Statistical applications of Random matrix theory: comparison of two populations II

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Abstract: This paper investigates a statistical procedure for testing the equality of two independent estimated covariance matrices when the number of potentially dependent data vectors is large and proportional to the size of the vectors, that is, the number of variables. Inspired by the spike models used in random matrix theory, we concentrate on the largest eigenvalues of the matrices in order to determine significance. To avoid false rejections we must guard against residual spikes and need a sufficiently precise description of the behaviour of the largest eigenvalues under the null hypothesis.

In this paper we propose some “invariant” theorems that allows us to extend the test of Mariétan and Morgenthaler (2019a) for perturbation of order 1 to some general tests for order k. The statistics introduced in this paper allow the user to test the equality of two populations based on high-dimensional multivariate data.

Simulations show that these tests have more power of detection than standard multivariate approaches.

Keywords and phrases: High dimension, equality test of two covariance matrices, Random matrix theory, residual spike, spike model, dependent data, eigenvector, eigenvalue.

1. Introduction

Random matrix theory (RMT) can be used to describe the asymptotic spectral properties of estimators of high-dimensional covariance matrices. The theory has been applied to multi-antenna channels in wireless communication engineering and to financial mathematics models. In other data-rich and high-dimensional areas where statistics is used, such as brain imaging or genetic research, it has not found widespread use. The main barrier to the adoption of RMT may be the lack of concrete statistical results from the probability side. Simply using classical multivariate theory in the high dimension setting can sometimes lead to success, but such procedures are valid only under strict assumptions about

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*This paper is constructed from the Thesis of Rémy Mariétan that will be divided in three parts.
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the data such as normality or independence. Even minor differences between the model assumptions and the actual data distribution typically lead to catastrophic results and such procedures do also often have little to no power.

This paper proposes a statistical procedure for testing the equality of two covariance matrices $\Sigma_X$ and $\Sigma_Y$ when the number of potentially dependent data vectors $n$ and the number of variables $m$ are large. RMT tells us what happens to the eigenvalues and eigenvectors of estimators of covariance matrices $\hat{\Sigma}$ when both $n$ and $m$ tend to infinity in such a way that $\lim \frac{m}{n} = c > 0$. The classical case, when $m$ is finite and $n$ tends to infinity, is presented in the books of Mardia, Kent and Bibby (1979), Muirhead (2005) and Anderson (2003) (or its original version Anderson (1958)). In the RMT case, the behaviour is more complex, but by now, results of interest are known. Anderson, Guionnet and Zeitouni (2009), Tao (2012) and more recently Bose (2018) contain comprehensive introductions to RMT and Bai and Silverstein (2010) covers the case of empirical (estimated) covariance matrices.

Although the existing theory builds a good intuition of the behaviour of these matrices, it does not provide enough of a basis to construct a statistical test with good power. Inspired by the existing theory, we extend the residual spikes introduced in Mariétan and Morgenthaler (2019a) and provide a description of the behaviour of diverse types of statistics under a null hypothesis when the perturbation is of order $k$. These results enable the user to test the equality of two populations as well as other null hypotheses such as the independence of two sets of variables. The remainder of the paper is organized as follows. First, we review the main theorem of Mariétan and Morgenthaler (2019a) and then indicate how to generalize the test (see Section 2). We next look at case studies and a compare the new test with alternatives. Finally, in Section 3, we present the main theorems. The proofs themselves are technical and presented in the supplementary material Mariétan and Morgenthaler (2019b).

2. Statistical test

2.1. Introduction

2.1.1. Hypotheses

We compare the spectral properties of two covariance estimators $\hat{\Sigma}_X$ and $\hat{\Sigma}_Y$ of dimension $m \times m$ which can be represented as

**Assumption 2.1.**

$$\hat{\Sigma}_X = P_X^{1/2} W_X P_X^{1/2} \text{ and } \hat{\Sigma}_Y = P_Y^{1/2} W_Y P_Y^{1/2}.$$ 

In this equation, $W_X$ and $W_Y$ are of the form

$$W_X = O_X \Lambda_X O_X \text{ and } W_Y = O_Y \Lambda_Y O_Y,$$

with $O_X$ and $O_Y$ being independent unit orthonormal random matrices whose distributions are invariant under rotations, while $\Lambda_X$ and $\Lambda_Y$ are independent...
positive random diagonal matrices, independent of $O_X, O_Y$ with trace equal to $m$ and a bound on the diagonal elements. Note that the usual RMT assumption, $\frac{m}{n} = c$ is replaced by this bound! The (multiplicative) spike model of order $k$ determines the form of the perturbation $P_X$ (and $P_Y$), which satisfies

$$P_X = I_m + \sum_{s=1}^{k} (\theta_{X,s} - 1)u_{X,s}u_{X,s}^t,$$

where $\theta_{X,1} > \theta_{X,2} > \ldots > \theta_{X,k}$ and the scalar product $(u_{X,s}, u_{X,r}) = \delta_{s,r}$. $P_Y$ is of the same form.

Some results require large value for $\theta$ and others not. To be precise, we will make use of the following types of hypotheses:

**Assumption 2.2.** (A1) $\frac{\theta}{\sqrt{m}} \to \infty$.

(A2) $\theta \to \infty$.

(A3) $\theta_i = p_i \theta$, where $p_i$ is fixed different from 1.

(A4) For $i = 1, \ldots, k_\infty$, $\theta_i = p_i \theta$, $\theta \to \infty$ according to (A1) or (A2).

For $i = k_\infty + 1, \ldots, k$, $\theta_i = p_i \theta_0$.

For all $i \neq j$, $p_i \neq p_j$.

The result of this paper will apply to finite eigenvalues $\theta_s$. However, they must be detectable.

**Definition 2.1.**

1. We assume that a perturbation $P = I_m + (\theta - 1)uu^t$ is detectable in $\hat{\Sigma} = P^{1/2}W P^{1/2}$ if the perturbation creates a largest isolated eigenvalue, $\hat{\theta}$.

2. We say that a finite perturbation of order $k$ is detectable if it creates $k$ largest eigenvalues separated from the spectrum of $W$.

Finally, we generalize the filtered estimator of the covariance matrix introduced in Mariétan and Morgenthaler (2019a).

**Definition 2.2.**

Suppose $\hat{\Sigma}$ is of the form given in Assumption 2.1.

The unbiased estimator of $\theta_s$ ($s = 1, \ldots, k$) is defined as

$$\hat{\theta}_s = 1 + \frac{1}{m-k} \sum_{i=k+1}^{m} \frac{\hat{\lambda}_{\hat{\Sigma},i}}{\hat{\theta}_s - \hat{\lambda}_{\hat{\Sigma},i}},$$

where $\hat{\lambda}_{\hat{\Sigma},i}$ is the $i^{th}$ largest eigenvalue of $\hat{\Sigma}$.

Suppose that $\hat{u}_i$ denotes the eigenvector of $\hat{\Sigma}$ corresponding to the $i^{th}$ largest eigenvalue, the filtered estimated covariance matrix is then defined as

$$\hat{\Sigma} = I_m + \sum_{i=1}^{k} (\hat{\theta}_i - 1)\hat{u}_i\hat{u}_i^t.$$
Under Assumption 2.1, this estimator is asymptotically equivalent to the theoretical estimator using

\[ \hat{\theta}_s = 1 + \frac{1}{m-k} \sum_{i=k+1}^{m} \frac{\lambda_{W,i}}{\hat{\theta}_s - \lambda_{W,i}} \]

where \( \lambda_{W,i} \) is the \( i \)-th eigenvalue of \( W \).

Our results will apply to any two centered data matrices \( X \in \mathbb{R}^{m \times n_X} \) and \( Y \in \mathbb{R}^{m \times n_Y} \) which are such that

\[ \hat{\Sigma}_X = \frac{1}{n_X} XX^t \text{ and } \hat{\Sigma}_Y = \frac{1}{n_Y} YY^t \]

can be decomposed in the manner indicated. This is the basic assumption concerning the covariance matrices.

We will assume throughout the paper that \( n_X \geq n_Y \).

Note also that because \( O_X \) and \( O_Y \) are independent and invariant by rotation we can assume without loss of generality that for \( s = 1, 2, ..., k \), \( u_{X,s} = e_s \) as in Benaych-Georges and Rao (2009). Under the null hypothesis, \( P_X = P_Y \), we use the simplified notation \( P_k \) for both matrices, where for \( s = 1, 2, ..., k \), \( \theta_{X,s} = \theta_{Y,s} = \theta_s \) and \( u_{X,s} = u_{Y,s}(= e_s) \).

2.2. The case of \( k = 1 \)

This paper generalise Mariétan and Morgenthaler (2019a), in which the following key result was established.

**Theorem 2.1.** Suppose \( W_X \) and \( W_Y \) satisfy 2.1 with \( P = P_X = P_Y \), a detectable perturbation of order \( k = 1 \). Moreover, we assume as known the spectra

\[ S_{W_X} = \{ \lambda_{W_X,1}, \lambda_{W_X,2}, ..., \lambda_{W_X,m} \} \text{ and } S_{W_Y} = \{ \lambda_{W_Y,1}, \lambda_{W_Y,2}, ..., \lambda_{W_Y,m} \}. \]

If \( (\hat{\theta}_X, \hat{\theta}_Y) \) converges to \((\rho_X, \rho_Y)\) in \( O\left(\frac{\theta}{\sqrt{m}}\right)\) and

\[ E\left[ \hat{\theta}_X \right] = \rho_X + o\left(\frac{\theta}{\sqrt{m}}\right) \text{ and } E\left[ \hat{\theta}_Y \right] = \rho_Y + o\left(\frac{\theta}{\sqrt{m}}\right), \]

then we have

\[ \begin{pmatrix} \hat{\theta}_X \\ \hat{\theta}_Y \end{pmatrix}_{(u_X, u_Y)^2} \big| S_{W_X}, S_{W_Y} \sim N\left( \begin{pmatrix} \theta \\ \rho_X \end{pmatrix}, \frac{1}{m} \begin{pmatrix} \sigma^2_{\theta,X} & \sigma_{\theta,\rho_X} \\ \sigma_{\rho_X,\theta} & \sigma^2_{\rho_X} \end{pmatrix} + \begin{pmatrix} \alpha_p & \alpha_p \left(\frac{\theta}{\sqrt{m}}\right) \\ \alpha_p & \alpha_p \left(\frac{\theta}{\sqrt{m}}\right) \end{pmatrix} \right) \],

where all the parameters in the limit law depend on

\[ M_{s,r,X}(\rho_X) = \frac{1}{m} \sum_{i=1}^{m} \frac{\hat{\lambda}_{W_X,i}}{(\rho_X - \hat{\lambda}_{W_X,i})^r} \text{ and } M_{s,r,Y}(\rho_Y) = \frac{1}{m} \sum_{i=1}^{m} \frac{\hat{\lambda}_{W_Y,i}}{(\rho_Y - \hat{\lambda}_{W_Y,i})^r}. \]
2.3. Generalization

Suppose $\hat{\Sigma}_X$ and $\hat{\Sigma}_Y$ are two random matrices that verify Assumption 2.1. We want to test

$$H_0 : P_X = P_Y, \text{ against } H_1 : P_X \neq P_Y.$$ 

When $P_X = P_Y = P_1$ are perturbation of order 1, we can use Theorem 2.1 to study any test statistic which is a function of the three statistics $\hat{\theta}_X, \hat{\theta}_Y, \langle \hat{u}_X, \hat{u}_Y \rangle^2$, where $\hat{\theta}_X$ and $\hat{\theta}_Y$ are asymptotic unbiased estimator of $\theta_X$ and $\theta_Y$ defined in 2.2 and $\langle \hat{u}_X, \hat{u}_Y \rangle$ is the dot product between the two largest eigenvectors of $\hat{\Sigma}_X$ and $\hat{\Sigma}_Y$.

In this paper we want to generalise such test statistics to perturbations of order $k$ by considering functions of $\hat{\theta}_X, 1, \ldots, \hat{\theta}_X,k, \hat{\theta}_Y, 1, \ldots, \hat{\theta}_Y,k, k \sum_{i=1}^{k} \langle \hat{u}_X, 1, \hat{u}_Y,i \rangle^2, \ldots, k \sum_{i=1}^{k} \langle \hat{u}_X,k, \hat{u}_Y,i \rangle^2$. (2.1)

Some possible tests are:

- $T_1 = m \sum_{i=1}^{k} \left( \frac{\hat{\theta}_X,i - \hat{\theta}_Y,i}{\sigma^2} \right)^2$, where $\sigma^2$ is the asymptotic variance of $\hat{\theta}_X,i - \hat{\theta}_Y,i$.
- $T_2 = \sum_{i=1}^{m} \left( \sum_{j=1}^{k} \langle \hat{u}_X,i, \hat{u}_Y,j \rangle^2 - \hat{\alpha}^2_{X,Y,i} \right)^{-1} \sum_{i=1}^{k} \langle \hat{u}_X,i, \hat{u}_Y,j \rangle^2 - \hat{\alpha}^2_{X,Y,i}$

where $\sum_{T_2}$ is the asymptotic variance of $\langle \hat{u}_X,i, \hat{u}_Y,j \rangle^2 - \hat{\alpha}^2_{X,Y,i}$.
- $T_3^\pm(s) = \lambda^\pm \left( \hat{\Sigma}_X^{-1/2} \left( \left( \hat{\theta}_Y,s - 1 \right) \hat{u}_Y,s \right) \hat{\Sigma}_X^{-1/2} + I_m \left( \frac{1}{\hat{\theta}_X,s} - 1 \right) \hat{u}_X,s \hat{u}_X,s \right)$

are also statistics of this form, where $\lambda^\pm()$ gives the extreme eigenvalues and $\hat{\Sigma}_X$ is the filtered estimator defined in 2.2.

- $\sum_{i=1}^{m} \lambda_i \left( \hat{\Sigma}_X^{-1/2} \hat{\Sigma}_Y \hat{\Sigma}_X^{-1/2} \right)$
- $\sum_{i=1}^{k} \lambda_i \left( \hat{\Sigma}_X^{-1/2} \hat{\Sigma}_Y \hat{\Sigma}_X^{-1/2} \right)$

In order to understand such statistics, we need to understand the joint behaviour of all the components in (2.1)

The theorems of this paper show that the distributions of $\hat{\theta}_X, \hat{\theta}_Y$ and $\langle \hat{u}_X, \hat{u}_Y \rangle^2$ we found for perturbation of order 1 describe also the general case.
2.4. Test statistic $T_1$

Based on Theorem 2.1, Theorem 3.1 and the fact that all the terms are uncorrelated by Theorem 3.1 of Marié etan and Morgenthaler (2019a), we can show that

$$T_1 \sim \chi^2_k + o_p(1),$$

where

$$\sigma^2 = \sigma^2_X + \sigma^2_Y = \frac{2(M_{2.2,X}(\rho) - M_{1.1,X}(\rho)^2)}{M_{1.1,X}(\rho)^4} + \frac{2(M_{2.2,Y}(\rho) - M_{1.1,Y}(\rho)^2)}{M_{1.1,Y}(\rho)^4},$$

Finally we can estimate $\sigma$ with $\hat{\sigma}$ by replacing $(\rho_{X,i}, \rho_{Y,i})$ by $(\hat{\theta}_{X,i}, \hat{\theta}_{Y,i})$.

2.5. Test statistic $T_2$

We can show that

$$\sum_{i=1}^{m} \left( \frac{\hat{\theta}_{X,i} - \hat{\theta}_{Y,i}}{\sum_{j=1}^{k} (\hat{u}_{X,i} \hat{u}_{Y,j})^2 - \hat{\alpha}^2_{X,Y,i}} \right)^2 \sum_{j=1}^{m} \left( \frac{\hat{\theta}_{X,i} - \hat{\theta}_{Y,i}}{\sum_{j=1}^{k} (\hat{u}_{X,i} \hat{u}_{Y,j})^2 - \hat{\alpha}^2_{X,Y,i}} \right) \sim \chi^2_{2k} + o(1),$$

where

$$M_{s_1,s_2,X}(\rho_{X}) = \frac{1}{m-k} \sum_{i=k+1}^{m} \frac{\hat{s}_{X_{i}}^{-1}}{(\rho_{X,i} - \hat{\lambda}_{X_{i}})^2}$$

and $M_{s_1,s_2,Y}(\rho_{Y}) = \frac{1}{m-k} \sum_{i=k+1}^{m} \frac{\hat{s}_{X_{i}}^{-1}}{(\rho_{Y,i} - \hat{\lambda}_{Y_{i}})^2}$.

Moreover

$$\Sigma_{T_2} = \nabla (G)^T \Sigma \nabla (G),$$

where $G : \mathbb{R}^3 \to \mathbb{R}^2$ is such that

$$\left( \sum_{j=1}^{k} (\hat{u}_{X,i} \hat{u}_{Y,j})^2 - \hat{\alpha}^2_{X,Y,i} \right) = G \left( \begin{array}{c} \hat{\theta}_{X,i} \\ \hat{\theta}_{Y,i} \end{array} \right).$$
and
\[
\left( \begin{array}{c}
\hat{\theta}_{X,i} \\
\hat{\theta}_{Y,i}
\end{array} \right)
\sim N\left( \begin{array}{c}
\rho_{X,i} \\
\rho_{Y,i}
\end{array} \right), \Sigma
\]

Using similar arguments as in the proof of Theorem 2.1, we can show that

Finally we can estimate \( \Sigma \) with \( \hat{\Sigma} \) by replacing \( (\rho_{X,i}, \theta_{X,i}, \rho_{Y,i}, \theta_{X,i}) \) by \( (\hat{\theta}_{X,i}, \hat{\theta}_{X,i}, \hat{\rho}_{Y,i}, \hat{\theta}_{X,i}) \) and \( \Sigma T_2 \) with

\[
\hat{\Sigma} T_2 = \nabla (G)^{t} \hat{\Sigma} \nabla (G)
\]

\section{2.6. Test statistic \( T_3 \)}

Elementary linear algebra in conjunction with the theorems of Mariétan and Morgenthaler (2019a) and this paper show that

\[
T_3(s) = \left[ \hat{\theta}_{Y,i} + \sum_{j=1}^{k} (\hat{\theta}_{Y,i} - \hat{\theta}_{Y,j})^2 \right] + o \left( \frac{1}{s} \right)
\]

This result can be obtained by looking at the trace and the square of the matrix. This statistic is the residual spike defined in Mariétan and Morgenthaler (2019a). Therefore \( T_3 \) is bounded by

\[
N \left( \lambda^+, \frac{\sigma^2}{m} \right) + o \left( \frac{1}{\sqrt{m}} \right) \quad \text{and} \quad N \left( \lambda^-, \frac{\sigma^2}{m} \right) + o \left( \frac{1}{\sqrt{m}} \right),
\]

with the parameters as defined in Theorem 2.1 of Mariétan and Morgenthaler (2019a).

\section{2.7. Simulation}

Assume \( X \in \mathbb{R}^{m \times n_X} \) and \( Y \in \mathbb{R}^{m \times n_Y} \) with \( X = (X_1, X_2, ..., X_{n_X}) \) and \( Y = (Y_1, Y_2, ..., Y_{n_Y}) \). The components of the random vectors are independent and the covariance between the vectors is as follows:

\[
X_i \sim N_m (\bar{0}, \sigma^2 I_m) \quad \text{with} \quad X_i = \epsilon_{X,i} + \mu X_i + \sqrt{1 - \rho^2} \epsilon_{X,i+1}, \quad \text{where} \quad \epsilon_{X,i} \overset{i.i.d}{\sim} N \left( 0, \sigma^2 I_m \right),
\]

\[
Y_i \sim N_m (\bar{0}, \sigma^2 I_m) \quad \text{with} \quad Y_i = \epsilon_{Y,i} + \mu Y_i + \sqrt{1 - \rho^2} \epsilon_{Y,i+1}, \quad \text{where} \quad \epsilon_{Y,i} \overset{i.i.d}{\sim} N \left( 0, \sigma^2 I_m \right)
\]
Let \( P_X = I_m + \sum_{i=1}^{k}(\theta X, i - 1)u X, i u X, i \) and \( P_Y = I_m + \sum_{i=1}^{k}(\theta Y, i - 1)u Y, i u Y, i \) be two perturbations in \( \mathbb{R}^{m \times m} \) and put

\[
X_P = P_X^{1/2} X \quad \text{and} \quad Y_P = P_Y^{1/2} Y,
\]

\[
\hat{\Sigma}_X = \frac{X_P^t X_P}{n_X} \quad \text{and} \quad \hat{\Sigma}_Y = \frac{Y_P^t Y_P}{n_Y}.
\]

### 2.7.1. Comparison with existing test

In the classical multivariate theory, the trace or the determinant of \( \hat{\Sigma}_X^{-1/2} \hat{\Sigma}_Y \hat{\Sigma}_X^{-1/2} \) are used to test the equality of two covariance matrices (see, for example, Anderson (1958)).

Suppose

\[
X_1, X_2, ..., X_{n_X} \overset{i.i.d.}{\sim} N_m(0, \Sigma_X), \quad Y_1, Y_2, ..., Y_{n_Y} \overset{i.i.d.}{\sim} N_m(0, \Sigma_Y).
\]

We want to test

\[ H_0 : \Sigma_X = \Sigma_Y \quad \text{against} \quad H_1 : \Sigma_X \neq \Sigma_Y, \]

In this section we show that any test statistic using either the log-determinant \( T_4 = \log |\hat{\Sigma}_X^{-1/2} \hat{\Sigma}_Y \hat{\Sigma}_X^{-1/2}| \) or \( T_5 = \text{Trace}(\hat{\Sigma}_X^{-1/2} \hat{\Sigma}_Y \hat{\Sigma}_X^{-1/2}) \) have difficulties to detect differences between the finite perturbations \( P_X \) and \( P_Y \). To explore this problem, we compare the performance of these tests with \( T_1, T_2 \) and \( T_3 \) by simulation. Table 1 shows the power of these tests to detect under a variety of alternatives and sample sizes. For \( T_1 \) and \( T_2 \) the critical values are based on the asymptotic chi-squared distributions, for \( T_3 \) the following two-sided power is used

\[
P_{025} \left( \max_{s=1,2,3} \left( \frac{\sqrt{v^2(\theta_X i, \theta_Y s) - \lambda_Y}}{\rho} \right) < q_{N(0,1)}(1 - 0.025/k) \right) \quad \text{or} \quad \min\limits_{s=1,2,3} \left( \frac{\sqrt{v^2(\theta_X i, \theta_Y s) - \lambda_Y}}{\rho} \right) < q_{N(0,1)}(0.025/k),
\]

with the parameters of Theorem 2.1 of Mariétan and Morgenthaler (2019a). For the tests \( T_4 \) and \( T_5 \) the critical values are determined by simulation. In order to apply these tests to degenerated matrices, the determinant is defined as the product of the non-null eigenvalues of the matrix and the inverse is the generalised inverse.

In the simulated cases, the trace and the determinant have difficulties to catch the alternatives. On the other hand, our procedures easily detect even small effects. These classical statistics \( T_4 \) and \( T_5 \) would presumably do well with global perturbations such as a multiplicative change of the covariance matrix.

**Remark 2.1.**

1. Under the assumption that \( \hat{\Sigma}_X = P_X^{1/2} W_X P_X^{1/2} \) and \( \hat{\Sigma}_Y = P_Y^{1/2} W_Y P_Y^{1/2} \) satisfy Assumption 2.1, the procedures \( T_1, T_2 \) and \( T_3 \) required the estimation of \( M_{s,r,X} = \frac{1}{m} \sum_{i=1}^{m} \frac{\lambda_{W_X, i}}{(\rho - \lambda_{W_X, i})} \) and \( M_{s,r,Y} = \frac{1}{m} \sum_{i=1}^{m} \frac{\lambda_{W_Y, i}}{(\rho - \lambda_{W_Y, i})} \).
3.1. Notation and definition

Notation 3.1.
We use a precise notation to enunciate the theorems, the proofs, however, often use a simpler notation when no confusion is possible. This difference is always specified at the beginning of the proofs.

- For any symmetric random matrix $A$ we denote by $(\hat{\lambda}_{A,i}, \hat{u}_{A,i})$ its $i^{th}$ eigenvalue and eigenvector.
A finite perturbation of order $k$ is denoted by $P_k = I_m + \sum_{i=1}^{k} (\theta_i - 1)u_i u_i^t \in \mathbb{R}^{m \times m}$ with $u_1, u_2, ..., u_k \in \mathbb{R}^{m \times m}$ orthonormal vectors.

$W \in \mathbb{R}^{m \times m}$ denotes a random matrix as defined in Assumption 2.1 which is invariant under rotation. Moreover, the estimated covariance matrix is $\hat{\Sigma} = P_k^{1/2} WP_k^{1/2}$.

When comparing two groups, we use $W_X$, $W_Y$ and $\hat{\Sigma}_X$, $\hat{\Sigma}_Y$.

When we consider only one group, $\hat{\Sigma}_P = P_k^{1/2} WP_k^{1/2}$ is the perturbation of order $r$ of the matrix $W$ and:

- $\hat{u}_{P,i}$ is its $i^{th}$ eigenvector. When $r = k$ we just use the simpler notation $\hat{u}_i = \hat{u}_{P,i}$ after an explicit statement.
- $\hat{u}_{P,i,j}$ is the $j^{th}$ component of the $i^{th}$ eigenvector.
- $\lambda_{P,i}$ is the $i^{th}$ eigenvalue. If $\theta_1 > \theta_2 > ... > \theta_r$, then for $i = 1, 2, ..., r$ we use also the notation $\hat{\lambda}_{P,i} = \lambda_{P,i}$. We call these eigenvalues the spikes. When $r = k$, we just use the simpler notation $\hat{\theta}_i = \hat{\lambda}_{P,i}$ after an explicit statement.
- $\hat{\alpha}_{P,i}^2 = \sum_{j=1}^{r} (\hat{u}_{P,i,j} \hat{u}_{P,i,j})^2$ is called the general angle.

With this notation, we have $\hat{\Sigma} = \hat{\Sigma}_P = P_k^{1/2} WP_k^{1/2}$.

When we consider two groups $X$ and $Y$, we use a notation similar to the above. The perturbation of order $r$ of the matrices $W_X$ and $W_Y$ are $\hat{\Sigma}_{X,P} = P_k^{1/2} W_X P_k^{1/2}$ and $\hat{\Sigma}_{Y,P} = P_k^{1/2} W_Y P_k^{1/2}$ respectively. Then, we define for the group $\hat{\Sigma}_{X,P}$ (and similarly for $\hat{\Sigma}_{Y,P}$):

- $\hat{u}_{\hat{\Sigma}_{X,P},i}$ is its $i^{th}$ eigenvector. When $r = k$ we use the simpler notation
  $\hat{u}_{X,i} = \hat{u}_{\hat{\Sigma}_{X,P},i}$.
- $\hat{u}_{\hat{\Sigma}_{X,P},i,j}$ is the $j^{th}$ component of the $i$ eigenvector.
- $\hat{\lambda}_{\hat{\Sigma}_{X,P},i}$ is its $i^{th}$ eigenvalue. If $\theta_1 > \theta_2 > ... > \theta_r$, then for $i = 1, 2, ..., r$ we use the notation $\hat{\lambda}_{\hat{\Sigma}_{X,P},i} = \hat{\lambda}_{\hat{\Sigma}_{X,P},i}$. When $r = k$, we use the simpler notation $\hat{\theta}_{X,i} = \hat{\lambda}_{\hat{\Sigma}_{X,P},i}$.
- $\hat{\alpha}_{\hat{\Sigma}_{X,P},i}^2 = \sum_{j=1}^{r} (\hat{u}_{\hat{\Sigma}_{X,P},i,j} \hat{u}_{\hat{\Sigma}_{X,P},i,j})^2$ is the double angle and, when no confusion is possible, we use the simpler notation $\hat{\alpha}_{P,i}^2$.

Some theorems assume the sign convention

$\hat{u}_{P,i,s} > 0$, for $s = 1, 2, ..., k$ and $i = 1, 2, ..., s$,

as in Theorem 3.4 or 3.5. Others assume the convention

$\hat{u}_{P,i,s} > 0$, for $s = 1, 2, ..., k$ and $i = 1, 2, ..., s$, 

as in Theorem 4.1.

Theorems that are not affected by this convention do not specify it precisely. Nevertheless, the convention will be mentioned in the proofs when confusion is possible.

- We define the function \( M_{s_1, s_2, X}(\rho_X) \), \( M_{s_1, s_2, Y}(\rho_Y) \) and \( M_{s_1, s_2}(\rho_X, \rho_Y) \) as

\[
M_{s_1, s_2, X}(\rho_X) = \frac{1}{m} \sum_{i=1}^{m} \frac{\hat{\lambda}_{W,X,i}}{\rho_X - \hat{\lambda}_{W,X,i}} \hat{W}_{X,i}^2,
\]

\[
M_{s_1, s_2, Y}(\rho_Y) = \frac{1}{m} \sum_{i=1}^{m} \frac{\hat{\lambda}_{W,Y,i}}{\rho_Y - \hat{\lambda}_{W,Y,i}} \hat{W}_{Y,i}^2,
\]

\[
M_{s_1, s_2}(\rho_X, \rho_Y) = \frac{M_{s_1, s_2, X}(\rho_X) + M_{s_1, s_2, Y}(\rho_Y)}{2}.
\]

In particular, when \( s_2 = 0 \), we use \( M_{s_1, X} = M_{s_1, 0, X} \). When we only study one group, we use the simpler notation \( M_{s_1, s_2}(\rho) \) when no confusion is possible.

- We use two transforms inspired by the T-transform:

\[
T_{W,u}(z) = \sum_{i=1}^{m} \frac{\hat{\lambda}_{W,i}}{z - \hat{\lambda}_{W,i}} \hat{u}_{W,i}^2
\]

is the T-transform in direction \( u \) using the random matrix \( W \).

\[
\hat{T}_{\Sigma_X}(z) = \frac{1}{m} \sum_{i=k+1}^{m} \frac{\hat{\lambda}_{W,i}}{z - \hat{\lambda}_{W,i}} \hat{W}_{i}^2, \quad \text{and} \quad \hat{T}_{W,X}(z) = \frac{1}{m} \sum_{i=1}^{m} \frac{\hat{\lambda}_{W,i}}{z - \hat{\lambda}_{W,i}} \hat{W}_{X,i}^2
\]

the estimated T-transforms using \( \hat{\Sigma}_X \) and \( W \) respectively.

- In some theorems we use the notation \( \sim_{ord} \) to describe the order size in probability of a positive random variable. For example, \( X_m \sim_{ord} 1/m \) if \( \frac{X_m}{1/m} \) tends to a random variable \( X \) independent of \( m \), with \( P\{X > \epsilon_j\} \to 1 \) for any sequences \( \epsilon_j \) tending to 0.

This paper extends previous results to perturbations of order \( k > 1 \) for some invariant statistics.

**Definition 3.1.**

Suppose \( W \) is a random matrix. Moreover, define \( P_1 = I_m + (\theta_1 - 1)u_1u_1^T \) and \( P_k = I_m + \sum_{i=1}^{k} (\theta_i - 1)u_iu_i^T \) some perturbations of order 1 and \( k > 1 \), respectively. We say that a statistic \( T(W_m, P_k) \) is invariant with respect to \( k \), if \( T(W_m, P_k) \) is such that

\[
T(W_m, P_k) = T(W_m, P_1) + \epsilon_m, \quad \text{where} \quad \max \left( \frac{\epsilon_m^2}{\text{var}(T(W_m, P_1))}, \frac{\epsilon_m^2}{\text{var}(T(W_m, P_1))} \right) \to 0.
\]

**3.2. Invariant Eigenvalue Theorem**

Theorem 2.1 provides distributions of statistics for perturbations of order 1. This estimated eigenvalue is an invariant statistics as defined in 3.1.
Theorem 3.1. Suppose that \( W \) satisfies Assumption 2.1 and
\[
\hat{P}_s = I_m + (\theta_s - 1)e_s e_s^t, \quad \text{for } s = 1, 2, ..., k,
\]
\[
P_k = I_m + \sum_{i=1}^{k} (\theta_i - 1)e_i e_i^t \quad \text{satisfies 2.2 (A4)},
\]
where \( \theta_1 > \theta_2 > ... > \theta_k \). We define
\[
\hat{\Sigma}_{\hat{P}_s} = \hat{P}_s^{1/2} W \hat{P}_s^{1/2},
\]
\[
\hat{\Sigma}_{P_k} = P_k^{1/2} W P_k^{1/2}.
\]
Moreover, for \( s = 1, 2, ..., k \), we define
\[
\hat{u}_{\hat{P}_s,1}, \hat{\theta}_{\hat{P}_s,1} \quad \text{s.t.} \quad \hat{\Sigma}_{\hat{P}_s} \hat{u}_{\hat{P}_s,1} = \hat{\theta}_{\hat{P}_s,1} \hat{u}_{\hat{P}_s,1},
\]
\[
\hat{u}_{P_k,s}, \hat{\theta}_{P_k,s} \quad \text{s.t.} \quad \hat{\Sigma}_{P_k} \hat{u}_{P_k,s} = \hat{\theta}_{P_k,s} \hat{u}_{P_k,s},
\]
where \( \hat{\theta}_{\hat{P}_s,1} = \hat{\lambda}_{\hat{\Sigma}_{\hat{P}_s,1}} \) and \( \hat{\theta}_{P_k,s} = \hat{\lambda}_{\hat{\Sigma}_{P_k,s}} \).

1. Then, for \( s > 1 \),
\[
\hat{\theta}_{P_k,s} - \hat{\theta}_{\hat{P}_s,1} \overset{d}{\sim} \frac{\theta_s}{m}
\]
and
\[
\hat{\theta}_{P_k,1} - \hat{\theta}_{\hat{P}_s,1} \overset{d}{\sim} \frac{\theta_2}{m}.
\]
The distribution of \( \hat{\theta}_{P_k,s} \) is therefore asymptotically the same as the distribution of \( \hat{\theta}_{\hat{P}_s,1} \) studied in Theorem 2.1.

2. More precisely we define for \( r, s \in \{1, 2, ..., k\} \) with \( r \neq s \),
\[
P_{r,s} = I_m + \sum_{i=1}^{k} (\theta_i - 1)e_i e_i^t.
\]

- If \( \theta_s > \theta_r \), then
\[
\hat{\theta}_{P_k,s} - \hat{\theta}_{P_{r,s}} = -\frac{\hat{\theta}_{P_{r,s}}}{\theta_s - 1} \hat{\Sigma}_{P_{r,s}} \hat{u}_{P_{r,s},s} \hat{u}_{P_{r,s},s}^t \hat{u}_{P_{r,s},s} + O_p \left( \frac{1}{m} \right) + O_p \left( \frac{\theta_s}{m^3} \right).
\]

- If \( \theta_s < \theta_r \), then
\[
\hat{\theta}_{P_k,s} - \hat{\theta}_{P_{r,s-1}} = -\frac{\hat{\theta}_{P_{r,s-1}}}{\theta_s - 1} \hat{\Sigma}_{P_{r,s-1}} \hat{u}_{P_{r,s-1},s} \hat{u}_{P_{r,s-1},s}^t \hat{u}_{P_{r,s-1},s} + O_p \left( \frac{1}{m} \right) + O_p \left( \frac{\theta_s}{m^3} \right).
\]

Remark 3.1.
In this manuscript, we are interested in the unbiased estimation of \( \hat{\theta}_{P_k,1} \). The invariance of \( \hat{\theta}_{P_k,1} \) is a direct consequence of the theorem. Moreover, Theorem 2.1 provides the distribution of \( \hat{\theta}_{P_k,1} \).

(Proof in supplement material Mariéton and Morgenthaler (2019b).)
3.3. Invariant Angle Theorem

The cosine of the angle between two vectors is linked to \( \langle u, v \rangle \). We need the more general notion of the angle between a vector and a subspace of dimension \( k \) associated with \( \sum_{i=1}^{k} \langle u, v_i \rangle^2 \), where \((v_1, \ldots, v_k)\) is an orthonormal basis of the subspace. This generalization of the angle used with the correct subspace leads to an invariance in the sense of Definition 3.1.

**Theorem 3.2.**

*Using the same notation as Theorem 3.1,*

1. The general angle is invariant in the sense of Definition 3.1,

\[
\sum_{i=1}^{k} \hat{u}_{P, s, i}^2 - \hat{u}_{P, 1, s}^2 + O_p \left( \frac{1}{\theta_1 m} \right).
\]

Therefore, the distribution of \( \sum_{i=1}^{k} \hat{u}_{P, s, i}^2 \) is asymptotically the same as the distribution of \( \hat{u}_{P, 1, s}^2 \) studied in Theorem 2.1.

2. Moreover,

\[
\hat{u}_{P, s, s}^2 - \hat{u}_{P, 1, s}^2 + O_p \left( \frac{1}{m} \right).
\]

**Remark 3.2.1.**

1. If \( \hat{u}_{P, 1, 1}^2 \sim N \left( \alpha^2, \frac{\sigma^2_{\alpha^2}}{\theta_1^2 m} \right) + o_p \left( \frac{1}{\theta_1 \sqrt{m}} \right) \),

then

\[
\sum_{i=1}^{k} \hat{u}_{P, 1, i}^2 \sim N \left( \alpha^2, \frac{\sigma^2_{\alpha^2}}{\theta_1^2 m} \right) + o_p \left( \frac{1}{\theta_1 \sqrt{m}} \right),
\]

where the parameter can be computed as in Theorem 2.1 in Marié etan and Morgenthaler (2019a).

2. Assuming that \( c = m/n \) and that \( W \) is a Wishart random matrix of dimension \( m \) with \( n \) degree of freedom, \( \alpha^2 = \frac{1}{\frac{\theta_1}{\theta_1 + 1}} \) and \( \sigma^2_{\alpha^2} = 2c^2 (c + 1) + o_p(1) \).

In particular if \( \frac{\theta_1}{\sqrt{m}} \) is large, then \( \alpha^2 \approx 1 - c/\theta_1 \).

3. In the general case, if \( \frac{\theta_1}{\sqrt{m}} \) is large,

\[
\alpha^2 \approx 1 + \frac{1 - M_{2, X}}{\theta_1} \quad \text{and} \quad \sigma^2_{\alpha^2} \approx 2 \left( 4M_{2, X}^3 - M_{2, X}^2 - 4M_{2, X}M_{3, X} + M_{4, X} \right).
\]

(Proof in supplement material Marié etan and Morgenthaler (2019b).)
3.4. Asymptotic distribution of the dot product

In this section, we compute the distribution of a dot product used in this paper to prove Theorem 3.1 and in a future work to compute the distributions of the residual spikes defined in Mariétan and Morgenthaler (2019a) for perturbation of order \(k\).

**Theorem 3.3.** Suppose that \(W\) satisfies Assumption 2.1 and \(P_2 = I + \sum_{i=1}^{2}(\theta_i - 1)e_ie_i^t\) with \(\theta_1 > \theta_2\). We define

\[
\hat{\Sigma}_P = P_2^{1/2}WP_2^{1/2} \quad \text{and} \quad \hat{\Sigma}_Q = P_1^{1/2}WP_1^{1/2}.
\]

Moreover, for \(s, k = 1, 2\) and \(s \leq k\), we define

\[
\hat{\hat{u}}_{P_{k,s}}, \hat{\hat{\theta}}_{P_{k,s}} \quad \text{s.t.} \quad \hat{\hat{\Sigma}}_{P_{k,s}} \hat{\hat{u}}_{P_{k,s}} = \hat{\hat{\theta}}_{P_{k,s}} \hat{\hat{u}}_{P_{k,s}},
\]

where \(\hat{\hat{\theta}}_{P_{k,s}} = \hat{\lambda}_{\hat{\hat{\Sigma}}_{P_{k,s}}}\). Finally the present theorem uses the convention:

For \(s = 1, 2, ..., k\) and \(i = 1, 2, ..., s\), \(\hat{\hat{u}}_{P_{s,i,i}} > 0\).

1. **Assuming that the conditions 2.2 (A2) and (A3) \((\theta_i = p_i \theta \rightarrow \infty)\) hold,** we have

\[
\sum_{s=3}^{m} \hat{u}_{P_{1,s}} \hat{u}_{P_{2,s}} = \hat{u}_{P_{1,2}} \left( \frac{1}{\theta_1} - \frac{1}{\theta_2} \right) - \frac{1}{\theta_2^2} \sum_{j=1}^{m} \lambda_{P_{1,j}} \hat{u}_{P_{1,j}} \hat{u}_{P_{1,2}}
\]

\[
+ O_p \left( \frac{1}{\theta_1^2 \theta_2^{1/2} m} \right) + O_p \left( \frac{1}{\theta_1^2 \theta_2^{1/2} m^{1/2}} \right)
\]

\[
= \sqrt{\theta_2} \theta_2^{-1/2} \left( W_{1,2} + (W_2)_{1,2} \right) + O_p \left( \frac{1}{\theta_1^{1/2} \theta_2^{1/2} m} \right) + O_p \left( \frac{1}{\theta_1^{1/2} \theta_2^{1/2} m^{1/2}} \right).
\]

Thus, we can estimate the distribution conditional on the spectrum of \(W\),

\[
\sum_{s=3}^{m} \hat{u}_{P_{1,s}} \hat{u}_{P_{2,s}} \sim N \left( \theta_1 (1 + M_2) (M_2 - 1) + (M_4 - (M_2^2)) - 2 (1 + M_2) (M_4 - M_2^2) \right)
\]

\[
+ O_p \left( \frac{1}{\theta_1^{1/2} \theta_2^{1/2} m} \right) + O_p \left( \frac{1}{\theta_1^{1/2} \theta_2^{1/2} m^{1/2}} \right).
\]

2. **If \(\theta_2\) is finite,** then

\[
\sum_{s=3}^{m} \hat{u}_{P_{1,s}} \hat{u}_{P_{2,s}} = O_p \left( \frac{1}{\sqrt{\theta_1 m}} \right).
\]

**Remark 3.2.**

1. We can easily show
where \( \theta_1 > \theta_2 > \ldots > \theta_k \). We define

\[
\hat{\Sigma}_{P_{s,r}} = P_{s,r}^{1/2} W P_{s,r}^{1/2}, \\
\hat{\Sigma}_{P_k} = P_k^{1/2} W P_k^{1/2}.
\]

Moreover, for \( s, r = 1, 2, \ldots, k \) with \( s \neq r \), we define

\[
\hat{u}_{P_{s,r},1}, \hat{\theta}_{P_{s,r},1} \quad \text{s.t.} \quad \hat{\Sigma}_{P_{s,r}} \hat{u}_{P_{s,r},1} = \hat{\theta}_{P_{s,r},1} \hat{u}_{P_{s,r},1}, \\
\hat{u}_{P_k,s}, \hat{\theta}_{P_k,s} \quad \text{s.t.} \quad \hat{\Sigma}_{P_k} \hat{u}_{P_k,s} = \hat{\theta}_{P_k,s} \hat{u}_{P_k,s},
\]

where \( \hat{\theta}_{P_{s,r},1} = \hat{\lambda}_{\hat{\Sigma}_{P_{s,r},1}} \) and \( \hat{\theta}_{P_k,s} = \hat{\lambda}_{\hat{\Sigma}_{P_k,s}} \).

Assuming the convention

\[
\text{For } s = 1, 2, \ldots, k \text{ and } i = 1, 2, \ldots, s, \hat{u}_{P_{s,i},1} > 0,
\]
leads to
\[
\sum_{i=1}^{m} \hat{u}_{p_{s},1,i} \hat{u}_{p_{s},2,i} = \sum_{i=k+1}^{m} \hat{u}_{p_{s},i} + O_p \left( \frac{1}{\sqrt{\theta_{s} \theta_{r} m}} \right).
\]

(Proof in supplement material Mariétan and Morgenthaler (2019b).)

### 3.6. Component distribution Theorem

**Theorem 3.5.** Suppose Assumption 2.1 holds with canonical \( P \) and 2.2 (A4). We define:

\[
U = \begin{pmatrix}
\hat{u}_{P_{k},1,1} \\
\hat{u}_{P_{k},2,1} \\
\vdots \\
\hat{u}_{P_{k},m,1}
\end{pmatrix} = \begin{pmatrix}
\hat{u}_{P_{k},1,k,1} & \hat{u}_{P_{k},1,k,2} & \cdots & \hat{u}_{P_{k},1,k,m} \\
\hat{u}_{P_{k},k+1,1,k} & \hat{u}_{P_{k},k+1,1,k} & \cdots & \hat{u}_{P_{k},k+1,1,k+1}
\end{pmatrix}
\]

To simplify the result we use the sign convention,

For \( s = 1, 2, ..., k \) and \( i = 1, 2, ..., s \), \( \hat{u}_{p_{s},i} > 0 \).

1. Without loss of generality on the \( k \) first components, the \( k^{th} \) element of the first eigenvector is

\[
\hat{u}_{p_{s},1,k} = \frac{\sqrt{\theta_{s}}}{\theta_{k} - \theta_{1}} \hat{u}_{p_{s-1},1,k} + O_p \left( \frac{\min(\theta_{1}, \theta_{k})}{\theta_{1}^{1/2} \theta_{k}^{1/2} m} \right) + O_p \left( \frac{1}{\sqrt{\theta_{s} \theta_{k} m}} \right)
\]

\[
= \frac{\theta_{1} \sqrt{\theta_{s}}}{|\theta_{k} - \theta_{1}|} \frac{1}{m} \sqrt{1 - \hat{\alpha}_{s}^{2}} Z + O_p \left( \frac{\min(\theta_{1}, \theta_{k})}{\theta_{1}^{1/2} \theta_{k}^{1/2} m} \right) + O_p \left( \frac{1}{\sqrt{\theta_{s} \theta_{k} m}} \right)
\]

\[
= \frac{\sqrt{\theta_{s}}}{|\theta_{k} - \theta_{1}|} \frac{1}{m} \sqrt{M_{2} - 1} Z + O_p \left( \frac{\min(\theta_{1}, \theta_{k})}{\theta_{1}^{1/2} \theta_{k}^{1/2} m} \right) + O_p \left( \frac{1}{\sqrt{\theta_{s} \theta_{k} m}} \right)
\]

where \( Z \) is a standard normal and \( M_{2} = \frac{1}{m} \sum_{i=1}^{m} \hat{\lambda}_{W,i}^{2} \) is obtained by conditioning on the spectrum.

- Thus, knowing the spectrum and assuming \( \theta_{1}, \theta_{k} \to \infty \),

\[
\hat{u}_{p_{s},1,k} \xrightarrow{Asy} N \left( 0, \frac{\theta_{1} \theta_{k}}{|\theta_{1} - \theta_{k}|} \frac{M_{2} - 1}{m} \right).
\]

- If \( \theta_{k} \) is finite,

\[
\hat{u}_{p_{s},1,k} = O_p \left( \frac{1}{\sqrt{\theta_{1} m}} \right)
\]

This result holds for any components \( \hat{u}_{p_{s},s,t} \) where \( s \neq t \in \{1, 2, ..., k\} \).
Remark 3.3.
The sign of $\hat{u}_{P_k,1,k}$ obtained by the construction using Theorem 4.1 is always positive. By convention ($\hat{u}_{P_k,1,i} > 0$, for $i = 1, 2, ..., k$), we multiply by \(\text{sign}(\hat{u}_{P_k,1,1})\) obtained in the construction. Thus, the remark of Theorem 4.1 describes the sign of the component assuming the convention.

\[
P \left\{ \text{sign}(\hat{u}_{P_k,1,k}) = \text{sign} \left( \left( \hat{\theta}_{P_k,1} - \hat{\theta}_{P_k-1,1} \right) \hat{u}_{P_{k-1},1,k} \hat{u}_{P_k-1,1,1} \right) \right\} = 1 + O \left( \frac{1}{m} \right).
\]

2. For $s = 1, ..., k$, the vector $\frac{\hat{u}_{s,k+1,m}}{\sqrt{1-\alpha_s^2}}$, where $\alpha_s^2 = \sum_{i=1}^{k} \hat{u}_{i,s}^2$, is unit invariant by rotation. Moreover, for $j > k$,

\[
\hat{u}_{j,s} \sim N \left( 0, \frac{1 - \alpha_s^2}{m} \right),
\]

where $\alpha_s^2$ is the limit of $\hat{\alpha}_s^2$.

Finally, the columns of $U^T[k+1:m, k+1:m]$ are invariant by rotation.

3. Assuming $P_k = I_m + \sum_{i=1}^{k} (\theta_i - 1) e_i e_i^T$ is such that

\[
\theta_1, \theta_2, ..., \theta_k
\]

are proportional, and

\[
\theta_k, \theta_{k+1}, \theta_{k+2}, ..., \theta_k
\]

are proportional,

then

\[
\sum \hat{u}_{k+1,m,1}^2 \leq \sum \hat{u}_{k+1,m,1,k}^2
\]

\[
\sim \text{RV} \left( O \left( \frac{1}{\theta_1} \right), O \left( \frac{1}{\theta_1^2 m} \right) \right) + O_p \left( \frac{\min(\theta_1, \theta_k)}{\max(\theta_1, \theta_k)m} \right).
\]

If $P$ satisfies Assumption 2.2(A4) with $\min \left( \frac{\theta_1}{\theta_k}, \frac{\theta_k}{\theta_1} \right) \rightarrow 0$, then

\[
\sum \hat{u}_{k+1,m,1}^2 \sim \text{RV} \left( O \left( \frac{1}{\theta_1} \right), O \left( \frac{1}{\theta_1^2 m} \right) \right) + O_p \left( \frac{1}{\theta_1 m} \right).
\]

(Proof in supplement material Mariétan and Morgenthaler (2019b).)

3.7. Invariant Double Angle Theorem

Finally, using the previous Theorem, we can prove the Invariant Theorem of the double angle.

Corollary 3.1. Suppose $W_X$ and $W_Y$ satisfies Assumption 2.1 and

\[
\bar{P}_s = I_m + (\theta_s - 1) e_s e_s^T, \text{ for } s = 1, 2, ..., k,
\]

\[
P_k = I_m + \sum_{i=1}^{k} (\theta_i - 1) e_i e_i^T \text{ respects } 2.2 \text{ (A4)},
\]

where $\theta_1 > \theta_2 > ... > \theta_k$. We define

\[
\Sigma_{X,P_s} = \bar{P}_s^{1/2} W_X P_s^{1/2} \text{ and } \Sigma_{X,\bar{P}_s} = \bar{P}_s^{1/2} W_X \bar{P}_s^{1/2};
\]

\[
\Sigma_{X,P_k} = P_k^{1/2} W_X P_k^{1/2} \text{ and } \Sigma_{Y,P_k} = P_k^{1/2} W_Y P_k^{1/2}.
\]
For \( s = 1, \ldots, k \), we define
\[
\hat{u}_{\Sigma X, P_k, s} \quad \text{s.t.} \quad \hat{\Sigma}_{X, P_k, s} \hat{u}_{\Sigma X, P_k, s} = \hat{\Sigma}_{X, P_k, s} \hat{u}_{\Sigma X, P_k, s},
\]
where \( \hat{\theta}_{\Sigma X, P_k, s} = \hat{\lambda}_{\Sigma X, P_k, s} \) and \( \hat{\theta}_{\Sigma X, P_k, s} = \hat{\lambda}_{\Sigma X, P_k, s} \). The statistics of the group \( Y \) are defined in analogous manner.

Then,
\[
\langle \hat{u}_{\Sigma X, P_k, 1}, \hat{u}_{\Sigma Y, P_k, 1} \rangle^2 = \sum_{i=1}^{k} \langle \hat{u}_{\Sigma X, P_k, i}, \hat{u}_{\Sigma Y, P_k, i} \rangle^2 + O_p \left( \frac{1}{\theta_s m} \right)
\]
\[
= \sum_{i=1}^{k+\epsilon} \langle \hat{u}_{\Sigma X, P_k, i}, \hat{u}_{\Sigma Y, P_k, i} \rangle^2 + O_p \left( \frac{1}{\theta_s m} \right),
\]
where \( \epsilon \) is a small integer.

Remark 3.4.
1. The procedure of the proof shows an interesting invariant:
   Assuming the sign convention \( \hat{u}_{P_s, i, i} > 0 \) for \( s = 1, 2, \ldots, k \) and \( i = 1, 2, \ldots, s \),
   \[
   \sum_{i=k+1}^{m} \hat{u}_{P_k, 1, i} \hat{u}_{P_k, 1, i} = \sum_{i=k}^{m} \hat{u}_{P_k, i, i} + O_p \left( \frac{1}{\theta_1 m} \right).
   \]

2. The distribution of \( \langle \hat{u}_{\Sigma X, P_k, 1}, \hat{u}_{\Sigma Y, P_k, 1} \rangle \) is computed in Theorem 2.1.
3. An error of \( \epsilon \) principal components does not affect the asymptotic distribution of the general double angle. This property allows us to construct a robust test.

(Proof in supplement material Mariétan and Morgenthaler (2019b).)

4. Tools for the proofs

In this section we present intermediary results necessary to prove the main theorems of this paper.

4.1. Characterization of eigenstructure

The next theorem concerns eigenvalues and eigenvectors. In order to show the result for \( u_1 \), without loss of generality we use the following condition for the other eigenvalues.
Notation 4.1. Usually we assume \( \theta_1 > \theta_2 > \ldots > \theta_k \) such that \( \hat\theta_{P_k,s} \), the \( s \)th largest eigenvalue of \( \hat\Sigma_{P_k} \) corresponds to \( \theta_s \).

We can relax the strict ordering \( \theta_1 > \theta_2 > \ldots > \theta_k \) in the following manner. The order of \( \theta_s \) in the eigenvalues \( \theta_1, \theta_2, \ldots, \theta_t, t \geq s \) is rank \( r_{t,s} = \rho_{t,s} \). Assuming a perturbation \( P_k \), \( \theta_s \) corresponds to the \( r_{t,s} \)th largest eigenvalue of \( \hat\Sigma_{P_k} \). In order to use simple notation, we again call this corresponding estimated eigenvalue, \( \hat\theta_{P_k,s} \).

We also change the notation for the eigenvector. For \( i = 1, 2, \ldots, t \), \( \hat u_{P_k,s} \) is the eigenvector corresponding to \( \hat\theta_{P_k,s} \).

Theorem 4.1. Using the same notation as in the Invariant Theorem (3.2, 3.1) and under Assumption 2.1 and 2.2(A4), we can compute the eigenvalues and the components of interest of the eigenvector of \( \hat\Sigma_{P_k} \). Using assumption 2.1, we can without loss of generality suppose the canonical form for the perturbation \( P_k \).

- **Eigenvalues:**

\[
\sum_{i=1}^{m} \frac{\lambda_{P_k,i} - \lambda_{P_k-1,i}}{\theta_{P_k,s} - \theta_{P_k-1,s}} \delta_{i,j} + \frac{\hat\theta_{P_k-1,s} - \theta_{P_k,s}}{\theta_{P_k,s} - \theta_{P_k-1,s}} \hat u_{P_k,s} \delta_{i,j} + \sum_{i\neq j}^{k} \frac{\hat\theta_{P_k-1,i} - \theta_{P_k,s}}{\theta_{P_k,s} - \theta_{P_k-1,i}} \hat u_{P_k,s} \delta_{i,j} = \frac{1}{\theta_k - 1} \]

for \( s = 1, 2, \ldots, k \).

**Remark 4.1.** If we do not assume canonical perturbations, then the formula is longer but the structure remains essentially the same. Assuming Condition 2.1 to hold, leads to matrices that are invariant under rotations. Elementary linear algebra methods extend the result to any perturbation.

- **Eigenvectors:**

We define \( \hat u_{P_k,i} \) such that \( WP_k \hat u_{P_k,i} = \hat\theta_{P_k,i} \hat u_{P_k,i} \) and \( \hat u_{P_k,i} \) such that \( P_k^{1/2} WP_k^{1/2} \hat u_{P_k,i} = \hat\theta_{P_k,i} \hat u_{P_k,i} \). To simplify notation we assume that \( \theta_i \) corresponds to \( \theta_{P_k,i} \). This notation is explained in 4.1 and allows us without loss of generality to describe only the eigenvector \( \hat u_{P_k,1} \).
Finally,

\[
\hat{u}_{P_k,1} = \left( \hat{u}_{P_k,1,1}, \hat{u}_{P_k,1,2}, \ldots, \sqrt{\theta_k} \hat{u}_{P_k,1,k}, \ldots, \hat{u}_{P_k,1} \right),
\]

where \( \sqrt{1 + (\theta - 1) \hat{u}_{P_k,1,k}^2} \) is the norm of \( P_{k}^{1/2} \hat{u}_{P_k,1} \) that we will call \( N_1 \).

**Remark 4.2.**

1. By construction, the sign of \( \hat{u}_{P_k,1,k} \) is always positive. This is, however, not the case of \( \hat{u}_{P_{k-1},1,i} \). We can show that:

\[
P \left\{ \text{sign} \left( \hat{u}_{P_{k-1},1} \right) = \text{sign} \left( \left( \hat{\theta}_{P_{k-1},1} - \hat{\theta}_{P_{k-1},1} \right) \hat{u}_{P_{k-1},1,1} \hat{u}_{P_{k-1},1,k} \right) \right\} \to 1.
\]

Moreover, the convergence to 1 is of order \( 1/m \). If \( \theta_1 \) tends to infinity, then

\[
P \left\{ \text{sign} \left( \hat{u}_{P_k,1,1} \right) = \text{sign} \left( (\theta_1 - \theta_k) \hat{u}_{P_{k-1},1,k} \right) \right\} \to 1.
\]

Thus, if we use a convention such as \( \text{sign} \left( \hat{u}_{P_k,i,i} \right) > 0 \) for \( i = 1, \ldots, k-1 \), then the sign of \( \hat{u}_{P_k,i,k} \) is distributed as a Bernoulli with parameter 1/2.

2. Without loss of generality, the other eigenvectors \( \hat{u}_{P_k,r} \) for \( r = 1, 2, \ldots, k-1 \) can be computed by the same formula thanks to the notation linking the estimated eigenvector to the eigenvalue \( \theta_{i,r} \). This formula does, however, not work for the vector \( \hat{u}_{P_k,k} \). Applying a different order of perturbation shows that similar formulas exist for
This observation leads to a problem in the proofs of the Dot Product Theorems 3.3 and 3.4. Deeper investigations are necessary to understand the two eigenvectors when \( k = 2 \).

\[
D_2 = \sum_{i=2}^{m} \frac{\hat{\lambda}_{P_{i}}}{\hat{\lambda}_{P_{i} - 1}} \hat{\theta}_{P_{i} - 1} \hat{u}_{P_{i}, 1, 2}^2 + \frac{\hat{\theta}_{P_{i}}}{\hat{\lambda}_{P_{i} - 1}} \hat{u}_{P_{i}, 1, 2}^2,
\]

\[
O_p \left( \frac{1}{\theta_2} \right)
\]

\[
N_2^2 = 1 + \frac{1}{(\theta_2 - 1)D_2}.
\]

\[
N_2D_2 = D_2 + \frac{1}{\theta_2 - 1}
\]

\[
= \frac{1}{\theta_2 - 1} + O_p \left( \frac{1}{\theta_2^2} \right) + O_p \left( \frac{\theta_1}{(\theta_2 - 1)m} \right).
\]

Furthermore, the theorem requires investigation of the \( m - k \) noisy components of the eigenvectors. For \( r = 1, 2 \) and \( s = 3, 4, ..., m \),

\[
\hat{u}_{P_{r}, i, s} = \sum_{i=1}^{m} \frac{\lambda_{P_{i} - 1}}{\theta_{P_{r}, i} - \lambda_{P_{i} - 1}} \hat{u}_{P_{i}, 1, s} \hat{u}_{P_{i}, 1, 2} \sqrt{D_r N_r}.
\]

The estimations using this last formula are difficult. It is beneficial to look at

\[
\hat{u}_{P_{r}, 1, t} / \sqrt{\sum_{s=3}^{m} \hat{u}_{P_{r}, 1, s}^2} \text{ and } \hat{u}_{P_{r}, 2, t} / \sqrt{\sum_{s=3}^{m} \hat{u}_{P_{r}, 2, s}^2}
\]

for \( t = 3, 4, ..., m \).

3. If the perturbation is not canonical, then we can apply a rotation \( U \), such that \( U \epsilon_s = \epsilon_s \), and replace \( \hat{u}_{P_{k-1}, i} \) by \( U \hat{\epsilon}_{P_{k-1}, i} \). Then, \( \langle \hat{u}_{P_{k-1}, 1}, \epsilon_s \rangle^2 \) is replaced by \( \langle \hat{\epsilon}_{P_{k-1}, 1}, \epsilon_s \rangle^2 \).

(Proof in supplement material Mariétan and Morgenthaler (2019b).)

4.2. Double dot product

**Theorem 4.2.** Suppose \( W_X \) and \( W_Y \) satisfies Assumption 2.1 and \( P_k = I_m + \sum_{i=1}^{k} (\theta_1 - 1) \epsilon_i \epsilon_i^T \) satisfies 2.2 (A4), where \( \theta_1 > \theta_2 > ... > \theta_k \). We set

\[
\hat{\Sigma}_X = \hat{\Sigma}_{X, P_k} = P_k^{1/2} W_X P_k^{1/2} \text{ and } \hat{\Sigma}_{Y, P_k} = P_k^{1/2} W_Y P_k^{1/2}.
\]

and for \( s = 1, ..., k \),

\[
\hat{\Sigma}_{X, s, p_s}, \hat{\Sigma}_{X, s}, \text{ s.t. } \hat{\Sigma}_{X, p_s} \hat{u}_{S_X, s} = \hat{\Sigma}_{X, s} \hat{u}_{S_X, s},
\]

\[
\hat{\Sigma}_{Y, s, p_s}, \hat{\Sigma}_{Y, s}, \text{ s.t. } \hat{\Sigma}_{Y, p_s} \hat{u}_{S_Y, s} = \hat{\Sigma}_{Y, s} \hat{u}_{S_Y, s}.
\]
Finally, we define
\[
\tilde{u}_s = \hat{U}_X \tilde{u}_s, 
\]
where,
\[
\hat{U}_X = (v_1, v_2, \ldots, v_m) = (\tilde{u}_{\Sigma Y, 1}, \tilde{u}_{\Sigma Y, 2}, \ldots, \tilde{u}_{\Sigma Y, k}, v_{k+1}, v_{k+2}, \ldots, v_m),
\]
where the vectors \(v_{k+1}, \ldots, v_m\) are chosen such that the matrix \(\hat{U}_X\) is orthonormal. Then,

1. If \(\theta_j, \theta_t \to \infty:\)
\[
\sum_{i=k+1}^{m} \tilde{u}_j, i \tilde{u}_{i, t} = \sum_{i=k+1}^{m} \tilde{u}_{\Sigma Y, j, i} \tilde{u}_{\Sigma Y, t, i} + \sum_{i=k+1}^{m} \tilde{u}_{\Sigma X, j, i} \tilde{u}_{\Sigma X, t, i} - \sum_{i=k+1}^{m} \tilde{u}_{\Sigma X, j, i} \tilde{u}_{\Sigma Y, t, i}
\]
\[
- \sum_{i=k+1}^{m} \tilde{u}_{\Sigma Y, j, i} \tilde{u}_{\Sigma X, t, i} - (\tilde{u}_{\Sigma X, t, j} + \tilde{u}_{\Sigma Y, j, i}) (\hat{\alpha}^2_{\Sigma Y, j} - \hat{\alpha}^2_{\Sigma X, j})
\]
\[
+ O_p \left( \frac{1}{\theta_t m} \right) + O_p \left( \frac{1}{\theta_t \sqrt{m}} \right),
\]
where \(\hat{\alpha}^2_{\Sigma X, t} = \sum_{i=1}^{k} \tilde{u}^2_{\Sigma X, t, i} \).

2. If \(\theta_t\) is finite:
\[
\sum_{i=k+1}^{m} \tilde{u}_j, i \tilde{u}_{i, t} = O_p \left( \frac{1}{\sqrt{m} \sqrt{\theta_t}} \right).
\]

Moreover, for \(s = 1, \ldots, k, t = 2, \ldots, k\) and \(j = k + 1, \ldots, m,\)
\[
\sum_{i=1}^{k} \tilde{u}^2_{s, i} = \sum_{i=1}^{k} \langle \tilde{u}_{\Sigma X, i, s}, \tilde{u}_{\Sigma Y, s} \rangle^2,
\]
\[
\tilde{u}_{s, s} = \hat{u}_{\Sigma X, s, s} \tilde{u}_{\Sigma Y, s, s} + O_p \left( \frac{1}{m} \right) + O_p \left( \frac{1}{\theta_s^{1/2} m^{1/2}} \right),
\]
\[
\tilde{u}_{s, t} = \hat{u}_{\Sigma X, s, t} + \hat{u}_{\Sigma X, t, s} + O_p \left( \frac{\sqrt{\min(\theta_s, \theta_t)}}{\sqrt{\max(\theta_s, \theta_t)}} \right) + O_p \left( \frac{1}{\theta_t m^{1/2}} \right),
\]
\[
\tilde{u}_{t, s} = O_p \left( \frac{\sqrt{\min(\theta_s, \theta_t)}}{m \sqrt{\max(\theta_s, \theta_t)}} \right) + O_p \left( \frac{1}{\theta_s m^{1/2}} \right),
\]
\[
\tilde{u}_{s, j} = \hat{u}_{\Sigma Y, s, j} - \hat{u}_{\Sigma X, s, j} \langle \tilde{u}_{\Sigma Y, j}, \tilde{u}_{\Sigma X, j} \rangle + O_p \left( \frac{1}{\theta_s^{1/2} m} \right).
\]

(Proof in supplement material Mariétan and Morgenthaler (2019b).)
4.3. Lemmas for Invariant Dot product Theorem

This section introduces a lemma used in the proof of the Dot Product Theorem 3.3.

Lemma 4.1. Assuming $W$ and $\hat{\Sigma}_P$ as in Theorem 3.3, then by construction of the eigenvectors using Theorem 4.1,

\[
\hat{u}_{P,1,2} = \frac{W_{1,2}}{\sqrt{\theta_1}} + O_p\left(\frac{1}{\theta_1 m^{1/2}}\right) + O_p\left(\frac{1}{\sqrt{\theta_2} m^{1/2}}\right),
\]

\[
\sum_{i=2}^{m} \hat{\lambda}_{P,i} \hat{u}_{P,1,2} = W_{2,2} + O_p\left(\frac{1}{m}\right).
\]

Remark 4.3.

Because the perturbation is of order 1, the two sign conventions defined in 3.1 are the same. (Proof in supplement material Mariétan and Morgenthaler (2019b).)

5. Conclusion

In this paper we extend results of Mariétan and Morgenthaler (2019a) to perturbation of order $k > 1$. Theorem 2.1 provides all the background results needed to build powerful test. The approach contains two deficiencies:

- We cannot treat the case with equal perturbing eigenvalues, $\theta_1 = \theta_2$. Indeed, all our theorems always assume different eigenvalues. In the case of equality, the procedures do not stay conservative.
- The distribution of the data before the perturbation is applied are assumed to be invariant under rotation. If we relax this assumption, then our procedure are no longer necessarily conservative.

In future work we will present a procedure based on the residual spikes introduced in Mariétan and Morgenthaler (2019a) for perturbations of order 1. These statistics seems to capture the differences between two populations very effectively and the problem of equal eigenvalues of the perturbation does not affect these tests. Relaxing the hypotheses of invariance under rotation still influences the properties of these alternative tests, but have a lesser impact.

Supplementary Material

Supplement A: Statistical applications of Random matrix theory: comparison of two populations II, Supplement () Proofs of Theorems in Mariétan and Morgenthaler (2019b)


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