

We recall that the accuracy of the sample eigenvectors also depends on how well separated the eigenvalues of the operator $\mathcal{K}$ are from each other. Under our assumptions on the covariance operator, we have control on the degree of separation. We can therefore derive the analogue of Theorem 4.3 of Section 4 for functional data, and state it below.

Theorem 5.2. *Assume the settings in Proposition 5.2 hold. Then, with η_f given by (5.6) above we define*

$$\eta_{\text{op}} = C_{1\lambda}\left(\frac{3\eta_f}{C_{3\lambda}\alpha}\right)^{\beta_1/\beta_3} + \eta_f.$$

Let

$$K_{\text{op}} = \max\{k : \widehat{\lambda}_k \geq \eta_{\text{op}}\}.$$

Then $\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\phi}_k\| \leq \alpha$, for all $k \leq \min\{K_{\text{op}}, m^{1/(\beta_1+\gamma_1)}\}$, and $|\widehat{\lambda}_k/\rho_k - 1| \leq \alpha/3$, for all $k \leq K_{\text{op}}$, with probability larger than $1 - 11n^{-1}$.

Remark 5.5. The proof is immediate, and identical to the one of Theorem 4.3 above. In light of Theorem 4.3, the result above continues to hold when η_f is replaced by an estimate; in order to keep the presentation clear we contented ourselves here with the usage of the theoretical level η_f. For the Brownian motion $\beta_1 = 2$, $\gamma_1 = 1$ and $\beta_3 = 3$, resulting in

$$\eta_f = \mathrm{O}\big\{(\ln n/n)^{1/2} + m^{-1/3}\big\} \quad \text{and} \quad \eta_{\text{op}} = \mathrm{O}\big\{(\ln n/n)^{1/3} + m^{-2/9}\big\}.$$

Reasoning as in Section 4, we conclude that a thresholding level that is larger than the minimal η_{op} guarantees the accuracy of the sample eigenvalues and eigenvectors. For the Brownian motion, the number of accurate sample eigenvectors is always upper-bounded by $m^{1/3}$, but it may be smaller, depending on the relative value of K_{op}.

Appendix A: Technical proofs

The proofs for the lemmas, propositions and theorems not included below are provided in the supplemental article ([8]).

A.1. Technical proofs of Section 2

A.1.1. *Three useful lemmas*

Lemma A.1. *Let $X \in \mathbb{R}^p$ be a generic vector. Let $\Delta = \{u = (u_1, \ldots, u_p)' \in \mathbb{R}^p : |u_1| = \cdots = |u_p| = 1\}$. Then for any positive integer d,*

$$\|X\|^{2d} \leq \frac{1}{2^p}\sum_{u\in\Delta}\big(u'X\big)^{2d}.$$

Remark A.1. In the following proofs, we will assume sometimes, without loss of generality, that Σ is a diagonal matrix. This can be immediately justified as follows. Consider the eigendecomposition $\Sigma = ODO'$, where O is an orthonormal matrix and D is a diagonal matrix. Then $\mathrm{cov}(O'X) = D$ and $\|X\| = \|O'X\|$. Similar arguments can be employed when we consider orthonormal transforms of matrices, and evaluate either their Frobenius or operator norm.

Lemma A.2. *Let $X \in \mathbb{R}^p$ be a zero-mean sub-Gaussian random vector that satisfies Assumption 1. For any positive integer d,*

$$\mathbb{E}\|X\|^{2d} \le \frac{(2d)^d}{c_0^d}\big[\operatorname{tr}(\Sigma)\big]^d.$$

Lemma A.3. *Let $X \in \mathbb{R}^p$ be a zero-mean sub-Gaussian random vector and satisfies Assumption 1. Then*

$$\big\|\|X\|\big\|_{\psi_2}^2 \le \frac{2\operatorname{tr}(\Sigma)}{c_0}.$$

A.1.2. Proof of the statements in Example 2.2

Proof of the statements in Example 2.2. We only need to show that X is sub-Gaussian and satisfies Assumption 1. Let $u \in \mathbb{R}^p$ be an arbitrary non-random vector. Then for any $t \ge 0$,

$$\mathbb{E}\exp\big(tu'X\big) = \prod_{j=1}^p \mathbb{E}\exp(tu_jX_j) \le \prod_{j=1}^p \exp\big\{(tu_j\sqrt{\Sigma_{jj}})^2\sigma^2/2\big\} = \exp\big\{t^2\big(u'\Sigma u\big)\sigma^2/2\big\},$$

where the last equality holds because Σ is a diagonal matrix as the components of X are independent. Hence, $u'X$ is sub-Gaussian and X is a sub-Gaussian random vector. The above inequality also implies

$$\mathbb{E}\exp\big\{t\big(u'X\big)/\sqrt{u'\Sigma u}\big\} \le \exp\big(t^2\sigma^2/2\big).$$

By Lemma 5.5 in [25], there exists a constant c_0 (depends only on σ^2) such that $\sqrt{c_0}\|(u'X)/\sqrt{u'\Sigma u}\|_{\psi_2} \le 1$. By the linearity of the sub-Gaussian norm, we have $c_0\|u'X\|_{\psi_2}^2 \le u'\Sigma u$ as desired. □

A.1.3. Proofs of Theorems 2.1 and 2.2

For our analysis, we write $\Sigma_n = \Sigma_n^* - \bar{X}\bar{X}'$, where $\Sigma_n^* = n^{-1}\sum_{i=1}^n X_iX_i'$. Then $\|\Sigma_n - \Sigma\|_F \le \|\Sigma_n^* - \Sigma\|_F + \|\bar{X}\|^2$ and $\|\Sigma_n - \Sigma\|_2 \le \|\Sigma_n^* - \Sigma\|_2 + \|\bar{X}\|^2$. Hence to derive the upper bounds for $\|\Sigma_n - \Sigma\|_F^2$ and $\|\Sigma_n - \Sigma\|_2^2$, we just need to obtain the upper bounds for $\|\Sigma_n^* - \Sigma\|_F^2$, $\|\Sigma_n^* - \Sigma\|_2^2$ and $\|\bar{X}\|^4$. Because of the fact that $\mathbb{P}(X + Y \ge c + d) \le \mathbb{P}(X \ge c) + \mathbb{P}(Y \ge d)$ for any two univariate random variables X and Y and arbitrary numbers c and d, to study the tail behaviors of $\|\Sigma_n - \Sigma\|_F$ and $\|\Sigma_n - \Sigma\|_2$, we only need to study those of $\|\Sigma_n^* - \Sigma\|_F$, $\|\Sigma_n^* - \Sigma\|_2$ and $\|\bar{X}\|^2$. As a result, Theorem 2.1 is proved by combining Propositions A.2 and A.3, and Theorem 2.2 is proved by combining Propositions A.2 and A.4. Materials that are needed for proving Propositions A.3 and A.3 are provided in the next two subsections.

We begin with the study of $\bar{X}\bar{X}'$. Since this is a rank 1 matrix, we make use of the basic fact $\|\bar{X}\bar{X}'\|_F = \|\bar{X}\bar{X}'\|_2 = \|\bar{X}\|^2$. The following proposition is instrumental in the proofs of Propositions A.2 and A.3.

Proposition A.1. *Let Assumption 1 hold. There exist two fixed positive constants C_*, c_* such that, if $|t| > c_*(4c_0^{-1} + 1)\operatorname{tr}(\Sigma)$,*

$$\mathbb{E}\exp\left\{\frac{\|X\|^2 - \operatorname{tr}(\Sigma)}{t}\right\} \le \exp\left\{C_*\left[\frac{(4c_0^{-1} + 1)\operatorname{tr}(\Sigma)}{t}\right]^2\right\}.$$

Proof. Let $\|\cdot\|_{\psi_1}$ be the sub-exponential norm of a sub-exponential random variable (see Definition 5.13 of [25]). We have

$$\begin{aligned}\big\|\|X\|^2 - \operatorname{tr}(\Sigma)\big\|_{\psi_1} &\le \big\|\|X\|^2\big\|_{\psi_1} + \big\|\operatorname{tr}(\Sigma)\big\|_{\psi_1} \\ &\le 2\|\|X\|\|_{\psi_2}^2 + \operatorname{tr}(\Sigma) \\ &\le \operatorname{tr}(\Sigma)\big(4c_0^{-1} + 1\big).\end{aligned} \tag{A.1}$$

For the second inequality above, we used Lemma 5.14 of [25] and for the third inequality we used Lemma A.3. Because $\|X\|^2 - \operatorname{tr}(\Sigma)$ is a zero-mean sub-exponential random variable, by Lemma 5.15 of [25], there exist two fixed constants C_*, c_* such that if $|t| \ge c_*\|\|X\|^2 - \operatorname{tr}(\Sigma)\|_{\psi_1}$,

$$\mathbb{E}\exp\left\{\frac{\|X\|^2 - \operatorname{tr}(\Sigma)}{t}\right\} \le \exp\left\{C_*\frac{\|\|X\|^2 - \operatorname{tr}(\Sigma)\|_{\psi_1}^2}{t^2}\right\}.$$

Combining (A.1) with the above inequality, we obtain the proposition. □

Proposition A.2. *Let Assumption 1 hold. For any $t \ge 0$,*

$$\mathbb{P}\left\{\|\bar{X}\|^2 \ge \frac{1 + c_1 t}{n} \cdot \operatorname{tr}(\Sigma)\right\} \le \exp(1 - t), \tag{A.2}$$

where $c_1 = \max\{\max(\sqrt{C_*}, c_*)(4c_0^{-1} + 1), 2\}$ is a constant. Furthermore,

$$\mathbb{E}\big(\|\bar{X}\|^4\big) \le \big\{1 + 2\big(c_1^2 + c_1\big)\exp(1)\big\}\frac{\operatorname{tr}(\Sigma)^2}{n^2}.$$

Proof. It is straightforward to verify that $\sqrt{n}\bar{X}$ is sub-Gaussian and satisfies Assumption 1 with the same c_0. Applying the Markov inequality to $\exp(n\|\bar{X}\|^2)$ we obtain, for any $a > 0$, $x \ge c_*(4c_0^{-1} + 1)\operatorname{tr}(\Sigma)$,

$$\begin{aligned}\mathbb{P}\big\{n\|\bar{X}\|^2 - \operatorname{tr}(\Sigma) \ge a\big\} &\le \exp\big(-at^{-1}\big)\mathbb{E}\exp\big\{x^{-1}\big[n\|\bar{X}\|^2 - \operatorname{tr}(\Sigma)\big]\big\} \\ &\le \exp\big(-ax^{-1}\big)\exp\left\{C_*\left[\frac{(4c_0^{-1} + 1)\operatorname{tr}(\Sigma)}{x}\right]^2\right\},\end{aligned}$$

where the last inequality holds by Proposition A.1. By letting $x = c_1\operatorname{tr}(\Sigma)$ and $a = tx$ we obtain (A.2). The expectation inequality is proved in the supplemental article ([8]). □

Next, we study $\Sigma_n^* - \Sigma$. Let $Z_i = X_i X_i' - \Sigma$. Then $\mathbb{E}(Z_i) = 0$ and $\Sigma_n^* - \Sigma = n^{-1}\sum_{i=1}^n Z_i$. We begin by stating the bounds with respect to the Frobenius norm.

Proposition A.3. *Let Assumption 1 hold. For all $n \geq 1$ and $t \geq 0$:*

$$\mathbb{P}\left\{\|\Sigma_n^* - \Sigma\|_F \geq \frac{2c_1[\sqrt{2\exp(1)} + 8\sqrt{t}]\cdot \operatorname{tr}(\Sigma)}{\sqrt{n}}\right\} \leq 2\exp\{-\min(t, 2\sqrt{nt})\}, \tag{A.3}$$

where c_1 is defined in Proposition A.2. Furthermore,

$$\mathbb{E}(\|\Sigma_n^* - \Sigma\|_F^2) \leq \left[\frac{4c_1 \operatorname{tr}(\Sigma)}{\sqrt{n}}\right]^2 c_2,$$

where $c_2 = \exp(1) + \int_0^\infty \exp\{-\frac{1}{64}\min(t, 16\sqrt{t})\}\,\mathrm{d}t$.

Proof. By Theorem A.2, the Frobenius norm is 2-smooth on the space $\mathbb{R}^{p\times p}$ of $p \times p$ real matrices. Hence by Proposition A.5 and Theorem A.1,

$$\mathbb{P}\left\{\|\Sigma_n^* - \Sigma\|_F \geq \frac{2c_1[\sqrt{2\exp(1)} + t]\cdot \operatorname{tr}(\Sigma)}{\sqrt{n}}\right\} \leq 2\exp\left\{-\frac{1}{64}\min(t^2, 16t\sqrt{n})\right\}.$$

Inequality (A.3) follows by changing t to $8\sqrt{t}$ in the above inequality. The expectation inequality is proved in the supplemental article ([8]). □

Proposition A.4. *Let Assumption 1 hold. For all $n \geq 1$ and $t \geq 0$:*

$$\mathbb{P}\left\{\|\Sigma_n^* - \Sigma\|_2 \geq c_3 \cdot \|\Sigma\|_2 \cdot \max\left\{\sqrt{\frac{r_e(\Sigma)(t + \ln p)}{n}}, \frac{r_e(\Sigma)(t + \ln p)}{n}\right\}\right\} \leq \exp(-t), \tag{A.4}$$

where c_3 is a fixed constant that depends only on c_0. Furthermore,

$$\mathbb{E}(\|\Sigma_n^* - \Sigma\|_2^2) \leq 5c_3^2 \cdot \|\Sigma\|_2^2 \cdot \max\left\{\frac{r_e(\Sigma)\cdot \ln p}{n}, \left(\frac{r_e(\Sigma)\cdot \ln p}{n}\right)^2\right\}.$$

Proof. Let $Z_i = X_i X_i' - \Sigma$, then $\mathbb{E}(Z_i) = 0$. We derive that $\Sigma_n^* = n^{-1}\sum_{i=1}^n X_i X_i' = n^{-1} \times \sum_{i=1}^n Z_i + \Sigma$ and hence $\|\Sigma_n^* - \Sigma\|_2 = \|n^{-1}\sum_{i=1}^n Z_i\|_2$. With Proposition A.6, the probability inequality (A.4) is proved by applying Theorem A.3. The expectation inequality is proved in the supplemental article ([8]). □

A.1.4. *Supplemental materials for proving Proposition A.3*

The proof of Proposition A.3 consists in adapting results in [18] to our context and verifying its hypotheses. For completeness, we state these results below.

Theorem A.1. *Let $(E, |||\cdot|||)$ be κ-smooth with a norm $|||\cdot|||$ on E. Let $\{Z_1, Z_2, \ldots\}$ be E-valued, zero-mean and independent. Assume that there exists a sequence of positive numbers $\{\sigma_1, \sigma_2, \ldots\}$ such that $\mathbb{E}\{\exp(\sigma_i^{-1}|||Z_i|||)\} \leq \exp(1)$, $i \geq 1$. Then for all $n \geq 1$ and $t \geq 0$:*

$$\mathbb{P}\left\{\left|\left|\left|\frac{Z_1 + \cdots + Z_n}{n}\right|\right|\right| \geq \frac{\sqrt{\exp(1)\kappa} + t}{n}\sqrt{\sum_{i=1}^{n} \sigma_i^2}\right\} \leq 2\exp\left\{-\frac{1}{64}\min\left(t^2, tt_n^*\right)\right\},$$

where $t_n^* = 16\sqrt{\sum_{i=1}^{n} \sigma_i^2}/\max_{1\leq i\leq n} \sigma_i$.

Remark A.2. Theorem A.1 is a special case of Theorem 4.1 in [18] and the definition of a κ-smooth space is on page 3 therein.

Theorem A.2. *Let $2 \leq p < \infty$. The Schatten norm $\|Z\|_p = \{\sum_j [d_j(Z)]^p\}^{1/p}$ on the space $\mathbb{R}^{m\times n}$ of $m \times n$ real matrices, where $d_1(Z) \geq d_2(Z) \geq \cdots$ are the singular values of Z, is $\kappa_p(m, n)$-smooth with*

$$\kappa_p(m, n) = \min_{2\leq\rho<\infty,\rho\leq p} \left\{\max(2, \rho - 1)\right\}\left\{\min(m, n)\right\}^{2/\rho-2/p}.$$

Remark A.3. Theorem A.2 is Example 3.3 in [18]. For $p = 2$ we have the Frobenius norm which is κ-smooth with $\kappa = 2$.

Proposition A.5. *Let $Z = XX' - \Sigma$. Then $\mathbb{E}\{\exp[t^{-1}\|Z_i\|_F]\} \leq \exp(1)$, for any $t \geq 2c_1 \operatorname{tr}(\Sigma)$, where c_1 is defined in Proposition A.2.*

Proof. First we have $\|Z\|_F = \|XX' - \Sigma\|_F \leq \|XX'\|_F + \|\Sigma\|_F = \|X\|^2 + \|\Sigma\|_F$. It is easy to show that $\|\Sigma\|_F \leq \operatorname{tr}(\Sigma)$. Hence,

$$\begin{aligned}\mathbb{E}\left\{\exp\left[t^{-1}\|Z\|_F\right]\right\} &\leq \exp\left\{t^{-1}\left[\|\Sigma\|_F + \operatorname{tr}(\Sigma)\right]\right\}\mathbb{E}\left\{\exp\left[t^{-1}\left(\|X\|^2 - \operatorname{tr}(\Sigma)\right)\right]\right\} \\ &\leq \exp\left\{2t^{-1}\operatorname{tr}(\Sigma)\right\}\exp\left\{C\left[\frac{(4c_0^{-1} + 1)\operatorname{tr}(\Sigma)}{t}\right]^2\right\} \\ &\leq \exp(1)\end{aligned}$$

as desired if $t > 2c_1 \operatorname{tr}(\Sigma)$. In the above derivation, we used Proposition A.1. □

A.1.5. Supplemental materials for proving Proposition A.4

To derive the set of bounds on $\|\Sigma_n - \Sigma\|_2$ presented in Proposition A.4, we will appeal to the following result, which is adapted from Theorem 6.2 in [24].

Theorem A.3. *Let $\{Z_i, i = 1, \ldots, n\}$ be a sequence of independent and identically distributed symmetric matrices of dimension p. Assume that there exist positive quantities R and σ such that*

$$\mathbb{E}(Z_i) = 0 \quad \textit{and} \quad \left\|\mathrm{E}\left(Z_i^d\right)\right\|_2 \leq \frac{d!}{2}\cdot R^{d-2}\sigma^2 \qquad \textit{for } d = 2, 3, \ldots. \tag{A.5}$$

Then for all $t \geq 0$, *with probability at least* $1 - \exp(-t)$,

$$\left\| \frac{Z_1 + \cdots + Z_n}{n} \right\|_2 < 3 \cdot \max\left\{ \sigma \sqrt{\frac{t + \ln p}{n}}, R \frac{t + \ln p}{n} \right\}.$$

The proof of Proposition A.4 consists in the non-trivial verification of condition (A.5). We do this in the following proposition and two lemmas.

Proposition A.6. *Let Assumption 1 hold, and define* $Z = XX' - \Sigma$, *where* Σ *is the covariance matrix of* X. *Let* $\tilde{c}_1 = \sup_{d \geq 1} \exp(-d) d^d / d!$, $\tilde{c}_2 = \tilde{c}_1 c_0^2 \exp(-1) + \tilde{c}_1 \exp(-1)/4 + 3$ *and* $\tilde{c}_3 = \max\{4 \exp(1)/c_0, 1\}$. *If we let* $R = 2\tilde{c}_3 \cdot \mathrm{tr}(\Sigma)$ *and* $\sigma^2 = \tilde{c}_2 \tilde{c}_3^2 \cdot \mathrm{tr}(\Sigma) \cdot \|\Sigma\|_2$, *then*

$$\left\| \mathbb{E}(Z^d) \right\|_2 \leq \frac{d!}{2} \cdot R^{d-2} \sigma^2 \qquad \text{for } d = 2, 3, \ldots.$$

Lemma A.4. *Suppose* $A, B \in \mathbb{R}^{p \times p}$ *are two positive semi-definite matrices. Let* ODO' *be an eigendecomposition of* $A - B$ *with* $D = \mathrm{diag}(\lambda_1, \ldots, \lambda_p)$. *Let* $D^+ = \mathrm{diag}(|\lambda_1|, \ldots, |\lambda_p|)$. *Then* $OD^+O' \leq A + 2\|B\|_2 \cdot I_p$, *where the notation "*$\leq$*" was used to compare two matrices and for two matrices* E_1 *and* E_2, $E_1 \leq E_2$ *implies* $E_2 - E_1$ *is psd.*

Lemma A.5. *Suppose* $A, B \in \mathbb{R}^{p \times p}$ *are two positive semi-definite matrices. Fix* $u \in \mathbb{R}^p$. *For an arbitrary positive integer* d,

$$u'(A - B)^d u \leq \|A - B\|_2^{d-1} \left\{ u'\left(A + 2\|B\|_2 \cdot I_p\right) u \right\}.$$

A.1.6. *Proof of Theorem 2.3*

Proof of Theorem 2.3. Observe that $\mathrm{tr}(\Sigma_n) = \mathrm{tr}(\Sigma_n^*) + \|\bar{X}\|^2$. With Proposition A.2, it suffices to show that

$$\mathbb{P}\left\{ \left| \mathrm{tr}\left(\Sigma_n^*\right) - \mathrm{tr}(\Sigma) \right| \geq 2c_1 \sqrt{t/n} \cdot \mathrm{tr}(\Sigma) \right\} \leq 2 \exp(-t)$$

for any $t \geq 0$. By the Markov inequality, if $nx \geq c_1 \mathrm{tr}(\Sigma)$,

$$\begin{aligned}
\mathbb{P}\left\{ \mathrm{tr}\left(\Sigma_n^*\right) - \mathrm{tr}(\Sigma) \geq a \right\} &\leq \exp\left(-ax^{-1}\right) \mathbb{E} \exp\left\{ x^{-1} \left[\mathrm{tr}\left(\Sigma_n^*\right) - \mathrm{tr}(\Sigma) \right] \right\} \\
&\leq \exp\left(-ax^{-1}\right) \left\{ \mathbb{E} \exp\left\{ n^{-1} x^{-1} \left[\|X\|^2 - \mathrm{tr}(\Sigma) \right] \right\} \right\}^n \\
&\leq \exp\left(-ax^{-1}\right) \exp\left\{ C^* \left[\frac{(4c_0^{-1} + 1) \mathrm{tr}(\Sigma)}{\sqrt{n}x} \right]^2 \right\},
\end{aligned}$$

where in the last inequality we used Proposition A.1. By letting $x = c_1 \mathrm{tr}(\Sigma)/\sqrt{nt}$ and $a = 2c_1 \mathrm{tr}(\Sigma) \cdot \sqrt{t/n}$ we obtain from the above inequality that

$$\mathbb{P}\left\{ \mathrm{tr}\left(\Sigma_n^*\right) - \mathrm{tr}(\Sigma) \geq 2c_1 \sqrt{t/n} \cdot \mathrm{tr}(\Sigma) \right\} \leq \exp(-t).$$

With a similar argument, we can obtain

$$\mathbb{P}\{\mathrm{tr}(\Sigma_n^*) - \mathrm{tr}(\Sigma) \le -2c_1\sqrt{t/n}\cdot\mathrm{tr}(\Sigma)\} \le \exp(-t)$$

which completes the proof. □

A.1.7. Bounds on $r_e(\Sigma_n)$

Theorem A.4. *Suppose X is a random vector that satisfies Assumption 1. Let $n > 1$. If $\Sigma \in \mathcal{P}_1(\varepsilon)$, then with probability $1 - 11n^{-1}$,*

$$\left|\frac{r_e(\Sigma_n)}{r_e(\Sigma)} - 1\right| \lesssim \max\left\{\sqrt{\frac{r_e(\Sigma)\cdot \ln pn}{2n}}, \frac{r_e(\Sigma)\cdot \ln pn}{n}\right\}.$$

If $\Sigma \in \mathcal{P}_2(\varepsilon)$, then with probability $1 - 11n^{-1}$,

$$\left|\frac{r_e(\Sigma_n)}{r_e(\Sigma)} - 1\right| \lesssim \frac{r_e(\Sigma)\cdot \ln n}{n}.$$

A.2. Technical proofs of Section 3

Proof of Theorem 3.1. The proof follows from arguments similar to those used in Theorem 2 of [7]. We sketch it here for completeness. Note that $\widehat{s}(\widetilde{\tau}) = s$ is equivalent to $\widehat{\lambda}_s \ge \widetilde{\tau}$ and $\widehat{\lambda}_{s+1} < \widetilde{\tau}$, or equivalently, $\lambda_s - \widehat{\lambda}_s \le \lambda_s - \widetilde{\tau}$ and $\widehat{\lambda}_{s+1} - \lambda_{s+1} \le \widetilde{\tau} - \lambda_{s+1}$. By Weyl's theorem, Theorem 2.1 and Theorem 2.2, with probability larger than $1 - 5n^{-1}$, $|\widehat{\lambda}_k - \lambda_k| \le \|\Sigma_n - \Sigma\|_2 \le \eta_j$, for all k. Therefore, with (3.5), it suffices to have $\lambda_s - \tau_1 \ge \eta_j$ and $\tau_2 - \lambda_{s+1} \ge \eta_j$, which is (3.4). □

Proof of Theorem 3.2. The proof is an application of Theorem 3.1 with $\tau_1 = 2(1+\varepsilon_1)\eta_j/C_j$ and $\tau_2 = 2C_j(1-\varepsilon_1)\eta_j$, and we just need to verify inequality (3.5) for appropriately chosen δ. By Theorem 2.3, with probability $1 - 5n^{-1}$, $|\mathrm{tr}(\Sigma_n) - \mathrm{tr}(\Sigma)| \le \varepsilon_1 \mathrm{tr}(\Sigma)$. Let $\varepsilon_2 = (1 + c_1 + c_3)\sqrt{\varepsilon}$. For $\Sigma \in \mathcal{P}_1(\varepsilon)$, by Theorem 2.2, with probability at least $1 - 4n^{-1}$, $\|\Sigma_n - \Sigma\|_2 \le \varepsilon_2\|\Sigma\|_2$. Therefore, it is easy to show that, for $\Sigma \in \mathcal{P}_1(\varepsilon)$, with probability at least $1 - 6n^{-1}$, $\sqrt{(1-\varepsilon_1)(1-\varepsilon_2)}\eta_1 \le \widetilde{\eta}_1 \le \sqrt{(1+\varepsilon_1)(1+\varepsilon_2)}\eta_1$, and $0.9(1-\varepsilon_1)\eta_1 \le \widetilde{\eta}_1 \le (1+\varepsilon_1)\eta_1/0.9$ with the assumption that $\varepsilon_2 \le 0.19$. For $\Sigma \in \mathcal{P}_2(\varepsilon)$, with probability at least $1 - 5n^{-1}$, $(1-\varepsilon_1)\eta_2 \le \widetilde{\eta}_2 \le (1+\varepsilon_1)\eta_2$. □

Proof of Theorem 3.3. The theorem is proved by combining Theorem 3.1 and the probability inequality $\mathbb{P}\{(1-\varepsilon_1)\eta_2 \le \widetilde{\eta}_2 \le (1+\varepsilon_1)\eta_2\} \ge 1 - 5n^{-1}$. □

A.3. Technical proofs of Section 4

Proof of Theorem 4.2. Note first that

$$\min_{\lambda \in EG(\Sigma), \lambda \ne \lambda_k} |\lambda - \lambda_k| = \min(\lambda_{k-1} - \lambda_k, \lambda_k - \lambda_{k+1}),$$

where we let $\lambda_0 = +\infty$ and $\lambda_{p+1} = 0$. By Weyl's theorem and the results in Section 4, it is easy to show that

$$\min(\lambda_{k-1} - \lambda_k, \lambda_k - \lambda_{k+1}) \geq \min(\widehat{\lambda}_{k-1} - \widehat{\lambda}_k, \widehat{\lambda}_k - \widehat{\lambda}_{k+1}) - 2\eta_{\min},$$

with probability larger than $1 - 5n^{-1}$. Because with probability larger than $1 - 6n^{-1}$, $\widetilde{\eta}_j \geq C_j(1-\varepsilon_1)\eta_{\min}$, the assumption (4.5) in the theorem implies with probability larger than $1 - 11n^{-1}$,

$$\min(\lambda_{k-1} - \lambda_k, \lambda_k - \lambda_{k+1}) \geq 3\eta_{\min}/\alpha,$$

and the theorem holds by Proposition 4.1. □

Proof of Theorem 4.3. Note that with probability larger than $1-6n^{-1}$, $\widetilde{\eta}_{\mathrm{ev}} \geq C_{1\lambda}(\frac{3\eta_2}{C_{3\lambda}\alpha})^{\beta_1/\beta_3} + \eta_2$. It follows that with probability larger than $1-11n^{-1}$, $\lambda_k \geq \widehat{\lambda}_k - \eta_2 \geq C_{1\lambda}(\frac{3\eta_2}{C_{3\lambda}\alpha})^{\beta_1/\beta_3}$, for all $k \leq \widetilde{K}_{\mathrm{ev}}$. By Assumption 2, we derive that $k \leq (\frac{3\eta_2}{C_{3\lambda}\alpha})^{-1/\beta_3}$ and $\lambda_k - \lambda_{k+1} \geq C_{3\lambda}k^{-\beta_3} \geq 3\eta_2/\alpha$. Therefore by Proposition 4.1, with probability larger than $1-11n^{-1}$, for all $k \leq \widetilde{K}_{\mathrm{ev}}$,

$$\|\widehat{\boldsymbol{\psi}}_k - \boldsymbol{\psi}_k\| \leq \frac{\eta_2}{3\eta_2/\alpha} + \frac{6\eta_2^2}{9\eta_2^2/\alpha^2} \leq \alpha,$$

and

$$\left|\frac{\widehat{\lambda}_k}{\lambda_k} - 1\right| \leq \frac{\eta_2}{\lambda_k} \leq \frac{\eta_2}{\lambda_k - \lambda_{k+1}} \leq \frac{\alpha}{3}. \qquad \square$$

A.4. Technical proofs of Section 5

A.4.1. *Proof of Proposition 5.1*

Proof of Proposition 5.1. First, notice that ρ_0 is the integral $\int K(t,t)\,\mathrm{d}t$, while $\mathrm{tr}(\mathbf{K}) = m^{-1}\sum_{j=1}^m K(t_j, t_j)$ is a finite approximation to the integral. Hence, equality (5.4) can be easily proved because of Assumption D.

To prove (5.3) and (5.5), we need some initial derivations. By Assumptions D, E and F, we have

$$\left|\boldsymbol{\phi}_{k_1}'\boldsymbol{\phi}_{k_2} - \delta_{k_1,k_2}\right| \leq C_{7\lambda}\max(k_1,k_2)^{\gamma_1}/m \tag{A.6}$$

for all k_1 and k_2. Here $C_{7\lambda}$ is a fixed constant that depends only on $C_{6\lambda}$ in Assumption D and δ_{k_1,k_2} equals 1 if $k_1 = k_2$ and 0 otherwise. Let $\lceil x \rceil$ be the smallest integer that is no smaller than x. Define $N = \lceil m^{1/(\beta_1+\gamma_1)} \rceil < m$. Let $A = [\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_N]$ be an $m \times N$ matrix and let $D = \mathrm{diag}(\lambda_1, \dots, \lambda_N)$. It follows that

$$\mathbf{K} = \sum_k \lambda_k \boldsymbol{\phi}_k \boldsymbol{\phi}_k' = ADA' + \sum_{k>N} \lambda_k \boldsymbol{\phi}_k \boldsymbol{\phi}_k',$$

and hence

$$\|\mathbf{K} - ADA'\|_F = \left\| \sum_{k>N} \lambda_k \boldsymbol{\phi}_k \boldsymbol{\phi}_k' \right\|_F \le \sum_{k>N} \lambda_k \|\boldsymbol{\phi}_k \boldsymbol{\phi}_k'\|_F = \sum_{k>N} \lambda_k \|\boldsymbol{\phi}_k\|^2.$$

By Assumption E, $\lambda_k \le C_{1\lambda} k^{-\beta_1}$. Hence,

$$\sum_{k>N} \lambda_k \le \int_N^\infty C_{1\lambda} x^{-\beta_1}\,\mathrm{d}x = \frac{C_{1\lambda}}{1-\beta_1} x^{1-\beta_1}\Big|_N^\infty = \frac{C_{1\lambda} N^{1-\beta_1}}{\beta_1 - 1}.$$

Combining the results above with (A.6), we obtain

$$\|\mathbf{K} - ADA'\|_F = \sum_{k>N} \lambda_k \|\boldsymbol{\phi}_k\|^2 \le C_{5\lambda}^2 \sum_{k>N} \lambda_k \le \frac{C_{5\lambda}^2 C_{1\lambda}}{\beta_1 - 1} N^{1-\beta_1}, \tag{A.7}$$

where $C_{5\lambda}$ is an upper bound for all ϕ_k (see Assumption B). Next, we study the term ADA'. Consider a QR decomposition of A, where Q is an $m \times N$ matrix with orthonormal columns and R is an $N \times N$ upper-triangular matrix. Then $ADA' = Q(RDR')Q'$. Let Q and R be given as in Lemma A.6 below. We can further derive for all $1 \le i, k \le N$,

$$\left|R_{ik}^2 - \delta_{i,k}(1+r_i)^2\right| \le \frac{5C_{7\lambda} k^{\gamma_1}}{m} \le \frac{5C_{7\lambda} N^{\gamma_1}}{m}$$

and for all $1 \le i, k, j \le N$ with $i \ne j$,

$$|R_{ik} R_{jk}| \le \frac{5C_{7\lambda} k^{\gamma_1}}{m} \le \frac{5C_{7\lambda} N^{\gamma_1}}{m}.$$

We let $\tilde{D} = RDR'$ and compute $\tilde{d}_{ij}$ below. First,

$$\tilde{d}_{ii} = \sum_k \lambda_k R_{ik}^2 = \sum_{1\le k\le N} \lambda_k \left\{R_{ik}^2 - \delta_{i,k}(1+r_i)^2\right\} + \sum_{1\le k\le N} \lambda_k \delta_{i,k}(1+r_i)^2$$

and hence

$$\left|\tilde{d}_{ii} - \lambda_i(1+r_i)^2\right| \le \sum_{1\le k\le N} \lambda_k \frac{5C_{7\lambda} N^{\gamma_1}}{m} = \frac{5C_{7\lambda}\rho_0 N^{\gamma_1}}{m}.$$

Furthermore,

$$\begin{aligned}(\tilde{d}_{ii} - \lambda_i)^2 &\le \left(\tilde{d}_{ii} - \lambda_i - 2\lambda_i r_i - \lambda_i r_i^2\right)^2 + \left(2\lambda_i r_i + \lambda_i r_i^2\right)^2 \\ &\le 25\rho_0^2 C_{7\lambda}^2 N^{2\gamma_1}/m^2 + 144\lambda_i^2 C_{7\lambda}^2 N^{2+2\gamma_1}/m^2.\end{aligned}$$

Next for $i \ne j$,

$$|\tilde{d}_{ij}| = \left|\sum_k \lambda_k R_{ik} R_{jk}\right| \le \frac{5\rho_0 C_{7\lambda} N^{\gamma_1}}{m}.$$

It follows that

$$\|\tilde{D}-D\|_F^2 = \sum_{ij}(\tilde{d}_{ij}-\lambda_i\delta_{ij})^2 = \sum_i(\tilde{d}_{ii}-\lambda_i)^2 + \sum_{i\neq j}\tilde{d}_{ij}^2$$
$$\leq m^{-2}\sum_{i=1}^N\{25\rho_0^2C_{7\lambda}^2 + 144\lambda_i^2C_{7\lambda}^2N^2\}N^{2\gamma_1} + m^{-2}\sum_{i\neq j}25\rho_0^2C_{7\lambda}^2N^{2\gamma_1}$$
$$\leq 169C_{7\lambda}^2\rho_0^2N^{2+2\gamma_1}/m^2,$$

and hence

$$\|ADA'-QDQ'\|_F = \|\tilde{D}-D\|_F \leq 13C_{7\lambda}\rho_0N^{1+\gamma_1}m^{-1}. \tag{A.8}$$

Inequalities (A.7) and (A.8) together lead to

$$\|\mathbf{K}-QDQ'\|_F \leq \frac{C_{5\lambda}^2C_{1\lambda}N^{1-\beta_1}}{\beta_1-1} + \frac{13C_{7\lambda}\rho_0N^{1+\gamma_1}}{m}. \tag{A.9}$$

Now we are ready to prove (5.3) and (5.5). First, we invoke Weyl's theorem ([16], page 181), to obtain, for each k,

$$\begin{aligned}|\tilde{\lambda}_k-\lambda_k| &\leq \|\mathbf{K}-QDQ'\|_2 + 1_{\{k>N\}}\lambda_k \\ &\leq \frac{C_{5\lambda}^2C_{1\lambda}N^{1-\beta_1}}{\beta_1-1} + \frac{13C_{7\lambda}\rho_0N^{1+\gamma_1}}{m} + C_{1\lambda}N^{-\beta_1} \\ &\leq C_{8\lambda}m^{(1-\beta_1)/(\beta_1+\gamma_1)},\end{aligned} \tag{A.10}$$

where $C_{8\lambda} = C_{5\lambda}^2C_{1\lambda}/(\beta_1-1) + C_{1\lambda} + 13C_{7\lambda}\rho_0$ is a fixed constant and recall that $N = \lceil m^{1/(\beta_1+\gamma_1)}\rceil$. Since the upper bound in the above derivation does not depend on k, we obtain (5.3).

Finally, we prove (5.5). As in Lemma A.6 below, we denote the columns of Q by $\mathbf{v}_1,\dots,\mathbf{v}_N$. Then for $1\leq k\leq N$, $\boldsymbol{\phi}_k = \sum_{j=1}^k R_{kj}\mathbf{v}_j$. It follows that

$$\begin{aligned}\|\boldsymbol{\phi}_k-\mathbf{v}_k\| &\leq \sum_{j=1}^k|R_{kj}-\delta_{k,j}| \leq |r_k| + \sum_{j=1}^k 3C_{7\lambda}j^{\gamma_1}/m \\ &\leq 7C_{7\lambda}k^{1+\gamma_1}/m \leq 7C_{7\lambda}N^{1+\gamma_1}/m.\end{aligned} \tag{A.11}$$

Next by Lemma A.1 in [20] (see also inequality (A.6) of [19]), we obtain from (A.9) that

$$\|\boldsymbol{\psi}_k-\mathbf{v}_k\| \leq \frac{C_{8\lambda}m^{(1-\beta)/(\beta+\gamma_1)}}{\min_{\lambda\in EG(\mathcal{K}),\lambda\neq\lambda_k}|\lambda-\lambda_k|} + 6\left\{\frac{C_{8\lambda}m^{(1-\beta)/(\beta+\gamma_1)}}{\min_{\lambda\in EG(\mathcal{K}),\lambda\neq\lambda_k}|\lambda-\lambda_k|}\right\}^2. \tag{A.12}$$

Inequalities (A.11) and (A.12) together gives (5.5) which completes the proof. □

Lemma A.6. *Suppose the assumptions in Proposition 5.1 hold. Let* $A = [\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_N]$ *be an* $m \times N$ *matrix. Let* (Q, R) *be a QR decomposition of* A *where* Q *is an* $m \times N$ *matrix with orthonormal columns and* R *is an* $N \times N$ *upper-triangular matrix. Denote the* (k, j)*th element of* R *by* R_{kj}*. Let* N *be a positive integer such that* $12C_{7\lambda}N^{1+\gamma_1} \le m$ *where* $C_{7\lambda}$ *is the constant as in inequality* (A.6)*. If* A *has full rank, then there exists a pair of* Q *and* R *such that if* $k > j$*,* $R_{kj} = 0$ *and if* $k \le j$*,*

$$|R_{kj} - \delta_{k,j} - \delta_{k,j} r_k| \le 3C_{7\lambda} j^{\gamma_1}/m,$$

where r_k *is defined in such a way that for all* $k \le N$

$$|r_k| \le 4C_{7\lambda} k^{1+\gamma_1}/m.$$

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Supplementary Material

Supplement to "On the sample covariance matrix estimator of reduced effective rank population matrices, with applications to fPCA" (DOI: 10.3150/14-BEJ602SUPP; .pdf). We provide proofs of all the lemmas, propositions and theorems stated, but not proved, in the Appendix of the main paper.

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