Topics on statistical methods for data with high dimension greater than the sample size

by

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Introduction

There is an increasing current interest in the statistical analysis of data arising in problems of genomics, medical image analysis, climatology, finance and functional data analysis, where one frequently observes multivariate data with high dimension greater than the sample size. It is then important to consider for this kind of data the behavior of classical multivariate statistical methodologies, which have been mainly developed for data with dimension d lower than the sample size n. This thesis is about the behavior of two classical methodologies of multivariate statistics in the High-Dimension, Low Sample Size (HDLSS) context: Principal Component Analysis (PCA) and Binary Discrimination Analysis.

In Chapter 1 we present some classical results and properties of the spectrum of the Wishart distribution in the classical and Random Matrix Theory contexts. They are useful to motivate, compare and develop some new asymptotic results for PCA in the HDLSS context. We also obtain an expression for the characteristic function of the ordered eigenvalues of a Wishart matrix in terms of the characteristic function of the gamma distribution. Furthermore, we consider the structure of the exact distribution of the largest eigenvalue of a Wishart matrix as a simultaneous mixture of scale and shape mixtures of gamma distributions.

In Chapter 2 we consider PCA in the HDLSS context. It is known that in the HDLSS framework PCA often fails to estimate the population eigenvalues and eigenvectors, since the sample covariance matrix is not a good approximation to the population covariance matrix. As pointed out in Johnstone [23], one often observes one or a small number of large sample eigenvalues well separated from the rest. In this case, the so-called spiked covariance model is of special interest. It has recently been studied the asymptotic behavior of the largest sample eigenvalues and their corresponding sample eigenvectors under the spiked covariance model in the HDLSS context. This line of work was initiated by Ahn, *et al.* [2] in the case of the largest eigenvalue when both the dimension of the data d and the sample size n go to infinity successively with d increasing at a much faster rate that n, i.e. $d \gg n$. Under the spiked covariance model where the $p \geq 2$ largest eigenvalues have different asymptotic order of magnitude as d increases, Jung and Marron [25] study the asymptotic behavior of the p largest sample eigenvalues and prove eigenvector consistency when d goes to infinity and n is fixed. As a contribution of this thesis, we consider the study of the spiked covariance model which has its p largest eigenvalues of the same asymptotic order of magnitude as d goes to infinity. Specifically, we find the joint asymptotic distribution of the nonzero sample eigenvalues when d tends to infinity and n is fixed. Then we show that the first p sample eigenvalues increase at the same speed as their population counterpart, in the sense that the vector of ratios of the sample and population eigenvalues converges to a multivariate distribution when $d \to \infty$ and n is fixed, and to the vector of ones when both $d, n \to \infty$ and $d \gg n$; and the subspace consistency of the corresponding sample eigenvectors when d tends to infinity and n is fixed. Moreover, we prove —under a Gaussian assumption— asymptotic results that allow us to consider hypothesis testing and confidence intervals for the first p largest population eigenvalues and, in particular, the test itself of a special case of our spiked covariance model.

In Chapter 3 we consider Binary Discrimination Analysis for data with dimension greater than the sample size. Here we focus on the behavior of the binary discrimination methods Mean Difference (MD), Support Vector Machine (SVM), Distance Weighted Discrimination (DWD) and Maximal Data Piling (MDP) when the dimension d of the training data set tends to infinity and the sample sizes m and n are fixed. It is worth mentioning that the last two methods are specially designed for the HDLSS context by Marron, *et al.* [28] and Ahn and Marron [1], respectively. The comparison of the MD, SVM and DWD methods was first studied in Hall, *et al.* [19], where the probability of correct classification of a new data point is considered when d tends to infinity and the sample sizes are fixed. The comparison of the four methods has been done by simulation studies in Marron, *et al.* [28], [29]. As contributions of this thesis, we extend the results of [19] and give theoretical proofs of some empirical results of [28] and [29]. Specifically, we show that when the data sets are spherical Gaussian where one set has mean zero and the other has mean v_d, then the orthogonal vectors of the separating hyperplanes of the methods tend to be in the same direction as v_d when $\| v_d \| \gg d^{1/2}$ and tend to be orthogonal to v_d when $\| v_d \| \ll d^{1/2}$. The case when $\| v_d \| \approx d^{1/2}$ is also considered. We also compare the MD method with the SVM when d is large but fixed. We see in a particular setting that generally the MD method is better than the SVM when d is large, in the sense that the angle between the orthogonal vector of the MD hyperplane and the optimal direction v_d is closer to zero than the angle between the orthogonal vector of the SVM hyperplane and v_d.

Chapter 1

On the spectrum of the Wishart distribution

In this chapter we gather some known properties of the spectrum of Wishart matrices in the classical and Random Matrix Theory (RMT) contexts. They are useful to motivate and develop some new asymptotic results in Chapter 2 for Principal Component Analysis in the HDLSS context. The classical case corresponds to the situation when data dimension p is fixed and less than or equal to the sample size n which is fixed or goes to infinity. On the other hand the RMT context considers p and n go to infinity simultaneously, in the sense that p/n goes to a constant.

We also give new expressions for the joint characteristic function of the ordered eigenvalues of a Wishart matrix and study the structure of the exact distribution of the largest eigenvalue. In particular we obtain an interpretation of this distribution as a simultaneous mixture of scale and shape mixtures of gamma distributions. We believe that these results may be useful to study some open problems in Random Matrices Theory, e.g. the characteristic functions of linear combinations of the ordered eigenvalues of a Wishart matrix and the infinite divisibility of the so-called Tracy-Widom distributions.

1.1 Definition and basic properties

The first matrix distribution was considered by John Wishart [42] in 1928, as a matrix generalization of the chi-square distribution. It is defined as follows.

Definition 1.1.1 *Let $X_1, X_2, \ldots, X_n$ be (real) random vectors from a p-multivariate normal distribution with mean zero and positive definite covariance matrix Σ, $N_p(0, \Sigma)$. Let $X = [X_1, X_2, \ldots, X_n]$. Then $A = XX^\top$ is said to have a* Wishart distribution *with n degrees of freedom and covariance matrix Σ. A common notation used is $A \sim \mathcal{W}(n, \Sigma)$.*

The density function of $A \sim \mathcal{W}(n, \Sigma)$, when $n \geq p$, can be found in [4, pp. 245] and is given by

$$f_A(B) = \frac{1}{2^{pn/2}\Gamma_p(\frac{n}{2})|\Sigma|^{n/2}} \exp\left[-\frac{1}{2}\text{tr}(\Sigma^{-1}B)\right] \det(B)^{(n-p-1)/2}, \quad B > 0,$$

where Γ_p is the *p-multivariate gamma function* given by

$$\Gamma_p(a) = \pi^{p(p-1)/4} \prod_{j=1}^{p} \Gamma(a - (j-1)/2).$$

When $n < p$, A is singular and the Wishart distribution $\mathcal{W}(n, \Sigma)$ does not have density function.

Let $A \sim \mathcal{W}(n, \Sigma)$. It can be seen that $E(A) = n\Sigma$. On the other hand the characteristic function of the random matrix A is given by

$$\varphi(\Theta) = E[\exp(i\text{tr}(A\Theta))] = \det(I_p - 2i\Theta\Sigma)^{-n/2},$$

for Θ a $p \times p$ symmetric matrix; see [4, pp. 253]. The following three facts are easily obtained from this characteristic function

1. When $p = 1$ and $\Sigma = 1$, the Wishart distribution $\mathcal{W}(n, \Sigma)$ is the chi-square distribution with n degrees of freedom, $\mathcal{X}_n^2$.
2. If C is a $q \times p$ matrix of rank q, then $CAC^\top \sim \mathcal{W}(n, C\Sigma C^\top)$.
3. If $A_i \sim \mathcal{W}(n_i, \Sigma)$ for $i = 1, 2, \ldots, r$ are independent, then $\sum_{i=1}^r A_i \sim \mathcal{W}(n, \Sigma)$ where $n = \sum_{i=1}^r n_i$.

The following two results give the distributions of functionals of the determinant and trace of a Wishart matrix A; see [31, pp. 100] and [31, pp. 107], respectively. They are useful in the study of some inference problems.

Theorem 1.1.1 *If $A \sim \mathcal{W}(n, \Sigma)$ where $n \geq p$, then $\det(A)/det(\Sigma)$ has the same distribution as $\prod_{i=1}^p \mathcal{X}_{n-i+1}^2$, where $\mathcal{X}_{n-i+1}^2$ for $i = 1, 2, \ldots, p$, are independent random variables with chi-squared distribution with $n - i + 1$ degrees of freedom.*

Theorem 1.1.2 *If $A \sim \mathcal{W}(n, cI_p)$ where $n \geq p$ and $c > 0$, then $\det(A)/[\text{tr}(A)/p]^p$ and $\text{tr}(A)$ are independent, and $\text{tr}(A)/c \sim \mathcal{X}_{pn}^2$.*

The next theorem is used to test the null hypothesis $H_0 : \Sigma = cI_p$ for the covariance matrix Σ in the context of large sample size; see [31, pp. 344].

Theorem 1.1.3 *Suppose $A \sim \mathcal{W}(n, cI_p)$ where $n \geq p$. Let $V = \det(A)/[\text{tr}(A)/p]^p$ and $\rho = 1 - (2p^2 + p + 2)/(6np)$. Then*

$$-n\rho \ln(V) \xrightarrow{w} \mathcal{X}_r^2 \qquad \text{as } n \to \infty,$$

where $\mathcal{X}_r^2$ is a random variable with chi-square distribution with $r = (p+2)(p-1)/2$ degrees of freedom.

1.2 Distribution of the spectrum: classical context

1.2.1 Joint density function of the eigenvalues

The number of nonzero eigenvalues of $A \sim \mathcal{W}(n, \Sigma)$ is $r = \min(n, p)$. The next theorem gives the joint density function of the nonzero eigenvalues of a Wishart matrix; see [31, pp. 106].

Theorem 1.2.1 *If $A \sim \mathcal{W}(n, \Sigma)$ with $n \geq p$, the joint density function of the eigenvalues of A, $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$, is given by*

$$f(\ell_1, \ldots, \ell_p) = \frac{\pi^{p^2/2}}{2^{pn/2}|\Sigma|^{n/2}\Gamma_p(\frac{p}{2})\Gamma_p(\frac{n}{2})} \prod_{i=1}^{p} \ell_i^{(n-p-1)/2} \prod_{i<j}^{p} (\ell_i - \ell_j)$$
$$* \int_{O(p)} \exp\left[-\frac{1}{2}\mathrm{tr}(\Sigma^{-1} H L H^\top)\right] (dH),$$

where $L = \mathrm{diag}(\ell_1, \ell_2, \ldots, \ell_p)$, and $O(p)$ is the Group of orthogonal $p \times p$ matrices, i.e.

$$O(p) = \{H \textit{ is a } p \times p \textit{ matrix}: \ H^\top H = I_p\}.$$

The product $\prod_{i<j}^{p}(\ell_i - \ell_j)$ is called the *Vandermonde determinant*. It is well known in Random Matrix Theory that due to the Vandermonde determinant there is a repulsion effect of the eigenvalues of a Wishart matrix. This says that these eigenvalues are strongly dependent.

As a consequence of this theorem we have the next corollary.

Corollary 1.2.1 *If $A \sim \mathcal{W}(n, cI_p)$ with $n \geq p$, the joint density function of the eigenvalues of A, $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$, is given by*

$$f(\ell_1, \ldots, \ell_p) = \frac{\pi^{p^2/2}}{(2c)^{pn/2}\Gamma_p(\frac{p}{2})\Gamma_p(\frac{n}{2})} \prod_{i=1}^{p} \ell_i^{(n-p-1)/2} \prod_{i<j}^{p} (\ell_i - \ell_j) \exp\left(-\frac{1}{2c}\sum_{i=1}^{p} \ell_i\right). \qquad (1.1)$$

Remark 1.2.1 *The density of the nonzero eigenvalues of the singular case ($p > n$) can be found in [15]. For the special case when $A \sim \mathcal{W}(n, cI_p)$ with $p > n$, the joint density function of the nonzero eigenvalues of A is given by (1.1) after interchanging n and p. That is because $A \stackrel{\mathcal{L}}{=} XX^\top$, where $X = [X_1, X_2, \ldots, X_n]$ and $X_1, X_2, \ldots, X_n$ are i.i.d. random vectors with distribution $N_p(0, cI_p)$ and if we define $B = X^\top X$, then $B \sim \mathcal{W}(p, cI_n)$ is a non-singular Wishart matrix having the same nonzero eigenvalues as A. Thus, the several results for the eigenvalues of B are also valid for the nonzero eigenvalues of A.*

In order to derive an expression for the characteristic function of the ordered eigenvalues of a Wishart matrix, we first point out an alternative form of the joint density function (1.1) in terms of the set of permutations S_p of the set $\{1, 2, \ldots, p\}$. A permutation $\alpha \in S_p$ will be represented by a vector $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_p)^\top$.

Lemma 1.2.1 *If $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p$ are the eigenvalues of $A \sim \mathcal{W}(n, cI_p)$ with $n \geq p$ and $c > 0$, then the joint density of $(\ell_1, \ell_2, \ldots, \ell_p)^\top$ is given by*

$$f_{\ell_1,\ell_2,\ldots,\ell_p}(\ell_1, \ell_2, \ldots, \ell_p) = \Delta \sum_{\alpha \in S_p} \mathrm{sign}(\alpha) \exp\left(-\frac{1}{2c}\sum_{k=1}^{p} \ell_k\right) \prod_{k=1}^{p} \ell_{p+1-k}^{\alpha_k+(n-p-1)/2-1}, \tag{1.2}$$

with $\ell_1 > \ell_2 > \cdots > \ell_p$, where

$$\Delta = \frac{\pi^{p^2/2}}{(2c)^{pn/2}\Gamma_p(\frac{p}{2})\Gamma_p(\frac{n}{2})}. \tag{1.3}$$

Proof. Let $l_k = \ell_{p+1-k}$ for $k = 1, 2, \ldots, p$. By Corollary 1.2.1, the joint density of $(l_1, l_2, \ldots, l_p)^\top$ is given by

$$f_{l_1,l_2,\ldots,l_p}(l_1, l_2, \ldots, l_p) = \Delta \exp\left(-\frac{1}{2c}\sum_{i=1}^{p} l_i\right) \prod_{i=1}^{p} l_i^{(n-p-1)/2} \prod_{i<j}^{p} (l_j - l_i), \quad l_p > \cdots > l_1, \tag{1.4}$$

where Δ is given as above. Note that the last product in the above expression is equal to the Vandermonde determinant

$$\begin{vmatrix} 1 & \cdots & 1 \\ l_1 & \cdots & l_p \\ l_1^2 & \cdots & l_p^2 \\ \vdots & \vdots & \vdots \\ l_1^{p-1} & \cdots & l_p^{p-1} \end{vmatrix} = \sum_{\alpha \in S_p} \mathrm{sign}(\alpha) \prod_{k=1}^{p} l_k^{\alpha_k - 1}.$$

Thus the density function $f_{\ell_1,\ell_2,\ldots,\ell_p}$ is given by the expression (1.2). □

1.2.2 Joint characteristic function of the eigenvalues

In this section we obtain an interesting representation for the joint characteristic function of the ordered eigenvalues of a Wishart random matrix with identity covariance matrix, in terms of characteristic functions of gamma distributions. We use the notation

$$g(x; a, b) = \frac{x^{a-1}\exp(-x/b)}{b^a\Gamma(a)}, \qquad x > 0, \text{ and} \tag{1.5}$$

$$\widehat{G}(t; a, b) = (1 - ibt)^{-a}, \qquad t \in \mathbb{R} \tag{1.6}$$

for the density and characteristic functions of the gamma distribution Gamma(a, b) with shape parameter $a > 0$ and scale parameter $b > 0$, respectively.

Proposition 1.2.1 *If $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p$ are the eigenvalues of $A \sim \mathcal{W}(n, cI_p)$ with $n \geq p$ and $c > 0$, then the characteristic function of $(\ell_1, \ell_2, \ldots, \ell_p)^\top$ is given by*

$$\varphi_{\ell_1,\ell_2,\ldots,\ell_p}(t_1, t_2, \ldots, t_p) = \Delta \left(\frac{2c}{p}\right)^{pn/2} \widehat{G}\left(\sum_{j=1}^{p} t_j; pn/2, 2c/p\right) \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-1}=0}^{\infty} \Gamma\left(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j\right)$$
$$* \, C_{n,p}(k_1, \ldots, k_{p-1}) \prod_{r=1}^{p-1} \left(\frac{r}{p}\right)^{k_r} \frac{\widehat{G}(\sum_{j=1}^{p} t_j; k_r, 2c/p)}{\widehat{G}(\sum_{j=p+1-r}^{p} t_j; k_r, 2c/r)}, \tag{1.7}$$

where $\widehat{G}(t; a, b)$ is the characteristic function of the gamma distribution $Gamma(a, b)$ and

$$C_{n,p}(k_1, \ldots, k_{p-1}) = \sum_{\alpha \in S_p} \operatorname{sign}(\alpha) \prod_{r=1}^{p-1} \frac{\Gamma(\sum_{j=1}^{r} \alpha_j + \frac{r(n-p-1)}{2} + \sum_{j=1}^{r-1} k_j)}{\Gamma(\sum_{j=1}^{r} \alpha_j + \frac{r(n-p-1)}{2} + \sum_{j=1}^{r} k_j + 1)}. \tag{1.8}$$

Proof. Let $l_k = \ell_{p+1-k}$ for $k = 1, 2, \ldots, p$. Using Lemma 1.2.1, we have that the characteristic function of $(l_1, l_2, \ldots, l_p)^\top$ is equal to

$$\begin{aligned}
\varphi(t_1, t_2, \ldots, t_p) &= E\left[\exp\left(i \sum_{k=1}^{p} t_k l_k\right)\right] \\
&= \Delta \sum_{\alpha \in S_p} \operatorname{sign}(\alpha) \int_0^{\infty} l_p^{\alpha_p + (n-p-1)/2 - 1} \exp(-(1/2c - it_p) l_p) \\
&\quad * \int_0^{l_p} l_{p-1}^{\alpha_{p-1} + (n-p-1)/2 - 1} \exp(-(1/2c - it_{p-1}) l_{p-1}) \cdots \\
&\quad * \int_0^{l_2} l_1^{\alpha_1 + (n-p-1)/2 - 1} \exp(-(1/2c - it_1) l_1) dl_1 dl_2 \cdots dl_p.
\end{aligned} \tag{1.9}$$

From equations 3.383(1), 9.212(1) and 9.210(1) of [18] it follows that

$$\int_0^m x^{\gamma - 1} \exp(-\beta x) dx = \exp(-\beta m) \sum_{k=0}^{\infty} \frac{\beta^k m^{\gamma + k}}{\gamma(\gamma + 1) \cdots (\gamma + k)}, \tag{1.10}$$

for $m > 0$, $Re(\gamma) > 0$ and any complex number β. Applying (1.10) several times in the last expression of (1.9) we have that it is equal to

$$\Delta \sum_{\alpha \in S_p} \operatorname{sign}(\alpha) \sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} \cdots \sum_{k_{p-1}=0}^{\infty} \prod_{r=1}^{p-1} \frac{(\frac{r}{2c} - i \sum_{s=1}^{r} t_s)^{k_r}}{\prod_{s=0}^{k_r} (\sum_{j=1}^{r} \alpha_j + \frac{r(n-p-1)}{2} + \sum_{j=1}^{r-1} k_j + s)}$$
$$* \int_0^{\infty} l_p^{\sum_{j=1}^{p} \alpha_j + p(n-p-1)/2 + \sum_{j=1}^{p-1} k_j - 1} \exp\left[-\left(\frac{p}{2c} - i \sum_{j=1}^{p} t_j\right) l_p\right] dl_p. \tag{1.11}$$

We recall that

$$\int_0^\infty x^{v-1}\exp(-ux)dx = \frac{\Gamma(v)}{u^v}, \qquad Re(u)>0,\ Re(v)>0.$$

Therefore we have that the integral in (1.11) is equal to

$$\frac{\Gamma(\sum_{j=1}^p \alpha_j + \frac{p(n-p-1)}{2} + \sum_{j=1}^{p-1} k_j)}{(\frac{p}{2c} - i\sum_{j=1}^p t_j)^{\sum_{j=1}^p \alpha_j + \frac{p(n-p-1)}{2} + \sum_{j=1}^{p-1} k_j}} = \frac{\Gamma(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j)}{(\frac{p}{2c} - i\sum_{j=1}^p t_j)^{pn/2 + \sum_{j=1}^{p-1} k_j}}.$$

Then, we obtain that (1.11) is given by

$$\begin{aligned}
&\Delta\left(\frac{2c}{p}\right)^{pn/2}\left(1 - i\frac{2c}{p}\sum_{j=1}^p t_j\right)^{-pn/2}\sum_{k_1=0}^\infty\cdots\sum_{k_{p-1}=0}^\infty \Gamma\left(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j\right)\\
&\quad * C_{n,p}(k_1,\dots,k_{p-1})\prod_{r=1}^{p-1}\left(\frac{r}{p}\right)^{k_r}\left(\frac{1 - i\frac{2c}{r}\sum_{j=1}^r t_j}{1 - i\frac{2c}{p}\sum_{j=1}^p t_j}\right)^{k_r}\\
&= \Delta\left(\frac{2c}{p}\right)^{pn/2}\widehat{G}\left(\sum_{j=1}^p t_j; pn/2, 2c/p\right)\sum_{k_1=0}^\infty\cdots\sum_{k_{p-1}=0}^\infty \Gamma\left(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j\right)\\
&\quad * C_{n,p}(k_1,\dots,k_{p-1})\prod_{r=1}^{p-1}\left(\frac{r}{p}\right)^{k_r}\frac{\widehat{G}(\sum_{j=1}^p t_j; k_r, 2c/p)}{\widehat{G}(\sum_{j=1}^r t_j; k_r, 2c/r)},
\end{aligned} \tag{1.12}$$

where $\widehat{G}(t;a,b)$ and $C_{n,p}(k_1,\dots,k_{p-1})$ are given as above. Thus we have

$$\begin{aligned}
\varphi_{\ell_1,\dots,\ell_p}(t_1,\dots,t_p) &= \varphi_{l_1,\dots,l_p}(t_p,\dots,t_1)\\
&= \Delta\left(\frac{2c}{p}\right)^{pn/2}\widehat{G}\left(\sum_{j=1}^p t_j; pn/2, 2c/p\right)\sum_{k_1=0}^\infty\cdots\sum_{k_{p-1}=0}^\infty \Gamma\left(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j\right)\\
&\quad * C_{n,p}(k_1,\dots,k_{p-1})\prod_{r=1}^{p-1}\left(\frac{r}{p}\right)^{k_r}\frac{\widehat{G}(\sum_{j=1}^p t_j; k_r, 2c/p)}{\widehat{G}(\sum_{j=p+1-r}^p t_j; k_r, 2c/r)}
\end{aligned}$$

which ends the proof. □

The next result follows by taking $(t_1, t_2, \cdots, t_p)^\top = \overrightarrow{\mathbf{0}}$ in (1.7). It may be useful to study in terms of characteristic functions the representation of the distribution of the largest eigenvalue of a Wishart matrix as a simultaneous mixture of scale and shape mixtures of gamma distributions, given in Section 1.4.

Corollary 1.2.2

$$\Delta\left(\frac{2c}{p}\right)^{pn/2}\sum_{k_1=0}^\infty\cdots\sum_{k_{p-1}=0}^\infty \Gamma\left(\frac{pn}{2} + \sum_{j=1}^{p-1} k_j\right) C_{n,p}(k_1,\dots,k_{p-1})\prod_{r=1}^{p-1}\left(\frac{r}{p}\right)^{k_r} = 1.$$

As an application of the last proposition, we can obtain the characteristic function $\varphi_{\ell_1}(t)$ of the largest eigenvalue ℓ_1 of a Wishart random matrix with distribution $\mathcal{W}(n, cI_p)$, simply by evaluating the vector $\overrightarrow{t_1} = te_1$ in (1.7), where e_i is the i-th p-dimensional unit vector, to get

$$\varphi_{\ell_1}(t) = \varphi_{\ell_1,\ldots,\ell_p}(\overrightarrow{t_1}) \quad \forall t \in \mathbb{R}.$$

We can do this for any eigenvalue ℓ_i, with $i = 2, \ldots, p$. Furthermore, we can obtain the characteristic function of any linear combination of the eigenvalues. In particular, for the level spacings $s_i = \ell_i - \ell_{i+1}$, for $i = 1, 2, \ldots, p-1$, we need to evaluate the vector $\overrightarrow{t_{i,i+1}} = t(e_i - e_{i+1})$ in (1.7) to obtain that the characteristic function of s_i is given by

$$\varphi_{s_i}(t) = \varphi_{\ell_1,\ldots,\ell_p}(\overrightarrow{t_{i,i+1}}) \quad \forall t \in \mathbb{R}.$$

1.2.3 Distribution of the eigenvectors

Before giving the distribution of the eigenvectors of a Wishart matrix we present the next definition given in Anderson [4]. We include it for the sake of completeness, but it is not used in this work.

Definition 1.2.1 *If the random orthogonal matrix E of order p has a distribution such that $EQ^\top$ has the same distribution for every orthogonal matrix Q, the distribution of E is said to have the* Haar invariant distribution.

If E has Haar invariant distribution the probability that E is such that $e_{i1} \geq 0$, $i = 1, 2, \ldots, p$, is $1/2^p$; see [4, pp. 536]. Then the conditional distribution of E given $e_{i1} \geq 0$, $i = 1, 2, \ldots, p$, is 2^p times the Haar invariant distribution over this part of the space. We call this distribution the *conditional Haar invariant distribution*. The next theorem is about the distribution of the matrix of eigenvectors of a Wishart matrix, it is taken from [4, pp. 537].

Theorem 1.2.2 *If $C = Y^\top$, where $Y = [Y_1, Y_2, \ldots, Y_p] = (y_{ij})$ is the orthogonal matrix of eigenvectors of $A \sim \mathcal{W}(n, I_p)$ with $y_{1j} \geq 0$ for all $j = 1, 2, \ldots, p$, then C has the conditional Haar invariant distribution and C is independent of the eigenvalues of A.*

1.2.4 Asymptotic distribution of the spectrum when p is fixed

In the case of a Wishart matrix with fixed dimension p, the asymptotic joint distribution of the normalized eigenvalues when n goes to infinity is given by the joint distributions of the eigenvalues of a symmetric standard Gaussian matrix, that is a symmetric matrix where the entries on and above the diagonal are independent, the elements in the diagonal are i.i.d. with distribution $N(0, 2)$ and the entries above the diagonal are i.i.d. with distribution $N(0, 1)$. Moreover the distribution of sample eigenvectors converges to a conditional Haar measure and the sample eigenvectors and eigenvalues are asymptotically independent; see [4, pp. 538].

Theorem 1.2.3 *Let $nS \sim \mathcal{W}(n, I_p)$, define the $p \times p$ matrices $L = \mathrm{diag}(l_1, l_2, \ldots, l_p)$ and $V = [V_1, V_2, \ldots, V_p] = (v_{ij})$ by $S = VLV^\top$ with $l_1 \geq l_2 \geq \cdots \geq l_p$, $V^\top V = I_p$ and $v_{1j} \geq 0$, $j = 1, 2, \ldots, p$. Then the density of the limiting distribution of $\sqrt{n}(L - I_p)$ as $n \to \infty$ is*

$$2^{-p/2}\pi^{p(p-1)/4}\Gamma_p^{-1}\left(\frac{p}{2}\right)\exp\left(-\frac{1}{2}\sum_{i=1}^{p}\varphi_i^2\right)\prod_{j<i}(\varphi_i - \varphi_j), \tag{1.13}$$

for $\varphi_1 > \cdots > \varphi_p$, which is the density of the eigenvalues of a symmetric standard Gaussian matrix. Furthermore, the matrix $V^\top$ is asymptotically distributed according to the conditional Haar measure and independent of L.

The next proposition can be consider an extension of the one-dimensional fact that if χ_n^2 is a chi-square random variable with n degrees of freedom, then χ_n^2/n converges to 1 in probability (almost surely and in distribution), as $n \to \infty$. It is a consequence of a more general result under a non-Gaussian assumption, the Proposition 2.2.1 in Chapter 2.

Proposition 1.2.2 *Let $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p$ be the eigenvalues of $W \sim \mathcal{W}(n, \Sigma)$ with $n \geq p$ and suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ are the eigenvalues of Σ. Then*

$$n^{-1}\left(\frac{\ell_1}{\lambda_1}, \frac{\ell_2}{\lambda_2}, \ldots, \frac{\ell_p}{\lambda_p}\right)^\top \xrightarrow{w} (1, 1, \ldots, 1)^\top \qquad \text{as } n \to \infty.$$

1.3 Asymptotic results for the spectrum: Random Matrix Theory context

1.3.1 Marchenko-Pastur distribution

Several results about the asymptotic behavior of eigenvalues of random matrices are given in terms of their empirical spectral distribution whose definition is the following.

Definition 1.3.1 *The* empirical spectral distribution *(ESD) of a $p \times p$ Hermitian matrix A with eigenvalues $l_1 \geq l_2 \geq \cdots \geq l_p$ is defined as*

$$\widehat{F}_A(x) = \frac{\sum_{i=1}^{p}\mathbf{I}_{(l_i,\infty)}(x)}{p} = \frac{\#\{1 \leq i \leq p : \ l_i \leq x\}}{p}.$$

The expectation of $F_A(x)$ is computed as follows

$$E(\widehat{F}_A(x)) = E\left(\frac{\sum_{i=1}^{p}\mathbf{I}_{(l_i,\infty)}(x)}{p}\right) = \frac{\sum_{i=1}^{p}E[\mathbf{I}_{(l_i,\infty)}(x)]}{p} = \frac{\sum_{i=1}^{p}P(l_i \leq x)}{p}.$$

The following theorem is due to Marchenko and Pastur [27]. It gives the limiting distribution of the ESD of (a sequence of) Wishart matrices, when the sample size n and the matrix dimension p go both to infinity at the same rate, in the sense that $p/n \to \gamma > 0$. It considers both the full ($\gamma \leq 1$) and non-full ($\gamma > 1$) rank cases.

Theorem 1.3.1 *Let $S_n = A_n/n$ where $A_n \sim \mathcal{W}(n, I_p)$, $p = p(n)$ and $p/n \to \gamma > 0$ as $n \to \infty$. Then for all $x \in \mathbb{R}$*

$$\widehat{F}_{S_n}(x) \longrightarrow F(x) \quad \text{as} \quad n \to \infty$$

almost surely, where F is the Marchenko-Pastur law *with density given by*

$$f(x) = \frac{1}{2\pi\gamma x}\sqrt{(b-x)(x-a)}\mathbf{I}_{(a,b)}(x) + \mathbf{I}_{(1,\infty)}(\gamma)\left(1 - \frac{1}{\gamma}\right)\delta_0(x), \tag{1.14}$$

where $a = (1-\sqrt{\gamma})^2$, $b = (1+\sqrt{\gamma})^2$ and δ_0 is the Dirac delta function in zero.

Note that when $\gamma > 1$ the Marchenko-Pastur law has an atom at $x = 0$ with mass $1 - \frac{1}{\gamma}$.

Remark 1.3.1 *The result of Theorem 1.3.1 holds for more general matrices of the form $B_n = YY^\top$, where the entries of the $p \times n$ matrix Y are i.i.d. random variables with mean zero and finite variance; see [6].*

Furthermore, by [17] and [38] we have the next result which says that when n and p tend to infinity and $p/n \to \gamma$ all the nonzero eigenvalues of S_n tend to be in the support of the Marchenko-Pastur density (1.14).

Proposition 1.3.1 *Under the same hypothesis as in Theorem 1.3.1, if l_1 and l_r are the largest and the smallest nonzero eigenvalue of S_n respectively, with $r = \min(n,p)$, then*

$$l_r \longrightarrow (1-\sqrt{\gamma})^2 \qquad \text{and} \qquad l_1 \longrightarrow (1+\sqrt{\gamma})^2$$

almost surely, when $p/n \to \gamma > 0$ and $n \to \infty$.

The next example is taken from [24]. It illustrates how Marchenko-Pastur's result explains the dispersion of sample eigenvalues in a simple case.

Example 1.3.1 *$n = 10$ independent observations are obtained from a distribution $N_p(0, I_p)$, with $p = 10$. In this case the eigenvalues of the population covariance matrix are all equal to one, but the eigenvalues of the sample covariance matrix, which is $1/n$ times a Wishart matrix, are*

$$(0.003, 0.036, 0.095, 0.16, 0.30, 0.51, 0.78, 1.12, 1.40, 3.07).$$

We can see an extreme spread in the sample eigenvalues and not all of them are close to one. This phenomenon can be explained by Theorem 1.3.1 because the limit of the ESD of the sample covariance matrix with $p = n$ (i.e. $\gamma = 1$) is the Marchenko-Pastur law with support

$$a = (1-\sqrt{1})^2 = 0 \quad \text{and} \quad b = (1+\sqrt{1})^2 = 4,$$

which corresponds to the range of the sample eigenvalues.

1.3.2 Tracy-Widom distribution

The asymptotic distribution of the largest eigenvalue of a Wishart matrix was obtained by Johnstone [23]. This distribution is the so-called Tracy-Widom distribution obtained by these authors [39] as the limiting law of the largest eigenvalue of Gaussian matrices; see [30, pp. 33].

Theorem 1.3.2 *Let us assume that the* $p \times n$ *matrix* X *has entries i.i.d. with distribution* $N(0,1)$. *Then, if* $p/n \to \gamma > 0$ *as* $n \to \infty$, *and if* l_1 *is the largest eigenvalue of* $S_n = XX^\top/n$, *we have*

$$P\left(n^{2/3}\frac{l_1 - (\sqrt{1-1/n}+\sqrt{p/n})^2}{(\sqrt{1-1/n}+\sqrt{p/n})(\sqrt{1+1/(n-1)}+\sqrt{n/p})^{1/3}} \leq s\right) \longrightarrow F_1(s)$$

as $n \to \infty$, *where* F_1 *is the* Tracy-Widom distribution of order 1 *defined by*

$$F_1(s) = \exp\left(-\frac{1}{2}\int_0^\infty q(x) + (x-s)q^2(x)dx\right), \quad s \in \mathbb{R},$$

with $q(x)$ *the solution of the Painlevé II differential equation*

$$q''^3(x), \quad q(x) \sim Ai(x) \text{ as } x \to \infty, \tag{1.15}$$

and where $Ai(x)$ *denotes the Airy function.*

Remark 1.3.2 *The complex case of Theorem 1.3.2 is study by Johansson [22], who shows that the limiting distribution of the largest sample eigenvalue in this case is the* Tracy-Widom distribution of order 2.

Theorem 1.3.2 can be used in hypothesis testing as we show in the next example taken from [24].

Example 1.3.2 *Suppose that the observed largest sample eigenvalue is equal to* 4.25 *and* $n = p = 10$. *Is this consistent with* $H_0 : \Sigma = I_p$?. *Let* l_1 *be largest sample eigenvalue. By Theorem 1.3.2 we have*

$$P\left(\frac{nl_1 - \mu_{n,p}}{\sigma_{n,p}} \leq s\right) \approx F_1(s),$$

where

$$\mu_{n,p} = (\sqrt{n-1}+\sqrt{p})^2 \qquad \text{and} \qquad \sigma_{n,p} = (\sqrt{n-1}+\sqrt{p})\left(\frac{1}{\sqrt{n-1}}+\frac{1}{\sqrt{p}}\right)^{1/3}.$$

Then

$$P(l_1 > 4.25) \approx 1 - F_1\left(\frac{n(4.25) - \mu_{n,p}}{\sigma_{n,p}}\right) = 0.06.$$

Therefore we do not reject H_0 *with significance level 5%.*

1.4 Exact distribution of the largest eigenvalue

In this section we obtain results that address the structure and properties of the exact distribution of the largest eigenvalue ℓ_1 of a Wishart matrix $\mathcal{W}(n, I_p)$. We show that this distribution is a simultaneous mixture of scale and shape mixtures of gamma distributions. We believe that these results could be useful to discover new properties of the Tracy-Widom distribution, e.g. its infinite divisibility, an open problem.

The notations $\Phi(a;c;z)$ and ${}_2F_1(a,b;c;z)$ will be used for the confluent hypergeometric function and the Gauss hypergeometric function of one variable, respectively. The integral and series representations of these functions can be found in [18] and are given by the expressions

$$ {}_2F_1(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}dt, \quad Re(c) > Re(b) > 0, |\arg(1-z)| < \pi; \tag{1.16} $$

$$ \Phi(a;b;z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 t^{a-1}(1-t)^{b-a-1}\exp(tz)dt, \quad Re(b) > Re(a) > 0; \tag{1.17} $$

$$ {}_2F_1(a,b;c;z) = \sum_{k=0}^{\infty} \frac{(a)_k(b)_k}{(c)_k}\frac{z^k}{k!}, \qquad |z| < 1; \tag{1.18} $$

$$ \Phi(a;b;z) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k}\frac{z^k}{k!}, \qquad b \neq 0, -1, -2, \ldots; \tag{1.19} $$

where $(a)_k = a(a+1)\cdots(a+k-1) = \frac{\Gamma(a+k)}{\Gamma(a)}$.

1.4.1 Mixtures of distributions

Let us recall some notions regarding mixtures of distributions.

Definition 1.4.1 *Let P be a probability measure on the measurable space $(\Theta, \mathcal{T})$ and let $\{F_\theta\}_{\theta\in\Theta}$ be a collection of distribution functions such that $\theta \mapsto F_\theta(x)$ is $\mathcal{T}$-measurable for all $x \in \mathbb{R}$. Then we say that the function*

$$ F(x) = \int_\Theta F_\theta(x)P(d\theta), \qquad x \in \mathbb{R}, \tag{1.20} $$

is a mixture of the distributions $\{F_\theta\}_{\theta\in\Theta}$.

Sometimes the space Θ can be a subset of $\mathbb{R}_+$ and P can be the Stieltjes measure induced by a distribution function H. Mixtures as in (1.20) can be written in terms of characteristic functions as follows

$$\varphi(t) = \int_\Theta \varphi_\theta(t)P(d\theta), \qquad t \in \mathbb{R}, \tag{1.21}$$

where φ_θ is the characteristic function of F_θ. If F_θ is absolutely continuous with density f_θ for every $\theta \in \Theta$, then the mixture F is absolutely continuous with density f given by

$$f(x) = \int_\Theta f_\theta(x)P(d\theta), \qquad x \in \mathbb{R}. \tag{1.22}$$

Let us recall two important types of mixtures. Suppose $\Theta \subset \mathbb{R}_+$ and let φ_1 be a characteristic function.

Definition 1.4.2 *The distribution of a random variable X is said to be a* scale mixture *if*

$$X \stackrel{\mathcal{L}}{=} ZY,$$

where Z and Y are independent and Z is non-negative. In terms of characteristics functions this is equivalent to

$$\varphi_X(t) = \int_\Theta \varphi_Y(\theta t)dF_Z(\theta), \qquad t \in \mathbb{R}. \tag{1.23}$$

Example 1.4.1 *Let $g(x; a, b)$ and $\widehat{G}(t; a, b)$ be the density and characteristic functions of the gamma distribution Gamma(a, b) given by (1.5) and (1.6), respectively. Suppose H_a is a distribution function for each $a \in \mathbb{R}_+$. Let $\varphi_1(t) = \widehat{G}(t; a, 1) = (1-it)^{-a}$ be the characteristic function of the gamma distribution Gamma$(a, 1)$. Then the distribution with density*

$$\widetilde{g}_a(x) = \int_{\mathbb{R}_+} g(x; a, \theta)dH_a(\theta)$$

is a scale mixture, called a scale mixture of gamma(a) distributions*. Its characteristic function is*

$$\varphi_a(t) = \int_{\mathbb{R}_+} \widehat{G}(t; a, \theta)dH_a(\theta) = \int_{\mathbb{R}_+} (1 - i\theta t)^{-a}dH_a(\theta) = \int_{\mathbb{R}_+} \varphi_1(\theta t)dH_a(\theta).$$

Now, suppose that B is a distribution function over $\mathbb{R}_+$, then

$$f(x) = \int_{\mathcal{R}_+} \widetilde{g}_a(x)dB(a)$$

is a mixture of the distributions $\{\widetilde{g}_a\}_{a\in\mathbb{R}_+}$ which we call a mixture of scale mixtures of gamma distributions*.*

1.4.2 The case $p = 2$

We calculate the density function of the largest eigenvalue of $\mathcal{W}(n, cI_2)$, ℓ_1, which has the expression of a density function given by Al-Zamel [3]. Also, it can be seen as a scale mixture of gamma(n) distributions as we show in the next proposition. For simplicity we take $c = 1$; the general case is analogous.

Proposition 1.4.1 *The density function of the largest eigenvalue of $A \sim \mathcal{W}(n, I_2)$, ℓ_1, is given by*

$$f_{\ell_1}(\ell_1) = \frac{\ell_1^{n-1}\exp(-\ell_1/2)\Phi(\frac{n-1}{2};\frac{n+3}{2};\frac{-\ell_1}{2})}{2^n\Gamma(n)_2F_1(n,\frac{n-1}{2};\frac{n+3}{2};-1)} \quad \textit{(Al-Zamel's density)} \tag{1.24}$$

$$= \int_1^2 g(\ell_1; n, y)h_n(y)dy, \quad \textit{(scale mixture of gamma(n) dist.)} \tag{1.25}$$

where $g(x; a, b)$ is as in (1.5) and

$$h_n(y) = (n-1)(y-1)(2-y)^{(n-3)/2}y^{(n-3)/2} \tag{1.26}$$

is a density function with support (1,2). Furthermore the characteristic function of ℓ_1 is

$$\varphi_{\ell_1}(t) = \frac{{}_2F_1(n, 2; \frac{n+3}{2}; \frac{1}{2(1-it)})}{(n+1)(1-it)^n}.$$

Proof. Let $l_k = \ell_{3-k}$ for $k = 1, 2$. Using Corollary 1.2.1 we have

$$f_{\ell_1}(\ell_1) = f_{l_2}(l_2) = \int_{\mathbb{R}} f_{(l_1,l_2)}(l_1, l_2)dl_1 = \frac{l_2^{(n-3)/2}\exp(-l_2/2)}{4\Gamma(n-1)}\int_0^{l_2} l_1^{(n-3)/2}(l_2 - l_1)\exp(-l_1/2)dl_1.$$

Under the change of variable $t = l_1/l_2$, the last expression is equal to

$$\frac{l_2^{n-1}\exp(-l_2/2)}{4\Gamma(n-1)}\int_0^1 t^{(n-3)/2}(1-t)\exp(-l_2t/2)dt. \tag{1.27}$$

In order to see that (1.27) is equal to (1.24) we only need to see that

$$\frac{\Phi(\frac{n-1}{2};\frac{n+3}{2};\frac{-l_2}{2})}{2^n\Gamma(n)_2F_1(n,\frac{n-1}{2};\frac{n+3}{2};-1)} = \frac{1}{4\Gamma(n-1)}\int_0^1 t^{(n-3)/2}(1-t)\exp(-l_2t/2)dt.$$

Before proving the last equality note the following:

$$\begin{aligned}
{}_2F_1\left(n, \frac{n-1}{2}; \frac{n+3}{2}; -1\right) &= \frac{\Gamma(\frac{n+3}{2})}{\Gamma(\frac{n-1}{2})\Gamma(2)}\int_0^1 u^{\frac{n-1}{2}-1}(1-u)(1+u)^{-n}du \\
&= \frac{\Gamma(\frac{n+3}{2})}{2^n\Gamma(\frac{n-1}{2})\Gamma(2)}\int_0^1 (1-y)^{\frac{n-1}{2}-1}y(1-y/2)^{-n}dy \\
&= \frac{1}{2^n}{}_2F_1\left(n, 2; \frac{n+3}{2}; 1/2\right) = \frac{2\Gamma(\frac{n+3}{2})}{2^n\Gamma(\frac{n+1}{2})}.
\end{aligned}$$

Thus we have

$$\frac{\Phi(\frac{n-1}{2};\frac{n+3}{2};\frac{-l_2}{2})}{2^n\Gamma(n)_2F_1(n,\frac{n-1}{2};\frac{n+3}{2};-1)} = \frac{\frac{\Gamma((n+3)/2)}{\Gamma((n-1)/2)\Gamma(2)}\int_0^1 t^{\frac{n-1}{2}-1}(1-t)\exp(-l_2t/2)dt}{2^n\Gamma(n)\frac{2\Gamma(\frac{n+3}{2})}{2^n\Gamma(\frac{n+1}{2})}}$$
$$= \frac{\Gamma(\frac{n+1}{2})}{2\Gamma(n)\Gamma(\frac{n-1}{2})}\int_0^1 t^{(n-3)/2}(1-t)\exp(-l_2t/2)dt$$
$$= \frac{1}{4\Gamma(n-1)}\int_0^1 t^{(n-3)/2}(1-t)\exp(-l_2t/2)dt.$$

To conclude the proof we will see that (1.25) is equal to (1.27). Adopting the change of variable $y=\frac{2}{2-t}$ we have that

$$\int_1^2 g(l_2;n,y)h_n(y)dy = \int_0^1 g\left(l_2;n,\frac{2}{2-t}\right)\widetilde{h}_n(t)dt,$$

where $g(x;a,b)$ and $h_n(y)$ are given by (1.5) and(1.26) respectively, and

$$\widetilde{h}_n(t) = \frac{n-1}{4}t(1-t)^{(n-3)/2}\left(1-\frac{t}{2}\right)^{-n}.$$

Furthermore, we have that

$$\int_0^1 g\left(l_2;n,\frac{2}{2-t}\right)\widetilde{h}_n(t)dt = \int_0^1 \frac{n-1}{4}t(1-t)^{(n-3)/2}\left(1-\frac{t}{2}\right)^{-n}\frac{l_2^{n-1}\exp(\frac{-l_2(2-t)}{2})}{(\frac{2}{2-t})^n\Gamma(n)}dt$$
$$= \frac{(n-1)l_2^{n-1}}{4\Gamma(n)}\int_0^1 t(1-t)^{(n-3)/2}\exp\left(\frac{-l_2(2-t)}{2}\right)dt$$
$$= \frac{l_2^{n-1}}{4\Gamma(n-1)}\int_0^1 y^{(n-3)/2}(1-y)\exp\left(\frac{-l_2(1+y)}{2}\right)dy$$
$$= \frac{l_2^{n-1}\exp(-l_2/2)}{4\Gamma(n-1)}\int_0^1 y^{(n-3)/2}(1-y)\exp(-l_2y/2)dy.$$

Therefore we have that (1.25) is equal to (1.27). The characteristic function of ℓ_1 is derived from Proposition 1.2.1 since

$$\varphi_{\ell_1}(t) = \varphi_{\ell_1,\ell_2}(t,0).\square$$

1.4.3 The case $p \geq 3$

In this section we prove that the distribution of the largest eigenvalue ℓ_1, when $p \geq 3$, is also related to mixtures of distributions involving mixtures of gamma distributions. In order to see this, we will obtain the density function of ℓ_1 for the case $p \geq 3$ differently from the way used in the case $p=2$. Let $(\Theta,\mathcal{T})$ be the measurable space where $\Theta=\mathbb{N}_0^{p-2}$ is the $(p-2)$-ary Cartesian product of the set $\mathbb{N}_0=\mathbb{N}\cup\{0\}$, and $\mathcal{T}$ is the power set of Θ.

Proposition 1.4.2 *The density function of the largest eigenvalue of $A \sim \mathcal{W}(n, I_p)$ with $p \geq 3$, ℓ_1, has the form*

$$f_{\ell_1}(\ell_1) = \int_\Theta \widetilde{g}(\ell_1; \theta, n, p) B_{n,p}(d\theta). \tag{1.28}$$

Here, $B_{n,p}$ is a probability measure on $(\Theta, \mathcal{T})$; the function $\widetilde{g}(\ell_1; \theta, n, p)$ is the density of a scale mixture of gamma(r) distributions, as defined in Example 1.4.1 with $r = r(\theta, n, p)$, given by

$$\widetilde{g}(x; \theta, n, p) = \int_{\mathbb{R}_+} g(x; r(\theta, n, p), z) dH_{(\theta,n,p)}(z)$$

and $H_{(\theta,n,p)}$ is a distribution function on $\mathbb{R}_+$. That is, f_{ℓ_1} is a simultaneous mixture of scale and shape mixtures of gamma distributions.

Proof. Let $l_k = \ell_{p+1-k}$ for $k = 1, 2, \ldots, p$. Using (1.4) we have the following:

$$\begin{aligned} f_{l_p}(l_p) &= \int_0^{l_p} \cdots \int_0^{l_2} f_{(l_1,\ldots,l_p)}(l_1, \ldots, l_p) dl_1 \cdots dl_{p-1} \\ &= \Delta \exp\left(-\frac{l_p}{2}\right) l_p^{(n-p-1)/2} \int_0^{l_p} \exp\left(-\frac{l_{p-1}}{2}\right) l_{p-1}^{(n-p-1)/2} (l_p - l_{p-1}) \cdots \\ &\qquad \int_0^{l_{i+1}} \exp\left(-\frac{l_i}{2}\right) l_i^{(n-p-1)/2} \prod_{j=i}^{p-1} (l_{j+1} - l_i) \cdots \\ &\qquad \int_0^{l_2} \exp\left(-\frac{l_1}{2}\right) l_1^{(n-p-1)/2} \prod_{j=1}^{p-1} (l_{j+1} - l_1) dl_1 \cdots dl_{p-1}. \end{aligned}$$

Doing the change of variable $y_i = l_i / l_{i+1}$, $i = 1, 2, \ldots, p-1$, iteratively in the last integrals we obtain that

$$\begin{aligned} f_{l_p}(l_p) = \Delta \exp\left(-\frac{l_p}{2}\right) l_p^{pn/2-1} &\int_0^1 \exp\left(-\frac{l_p y_{p-1}}{2}\right) y_{p-1}^{(p-1)(n-1)/2-1} (1 - y_{p-1}) \cdots \\ &\int_0^1 \exp\left(-\frac{l_p \prod_{j=i}^{p-1} y_j}{2}\right) y_i^{i(n-p+i)/2-1} \prod_{j=i}^{p-1} \left(1 - \prod_{r=i}^{j} y_r\right) \cdots \\ &\int_0^1 \exp\left(-\frac{l_p \prod_{j=1}^{p-1} y_j}{2}\right) y_1^{(n-p+1)/2-1} \prod_{j=1}^{p-1} \left(1 - \prod_{r=1}^{j} y_r\right) dy_1 \cdots dy_{p-1}. \end{aligned} \tag{1.29}$$

Now, writing $t_1 = 1 - y_1$ in the internal integral of (1.29) and taking in to account that

$$\begin{aligned} &\prod_{j=i+1}^{p-1} \left(1 - \prod_{r=i+1}^{j} y_r + t_i \prod_{r=i+1}^{j} y_r\right)^{n_j} \\ &\quad = \sum_{x_{i+1}=0}^{n_{i+1}} \cdots \sum_{x_{p-1}=0}^{n_{p-1}} t_i^{\sum_{r=i+1}^{p-1} x_r} \prod_{j=i+1}^{p-1} \left[\binom{n_j}{x_j} (1 - \prod_{r=i+1}^{j} y_r)^{n_j - x_j} y_j^{\sum_{r=j}^{p-1} x_r} \right], \end{aligned} \tag{1.30}$$

for i and n_j positive integers (in this case $i = 1$ and $n_j = 1$ for all $j = 2, 3, \ldots, p-1$), we have that the internal integral of (1.29) is equal to

$$\exp\left(-\frac{l_p \prod_{j=2}^{p-1} y_j}{2}\right) \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} \prod_{j=2}^{p-1} \left[\left(1 - \prod_{r=2}^{j} y_r\right)^{1-x_j^{(1)}} y_j^{\sum_{r=j}^{p-1} x_r^{(1)}} \right]$$
$$* \int_0^1 \exp\left(\frac{l_p \prod_{j=2}^{p-1} y_j t_1}{2}\right) (1-t_1)^{(n-p+1)/2-1} t_1^{2-\sum_{r=2}^{p-1} x_r^{(1)}-1} dt_1. \tag{1.31}$$

By (1.17) the integral in (1.31) is equal to

$$B\left(2 + \sum_{r=2}^{p-1} x_r^{(1)}, \frac{n-p+1}{2}\right) \Phi\left(2 + \sum_{r=2}^{p-1} x_r^{(1)}; 2 + \frac{n-p+1}{2} + \sum_{r=2}^{p-1} x_r^{(1)}; \frac{l_p \prod_{j=2}^{p-1} y_j}{2}\right).$$

Hence using (1.19) we can write (1.31) as

$$\exp\left(-\frac{l_p \prod_{j=2}^{p-1} y_j}{2}\right) \sum_{k_1=0}^{\infty} \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} a^{(1)}(x^{(1)}, k_1, n, p) l_p^{k_1}$$
$$* \prod_{j=2}^{p-1} \left[\left(1 - \prod_{r=2}^{j} y_r\right)^{1-x_j^{(1)}} y_j^{\sum_{r=j}^{p-1} x_r^{(1)} + k_1} \right], \tag{1.32}$$

where $a^{(1)}$ is a non-negative constant that depends only on $x^{(1)} := (x_2^{(1)}, \ldots, x_{p-1}^{(1)})^\top$, k_1, n and p. Therefore (1.29) can be written as

$$f_{l_p}(l_p) = \Delta \exp\left(-\frac{l_p}{2}\right) l_p^{pn/2-1} \int_0^1 \exp\left(-\frac{l_d y_{p-1}}{2}\right) y_{p-1}^{(p-1)(n-1)/2-1} (1-y_{p-1}) \cdots$$
$$\int_0^1 \exp\left(-\frac{l_p \prod_{j=i}^{p-1} y_j}{2}\right) y_i^{i(n-p+i)/2-1} \prod_{j=i}^{p-1} \left(1 - \prod_{r=i}^{j} y_r\right) \cdots$$
$$\sum_{k_1=0}^{\infty} \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} a^{(1)}(x^{(1)}, k_1, n, p) l_p^{k_1} \prod_{j=3}^{p-1} \left[y_j^{\sum_{r=j}^{p-1} x_r^{(1)} + k_1} \right]$$
$$\int_0^1 \exp\left(-\frac{2 l_p \prod_{j=2}^{p-1} y_j}{2}\right) y_2^{2(n-p+1)/2 + \sum_{r=2}^{p-1} x_r^{(1)} + k_1 - 1} \prod_{j=2}^{p-1} \left(1 - \prod_{r=2}^{j} y_r\right)^{2-x_j^{(1)}} dy_2 \cdots dy_{p-1} \tag{1.33}$$

after interchanging the order of the sums with the integral respect to y_2. Similarly, doing the change of variable $t_i = 1 - y_i$, $i = 2, 3, \ldots, p-2$, in (1.33) iteratively and using (1.30) we see that

$$f_{l_p}(l_p) = \Delta \exp\left(-\frac{l_p}{2}\right) l_p^{pn/2-1} \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} \sum_{x_3^{(2)}=0}^{2-x_3^{(1)}} \cdots \sum_{x_{p-1}^{(2)}=0}^{2-x_{p-1}^{(1)}} \cdots \sum_{x_{p-1}^{(p-2)}=0}^{p-2-\sum_{i=1}^{p-3} x_{p-1}^{(i)}}$$

$$a^{(p-2)}(x^{(1)}, \ldots, x^{(p-2)}, k^{(p-2)}, n, p) l_p^{\sum_{r=1}^{p-2} k_r} \int_0^1 \exp\left(-\frac{(p-1)l_p y_{p-1}}{2}\right)$$

$$* (1-y_{p-1})^{p-\sum_{i=1}^{p-2} x_{p-1}^{(i)}-1} y_{p-1}^{(p-1)(n-1)/2+\sum_{i=1}^{p-2}(x_{p-1}^{(i)}+k_i)-1} dy_{p-1}, \quad (1.34)$$

where $a^{(p-2)}$ is a non-negative constant that depends only on the vectors

$$x^{(i)} := (x_{i+1}^{(i)}, x_{i+2}^{(i)}, \ldots, x_{p-1}^{(i)})^\top, \quad \text{for} \quad i = 1, 2, \ldots, p-2,$$

$k^{(p-2)} := (k_1, k_2, \ldots, k_{p-2})^\top$ and the numbers n, p. Performing the change of variable $t = 1 - y_{p-1}$ in (1.34) we obtain that

$$f_{l_p}(l_p) = \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} \sum_{x_3^{(2)}=0}^{2-x_3^{(1)}} \cdots \sum_{x_{p-1}^{(2)}=0}^{2-x_{p-1}^{(1)}} \cdots \sum_{x_{p-1}^{(p-2)}=0}^{p-2-\sum_{i=1}^{p-3} x_{p-1}^{(i)}}$$

$$\Delta a^{(p-2)}(x^{(1)}, \ldots, x^{(p-2)}, k^{(p-2)}, n, p) \int_0^1 \exp\left(-\frac{l_p(p-(p-1)t)}{2}\right) l_p^{pn/2+\sum_{r=1}^{p-2} k_r - 1}$$

$$* t^{p-\sum_{i=1}^{p-2} x_{p-1}^{(i)}-1} (1-t)^{(p-1)(n-1)/2+\sum_{i=1}^{p-2}(x_{p-1}^{(i)}+k_i)-1} dt. \quad (1.35)$$

A further change of variable $z = \frac{2}{p-(p-1)t}$ in the integral of (1.35), yields that this integral is equal to

$$\int_{2/p}^{2} \exp\left(-\frac{l_p}{z}\right) l_p^{pn/2+\sum_{r=1}^{p-2} k_r - 1} \left(1 - \frac{pz-2}{(p-1)z}\right)^{(p-1)(n-1)/2+\sum_{i=1}^{p-2}(x_{p-1}^{(i)}+k_i)-1}$$

$$* \left(\frac{pz-2}{(p-1)z}\right)^{p-\sum_{i=1}^{p-2} x_{p-1}^{(i)}-1} \frac{2}{(p-1)z^2} dz$$

$$= \Gamma\left(\frac{pn}{2} + \sum_{r=1}^{p-2} k_r\right) \int_{2/p}^{2} g\left(l_p; \frac{pn}{2} + \sum_{r=1}^{p-2} k_r, z\right) h(z; x_{p-1}^{(1)}, \ldots, x_{p-1}^{(p-2)}, k^{(p-2)}, n, p) dz, \quad (1.36)$$

where g is the gamma density given in (1.5) and

$$h(z; x_{p-1}^{(1)}, \ldots, x_{p-1}^{(p-2)}, k^{(p-2)}, n, p) = z^{pn/2+\sum_{r=1}^{p-2} k_r} \left(1 - \frac{pz-2}{(p-1)z}\right)^{(p-1)(n-1)/2+\sum_{i=1}^{p-2}(x_{p-1}^{(i)}+k_i)-1}$$

$$* \left(\frac{pz-2}{(p-1)z}\right)^{p-\sum_{i=1}^{p-2} x_{p-1}^{(i)}-1} \frac{2}{(p-1)z^2}.$$

Then, interchanging the integral in (1.35) by the last expression of (1.36) we have

$$\begin{aligned} f_{l_p}(l_p) &= \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} \int_{2/p}^{2} g\left(l_p; \frac{pn}{2} + \sum_{r=1}^{p-2} k_r, z\right) \overline{h}(z; k^{(p-2)}, n, p) dz \\ &= \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} b(k^{(p-2)}, n, p) \int_{2/p}^{2} g\left(l_p; \frac{pn}{2} + \sum_{r=1}^{p-2} k_r, z\right) \widetilde{h}(z; k^{(p-2)}, n, p) dz, \end{aligned} \tag{1.37}$$

where

$$\overline{h}(z; k^{(p-2)}, n, p) = \sum_{x_2^{(1)}=0}^{1} \cdots \sum_{x_{p-1}^{(1)}=0}^{1} \sum_{x_3^{(2)}=0}^{2-x_3^{(1)}} \cdots \sum_{x_{p-1}^{(2)}=0}^{2-x_{p-1}^{(1)}} \cdots \sum_{x_{p-1}^{(p-2)}=0}^{p-2-\sum_{i=1}^{p-3} x_{p-1}^{(i)}}$$

$$\Delta a^{(p-2)}(x^{(1)}, \ldots, x^{(p-2)}, k^{(p-2)}, n, p) \Gamma\left(\frac{pn}{2} + \sum_{r=1}^{p-2} k_r\right) h(z; x_{p-1}^{(1)}, \ldots, x_{p-1}^{(p-2)}, k^{(p-2)}, n, p),$$

$$b(k^{(p-2)}, n, p) = \int_{2/p}^{2} \overline{h}(z; k^{(p-2)}, n, p) dz, \tag{1.38}$$

$$\widetilde{h}(z; k^{(p-2)}, n, p) = \frac{\overline{h}(z; k^{(p-2)}, n, p)}{b(k^{(p-2)}, n, p)}.$$

Let

$$\widetilde{g}(l_p; k^{(p-2)}, n, p) = \int_{2/p}^{2} g\left(l_p; \frac{pn}{2} + \sum_{r=1}^{p-2} k_r, z\right) \widetilde{h}(z; k^{(p-2)}, n, p) dz. \tag{1.39}$$

Then by the last expression in (1.37) we have

$$f_{l_p}(l_p) = \sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} b(k^{(p-2)}, n, p) \widetilde{g}(l_p; k^{(p-2)}, n, p). \tag{1.40}$$

Since f_{l_p} and $\widetilde{g}$ are density functions depending on l_p, integrating both size of (1.40) respect to l_p we see that

$$\sum_{k_1=0}^{\infty} \cdots \sum_{k_{p-2}=0}^{\infty} b(k^{(p-2)}, n, p) = 1$$

and since $b(k^{(p-2)}, n, p) \geq 0$ we can define a probability measure, $B_{n,p}$, over the space $\Theta = \mathbb{N}_0^{p-2}$ by

$$B_{n,p}(\theta) = b(\theta, n, p), \quad \theta \in \Theta. \tag{1.41}$$

Finally, by (1.40) we obtain (1.28). □

Chapter 2

Principal component analysis for the spiked covariance model in HDLSS

An important methodology in multivariate statistical analysis for reduction of dimensionality is Principal Component Analysis (PCA), which is based on the estimation of the population covariance matrix by the sample eigenvalues and eigenvectors of the sample covariance matrix. In this chapter we study the asymptotic behavior of the p largest sample eigenvalues and their corresponding sample eigenvectors under the so-called spiked covariance model. We assume for this model that its $p \geq 2$ largest population eigenvalues have the same asymptotic order of magnitude, as the data dimension d tends to infinity, while the rest of the eigenvalues are constant, as explained in Section 2.1.2. We also propose hypotesis testing for a particular case of our model and confidence intervals for the p largest population eigenvalues under this model.

In Section 2.1 the definition of the spiked covariance model is given, as well as the ways it has been considered in PCA under the the High-Dimension, Low Sample Size framework. Section 2.2 is dedicated to study PCA for the spiked covariance model where the p largest population eigenvalues have the same asymptotic order of magnitude. Specifically, in Section 2.2.1 we find the asymptotic joint distribution of the nonzero sample eigenvalues when $d \to \infty$ and with the sample size n fixed. We then obtain that the p largest sample eigenvalues increase jointly at the same speed as their population counterpart, in the sense that the vector of ratios of the sample and population eigenvalues converges to a multivariate distribution when $d \to \infty$ and n is fixed, and to the vector of ones when both $d, n \to \infty$ and $d \gg n$. It is proved in Section 2.2.2 that the sample eigenvectors corresponding to the p largest sample eigenvalues are not consistent but they are subspace consistent when d tends to infinity and n is fixed, in the sense of Jung and Marron [25]. In Section 2.3 we consider some inference problems for the spiked covariance model under a Gaussian assumption, in particular, the hypothesis testing of a special case of our spiked covariance model and confidence intervals for the p largest population eigenvalues. Detailed comparisons of our results with those found in the literature for PCA under different settings are done in Section 2.4, also including some open problems of interest in statistical inference.

2.1 Spiked covariance model

An important problem in multivariate statistical analysis is the estimation of the population covariance matrix. When the data dimension is greater than the sample size, PCA often fails to estimate the population eigenvalues and eigenvectors, since the sample covariance matrix is not a good approximation to the population covariance matrix. Therefore, it is important to know conditions under which PCA has good properties in this context. One way to approach this problem is considering a particular covariance model and to study the behavior of PCA under this model. As pointed out in Johnstone [23], one often observes one or a small number of large sample eigenvalues well separated from the rest. The so-called *spiked covariance model* has attracted attention in this situation.

More specifically, suppose $X = [X_1, X_2, \dots, X_n]$ is a $d \times n$ data matrix with $n < d$, where the sample $X_j = (x_{1j}, \dots, x_{dj})^\top$, $j = 1, 2, \dots, n$, are independent and identically distributed random vectors with mean zero and unknown covariance matrix Σ, and X has rank n with probability one (it is not assumed that the X_j's have a multivariate Gaussian distribution). The spiked covariance model considers a covariance matrix of the type

$$\Sigma = O\Lambda O^\top \text{ where } \Lambda = \operatorname{diag}(\tau_1, \tau_2, \dots, \tau_p, \sigma, \dots, \sigma), \tag{2.1}$$

with $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_p > \sigma > 0$, for some $1 \leq p < d$, and O is a $d \times d$ orthogonal matrix.

The spiked covariance model is a kind of covariance matrix that may achieve few sample eigenvalues well separated from the rest, the latter being in the support of the Marchenko-Pastur distribution. This is showed in Baik and Silverstein [9]. They prove that when $d, n \to \infty$, $d/n \to \gamma > 0$ and there are population eigenvalues of the spiked covariance model outside the interval $[1 - \sqrt{\gamma}, 1 + \sqrt{\gamma}]$, precisely the same number of sample eigenvalues will converge almost surely to values outside the support $[(1-\sqrt{\gamma})^2, (1+\sqrt{\gamma})^2]$ of the Marchenko-Pastur distribution as $d/n \to \gamma$. Thus, although Theorem 1.3.1 is also true for the spiked covariance model (see [27], [5]) we can not guarantee the result of Proposition 1.3.1 and some sample eigenvalues may be outside the support of the Marchenko-Pastur distribution and well separated from the rest.

Many aspects of the spiked covariance model have been considered in several papers; see for example [7], [8], [9], [16], [33], [35]. In particular, Principal Component Analysis for the spiked covariance model has been considered in [2], [20], [23], [25], [32].

2.1.1 Different asymptotic contexts

There are three different asymptotic contexts in which the study of the sample spectrum of the spiked covariance model arises: (i) the Classical case, (ii) the Random Matrix Theory (RMT) context and (iii) the High-Dimension, Low Sample Size (HDLSS) context. Each context depends on the particular data analytic setting and the way the corresponding asymptotics are considered with respect to the data dimension d and the sample size n.

In the classical case, one considers d fixed and n goes to infinity. In the RMT situation one considers d and n go to infinity simultaneously, in the sense that $d/n \to \gamma$, where $\gamma > 0$, $\gamma = 0$ or $\gamma = \infty$. This framework has been considered in Bai and Yao [7], Baik and Silverstein [9] and references therein. The limiting distribution of the sample spiked eigenvalues is considered in [7], when $\gamma < 1$ (data dimension d lower than sample size), and as we have mentioned before almost sure limits are considered in [9], when $\gamma > 0$. In this context the population eigenvalues of the covariance matrix Σ do not depend on d and the basic analytic tool is the so-called Marchenko-Pastur theorem.

On the other hand, in the so-called HDLSS context the asymptotic results are developed by letting the data dimension $d \to \infty$ while keeping fixed the sample size n. The main references on this framework are Ahn, Marron, Muller and Chi [2], Hall, Marron and Neeman [19] and Jung and Marron [25]. One can also consider in this framework the case of letting first the data dimension $d \to \infty$ while keeping fixed the sample size n and in a second step, letting $n \to \infty$; see [2] and [25]. In other words d, n tend to infinity successively with d increasing at a much faster rate than n, i.e. $d, n \to \infty$ and $d \gg n$. In contrast to the RMT context, [2] and [25] assume that the p largest population eigenvalues of the covariance Σ depend also on the data dimension d. Furthermore, the Marchenko-Pastur theorem does not hold in the HDLSS context because we do not have the convergence of d/n to a positive constant.

In this work we study the behavior of PCA, in the HDLSS context, for considering the asymptotic behavior of largest population eigenvalues and their corresponding eigenvectors under the spiked covariance model. We also study some inference problems for the spiked covariance model and propose hypothesis testing for a particular case of this model and confidence intervals for the largest eigenvalues.

2.1.2 Asymptotic behavior of the sample eigenvalues and eigenvectors

Since the sample covariance matrix $S = n^{-1}XX^\top$ has rank n with probability one, it has exactly n nonzero sample eigenvalues which are denoted by $\widehat{\tau}_1 \geq \widehat{\tau}_2 \geq \cdots \geq \widehat{\tau}_n$. Suppose that $v_1, \ldots, v_d$ are the orthonormal sample eigenvectors corresponding to the orthonormal population eigenvectors $o_1, \ldots, o_d$, respectively. We consider that the direction of v_i is close to that of o_i if

$$\text{Angle}(v_i, o_i) = \arccos\left(\frac{v_i^\top o_i}{\| v_i \| \| o_i \|}\right)$$

is near zero. As mentioned in [25], in the case when several population eigenvalues indexed by the elements of a set J are similar, their corresponding sample eigenvectors may not be distinguishable. Therefore, for $j \in J$ the sample eigenvector v_j, corresponding to the j-th sample eigenvalue, will not be close to its corresponding population eigenvector o_j but rather may asymptotically be in $E_J = \text{span}\{o_j : j \in J\}$, the linear span generated by $\{o_j : j \in J\}$. For this case it is needed to consider the angle between v_j, for $j \in J$, and E_J, which is defined as

$$\begin{aligned}\text{Angle}(v_j, E_J) &= \arccos\left(\frac{v_j^\top[\text{Proj}_{E_J} v_j]}{\| v_j \| \| \text{Proj}_{E_J} v_j \|}\right) \\ &= \arccos\left(\frac{v_j^\top(\sum_{i\in J}(o_i^\top v_j)o_i)}{\| v_j \| \| \sum_{i\in J}(o_i^\top v_j)o_i \|}\right).\end{aligned}$$

We say that v_i is *consistent* if

$$\text{Angle}(v_i, o_i) \xrightarrow{w} 0;$$

it is *strongly inconsistent* if

$$\text{Angle}(v_i, o_i) \xrightarrow{w} \frac{\pi}{2};$$

and it is *subspace consistent* if

$$\text{Angle}(v_i, E_J) \xrightarrow{w} 0,$$

for some set of indices J with $i \in J$; when $d, n \to \infty$ and $d \gg n$ or when $d \to \infty$ and n is fixed.

Under a sample Gaussian assumption on X_j, Ahn, *et al.* [2] show for $p = 1$ and $\Sigma = \text{diag}(d^\alpha, 1, \ldots, 1)$ with $\alpha > 1$, that the largest sample eigenvalue increases at the same speed as its population eigenvalue, in the sense that its ratio converges to the distribution $\mathcal{X}_n^2/n$ when $d \to \infty$ and n is fixed. Moreover, they show that this ratio converges to one and the first sample eigenvector is consistent when $d, n \to \infty$ and $d \gg n$. A natural question is whether these results can be generalized for the case $p \geq 2$.

In this thesis we assume for the population covariance matrix the spiked covariance model (2.1) where the $p \geq 2$ largest population eigenvalues, $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_p$, have the *same asymptotic order of magnitude* as d goes to infinity, that is $\tau_i = \tau_i(d)$ and

$$\frac{\tau_i}{d^\alpha} \longrightarrow c_i \qquad \text{as } d \to \infty, \tag{2.2}$$

for some $\alpha > 1$ and $c_i > 0$, $i = 1, 2, \ldots, p$. Then we show, under certain assumptions for the data, that the p largest sample eigenvalues increase jointly at the same speed as their population counterpart, in the sense that the vector of ratios of the sample and population eigenvalues converges to a multivariate distribution when $d \to \infty$ and n is fixed, and to the vector of ones when both $d, n \to \infty$ and $d \gg n$. We also show that the corresponding sample eigenvectors are subspace consistent as $d \to \infty$ and n is fixed.

Recently, Jung and Marron [25] studied the spiked covariance model (2.1) for the case when each of the p largest population eigenvalues has a *different asymptotic order of magnitude* when dimension increases, that is $\tau_i = \tau_i(d)$ and

$$\frac{\tau_i}{d^{\alpha_i}} \longrightarrow c_i \qquad \text{as } d \to \infty, \tag{2.3}$$

where $\alpha_1 > \alpha_2 > \cdots > \alpha_p > 1$ and $c_i > 0$, $i = 1, 2, \ldots, p$. Taking into account a ρ-mixing condition, they studied the asymptotic behavior of the p largest sample eigenvalues and the consistency of the corresponding sample eigenvectors.

2.2 PCA under same asymptotic order of magnitude

Consider the spiked covariance model (2.1) where the p largest population eigenvalues have the same asymptotic order of magnitude as d goes to infinity, together with the following assumptions for the matrix X:

(a) Let $Z = \Lambda^{-1/2} O^\top X$ and assume that its entries have uniformly bounded fourth moments with respect to d, in the sense that for each $n = p+1, p+2, \ldots$ we have $E(z_{ij}^4) \leq K_n$ for all $i = 1, 2, \ldots, d$, $j = 1, 2, \ldots, n$ and $d = n+1, n+2, \ldots$.

(b) Let Z_i be the i-th row of Z and define $\widetilde{Z}_p = [Z_1^\top, \ldots, Z_p^\top]^\top$. Assume that $\widetilde{Z}_p$ converges in distribution to some $p \times n$ matrix $\widetilde{Y}_n$ as $d \to \infty$, which has rank p with probability one.

We observe that the columns of Z are independent and identically distributed random vectors with mean zero and identity covariance matrix. These assumptions do not cover all random matrices but are still very general and include some interesting settings. In the case when the independent columns of X have the Gaussian distribution $N_d(0, \Sigma)$, assumptions (a) and (b) are automatically satisfied and the $W_1 = Z_i^\top Z_i$'s have a Wishart distribution with one degree of freedom. The assumption (b) is also satisfied in the case when the $\widetilde{Z}_p$'s have a stationary distribution in d, that is the distribution of $\widetilde{Y}_n$ is the distribution of the $\widetilde{Z}_p$'s for all $d > n$. Assumption (b) also holds in the case considered by Jung and Marron [25] where a ρ-mixing condition is assumed; see proof of Lemma 1 in [25].

Considering the above assumptions for the covariance matrix Σ and for the data matrix X, we study the asymptotic behavior of the p largest sample eigenvalues under the two different limiting schemes of HDLSS; and we show the subspace consistency of the corresponding sample eigenvectors when d tends to infinity and n is fixed.

2.2.1 Asymptotic behavior of the sample eigenvalues

As we have mentioned before, Ahn, *et al.* [2] show under the Gaussian setting, that for $p = 1$ and $\Sigma = \mathrm{diag}(d^\alpha, 1, \ldots, 1)$ with $\alpha > 1$, the largest sample eigenvalue increases at the same speed as its population eigenvalue. Specifically, they showed that if $\widehat{\tau}_1$ is the largest sample eigenvalue of the sample covariance matrix $S = n^{-1} X X^\top$ then

$$\frac{\widehat{\tau}_1}{d^\alpha} \xrightarrow{w} \frac{\mathcal{X}_n^2}{n} \qquad \text{as } d \to \infty, \tag{2.4}$$

where $\mathcal{X}_n^2$ is a r.v. with a chi-square distribution with n degrees of freedom. Therefore, since $\mathcal{X}_n^2/n \xrightarrow{w} 1$ as $n \to \infty$ we have that the largest sample and population eigenvalue increase at the same speed. This result can be derived also from Corollary 3 of Jung and Marron [25] and can be extended for the $p \geq 2$ largest population eigenvalues under certain assumptions as we will see in Section 2.4.

We show that the p largest eigenvalues, with $p \geq 2$, increase jointly at the same speed as their population counterpart under our model under two different limiting schemes. We begin with the case when d goes to infinity and n is fixed. The first result is an analogue of Lemma 1 of [25]. In the next theorem we observe the joint convergence in distribution of the vector of nonzero sample eigenvalues, while Lemma 1 of [25] states only the convergence in distribution of each component of this vector (marginal convergence).

Theorem 2.2.1 *Suppose that the unknown covariance matrix Σ of the columns of X is given by the spiked covariance model (2.1), with $p < n < d$ and where $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_p$ have the same asymptotic order of magnitude in the sense of (2.2). Consider the assumptions (a) and (b) for the matrix X. Then when n is fixed*

$$d^{-\alpha}(\widehat{\tau}_1, \widehat{\tau}_2, \ldots, \widehat{\tau}_n)^\top \xrightarrow{w} n^{-1}(\ell_1, \ell_2, \ldots, \ell_p, 0, \ldots, 0)^\top$$

as $d \to \infty$, where $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of the random matrix $\widetilde{U}_0 = \mathcal{C}_p^{1/2}\widetilde{Y}_n\widetilde{Y}_n^\top\mathcal{C}_p^{1/2}$, where $\mathcal{C}_p = \mathrm{diag}(c_1, c_2, \ldots, c_p)$.

Proof. The proof is based on the ideas of Section 4.2 of [2] where the case $p = 1$ was considered. We have $\Sigma = O\Lambda O^\top$ where $\Lambda = \mathrm{diag}(\tau_1, ..., \tau_p, \sigma, \ldots, \sigma)$ is the diagonal matrix of the eigenvalues of Σ and the corresponding eigenvectors are the column vectors of the matrix O. The sample covariance matrix S and the dual sample covariance matrix $S_D = n^{-1}X^\top X$ have the same nonzero eigenvalues. Moreover, the following representation holds

$$nS_D = Z^\top \Lambda Z = \sum_{i=1}^{d} \lambda_i W_i = \sum_{i=1}^{p} \tau_i W_i + \sigma \sum_{i=p+1}^{d} W_i,$$

where $W_i = Z_i^\top Z_i$ and Z_i, $i = 1, 2, \ldots, d$, are the row vectors of Z. Hence

$$d^{-\alpha} nS_D = d^{-\alpha} \sum_{i=1}^{p} \tau_i W_i + d^{-\alpha}\sigma \sum_{i=p+1}^{d} W_i = U + \sigma d^{-\alpha} V, \tag{2.5}$$

where $U = \sum_{i=1}^{p} d^{-\alpha}\tau_i W_i$ and $V = \sum_{i=p+1}^{d} W_i$.

Let $\widetilde{\tau}_p = \mathrm{diag}(\tau_1, \ldots, \tau_p)$ and $\mathcal{C}_p = \mathrm{diag}(c_1, c_2, \ldots, c_p)$. Note that $U = \widetilde{Z}_p^\top(d^{-\alpha}\widetilde{\tau}_p)\widetilde{Z}_p$ converges in distribution to $\widetilde{U} = \widetilde{Y}_n^\top \mathcal{C}_p \widetilde{Y}_n$ as $d \to \infty$. On the other hand, we can show that $d^{-\alpha}V$ converges to the zero matrix in distribution as $d \to \infty$. In order to see that, consider the norm $\| A \| = [\mathrm{tr}(A^\top A)]^{1/2}$ for the $n \times n$ matrix A. By the Markov's inequality we have that for any $\epsilon > 0$

$$P(\| d^{-\alpha}V \| > \epsilon) = P(\| d^{-\alpha}V \|^2 > \epsilon^2) \leq (d^\alpha \epsilon)^{-2} E(\| V \|^2).$$

Using properties of the trace and the fact that the W_i's are symmetric, it can be seen that the right side of the last inequality is equal to

$$(d^\alpha \epsilon)^{-2} \sum_{i=p+1}^{d} \sum_{j=p+1}^{d} E[(Z_i Z_j^\top)^2] = (d^\alpha \epsilon)^{-2} \sum_{i=p+1}^{d} \sum_{j=p+1}^{d} \sum_{k=1}^{n} \sum_{r=1}^{n} E(z_{ik}^2 z_{jr}^2).$$

Since there exist $K_n > 0$ such that $E(z_{ij}^4) \leq K_n$ for all i, j, and by the Holder's inequality $E(z_{ik}^2 z_{jr}^2) \leq E(z_{ik}^4)^{1/2} E(z_{jr}^4)^{1/2}$, we have that the right side of the last equation is less than or equal to $(d^\alpha \epsilon)^{-2}(d-p)^2 n^2 K_n$. Then

$$P(\| d^{-\alpha} V \| > \epsilon) \leq \frac{(d-p)^2 n^2 K_n}{d^{2\alpha}\epsilon^2} = \left(\frac{d-p}{d}\right)^2 \left(\frac{1}{d^{\alpha-1}}\right)^2 \frac{n^2 K_n}{\epsilon^2} \tag{2.6}$$

and the right side of the inequality tends to zero when $d \to \infty$ because $\alpha > 1$. Thus the second term in the right hand side of (2.5) goes to the zero matrix in probability, and therefore in distribution, as d increases. Hence

$$d^{-\alpha} n S_D \xrightarrow{w} \widetilde{U} \qquad \text{as } d \to \infty.$$

Then the vector of the roots of the characteristic polynomial of $d^{-\alpha} n S_D$ converge in distribution to the vector of the roots of the characteristic polynomial of $\widetilde{U}$ as $d \to \infty$.

Since $\widetilde{U} = \widetilde{Y}_n^\top \mathcal{C}_p \widetilde{Y}_n$ has rank p with probability one, the nonzero eigenvalues of $\widetilde{U}$ are the p nonzero eigenvalues $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p$ of $\widetilde{U}_0 = (\mathcal{C}_p^{1/2}\widetilde{Y}_n)(\mathcal{C}_p^{1/2}\widetilde{Y}_n)^\top = \mathcal{C}_p^{1/2}\widetilde{Y}_n\widetilde{Y}_n^\top\mathcal{C}_p^{1/2}$. Hence, if $\widehat{\tau}_1 \geq \widehat{\tau}_2 \geq \cdots \geq \widehat{\tau}_n$ are the nonzero eigenvalues of S_D, or of S, we have

$$d^{-\alpha} n (\widehat{\tau}_1, \widehat{\tau}_2, \ldots, \widehat{\tau}_n)^\top \xrightarrow{w} (\ell_1, \ldots \ell_p, 0, \ldots, 0)^\top$$

when $d \to \infty$. □

The following consequence of Theorem 2.2.1 shows the usefulness of the joint convergence in distribution of the sample eigenvalues when the dimension d goes to infinity and n is fixed. The result is a multivariate extension of (2.4). It gives the joint convergence in distribution of the ratios of the sample and population eigenvalues to a random vector of multiples of the eigenvalues corresponding to the random matrix $\widetilde{U}_0$.

Corollary 2.2.1 *Under the assumptions of Theorem 2.2.1 and for n fixed, we have the joint weak convergence*

$$\left(\frac{\widehat{\tau}_1}{\tau_1}, \frac{\widehat{\tau}_2}{\tau_2}, \ldots, \frac{\widehat{\tau}_p}{\tau_p}\right)^\top \xrightarrow{w} n^{-1}\left(\frac{\ell_1}{c_1}, \frac{\ell_2}{c_2}, \ldots, \frac{\ell_p}{c_p}\right)^\top,$$

when $d \to \infty$, *where* $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ *are the eigenvalues of the random matrix* $\widetilde{U}_0$.

Proof. Note that

$$\left(\frac{\widehat{\tau}_1}{\tau_1}, \frac{\widehat{\tau}_2}{\tau_2}, \ldots, \frac{\widehat{\tau}_p}{\tau_p}\right)^\top = \operatorname{diag}\left(\frac{d^\alpha}{\tau_1}, \frac{d^\alpha}{\tau_2}, \ldots, \frac{d^\alpha}{\tau_p}\right)\left(\frac{\widehat{\tau}_1}{d^\alpha}, \frac{\widehat{\tau}_2}{d^\alpha}, \ldots, \frac{\widehat{\tau}_p}{d^\alpha}\right)^\top \tag{2.7}$$

which by Theorem 2.2.1 tends in distribution to

$$\operatorname{diag}\left(\frac{1}{c_1},\frac{1}{c_2},\ldots,\frac{1}{c_p}\right)\left(\frac{\ell_1}{n},\frac{\ell_2}{n},\ldots,\frac{\ell_p}{n}\right)^\top = n^{-1}\left(\frac{\ell_1}{c_1},\frac{\ell_2}{c_2},\ldots,\frac{\ell_p}{c_p}\right)^\top . \square$$

Remark 2.2.1 *Suppose $\tau_1 \geq \cdots \geq \tau_p \geq \sigma_{p+1} \geq \cdots \geq \sigma_d > 0$ are functions of d. The two previous results hold if we consider the covariance matrix*

$$\Sigma = O\Lambda O^\top \text{ where } \Lambda = \operatorname{diag}(\tau_1,\ldots,\tau_p,\sigma_{p+1},\ldots,\sigma_d), \tag{2.8}$$

where $\tau_1,\ldots,\tau_p$ satisfy (2.2), $\max(\sigma_{p+1},\ldots,\sigma_d)/d^{\alpha-1} \to 0$ as $d \to \infty$, and O is a $d \times d$ orthogonal matrix. The proof is similar to that of Theorem 2.2.1; we only need to prove that

$$d^{-\alpha}\sum_{i=p+1}^{d}\sigma_i W_i \xrightarrow{w} \mathbf{0} \qquad \text{as } d \to \infty, \tag{2.9}$$

where W_i is as in the proof of Theorem 2.2.1 and $\mathbf{0}$ is the $n \times n$ matrix of zeros. We use the result that if A_d, B_d and $A_d - B_d$ are non-negative definite matrices and $A_d \to \mathbf{0}$ as $d \to \infty$, then $B_d \to \mathbf{0}$ as $d \to \infty$. Let $M_d = \max(\sigma_{p+1},\ldots,\sigma_d)$ and $V = \sum_{i=p+1}^{d} W_i$. Since W_i is non-negative definite and $M_d - \sigma_i > 0$ for $i = p+1,\ldots,d$, we have that $A_d = d^{-\alpha}M_d V$, $B_d = d^{-\alpha}\sum_{i=p+1}^{d}\sigma_i W_i$ and $A_d - B_d$ are non-negative definite matrices. Let $\epsilon > 0$; analogously to the proof of (2.6) it can be seen that

$$P(\| A_d \| > \epsilon) \leq \frac{(d-p)^2 M_d^2 n^2 K_n}{d^{2\alpha}\epsilon^2} = \left(\frac{d-p}{d}\right)^2\left(\frac{M_d}{d^{\alpha-1}}\right)^2\frac{n^2 K_n}{\epsilon^2}$$

and the right side of the last inequality tends to zero as $d \to \infty$ since $d^{-(\alpha-1)}M_d \to 0$. Therefore $A_d \to \mathbf{0}$ in probability and in distribution as $d \to \infty$. Then we have (2.9).

Theorem 2.2.1 can also be used to obtain the asymptotic distribution of the differences $\widehat{\tau}_i - \widehat{\tau}_j$ for $1 \leq i < j \leq p$, when $d \to \infty$. More precisely we have the following result.

Theorem 2.2.2 *Under the same assumptions as in Theorem 2.2.1, for $1 \leq i < j \leq p$ we have, for n fixed,*

$$d^{-\alpha}(\widehat{\tau}_i - \widehat{\tau}_j) \xrightarrow{w} n^{-1}(\ell_i - \ell_j) \qquad \text{as } d \to \infty,$$

where $\ell_1 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of the random matrix $\widetilde{U}_0$.

As a direct application of Proposition 1.2.1 we can also obtain the characteristic function of the limiting distribution of the last theorem when the column vectors of X are Gaussian. Note that when $\mathcal{C}_p = cI_p$ with $c > 0$, the characteristic function of $\delta_{i,j} = n^{-1}(\ell_i - \ell_j)$ is

$$\varphi_{\delta_{i,j}}(t) = \varphi_\ell(\overrightarrow{t_{i,j}}/n)$$

where φ_ℓ is the characteristic function of $\ell = (\ell_1,\ldots,\ell_p)^\top$ given by (1.7), $\overrightarrow{t_{i,j}}/n = (t/n)(e_i - e_j)$ with e_i the p-dimensional unit vectors for $i = 1,2,\ldots,p$.

We now consider the limiting scheme when $d, n \to \infty$ and $d \gg n$. The next theorem is a generalization of the result of Section 4.2 of [2] which considers the case $p = 1$.

Theorem 2.2.3 *Suppose that the unknown covariance matrix of the columns of X is given by the spiked covariance model (2.1), with $p < n < d$ and where $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_p$ have the same asymptotic order of magnitude in the sense of (2.2). Suppose that X satisfies (a) and the following assumption:*

(b') *Let Z_i be the i-th row of Z and define $\widetilde{Z}_p = [Z_1^\top, \ldots, Z_p^\top]^\top$. Assume that $\widetilde{Z}_p$ converges in distribution to some $p \times n$ matrix $\widetilde{Y}_n = (y_{ij,n})$ as $d \to \infty$, which has rank p with probability one and its entries have uniformly bounded fourth moments with respect to n, that is for some $M > 0$ we have $E(y_{ij,n}^4) \leq M$ for all $i = 1, 2, \ldots p$, $j = 1, 2, \ldots, n$ and $n = p+1, p+2, \ldots$. Furthermore, suppose that the matrix distribution of $\widetilde{Y}_n \widetilde{Y}_n^\top$ is continuous.*

Then we have that

$$\left(\frac{\widehat{\tau}_1}{\tau_1}, \frac{\widehat{\tau}_2}{\tau_2}, \ldots, \frac{\widehat{\tau}_p}{\tau_p} \right)^\top \xrightarrow{w} (1, 1, \ldots, 1)^\top \quad \text{as } d \to \infty, n \to \infty, \tag{2.10}$$

where the limits are applied successively.

For the proof of this theorem, we first give the following Law of Large Numbers for random matrices and vector of eigenvalues.

Proposition 2.2.1 *Let Y_n be a sequence of $p \times n$ random matrices with $p < n$, such that its columns are independent with mean zero and identity covariance matrix. Assume that the rank of Y_n is p with probability one and that the entries of $Y_n = (y_{ij,n})$ have uniformly bounded fourth moments with respect to n, that is $E(y_{ij,n}^4) \leq K$ for all $i = 1, 2, \ldots p$, $j = 1, 2, \ldots, n$ and $n = p+1, p+2, \ldots$. Let $A_n = Y_n Y_n^\top$. Then we have the following:*

(i)

$$n^{-1} A_n \xrightarrow{w} I_p \quad \text{as } n \to \infty.$$

(ii) *If we suppose that $\Sigma = O \Lambda O^\top$ is a $p \times p$ positive definite matrix, where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_p)$ is the diagonal matrix of its eigenvalues and O is the $p \times p$ orthogonal matrix of its eigenvectors, then if $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p$ are the eigenvalues of $W_n = O \Lambda^{1/2} A_n \Lambda^{1/2} O^\top$ we have*

$$n^{-1} \left(\frac{\ell_1}{\lambda_1}, \frac{\ell_2}{\lambda_2}, \ldots, \frac{\ell_p}{\lambda_p} \right)^\top \xrightarrow{w} (1, 1, \ldots, 1)^\top \qquad \text{as } n \to \infty.$$

Proof. (i) We have that $Y_n Y_n^\top = (\sum_{k=1}^n y_{ik,n} y_{jk,n})$; therefore

$$n^{-1} Y_n Y_n^\top - I_p = (n^{-1} \sum_{k=1}^n y_{ik,n} y_{jk,n} - \delta_{i,j}),$$

where $\delta_{i,j}$ is one if $i = j$ and zero otherwise. It is sufficient to prove that for all $\epsilon > 0$

$$P(|\sum_{k=1}^{n} n^{-1} y_{ik,n} y_{jk,n} - \delta_{i,j}| > \epsilon) \longrightarrow 0 \qquad \text{as } n \to \infty. \tag{2.11}$$

For the case $i = j$, by Chebyshev's inequality and the assumptions for Y_n we have that

$$\begin{aligned} P(|n^{-1}\sum_{k=1}^{n} y_{ik,n}^2 - 1| > \epsilon) &\leq \epsilon^{-2}\text{Var}(n^{-1}\sum_{k=1}^{n} y_{ik,n}^2) = (n\epsilon)^{-2} E[(\sum_{k=1}^{n} y_{ik,n}^2 - n)^2] \\ &= (n\epsilon)^{-2} E[\sum_{k=1}^{n} y_{ik,n}^4 + 2\sum_{k_1<k_2}^{n} y_{ik_1,n}^2 y_{ik_2,n}^2 - 2n\sum_{k=1}^{n} y_{ik,n}^2 + n^2] \\ &= (n\epsilon)^{-2}[\sum_{k=1}^{n} E(y_{ik,n}^4) - n]. \end{aligned} \tag{2.12}$$

Since $E(y_{ik,n}^4) \leq K$ for all i, k and $n = p+1, p+2, \ldots$, the last expression of (2.12) is less than or equal to $(n\epsilon)^{-2}(nK - n) = n^{-1}\epsilon^{-2}(K-1)$ which tends to zero as $n \to \infty$. Thus we have (2.11).

Analogously, for the case $i \neq j$, by Chebyshev's inequality and the assumptions for Y_n we have

$$\begin{aligned} P(|n^{-1}\sum_{k=1}^{n} y_{ik,n}^2| > \epsilon) &\leq (n\epsilon)^{-2}\text{Var}(\sum_{k=1}^{n} y_{ik,n} y_{jk,n}) \\ &= (n\epsilon)^{-2}\sum_{k_1=1}^{n}\sum_{k_2=1}^{n} E(y_{ik_1,n} y_{jk_1,n} y_{ik_2,n} y_{jk_2,n}) = (n\epsilon)^{-2}\sum_{k=1}^{n} E(y_{ik,n}^2 y_{jk,n}^2). \end{aligned} \tag{2.13}$$

By Holder's inequality we have $E(y_{ik,n}^2 y_{jk,n}^2) \leq E(y_{ik,n}^4)^{1/2} E(y_{jk,n}^4)^{1/2} \leq K$, thus the last expression of (2.13) is less than or equal to $n^{-1}\epsilon^{-2}M$ which tends to zero as $n \to \infty$.

(ii) Suppose that $W_n = V_n \ell_n V_n^\top$, where $\ell_n = \text{diag}(\ell_1, \ldots, \ell_p)$ is the diagonal matrix of the eigenvalues of W_n and V_n is the orthogonal matrix of its eigenvectors. Since $n^{-1}A_n \xrightarrow{w} I_p$ as $n \to \infty$ by (i), we have that $V_n(n^{-1}\ell_n)V_n^\top = n^{-1}W_n \xrightarrow{w} \Sigma = O\Lambda O^\top$ and therefore $n^{-1}\ell_n \xrightarrow{w} \Lambda$ as $n \to \infty$. It follows that $n^{-1}\Lambda^{-1}\ell_n \xrightarrow{w} I_p$ as $n \to \infty$. □

Proof of Theorem 2.2.3. Let $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ be the eigenvalues of the matrix $\widetilde{U}_0 = \mathcal{C}_p^{1/2}\widetilde{Y}_n\widetilde{Y}_n^\top\mathcal{C}_p^{1/2}$ with $\mathcal{C}_p = \text{diag}(c_1, \ldots, c_p)$. Let $F_{\mathbf{1}_p}$, $F_{\widehat{\tau}/\tau}$ and $F_{n^{-1}\ell/\mathcal{C}_p}$ be the distribution functions of $\mathbf{1}_p = (1, 1, \ldots, 1)^\top$, $\widehat{\tau}/\tau = (\frac{\widehat{\tau}_1}{\tau_1}, \frac{\widehat{\tau}_2}{\tau_2}, \ldots, \frac{\widehat{\tau}_p}{\tau_p})^\top$ and $n^{-1}\ell/\mathcal{C}_p = n^{-1}(\frac{\ell_1}{c_1}, \frac{\ell_2}{c_2}, \ldots, \frac{\ell_p}{c_p})^\top$, respectively. Since $\widetilde{Y}_n\widetilde{Y}_n^\top$ has continuous matrix distribution then $\widetilde{U}_0$ and $n^{-1}\ell/\mathcal{C}_p$ have continuous distributions. Therefore the continuity set of $F_{n^{-1}\ell/\mathcal{C}_p}$ is given by $\mathcal{C}(F_{n^{-1}\ell/\mathcal{C}_p}) = \mathbb{R}^p$. By Corollary 2.2.1

$$\lim_{d\to\infty} |F_{\widehat{\tau}/\tau}(t) - F_{n^{-1}\ell/\mathcal{C}_p}(t)| = 0,$$

for all $t \in \mathbb{R}^p$. Therefore

$$\lim_{d\to\infty} |F_{\widehat{\tau}/\tau}(t) - F_{\mathbf{1}_p}(t)| = |F_{n^{-1}\ell/\mathcal{C}_p}(t) - F_{\mathbf{1}_p}(t)| \quad \forall t \in \mathbb{R}^p.$$

Since $\widetilde{Z}_p$ has independent column vectors and it converges in distribution to $\widetilde{Y}_n$, the column vectors of $\widetilde{Y}_n$ are also independent. Because $\widetilde{Z}_p$ has uniformly fourth moment with respect to d, by Theorem 4.5.2 of [12] we have $E(z_{ij}) = 0 \to E(y_{ij,n})$, $E(z_{ij}^2) = 1 \to E(y_{ij,n}^2)$ $\forall\ i = 1, 2, \ldots, p$, $j = 1, 2, \ldots, n$, and $E(z_{ik}z_{jk}) = 0 \to E(y_{ik,n}y_{jk,n})$ $\forall k = 1, 2, \ldots, n$, $i \neq j$, as $d \to \infty$. Therefore, $\widetilde{Y}_n$ has mean zero and its column vectors have identity covariance matrix. Thus by Proposition 2.2.1(ii)

$$\lim_{n\to\infty} |F_{n^{-1}\ell/\mathcal{C}_p}(t) - F_{\mathbf{1}_p}(t)| = 0,$$

for all t in the continuity set of $F_{\mathbf{1}_p}$, namely $\mathcal{C}(F_{\mathbf{1}_p})$. Thus

$$\lim_{n\to\infty} \lim_{d\to\infty} |F_{\widehat{\tau}/\tau}(t) - F_{\mathbf{1}_p}(t)| = 0,$$

for all $t \in \mathcal{C}(F_{\mathbf{1}_p})$. □

2.2.2 Subspace consistency of the sample eigenvectors

From the results of [25], under our spiked covariance model the first p sample eigenvectors $v_1, v_2, \ldots, v_p$ are subspace consistent and the sample eigenvectors $v_{p+1}, v_{p+2}, \ldots, v_n$ are strongly inconsistent, when $d \to \infty$ and n is fixed. We give a similar proof of the subspace consistency of the first p sample eigenvectors using the results of Section 2.2.1 when $d \to \infty$ and n is fixed. We recall that the population eigenvectors of the spiked covariance model (2.1) are the column vectors, $o_1, o_2, \ldots, o_d$, of the matrix O.

Theorem 2.2.4 *Under the same assumptions of Theorem 2.2.1, let $v_1, v_2, \ldots, v_p$ be the sample eigenvectors corresponding to the p largest sample eigenvalues $\widehat{\tau}_1 \geq \widehat{\tau}_2 \geq \cdots \geq \widehat{\tau}_p$. Then for $i = 1, 2, \ldots, p$,*

$$\text{Angle}(v_i, E_J) \xrightarrow{w} 0 \qquad \textit{as } d \to \infty, \tag{2.14}$$

where $E_J = \text{span}\{o_1, o_2, \ldots, o_p\}$.

Proof. We follow closely the ideas in [2] and [25]. Consider the eigenvalue decomposition of the sample covariance matrix $S = VLV^\top$, where $L = \text{diag}(\widehat{\tau}_1, \ldots, \widehat{\tau}_n, 0, \ldots, 0)$ is the diagonal matrix of the sample eigenvalues and $V = [v_1, v_2, \ldots, v_d]$ is the matrix of the sample eigenvectors $v_j = (v_{1j}, \ldots, v_{dj})^\top$, $j = 1, 2, \ldots, d$. We assume that V is orthogonal, that is $V^\top V = I_d$. We have $\Sigma = O\Lambda O^\top$, where $\Lambda = \text{diag}(\tau_1, \ldots, \tau_p, \sigma, \ldots, \sigma)$ is the diagonal matrix of eigenvalues of Σ and $O = [o_1, \ldots, o_d]$ the $d \times d$ orthogonal matrix of its eigenvectors. A standardized version of the sample covariance matrix S is given by

$$\widetilde{S} = \Lambda^{-1/2} O^\top S O \Lambda^{-1/2} = \Lambda^{-1/2} O^\top V L V^\top O \Lambda^{-1/2}. \tag{2.15}$$

Thus we have $S = n^{-1} X X^\top = n^{-1} O \Lambda^{1/2} Z Z^\top \Lambda^{1/2} O^\top$ and

$$\widetilde{S} = n^{-1} \Lambda^{-1/2} O^\top O \Lambda^{1/2} Z Z^\top \Lambda^{1/2} O^\top O \Lambda^{-1/2} = n^{-1} Z Z^\top. \tag{2.16}$$

From (2.15) we have that the j-th diagonal entry of $\widetilde{S}$ is given by $\widetilde{s}_{jj} = \lambda_j^{-1} \sum_{i=1}^n \widehat{\tau}_i (v_i^\top o_j)^2$, where λ_j is the j-th diagonal entry of Λ, for $j = 1, 2, \ldots, d$. Therefore $\lambda_j^{-1} \widehat{\tau}_i (v_i^\top o_j)^2 \leq \widetilde{s}_{jj}$, for $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, d$. Furthermore, from (2.16) we also have $\widetilde{s}_{jj} = n^{-1} Z_j Z_j^\top = n^{-1} \sum_{k=1}^n z_{jk}^2$. Thus for $i = 1, 2, \ldots, n$

$$\sum_{j=p+1}^{d} (v_i^\top o_j)^2 \leq \sum_{j=p+1}^{d} \frac{\lambda_j}{\widehat{\tau}_i} \widetilde{s}_{jj} = \frac{\sigma}{n \widehat{\tau}_i} \sum_{j=p+1}^{d} \sum_{k=1}^{n} z_{jk}^2 = \frac{\sigma}{n} \frac{d^\alpha}{\widehat{\tau}_i} \sum_{k=1}^{n} \sum_{j=p+1}^{d} \frac{z_{jk}^2}{d^\alpha}. \tag{2.17}$$

By Theorem 2.2.1 we have $\widehat{\tau}_i / d^\alpha \xrightarrow{w} \ell_i / n$ as $d \to \infty$, for $i = 1, 2, \ldots, p$. Since the entries of Z have uniformly bounded fourth moments in d, we have that there exist $K_n^* > 0$ such that $E(z_{jk}^2) \leq K_n^*$ for all $j = 1, 2, \ldots, d$, $k = 1, 2, \ldots, n$ and $d = n+1, n+2, \ldots$. Let $\epsilon > 0$ and observe that

$$P\left(\left| \sum_{j=p+1}^{d} \frac{z_{jk}^2}{d^\alpha} \right| > \epsilon \right) \leq \frac{E(\sum_{j=p+1}^d z_{jk}^2)}{d^\alpha \epsilon} \leq \frac{(d-p) K_n^*}{d^\alpha \epsilon} \longrightarrow 0 \qquad \text{as } d \to \infty,$$

that is $\sum_{j=p+1}^d d^{-\alpha} z_{jk}^2 \xrightarrow{P} 0$ as $d \to \infty$. Hence, it follows from (2.17) that

$$\sum_{j=p+1}^{d} (v_i^\top o_j)^2 \xrightarrow{w} 0 \qquad \text{as } d \to \infty, \tag{2.18}$$

for $i = 1, 2, \ldots, p$. Since $V^\top O O^\top V = I_d$ we have $\sum_{j=1}^d (v_i^\top o_j)^2 = 1$, and thus (2.18) implies

$$\sum_{j=1}^{p} (v_i^\top o_j)^2 \xrightarrow{w} 1 \qquad \text{as } d \to \infty, \tag{2.19}$$

for $i = 1, 2, \ldots, p$.

Finally, following the arguments in Section 5.2.2 of [25], we have that for $i = 1, 2, \ldots, p$,

$$\text{Angle}(v_i, E_J) = \arccos([\sum_{j=1}^{p} (v_i^\top o_j)^2]^{1/2}).$$

Then from (2.19) it follows that

$$\text{Angle}(v_i, E_J) \xrightarrow{w} 0 \qquad \text{as } d \to \infty,$$

for $i = 1, 2, \ldots, p$. □

Remark 2.2.2 *The result of Theorem 2.2.4 holds if we consider that the population covariance matrix is as in Remark 2.2.1. The proof is similar to that of Theorem 2.2.4.*

2.3 The Gaussian case and some statistical eigen-inference

In this section we assume that the data matrix X is a sample from the multivariate Gaussian distribution $N_d(0, \Sigma)$ where the matrix Σ is a spiked covariance matrix under the assumption that the p largest eigenvalues are of the same order of magnitude when d goes to infinity, as in (2.2) with $c_1 = \cdots = c_p = c > 0$. In this case the matrix $\widetilde{U}_0$ of Theorem 2.2.1 follows a Wishart random matrix distribution $\mathcal{W}(n, cI_p)$.

We now use the asymptotic results in Section 2.2.1, specially the joint convergence in distribution of the nonzero sample eigenvalues given in Theorem 2.2.1, to consider some inference problems for the population eigenvalues and show that some of the classical statistics are also useful in the cases when d goes to infinity and n is fixed and when d, n go to infinity with $d \gg n$.

We first point out some asymptotic results. The first one is a kind of Central Limit Theorem for the vector of the ratios of the sample and population eigenvalues under our model and when d and n go to infinity successively.

Theorem 2.3.1 *Under the same assumptions as in Theorem 2.2.1, suppose* $c_1 = c_2 = \cdots = c_p = c > 0$ *in (2.2) and the columns of* X *are Gaussian. Let* $\frac{\widehat{\tau}}{\tau} = (\frac{\widehat{\tau}_1}{\tau_1}, \ldots, \frac{\widehat{\tau}_p}{\tau_p})^\top$ *and denote by* φ *the random vector with density function given by (1.13), that is* φ *is the vector of the eigenvalues of a symmetric standard Gaussian matrix. Then we have that*

$$n^{1/2}\left(\frac{\widehat{\tau}}{\tau} - \mathbf{1}_p\right)^\top \xrightarrow{w} \varphi \qquad \text{as } d \to \infty, n \to \infty \tag{2.20}$$

where the limits are applied successively.

Proof. Without losing generality we can assume $c = 1$. Let $L = n^{-1}(\ell_1, \ldots, \ell_p)^\top$, where $\ell_1 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of the matrix $\widetilde{U}_0$ with distribution $\mathcal{W}(n, I_p)$. By Corollary 2.2.1 we have $\widehat{\tau}/\tau \xrightarrow{w} L$ as $d \to \infty$ and by Theorem 1.2.3 we have $n^{1/2}(L - \mathbf{1}_p)^\top \xrightarrow{w} \varphi$ as $n \to \infty$, where the random vector φ has density function given by (1.13). Thus we have (2.20). $\square$

The next two propositions are consequences of Theorem 2.2.1 and they are useful to study some inference problems in the context of data with dimension greater than the sample size.

Proposition 2.3.1 *Under the same assumptions as in Theorem 2.2.1, suppose* $c_1 = c_2 = \cdots = c_p = c > 0$ *in (2.2) and the columns of* X *are Gaussian. Let* $T = \operatorname{diag}(\widehat{\tau}_1, \widehat{\tau}_2, \ldots, \widehat{\tau}_p)$ *be the diagonal matrix of the* p *largest sample eigenvalues and* $\ell = \operatorname{diag}(\ell_1, \ell_2, \ldots, \ell_p)$*, where* $\ell_1, \ell_2, \ldots, \ell_p$ *are the nonzero eigenvalues of a Wishart matrix with distribution* $\mathcal{W}(n, cI_p)$*. Then we have the following when* n *is fixed:*

(a) $\operatorname{tr}(T)/\tau_i \xrightarrow{w} \mathcal{X}^2_{np}/n$ *as* $d \to \infty$*, for* $i = 1, 2, \ldots, p$*.*

(b) $\widetilde{V} = \det(T)/[\mathrm{tr}(T)/p]^p \xrightarrow{w} V = \det(\ell)/[\mathrm{tr}(\ell)/p]^p$; *furthermore* $\widetilde{V}$ *is asymptotically independent of* $\mathrm{tr}(T)/d^\alpha$ *as* $d \to \infty$.

(c) $\det(T)/\tau_i^p \xrightarrow{w} (\prod_{j=1}^p \mathcal{X}_{n-j+1}^2)/n^p$ *as* $d \to \infty$ *for* $i = 1, 2, \ldots, p$, *where* $\mathcal{X}_{n-j+1}^2$ *are independent random variables with chi-square distribution with* $n-j+1$ *degrees of freedom, for* $j = 1, 2, \ldots, p$.

Proof. Using the continuity of the trace and determinant, from the joint weak convergence of the eigenvalues in Theorem 2.2.1 and the assumption (2.2) we have that for n fixed

$$\mathrm{tr}(T)/\tau_i = [\mathrm{tr}(T)/(cd^\alpha)][cd^\alpha/\tau_i] \xrightarrow{w} \mathrm{tr}(\ell)/cn, \tag{2.21}$$

$$\widetilde{V} = \frac{\det(T/d^\alpha)}{[\mathrm{tr}(T/d^\alpha)/p]^p} \xrightarrow{w} \frac{\det(\ell/n)}{[\mathrm{tr}(\ell/n)/p]^p} = V, \text{ and} \tag{2.22}$$

$$\det(T)/\tau_i^p = [\det(T)/(cd^\alpha)^p][cd^\alpha/\tau_i]^p \xrightarrow{w} \det(\ell)/(nc)^p, \tag{2.23}$$

as $d \to \infty$. By Theorem 1.1.2 $\mathrm{tr}(\ell)/cn \sim \mathcal{X}_{np}^2/n$ and $\det(\ell)/[\mathrm{tr}(\ell)/p]^p$ is independent of $\mathrm{tr}(\ell)/n$; therefore using (2.21) and (2.22) we have (a) and (b). It follows from Theorem 1.1.1 that $\det(\ell)/(nc)^p$ is equal in distribution to $(\prod_{j=1}^p \mathcal{X}_{n-j+1}^2)/n^p$, where $\mathcal{X}_{n-j+1}^2$ for $j = 1, 2, \ldots, p$, are independent random variables with chi-square distribution with $n-j+1$ degrees of freedom. Thus from (2.23) we have (c). □

Proposition 2.3.2 *Under the same assumptions as in Theorem 2.2.1, suppose* $c_1 = c_2 = \cdots = c_p = c > 0$ *in (2.2) and the columns of* X *are Gaussian. Let* $T = \mathrm{diag}(\widehat{\tau}_1, \widehat{\tau}_2, \ldots, \widehat{\tau}_p)$ *be the diagonal matrix of the* p *largest sample eigenvalues. Then we have the following results:*

(a) $(np/2)^{1/2}[\mathrm{tr}(T)/p - \tau_i]/\tau_i \xrightarrow{w} N(0,1)$ *as* $d \to \infty$, $n \to \infty$, *where the limits are applied successively, for* $i = 1, 2, \ldots, p$.

(b) *Let* $\widetilde{V} = \det(T)/[\mathrm{tr}(T)/p]^p$ *and* $\rho = 1 - (2p^2 + p + 2)/(6np)$, *then* $\widetilde{U} = -n\rho \ln(\widetilde{V}) \xrightarrow{w} \mathcal{X}_r^2$ *as* $d \to \infty$, $n \to \infty$, *where the limits are applied successively and* $\mathcal{X}_r^2$ *is a chi-square r.v. with* $r = (p+2)(p-1)/2$ *degrees of freedom.*

Proof. By Proposition 2.3.1(a) it follows that

$$\left(\frac{np}{2}\right)^{1/2} \left(\frac{\mathrm{tr}(T)/p - \tau_i}{\tau_i}\right) = \frac{n\mathrm{tr}(T)/\tau_i - np}{(2np)^{1/2}} \xrightarrow{w} \frac{\mathcal{X}_{np}^2 - np}{(2np)^{1/2}} \tag{2.24}$$

as $d \to \infty$, where $\mathcal{X}_{np}^2$ is a chi-square r.v. with np degrees of freedom. Since $\mathcal{X}_{np}^2$ is equal in distribution to $\sum_{j=1}^n \mathcal{X}_{p,j}^2$, where $\mathcal{X}_{p,j}^2$ for $j = 1, 2, \ldots, n$ are independent r.v.'s with chi-square distribution with p degrees of freedom, we have by the Central Limit Theorem (see [36, pp. 313]) that

$$\frac{\mathcal{X}_{np}^2 - np}{(2np)^{1/2}} \xrightarrow{w} N(0,1) \tag{2.25}$$

as $n \to \infty$. Thus, from (2.24) and (2.25) we have (a). From Proposition 2.3.1(b) and Theorem 1.1.3, (b) follows. □

2.3.1 Hypothesis testing for the p largest population eigenvalues

Let M_d be the maximum of the $d - p$ smaller population eigenvalues and suppose that we have evidence that the sequence $\{M_d\}_{d \in \mathbb{N}}$ is bounded by a constant number M, that is $0 < M_d \leq M$ for all $d > n$ and $d \in \mathbb{N}$. Consider the null hypothesis

$$H_0 : \tau_i / d^\alpha \to c \quad \text{as } d \to \infty, \text{ for all } i = 1, 2, \ldots, p, \tag{2.26}$$

where $\alpha > 1$ and $c > 0$ are unspecified numbers. Under H_0 we have a population covariance matrix as in Remark 2.2.1; therefore all the results of Section 2.2.1 are valid in this case.

In order to test the null hypothesis H_0 that the p largest population eigenvalues have the same asymptotic order of magnitude and $c_1 = c_2 = \cdots = c_p = c > 0$, we can use the *ellipticity statistic* $\widetilde{V} = \det(T)/[\mathrm{tr}(T)/p]^p$, where $T = \mathrm{diag}(\widehat{\tau}_1, \widehat{\tau}_2, \ldots, \widehat{\tau}_p)$ is the diagonal matrix of the p largest sample eigenvalues. The null hypothesis (2.26) can be tested in the following two situations:

- WHEN $d \to \infty$ AND n IS FIXED. By Proposition 2.3.1(b) $\widetilde{V} \overset{w}{\to} V = \det(\ell)/[\mathrm{tr}(\ell)/p]^p$ as $d \to \infty$, where $\ell = \mathrm{diag}(\ell_1, \ell_2, \ldots, \ell_p)$ and $\ell_1, \ell_2, \ldots, \ell_p$ are the eigenvalues of a Wishart matrix with distribution $\mathcal{W}(n, cI_p)$. The explicit expression of the moments of V are well known and using the Mellin transform approach (see [31, pp. 302]) they may be used to obtain the exact expression for the density function of V; see [26]. It is also possible to calculate numerically the values of the distribution of V; see [34]. Therefore if $\widetilde{V}_0$ is the observed value of $\widetilde{V}$, a test of asymptotic significance level β is to reject H_0 if $\widetilde{V}_0 \leq k_\beta$, where k_β is the lower $100\beta\%$ point of the distribution of V. We expect that this rejection region works very well, because if A is a $p \times p$ random matrix with distribution $\mathcal{W}(n, \Psi)$ and W_0 is the observed value of $W = \det(A)/(\mathrm{tr}(A)/p)^p$, then the test that rejects $H_1 : \Psi = cI_n$ if $W_0 \leq k_\beta$ is unbiased; see [31, pp. 336].

- WHEN $d, n \to \infty$ AND $d \gg n$. By Proposition 2.3.2(b) the statistic $\widetilde{U} = -n\rho \ln(\widetilde{V}) \overset{w}{\to} \mathcal{X}_r^2$, where $\mathcal{X}_r^2$ is a chi-square r.v. with $r = (p+2)(p-1)/2$ degrees of freedom. Thus, if $\widetilde{U}_0$ is the observed value of $\widetilde{U}$, a test of asymptotic significance level β is to reject H_0 if $\widetilde{U}_0 > k_\beta$, where k_β is the upper $100\beta\%$ point of the chi-square distribution with r degrees of freedom.

2.3.2 Confidence intervals for the p largest population eigenvalues

Under the hypothesis H_0 given in (2.26) we may be interested in a confidence interval for the population eigenvalue τ_i, for $i = 1, 2, \ldots, p$. Again we have two situations in which we may address this problem:

- When $d \to \infty$ and n is fixed. From Proposition 2.3.1(a), for $0 < \beta < 1$ and d is large enough,
$$P\left(\frac{k_{\beta/2}}{n} \le \frac{\mathrm{tr}(T)}{\tau_i} \le \frac{u_{\beta/2}}{n}\right) \approx 1 - \beta,$$
where $k_{\beta/2}$ and $u_{\beta/2}$ are the lower and upper $100(\beta/2)\%$ points of the chi-square distribution with np degrees of freedom, respectively. Therefore, a confidence interval with asymptotic confidence level $1-\beta$ for τ_i is
$$\left[\frac{n\mathrm{tr}(T)}{u_{\beta/2}}, \frac{n\mathrm{tr}(T)}{k_{\beta/2}}\right].$$

- When $d, n \to \infty$ and $d \gg n$. From Proposition 2.3.2(a), for $0 < \beta < 1$ and d, n sufficiently large with $d \gg n$ we have
$$P\left(-z_{\beta/2} \le \left(\frac{np}{2}\right)^{1/2}\left(\frac{\mathrm{tr}(T)/p - \tau_i}{\tau_i}\right) \le z_{\beta/2}\right) \approx 1 - \beta,$$
where $z_{\beta/2}$ is the upper $100(\beta/2)\%$ point of the standard normal distribution. Thus, a confidence interval with asymptotic confidence level $1-\beta$ for τ_i is
$$\left[\frac{\mathrm{tr}(T)/p}{1 + z_{\beta/2}[2/(np)]^{1/2}}, \frac{\mathrm{tr}(T)/p}{1 - z_{\beta/2}[2/(np)]^{1/2}}\right].$$

2.4 PCA under different settings

The study of the asymptotic behavior of the sample eigenvalues and their corresponding eigenvectors under more general settings than the spiked covariance model (2.1) is considered in [25]. In this section we present some results of [25] for several kinds of spiked covariance models and discuss the differences with our results obtained in Section 2.2.

Suppose that the $d \times n$ matrix X satisfies the assumptions (a) and (b) of Section 2.2. Let $1 \le p < n$ and let $\alpha_1 > \alpha_2 > \cdots > \alpha_r > 1$ for some $r \le p$. Let $k_1, \dots, k_r \in \mathbb{N}$ such that $\sum_{i=1}^r k_i = p$. Define $k_0 = 0$ and $k_{r+1} = d - p$. Let $s_l = \sum_{j=0}^{l-1} k_j$ and
$$J_l = \{s_l + 1, \dots, s_l + k_l\}, \qquad \text{for } l = 1, 2, \dots, r+1.$$

In this section we consider the spiked covariance model (2.1) where $\tau_i = \tau_i(d)$ and
$$\frac{\tau_i}{d^{\alpha_l}} \longrightarrow c_i \qquad \text{as } d \to \infty, \tag{2.27}$$
for some $c_i > 0$, $\forall i \in J_l$, $\forall l = 1, 2, \dots, r$.

Observe that when $r = 1$, we get the spiked covariance model with the p largest eigenvalues with the same asymptotic order of magnitude (2.2), studied in Section 2.2.

2.4.1 Asymptotic behavior of the sample eigenvalues

The following result is a special case of Lemma 1 of [25] for the spiked covariance model with the assumption (2.27). Suppose that the $p \times n$ matrix $\widetilde{Y}_n$ of assumption (b) is given by $\widetilde{Y}_n = [Y_1^\top, \ldots, Y_p^\top]^\top$. We define the matrix $\widetilde{Y}_{l,n}$ as the $k_l \times n$ matrix whose row vectors are given by $\{Y_j : j \in J_l\}$, for $l = 1, 2, \ldots, r$.

Lemma 2.4.1 *Assume that the covariance matrix Σ of the columns of X is given by the spiked covariance model (2.1) where $\tau_1 \geq \cdots \geq \tau_p$ satisfy (2.27). Consider the assumptions (a) and (b) for X. Let $\widehat{\tau}_1 \geq \cdots \geq \widehat{\tau}_p$ be the p largest sample eigenvalues. Then for n fixed*

$$\frac{\widehat{\tau}_i}{d^{\alpha_l}} \xrightarrow{w} \frac{\eta_{l,i-s_l}}{n} \qquad \text{as } d \to \infty \text{ if } i \in J_l,\ \forall l = 1, 2, \ldots, r,$$

$$\frac{\widehat{\tau}_i}{d^{\alpha_l}} \xrightarrow{P} 0 \qquad \text{as } d \to \infty \text{ if } i = p+1, \ldots, n$$

where $\eta_{l,1} \geq \eta_{l,2} \geq \cdots \geq \eta_{l,k_l}$ are the eigenvalues of the random matrix $\widetilde{U}_l = \mathcal{C}_l^{1/2} \widetilde{Y}_{l,n} \widetilde{Y}_{l,n}^\top \mathcal{C}_l^{1/2}$, where $C_l = \operatorname{diag}\{c_j : j \in J_l\}$.

Remark 2.4.1 *This result is analogous to that of Theorem 2.2.1, but here only the marginal convergence is taken into account. The advantage of considering the joint convergence in distribution of the vector of nonzero sample eigenvalues is that it is possible to derive asymptotic results for functions of them, as we did in Section 2.3 using Theorem 2.2.1. Furthermore, these asymptotic results are useful to consider inference problems as we have done in sections 2.3.1 and 2.3.2. The joint convergence of the vector $(\widehat{\tau}_i / d^{\alpha_l} : i \in J_l)^\top$ to the vector $(\eta_{l,i-s_l}/n : i \in J_l)^\top$ as $d \to \infty$, for $l = 1, 2, \ldots, r$, follows from the proof of Lemma 1 in [25]. Therefore, analogously as we did in Section 2.3.1 it is possible to test the hypothesis*

$$H_0 : \ \frac{\widehat{\tau}_i}{d^{\alpha_l}} \to c_l^* \qquad \text{as } d \to \infty, \text{ for all } i \in J_l$$

where $\alpha_l > 1$ and $c_l^* > 0$ are unspecified numbers.

In the Gaussian case, by Corollary 3 of [25] it follows that when $k_l = 1$ and $i \in J_l$

$$\frac{\widehat{\tau}_i}{\tau_i} \xrightarrow{w} \frac{\mathcal{X}_n^2}{n} \qquad \text{as } d \to \infty,$$

where $\mathcal{X}_n^2$ is a r.v. with chi-square distribution with n degrees of freedom. Thus, since $\mathcal{X}_n^2/n \xrightarrow{w} 1$ as $n \to \infty$, in this case we have that the i-th sample eigenvalue increases at the same speed as its population eigenvalue under the two different limiting schemes considered here. Therefore, if the p largest population eigenvalues have different asymptotic order of magnitude, i.e. $k_l = 1$ for all $l = 1, 2, \ldots, p$, the p largest sample eigenvalues have this property. However, the work in [25] does not address this asymptotic behavior of the p largest sample eigenvalues in the non-Gaussian case and neither when the p largest population eigenvalues have same asymptotic order of magnitude; only the convergence in distribution of these sample eigenvalues given in Lemma 2.4.1 is shown.

We have shown in Section 2.2.1 that the p largest sample eigenvalues increase jointly at the same speed as their population eigenvalues, with $r = 1$ and $k_1 > 1$, under a non-Gaussian assumption. Specifically, by our Corollary 2.2.1 we have

$$\left(\frac{\widehat{\tau}_1}{\tau_1}, \frac{\widehat{\tau}_2}{\tau_2}, \ldots, \frac{\widehat{\tau}_p}{\tau_p}\right)^\top \xrightarrow{w} n^{-1}\left(\frac{\ell_1}{c_1}, \frac{\ell_2}{c_2}, \ldots, \frac{\ell_p}{c_p}\right)^\top \qquad \text{as } d \to \infty,$$

where $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of the random matrix $\widetilde{U}_0$. Thus, by Theorem 2.2.3 we have that the vector of ratios of the p largest sample and population eigenvalues converges to the vector of ones when $d, n \to \infty$ and $d \gg n$, without considering the Gaussian assumption for the columns of X and when the p largest population eigenvalues have same asymptotic order of magnitude.

An open problem is to obtain the joint weak convergence in the case of more general spiked covariance models. As a first step we obtain the joint weak convergence of the vector of nonzero eigenvalues of a linear transform of the sample covariance matrix. This result is presented in the next theorem.

Theorem 2.4.1 *Under the same assumptions as in Lemma 2.4.1, let β be the $d \times d$ diagonal matrix where the i-th diagonal element for $1 \leq i \leq p$ is $\beta_{i,i} = d^{-\alpha_l}$ if $i \in J_l$ and for $p+1 \leq i \leq d$ is $\beta_{i,i} = d^{-\alpha_r}$. Let O be the $d \times d$ matrix of eigenvectors of Σ given by (2.1) and define $B^{1/2} = O\beta^{1/2}O^\top$. Let $\widetilde{\tau}_1 \geq \cdots \geq \widetilde{\tau}_n$ be the nonzero eigenvalues of $B^{1/2}SB^{1/2}$, where $S = n^{-1}XX^\top$ is the sample covariance matrix. Then for n fixed,*

$$(\widetilde{\tau}_1, \widetilde{\tau}_2, \ldots, \widetilde{\tau}_n)^\top \xrightarrow{w} n^{-1}(\ell_1, \ell_2, \ldots, \ell_p, 0, \ldots, 0)^\top \qquad d \to \infty$$

where $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of $\widetilde{U}_0 = \mathcal{C}_p^{1/2}\widetilde{Y}_n\widetilde{Y}_n^\top\mathcal{C}_p^{1/2}$, where $\mathcal{C}_p = \operatorname{diag}(c_1, c_2, \ldots, c_p)$.

Proof. Let $Z = \Lambda^{-1/2}O^\top X$, $\widetilde{X} = B^{1/2}X$ and $\widetilde{Z} = \Lambda^{-1/2}\widetilde{X}$. Define $\widetilde{S}_D = n^{-1}\widetilde{X}^\top\widetilde{X}$ and note that $\widetilde{S}_D$ has the same nonzero eigenvalues as $B^{1/2}SB^{1/2} = n^{-1}\widetilde{X}\widetilde{X}^\top$. Observe that

$$\begin{aligned} n\widetilde{S}_D &= X^\top O\beta^{1/2}O^\top O\beta^{1/2}O^\top X = X^\top O\beta O^\top X \\ &= Z^\top\Lambda^{1/2}O^\top O\beta O^\top O\Lambda^{1/2}Z = Z^\top\beta\Lambda Z \\ &= \sum_{i=1}^{p}\beta_{i,i}\tau_i W_i + d^{-\alpha_r}\sigma\sum_{i=p+1}^{d}W_i, \end{aligned}$$

where $W_i = Z_i^\top Z_i$, $Z_i = 1, 2, \ldots, d$, are the row vectors of Z. Since $\beta_{i,i}\tau_i \to c_i$ as $d \to \infty$, following the same ideas as in the proof of Theorem 2.2.1 we have

$$n\widetilde{S}_D \xrightarrow{w} \widetilde{U} = \widetilde{Y}_n^\top\mathcal{C}_p\widetilde{Y}_n \qquad \text{as } d \to \infty,$$

where $\mathcal{C}_p = \text{diag}(c_1, \ldots, c_p)$. Furthermore $\widetilde{U}$ has the same nonzero eigenvalues as the random matrix $\widetilde{U}_0 = \mathcal{C}_p^{1/2} \widetilde{Y}_n \widetilde{Y}_n^\top \mathcal{C}_p^{1/2}$. Thus, the vector of nonzero eigenvalues of $\widetilde{S}_D$, or of $B^{1/2}SB^{1/2}$, converges in distribution to the vector $n^{-1}(\ell_1, \ell_2, \ldots, \ell_p, 0, \ldots, 0)^\top$ as $d \to \infty$, where $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_p > 0$ are the eigenvalues of $\widetilde{U}_0$. □

Observe that in the particular case when $r = 1$, Theorem 2.4.1 becomes Theorem 2.2.1 since $\widetilde{\tau}_i = d^{-\alpha}\widehat{\tau}_i$ for $i = 1, 2, \ldots n$.

2.4.2 Subspace consistency of the sample eigenvectors

Recall that the spiked covariance model (2.1) has population eigenvectors the column vectors of the matrix O. The next result follows from [25].

Theorem 2.4.2 *Under the same assumptions as in Lemma 2.4.1 we have for n fixed*

$$\text{Angle}(v_i, E_{J_l}) \xrightarrow{P} 0 \qquad \textit{as } d \to \infty \textit{ if } i \in J_l,\ \forall l = 1, 2, \ldots, r, \tag{2.28}$$

$$\text{Angle}(v_i, o_i) \xrightarrow{P} \frac{\pi}{2} \qquad \textit{as } d \to \infty\ \forall i = p+1, \ldots, n. \tag{2.29}$$

That is, the first p sample eigenvectors are subspace consistent and the rest of the eigenvectors, corresponding to the nonzero sample eigenvalues, are strongly inconsistent when $d \to \infty$. Note that if $k_l = 1$ then v_i for $i \in J_l$ is consistent when $d \to \infty$. In Theorem 2.2.4 we give the proof of (2.28) under our spiked covariance model. This proof shows that (2.28) holds when $d, n \to \infty$ and $d \gg n$. The conjecture is that (2.29) is also true if $d, n \to \infty$ and $d \gg n$.

Most of the results in [25] are for the case when $d \to \infty$ and n is fixed. However, it is shown in [25] that if $c_i > c_j$ for $i > j$ and $i, j \in J_l$, $\forall l = 1, 2, \ldots, r$, then $\forall i \leq p$

$$\text{Angle}(v_i, o_i) \xrightarrow{P} 0 \qquad \text{as } d \to \infty, n \to \infty,$$

where the limits are applied successively. That is, in this case the sample eigenvectors are distinguishable and consistent. They conjecture that the inconsistent sample eigenvectors are still strongly inconsistent when $d, n \to \infty$ and $d \gg n$.

Chapter 3

Binary discrimination analysis for high dimensional data

This chapter deals with Binary Discrimination Analysis in the High-Dimension, Low Sample Size (HDLSS) framework. We focus on the study of asymptotic behavior of four methods for two-class discrimination: Support Vector Machine (SVM), Mean Difference (MD), Distance Weighted Discrimination (DWD) and Maximal Data Piling (MDP). The HDLSS asymptotics of the first three methods have been previously studied in Hall, Neeman and Marron [19], where the probability of correct classification of a new data is considered when the dimension d of the data sets tends to infinity. The comparison of the four methods has been done by simulation studies in Marron, Todd and Ahn [28], [29]. As contributions of this work we extend the results of [19] and give theoretical proofs of some empirical results of [28] and [29], by specifically studying the asymptotic behavior of the orthogonal vectors to the separating hyperplanes of the four methods, as data dimension increases. We also compare the Mean Difference method with the Support Vector Machine method when the dimension of the data is large but fixed.

In Section 3.1 we give a brief description of the four methods mentioned above. In Section 3.2 we show that these methods have asymptotically the same behavior when d tends to infinity. Specifically, we see that when the data sets are spherical Gaussian and one set has mean zero and the other has mean v_d, then the orthogonal vectors of the separating hyperplanes tend to be in the same direction as v_d when $\| v_d \| \gg d^{1/2}$ and tend to be orthogonal to v_d when $\| v_d \| \ll d^{1/2}$. This section also contains the HDLSS analysis of behavior in the interesting boundary case $\| v_d \| \approx d^{1/2}$. Since the data are Gaussian and the only difference between the two data sets is the mean v_d, this vector is the optimal direction (the best direction) for the orthogonal vector of the separating hyperplane. In Section 3.3 we show in a particular setting that in the case when the data sets are very well separated, that is $\| v_d \| \gg d^{1/2}$, MD is better than the SVM method when d is large, in the sense that A_{MD}, the angle between the MD orthogonal vector and the optimal direction v_d, is always smaller than A_{SVM}, the angle between the SVM orthogonal vector and v_d. In the case when $\| v_d \| \ll d^{1/2}$ we conclude that the MD method is a little better than the SVM method when d is large, meaning that generally (but not always) A_{MD} is smaller than A_{SVM}; but the methods are almost indistinguishable when d grows, this means that half of the time A_{MD} is smaller than A_{SVM} when d increases.

3.1 Binary discrimination methods

In this section we present the linear classification methods treated in this chapter, which are based on separating hyperplanes. Suppose that we have the following training data set

$$(x_1, w_1), (x_2, w_2), \ldots, (x_N, w_N), \tag{3.1}$$

where $x_i \in \mathbb{R}^d$ and $w_i \in \{-1, 1\}$, for $i = 1, 2, \ldots, N$. In particular, we have two classes of data, the classes C_+ and C_- corresponding to the vectors with $w_i = 1$ and $w_i = -1$, respectively. Let $X = [x_1, x_2 \ldots, x_N]$ be the $d \times N$ matrix of the training data and $w = (w_1, w_2, \ldots, w_N)^\top$ be the vector of the labels. The following notation will be used:

- W is the $N \times N$ diagonal matrix with the elements of w in its diagonal,
- X_+ (X_-) is the sub-matrix of X corresponding to the class C_+ (C_-),
- m (n) is the cardinality of the class C_+ (C_-),
- $\mathbf{1}_k$ is the k-dimensional vector of ones.

We say that the training data set (3.1) is *linearly separable* if there exists a hyperplane for which all the data of the class C_+ are on one side of the hyperplane and all the data of the class C_- are on the other side. In this case a hyperplane with such property is called a *separating hyperplane* of the training data set.

3.1.1 Support Vector Machine

A brief introduction to the Support Vector Machine (SVM) method for Binary Discrimination Analysis is given in this section. For a more comprehensive and detailed study see for example [11], [13], [14], [21], [40], [41].

The SVM method was proposed by Vapnik in [40] and [41]. It is one of the most useful binary discrimination methods in the literature. In the linearly separable case, the SVM method consists in finding a separating hyperplane that maximizes the distances of the hyperplane to the nearest vector of each class.

More specifically, suppose that there exists a vector v and a scalar b such that the following inequalities hold:

$$\begin{aligned} &v^\top x_i + b \geq 1, \quad if\ w_i = 1, \\ &v^\top x_i + b \leq -1, \quad if\ w_i = -1. \end{aligned} \tag{3.2}$$

In this case the hyperplane

$$v^\top x + b = 0$$

is a separating hyperplane of the training data set. Note that the inequalities in (3.2) can be written as

$$w_i(v^\top x_i + b) \geq 1, \quad i = 1, 2, \ldots, N. \tag{3.3}$$

The vectors x_i that satisfy the equality in (3.3) are called *support vectors*. That is, the support vectors are the training vectors that belong to one of the hyperplanes

$$v^\top x + b = -1 \quad \text{or} \quad v^\top x + b = 1. \tag{3.4}$$

The set of support vectors will be denoted by SV.

Let d_+ and d_- be the shortest distances from the separating hyperplane to the nearest vector in C_+ and C_-, respectively. Then the *margin* of the separating hyperplane is defined as $d_0 = d_+ + d_-$. Hence, the margin of the separating hyperplane is the distance between the hyperplanes given in (3.4) which is

$$d_0 = \frac{2}{\| v \|}.$$

In the separable case the *optimal separating hyperplane* or *SVM hyperplane*

$$v_0^\top x + b_0 = 0$$

is the unique separating hyperplane with a maximal margin. Thus, the SVM hyperplane maximizes $2/ \| v \|$ subject to the conditions (3.3). Equivalently, the SVM hyperplane solves the optimization problem

$$\begin{aligned} &\textit{minimize} \quad \frac{\| v \|^2}{2}, \\ &\textit{subject to} \quad w_i(v^\top x_i + b) \geq 1, \quad i = 1, 2, \ldots, N. \end{aligned} \tag{3.5}$$

According to [11], [13] and [21], the optimal vector is given by

$$v_0 = XW\widehat{\alpha}, \tag{3.6}$$

where $\widehat{\alpha}$ solves the optimization problem

$$\begin{aligned} &\textit{maximize} \quad \mathbf{1}_N^\top \alpha - \frac{1}{2} \| XW\alpha \|, \\ &\textit{subject to} \quad \alpha \geq \mathbf{0}, \ \alpha^\top w = 0. \end{aligned} \tag{3.7}$$

Furthermore we have that $\widehat{\alpha}_i \neq 0$ only if x_i is a support vector, hence by (3.6) v_0 is a linear function only of the support vectors. Since the support vectors satisfy the equality (3.3), the bias b_0 can be calculated as

$$b_0 = w_i - v_0^\top x_i, \tag{3.8}$$

for any $x_i \in SV$.

From [29] we have that the optimization problem (3.7) is equivalent to the following

$$\begin{aligned} &\textit{maximize} \quad \frac{2}{\| XW\alpha^* \|^2} \\ &\textit{subject to} \quad \mathbf{1}_m^\top \alpha_+^* = \mathbf{1}_n^\top \alpha_-^* = 1, \quad \alpha_+^*, \alpha_-^* \geq 0, \end{aligned} \tag{3.9}$$

where α_+^* and α_-^* are the sub-vectors of α^* corresponding to the class C_+ and C_-. respectively. Note that $XW\alpha^* = X_+\alpha_+^* - X_-\alpha_-^*$; thus we are minimizing the distance between points in the convex hulls of the classes C_+ and C_-. Therefore, if $\widehat{\alpha}^*$ solves the optimization problem (3.9), the orthogonal vector of the SVM hyperplane can be taken as

$$v_0^* = XW\widehat{\alpha}^* = X_+\widehat{\alpha}_+^* - X_-\widehat{\alpha}_-^*, \tag{3.10}$$

which is the difference of a pair of closest points of the convex hulls of the classes and is proportional to the vector v_0 given by (3.6).

For the non-separable case see [11], [13] and [21].

3.1.2 Distance Weighted Discrimination

In the HDLSS situation Marron, Todd and Ahn [28] observe that the projection of the data onto the orthogonal vector of the SVM separating hyperplane produces substantial data piling (that is, many of these projections are the same), and they show that data piling may affect the *generalization performance* (how well new data from the same distributions can be discriminated). Therefore, they propose the Distance Weighted Discrimination (DWD) method, which avoids the data piling problem and improves generalizability. The idea of this method is to find a separating hyperplane that minimizes the sum of the reciprocals of the distances of the training data to the hyperplane. Thus, all the training data have a role in finding the hyperplane, but data close to the hyperplane have a bigger impact than the data that are farther away. Here we describe briefly how this method works for the case when training data are linearly separable. The non-separable case can be found in [28] and [29].

Let $v \in \mathbb{R}^d$ be the orthogonal vector of the separating hyperplane and $b \in \mathbb{R}$ its bias. Define the *residual* of the i-th data vector as

$$r_i = w_i(v^\top x_i + b). \tag{3.11}$$

The *DWD hyperplane*

$$v_1^\top x + b_1 = 0,$$

solves the optimization problem

$$\begin{aligned} &\textit{minimize} \quad \sum_{i=1}^{N} \frac{1}{r_i} \\ &\textit{subject to} \quad \| v \| = 1, \; r_i \geq 0, \, i = 1, 2, \ldots, N. \end{aligned} \tag{3.12}$$

As can be seen in [29], the optimal vector v_1 is given by

$$v_1 = \frac{XW\widehat{\beta}}{\parallel XW\widehat{\beta} \parallel} \tag{3.13}$$

where $\widehat{\beta}$ solves the optimization problem

$$\begin{aligned} &\textit{maximize} \quad 2\mathbf{1}_N^\top \sqrt{\beta} - \parallel XW\beta \parallel, \\ &\textit{subject to} \quad \beta \geq \mathbf{0},\ \beta^\top w = 0, \end{aligned} \tag{3.14}$$

with $\sqrt{\beta}$ denoting the vector whose components are the square roots of the components of β. Note that the optimization problem (3.14) is similar to that of (3.7) for the SVM method. On the other hand, from [29] the residuals are given by

$$r_i = \frac{1}{\sqrt{\widehat{\beta}_i}}, \quad i = 1, 2, \ldots, N. \tag{3.15}$$

Thus, from the equation (3.11) the bias can be calculated as

$$b_1 = \frac{w_i}{\sqrt{\widehat{\beta}_i}} - v_1^\top x_i, \tag{3.16}$$

for any data vector x_i.

Similar to the case of the SVM method, it is shown in [29] that the optimization problem (3.14) is equivalent to

$$\begin{aligned} &\textit{maximize} \quad \frac{(\mathbf{1}_m^\top \sqrt{\beta_+^*} + \mathbf{1}_n^\top \sqrt{\beta_-^*})^2}{\parallel X_+\beta_+^* - X_-\beta_-^* \parallel}, \\ &\textit{subject to} \quad \mathbf{1}_m^\top \beta_+^* = \mathbf{1}_n^\top \beta_-^* = 1, \quad \beta_+^*, \beta_-^* \geq \mathbf{0}. \end{aligned} \tag{3.17}$$

Hence we are trying to minimize the distance between points in the two convex hulls, but divided by the square of the sum of the square roots of the convex weights. Therefore, if $\widehat{\beta}^*$ solves the optimization problem (3.17), the orthogonal vector of the DWD hyperplane is proportional to

$$v_1^* = X_+\widehat{\beta}_+^* - X_-\widehat{\beta}_-^*. \tag{3.18}$$

3.1.3 Mean Difference Method

In the Mean Difference (MD) method, also called the nearest centroid method (see [37]), the separating hyperplane is the one that orthogonally bisects the segment joining the centroids or means of the two classes. That is, if the means of the classes C_+ and C_- are given by

$$\overline{x}_+ = \frac{1}{m} \sum_{x_i \in C_+} x_i \quad \text{and} \quad \overline{x}_- = \frac{1}{n} \sum_{x_i \in C_-} x_i, \tag{3.19}$$

respectively, then the *MD hyperplane* has orthogonal vector

$$v = \overline{x}_+ - \overline{x}_- \tag{3.20}$$

and bisects the segment joining the means $\overline{x}_+$ and $\overline{x}_-$. Thus, as in the case of the SVM and DWD hyperplanes the orthogonal vector of the MD hyperplane is the difference between two points on the convex hulls of the two classes.

3.1.4 Maximal Data Piling

The Maximal Data Piling (MDP) method for binary discrimination was proposed by Ahn and Marron [1]. This method was specially designed for the HDLSS context and we need to assume $d \geq N-1$ and that the subspace generated by the dataset has dimension $N-1$. Under these assumptions there exist direction vectors onto which the projection of the training data are piled completely at two distinct points, one for each class. The orthogonal vector of the MDP method is the direction vector for which the distance between these two points is maximal. On the other hand, in [1] it is shown that the MDP method is equivalent to the Fisher Linear Discrimination (FLD) in the non-HDLSS situation. However, Bickel and Levina [10] have demonstrated that FLD has very poor HDLSS properties, while in [1] is shown that, although data piling may not be desirable, the MDP method can work very well and better than FLD under some settings in the HDLSS context.

In order to explain how to build the separating hyperplane for this method, let $u = \overline{x}_+ - \overline{x}_-$ be the difference of the means of the two classes, where $\overline{x}_+$ and $\overline{x}_-$ are given in (3.19). Define $C = [X_c^+, X_c^-]$, where X_c^+ and X_c^- are the centered versions of X_+ and X_- respectively, that is

$$X_c^+ = X_+ - \overline{x}_+ \mathbf{1}_d^\top, \quad X_c^- = X_- - \overline{x}_- \mathbf{1}_d^\top.$$

The symmetric projection matrix onto the orthogonal complement of the column space of C is given by $Q = I_d - CC^\dagger$, where $A^\dagger$ is the Moore-Penrose generalized inverse of A.

The *MDP hyperplane*

$$v_2^\top x + b_2 = 0$$

has the property that its unit orthogonal vector v_2 is the direction for which the projections of the two class means have maximal distance, subject to the constraint that the projection of each training data onto the vector is the same as its class mean. In other words, v_2 solves the optimization problem

$$\begin{aligned} &\textit{maximize} \quad (v^\top u)^2, \\ &\textit{subject to} \quad C^\top v = 0, \ v^\top v = 1. \end{aligned} \tag{3.21}$$

It is seen in [1] that the orthogonal vector is given by

$$v_2 = \frac{Qu}{\| Qu \|}. \tag{3.22}$$

This means that v_2 is orthogonal to the $N-2$ dimensional subspace generated by the columns of C. Furthermore, the expression (3.22) is equivalent to

$$v_2 = \frac{(X_c X_c^\top)^\dagger u}{\| (X_c X_c^\top)^\dagger u \|}, \tag{3.23}$$

where X_c is the centered version of the the data matrix X. Therefore, v_2 is also in the $N-1$ dimensional subspace generated by the globally centered data vectors. Finally, the bias b_2 can be calculated as

$$b_2 = -v_2^\top (m\overline{x}_+ + n\overline{x}_-)/N. \tag{3.24}$$

3.2 Asymptotic results for the orthogonal vectors

In this section we consider the $d \times N$ matrix $X = [x_1, x_2, \ldots, x_N]$ whose columns are a training data set for two classes. Suppose the first m columns of X are the vectors of the class C_+ and the remaining $n = N - m$ columns are the vectors of the class C_-. Therefore, the matrices

$$\begin{aligned} X_+ &= [x_1, x_2 \ldots, x_m], \\ X_- &= [x_{m+1}, x_{m+2}, \ldots, x_{m+n}] \end{aligned}$$

are the sub-matrices of X corresponding to the class C_+ and C_-, respectively. We assume that the random vectors in C_+ and C_- are independent with d-multivariate normal distributions $N_d(v_d, I_d)$ and $N_d(0, I_d)$, respectively. Note that the difference between these classes is made by the mean vector v_d. So the length of v_d, $\| v_d \|$, is crucial for classification performance.

Because the separating hyperplanes of the discrimination methods described in Section 3.1 are determined by their orthogonal vectors, the behavior of classification is studied considering the direction of these vectors. When the dimension grows and the sample size is fixed (HDLSS framework) asymptotic performance of all these methods will be related with the distance between the two class distributions, in particular by $\| v_d \|$. Before giving the main theorem of this section, we state the next lemma which tells us that when $\| v_d \| d^{-1/2} \to c$ with $c \geq 0$, the orthogonal vectors of the three methods MD, SVM and DWD converge to the same direction as $d \to \infty$.

Lemma 3.2.1 *Let X_+ and X_- be as before and assume $\| v_d \| d^{-1/2} \to c$, with $c \geq 0$. If the vector $\widetilde{v} = X_+\alpha_+ - X_-\alpha_-$, where $\alpha \geq \mathbf{0}$ and $\mathbf{1}_m^\top \alpha_+ = \mathbf{1}_n^\top \alpha_- = 1$, is proportional to the orthogonal vector of the MD, SVM or DWD hyperplane we have*

$$\alpha_{i,+} \xrightarrow{w} \frac{1}{m}, \quad \alpha_{j,-} \xrightarrow{w} \frac{1}{n}, \tag{3.25}$$

for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$, as $d \to \infty$.

Proof. Let $y_j = x_{m+j}$ for $j = 1, 2, \dots, n$. By the Law of Large Numbers (LLN), see [36, pp. 220], we have the following

$$\frac{\| x_i - x_j \|}{d^{1/2}} \xrightarrow{P} 2^{1/2}, \qquad \frac{\| y_i - y_j \|}{d^{1/2}} \xrightarrow{P} 2^{1/2} \tag{3.26}$$

for $i \neq j$, as $d \to \infty$. We also have

$$\frac{\sum_{k=1}^{d} \mathrm{Var}(x_i^{(k)})}{d} = 1 \longrightarrow 1, \quad \frac{\sum_{k=1}^{d} \mathrm{Var}(y_i^{(k)})}{d} = 1 \longrightarrow 1,$$

$$\frac{\sum_{k=1}^{d} (E(x_i^{(k)}) - E(y_j^{(k)}))^2}{d} = \frac{\| v_d \|^2}{d} \longrightarrow c^2,$$

as $d \to \infty$; then by Section 3.2 of [19]

$$\frac{\| x_i - y_j \|}{d^{1/2}} \xrightarrow{P} \ell = (2 + c^2)^{1/2}, \tag{3.27}$$

as $d \to \infty$. By [19], (3.26) and (3.27) imply that the data $x_1, \dots, x_N$ tend to be the vertices of an N-polyhedron (a figure in $(N-1)$-dimensional space with just N vertices and all its faces given by hyperplanes in $(N-1)$-variate space) as $d \to \infty$. This polyhedron has m of its vertices arranged as those of an m-simplex (an m-polyhedron with all edges of equal length) and the other n vertices arranged in an n-simplex. The data in C_+ and C_- tend to be the vertices of the m-simplex and n-simplex respectively as $d \to \infty$. Let $x_1^*, \dots, x_m^*$ be the vertices of the m-simplex and let $y_1^*, \dots, y_n^*$ be the vertices of the n-simplex.

If $\widetilde{v} = X_+\alpha_+ - X_-\alpha_-$ is proportional to the SVM orthogonal vector, as explained in Section 3.1.1, $\widetilde{v}$ is the difference between the two closest vectors of the convex hulls of the classes C_+ and C_-. When $d \to \infty$ these convex hulls tend to be the m-simplex and n-simplex, respectively. We will show that the closest points of these simplices are the means $\overline{x}^* = \sum_{i=1}^{m} x_i^*/m$ and $\overline{y}^* = \sum_{i=1}^{n} y_i^*/n$. For the N-polyhedron we have

$$\| x_i^* - y_j^* \| = \ell,$$

for $i = 1, 2, \dots, m$ and $j = 1, 2, \dots, n$. Since the distance from x_i^* to any vertex of the n-simplex is the same, we have that for any j, x_i^*, y_j^* and $\overline{y}^*$ are the vertices of a right-angled triangle where the hypotenuse is the line joining x_i^* to y_j^*. Thus, $\overline{y}^*$ is the closest point in the n-simplex to x_i^*, for $i = 1, 2, \dots, m$. Similarly, because the distance from $\overline{y}^*$ to x_i^* for $i = 1, 2, \dots, m$ is constant, the closest point in the m-simplex to $\overline{y}^*$ is $\overline{x}^*$, hence the closest points in the simplices are $\overline{x}^*$ and $\overline{y}^*$. Thus we have (3.25).

In the case when $\widetilde{v}$ is proportional to the DWD orthogonal vector, by Section 3.1.2 we have that α solves the optimization problem (3.17). For the N-polyhedron this α is given by

$$\widehat{\alpha}_{i,+} = \frac{1}{m}, \quad \widehat{\alpha}_{j,-} = \frac{1}{n}, \quad i = 1, 2, \dots, m, \; j = 1, 2, \dots, n.$$

This is because if β satisfies $\mathbf{1}_m^\top \beta_+ = \mathbf{1}_n^\top \beta_+ = 1$ then

$$\| X_+^* \beta_+ - X_-^* \beta_- \| \geq \| \overline{x}^* - \overline{y}^* \| = \| X_+^* \widehat{\alpha}_+ - X_-^* \widehat{\alpha}_- \|$$

where $X_+^* = [x_1^*, \ldots, x_m^*]$ and $X_-^* = [y_1^*, \ldots, y_n^*]$, since $\overline{x}^*$ and $\overline{y}^*$ are the closest points of the simplices. Furthermore

$$(\mathbf{1}_m^\top \sqrt{\beta_+} - \mathbf{1}_n^\top \sqrt{\beta_-})^2 \leq (\sqrt{m} + \sqrt{n})^2 = (\mathbf{1}_m \sqrt{\widehat{\alpha}_+} + \mathbf{1}_n \sqrt{\widehat{\alpha}_-})^2,$$

thus

$$\frac{(\mathbf{1}_m \sqrt{\beta_+} + \mathbf{1}_n \sqrt{\beta_-})^2}{\| X_+^* \beta_+ - X_-^* \beta_- \|} \leq \frac{(\mathbf{1}_m \sqrt{\widehat{\alpha}_+} + \mathbf{1}_n \sqrt{\widehat{\alpha}_-})^2}{\| X_+^* \widehat{\alpha}_+ - X_-^* \widehat{\alpha}_- \|},$$

and $\widehat{\alpha}$ solves the optimization problem (3.17) for the N-polyhedron, hence we have (3.25).

For the case of the MD method $\widetilde{v} = \overline{x}_+ - \overline{x}_-$ and

$$\alpha_{i,+} = \frac{1}{m}, \quad \alpha_{j,-} = \frac{1}{n}, \quad i = 1, 2, \ldots, m, \; j = 1, 2, \ldots, n.$$

Then we have (3.25). □

When $\| v_d \|$ is large the classification becomes easy, and it is rather challenging when $\| v_d \|$ is small. In view of the results of Hall, Marron and Neeman [19], who showed that spherical Gaussian data tend to lie at a distance $d^{1/2}$ from the mean when d is large, it is not surprising that $\| v_d \| \approx d^{1/2}$ is a critical boundary. This is confirmed by the next theorem where we show that all the linear methods are *consistent* in the sense that the angles between the orthogonal vectors of the hyperplanes and the optimal vector v_d converge to zero, in the case $\| v_d \| \gg d^{1/2}$, while for the case $\| v_d \| \ll d^{1/2}$ the orthogonal vectors do not converge to the optimal direction. Furthermore they are *strongly inconsistent*, in the sense that they are asymptotically orthogonal.

Theorem 3.2.1 *If v represents the orthogonal vector of the Mean Difference (MD), Support Vector Machine (SVM), Distance Weighted Discrimination (DWD) or Maximal Data Piling (MDP) hyperplane we have that*

$$\text{Angle}(v, v_d) \xrightarrow{w} \begin{cases} 0, & \text{if } \| v_d \| d^{-1/2} \to \infty; \\ \frac{\pi}{2}, & \text{if } \| v_d \| d^{-1/2} \to 0; \\ \arccos(c/(\gamma + c^2)^{1/2}), & \text{if } \| v_d \| d^{-1/2} \to c, \; c > 0, \end{cases}$$

as $d \to \infty$, where $\gamma = \frac{1}{m} + \frac{1}{n}$.

Proof. <u>Case 1</u>: *When v is the orthogonal vector of the MD, SVM or DWD hyperplane.* We have seen in Section 3.1 that v is proportional to the vector $\widetilde{v} = X_+ \alpha_+ - X_- \alpha_-$ given in Lemma 3.2.1. We also have

$$\cos(\text{Angle}(\widetilde{v}, v_d)) = \frac{\langle \widetilde{v}, v_d \rangle}{\| \widetilde{v} \| \| v_d \|}.$$

Let $z_i = x_i - v_d$ be the centered version of the data x_i and let $y_j = x_{m+j}$, for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. It can be seen that

$$\begin{aligned}\langle \widetilde{v}, v_d \rangle &= \sum_{k=1}^{d} \left(\sum_{i=1}^{m} z_i^{(k)} \alpha_{i,+} - \sum_{i=1}^{n} y_i^{(k)} \alpha_{i,-} \right) v_d^{(k)} + \| v_d \|^2 \\ &= \sum_{i=1}^{m} \alpha_{i,+} \sum_{k=1}^{d} z_i^{(k)} v_d^{(k)} - \sum_{i=1}^{n} \alpha_{i,-} \sum_{k=1}^{d} y_i^{(k)} v_d^{(k)} + \| v_d \|^2 .\end{aligned}$$

Therefore

$$\langle \widetilde{v}, v_d \rangle = \| v_d \| \left(\sum_{i=1}^{m} \alpha_{i,+} N_{i,+} - \sum_{i=1}^{n} \alpha_{i,-} N_{i,-} \right) + \| v_d \|^2, \tag{3.28}$$

where $N_{i,+} = \| v_d \|^{-1} \sum_{k=1}^{d} z_i^{(k)} v_d^{(k)}$ and $N_{j,-} = \| v_d \|^{-1} \sum_{k=1}^{d} y_j^{(k)} v_d^{(k)}$, for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$, are independent random variables with the standard normal distribution. Furthermore

$$\begin{aligned}\| \widetilde{v} \|^2 &= \sum_{k=1}^{d} \left(\sum_{i=1}^{m} z_i^{(k)} \alpha_{i,+} - \sum_{i=1}^{n} y_i^{(k)} \alpha_{i,-} \right)^2 + 2 \sum_{k=1}^{d} \left(\sum_{i=1}^{m} z_i^{(k)} \alpha_{i,+} - \sum_{i=1}^{n} y_i^{(k)} \alpha_{i,-} \right) v_d^{(k)} + \| v_d \|^2 \\ &= \sum_{i=1}^{m} \alpha_{i,+}^2 \sum_{k=1}^{d} z_i^{(k)2} + 2 \sum_{i<j} \alpha_{i,+} \alpha_{j,+} \sum_{k=1}^{d} z_i^{(k)} z_j^{(k)} + \sum_{i=1}^{n} \alpha_{i,-}^2 \sum_{k=1}^{d} y_i^{(k)2} \\ &\quad + 2 \sum_{i<j} \alpha_{i,-} \alpha_{j,-} \sum_{k=1}^{d} y_i^{(k)} y_j^{(k)} - 2 \sum_{i=1}^{m} \sum_{j=1}^{n} \alpha_{i,+} \alpha_{j,-} \sum_{k=1}^{d} z_i^{(k)} y_j^{(k)} \\ &\quad + 2 \| v_d \| \left(\sum_{i=1}^{m} \alpha_{i,+} N_{i,+} - \sum_{i=1}^{n} \alpha_{i,-} N_{i,-} \right) + \| v_d \|^2 .\end{aligned} \tag{3.29}$$

Note that by the LLN we have

$$\begin{aligned} &\frac{\sum_{k=1}^{d} z_i^{(k)2}}{d} \xrightarrow{w} 1, \quad \frac{\sum_{k=1}^{d} y_j^{(k)2}}{d} \xrightarrow{w} 1, \quad \frac{\sum_{k=1}^{d} z_i^{(k)} y_j^{(k)}}{d} \xrightarrow{w} 0, \qquad \forall i, \forall j, \\ &\frac{\sum_{k=1}^{d} z_i^{(k)} z_j^{(k)}}{d} \xrightarrow{w} 0, \quad \frac{\sum_{k=1}^{d} y_i^{(k)} y_j^{(k)}}{d} \xrightarrow{w} 0, \qquad i \neq j, \end{aligned} \tag{3.30}$$

as $d \to \infty$. It is also true that

$$\frac{N_{i,+}}{d^{1/2}} \xrightarrow{w} 0, \qquad \frac{N_{j,-}}{d^{1/2}} \xrightarrow{w} 0 \quad as\ d \to \infty. \tag{3.31}$$

For the case when $\| v_d \| d^{-1/2} \to \infty$, from (3.28)-(3.31) and since $0 \leq \alpha_{i,+}, \alpha_{j,-} \leq 1$ we have

$$\frac{\| \widetilde{v} \|^2}{\| v_d \|^2} \xrightarrow{w} 1, \qquad \frac{\langle \widetilde{v}, v_d \rangle}{\| v_d \|^2} \xrightarrow{w} 1 \tag{3.32}$$

as $d \to \infty$. Thus,

$$\frac{\langle \widetilde{v}, v_d \rangle}{\| \widetilde{v} \| \| v_d \|} = \frac{\langle \widetilde{v}, v_d \rangle / \| v_d \|^2}{\| \widetilde{v} \| / \| v_d \|} \xrightarrow{w} 1$$

and

$$\text{Angle}(\widetilde{v}, v_d) = \arccos\left(\frac{\langle \widetilde{v}, v_d \rangle}{\| \widetilde{v} \| \| v_d \|} \right) \xrightarrow{w} 0,$$

as $d \to \infty$.

For the case when $\| v_d \| d^{-1/2} \to c$, with $c \geq 0$, from (3.28)-(3.31) and Lemma 3.2.1 it can be seen that

$$\frac{\| \widetilde{v} \|^2}{d} \xrightarrow{w} \gamma + c^2, \qquad \frac{\langle \widetilde{v}, v_d \rangle}{d^{1/2} \| v_d \|} \xrightarrow{w} c, \tag{3.33}$$

as $d \to \infty$, where $\gamma = \frac{1}{m} + \frac{1}{n}$. Therefore,

$$\frac{\langle \widetilde{v}, v_d \rangle}{\| \widetilde{v} \| \| v_d \|} = \frac{\langle \widetilde{v}, v_d \rangle / (d^{1/2} \| v_d \|)}{\| \widetilde{v} \| / d^{1/2}} \xrightarrow{w} \frac{c}{(\gamma + c^2)^{1/2}}$$

and

$$\text{Angle}(\widetilde{v}, v_d) = \arccos\left(\frac{\langle \widetilde{v}, v_d \rangle}{\| \widetilde{v} \| \| v_d \|} \right) \xrightarrow{w} \arccos\left(\frac{c}{(\gamma + c^2)^{1/2}} \right)$$

as $d \to \infty$. In particular, for $c = 0$ we have $\arccos(\frac{c}{(\gamma+c^2)^{1/2}}) = \frac{\pi}{2}$.

<u>Case 2</u>: *When v is the orthogonal vector of the MDP hyperplane.* Let $\overline{x} = \sum_{i=1}^{m} x_i/m$, $\overline{z} = \sum_{i=1}^{m} z_i/m$, $\overline{y} = \sum_{i=1}^{n} y_i/n$, where z_i and y_j, for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$, are as in Case 1. Note that

$$\begin{aligned}
\| x_i - \overline{x} \|^2 &= \langle z_i - \overline{z}, z_i - \overline{z} \rangle = \left\langle \left(1 - \frac{1}{m}\right) z_i - \sum_{j \neq i} \frac{z_j}{m}, \left(1 - \frac{1}{m}\right) z_i - \sum_{j \neq i} \frac{z_j}{m} \right\rangle \\
&= \left(1 - \frac{1}{m}\right)^2 \sum_{k=1}^{d} z_i^{(k)2} - 2\left(1 - \frac{1}{m}\right) \sum_{k=1}^{d} z_i^{(k)} \sum_{j \neq i} \frac{z_j^{(k)}}{m} + \sum_{k=1}^{d} \left(\sum_{j \neq i} \frac{z_j^{(k)}}{m} \right)^2 \\
&= \left(1 - \frac{1}{m}\right)^2 \sum_{k=1}^{d} z_i^{(k)2} - 2\left(1 - \frac{1}{m}\right) \frac{(m-1)^{1/2}}{m} \sum_{k=1}^{d} z_i^{(k)} N_{-i}^{(k)} + \frac{m-1}{m^2} \sum_{k=1}^{d} N_{-i}^{(k)2}
\end{aligned} \tag{3.34}$$

where $N_{-i}^{(k)} = (m-1)^{-1/2} \sum_{j \neq i} z_j^{(k)}$, for $k = 1, 2, \ldots, d$, are independent random variables with standard normal distribution and they are independent of z_i. Let $u = \overline{x} - \overline{y}$, if $\| v_d \| d^{-1/2} \to \infty$ using (3.29), (3.34) and the LLN we can see that $\cos(\text{Angle}(x_i - \overline{x}, u)) \xrightarrow{w} 0$ as $d \to \infty$. Analogously, $\cos(\text{Angle}(y_i - \overline{y}, u)) \xrightarrow{w} 0$ as $d \to \infty$. Thus

$$\text{Angle}(x_i - \overline{x}, u) \xrightarrow{w} \frac{\pi}{2}, \qquad \text{Angle}(y_j - \overline{y}, u) \xrightarrow{w} \frac{\pi}{2} \tag{3.35}$$

as $d \to \infty$. The same is true if $\| v_d \| d^{-1/2} \to c$, with $c \geq 0$.

Let C be the matrix whose columns are the vectors $x_i - \overline{x}$, $y_j - \overline{y}$, for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. By Section 3.1.4 the orthogonal vector of the MDP method is given by $v = Qu/ \parallel Qu \parallel$ where Q is the symmetric projection matrix on the orthogonal complement of the column space of C. According to (3.35), u tends to be in the orthogonal complement of the column space of C. Thus, when d is large Qu can be approximated by u and v can be approximated by $u/ \parallel u \parallel$. Therefore,

$$\cos(\text{Angle}(v, v_d)) = \frac{\langle v, v_d \rangle}{\parallel v \parallel \parallel v_d \parallel} \tag{3.36}$$

can be approximated by $\langle u, v_d \rangle /(\parallel u \parallel \parallel v_d \parallel)$. Hence by Case 1, this converges to 1 if $\parallel v_d \parallel d^{-1/2} \to \infty$ and converges to $c/(\gamma + c^2)^{1/2}$ if $\parallel v_d \parallel d^{-1/2} \to c$ with $c \geq 0$. □

Remark 3.2.1 *Recall that by Lemma 3.2.1 the MD, SVM and DWD orthogonal vectors converge to the same direction when $\parallel v_d \parallel d^{-1/2} \to c \geq 0$ as $d \to \infty$. Due to the proof of the last theorem, the unitary MDP orthogonal vector converges to the same direction as the other three methods as $d \to \infty$, since it can be approximated by the unitary MD orthogonal vector when d is large.*

3.3 Comparison of the MD and SVM methods

In the case when $\parallel v_d \parallel d^{-1/2} \to \infty$, by Theorem 3.2.1 we have that all the orthogonal vectors converge to the optimal vector, but an interesting question is which of them is better in the HDLSS context. In the case when $\parallel v_d \parallel d^{-1/2} \to 0$ and the orthogonal vectors are strongly inconsistent, another interesting question is which of them is closer to the optimal direction v_d. In order to compare the SVM and the MD methods in these cases we first obtain a useful result that gives an explicit form for the orthogonal vector of the SVM hyperplane in some particular settings.

Lemma 3.3.1 *Suppose $\parallel v_d \parallel = d^\delta$, with $\delta > 0$. Let x_1 be a vector in the class C_+ and let y_1, y_2 be vectors in the class C_-. If ρ is the probability that the orthogonal projection of x_1 onto the line passing through y_1 and y_2 is on the segment joining these vectors, then*

$$\rho \longrightarrow \begin{cases} 1, & \text{if } \delta < 1; \\ 2\Phi(2^{-1/2}) - 1 \approx 0.52, & \text{if } \delta = 1; \\ 0, & \text{if } \delta > 1, \end{cases}$$

as $d \to \infty$, where $\Phi(\cdot)$ is the standard normal distribution function.

Proof. Let $z_1 = x_1 - v_d$. Note that the orthogonal projection of x_1 into the line passing through y_1 and y_2 is on the segment joining these vectors if and only if $\text{Angle}(x_1 - y_1, y_2 - y_1) \leq \pi/2$ and $\text{Angle}(x_1 - y_2, y_1 - y_2) \leq \pi/2$, if and only if

$$\langle x_1 - y_1, y_2 - y_1 \rangle \geq 0 \quad \text{and} \quad \langle x_1 - y_2, y_1 - y_2 \rangle \geq 0.$$

Thus,

$$\begin{aligned}\rho &= P([\langle x_1 - y_1, y_2 - y_1\rangle \geq 0] \cap [\langle x_1 - y_2, y_1 - y_2\rangle \geq 0]) \\ &= 1 - P([\langle x_1 - y_1, y_2 - y_1\rangle < 0] \cup [\langle x_1 - y_2, y_1 - y_2\rangle < 0]) \\ &= 1 - [P(\langle x_1 - y_1, y_2 - y_1\rangle < 0) + P(\langle x_1 - y_2, y_1 - y_2\rangle < 0)] \\ &= 1 - 2P(\langle x_1 - y_1, y_2 - y_1\rangle < 0). \end{aligned} \tag{3.37}$$

One can see that

$$\begin{aligned} P(\langle x_1 - y_1, y_2 - y_1\rangle < 0) &= P\left(\frac{\langle x_1 - y_1, y_2 - y_1\rangle}{\| y_2 - y_1 \|} < 0\right) \\ &= P\left(\frac{\langle z_1 - y_1, y_2 - y_1\rangle}{\| y_2 - y_1 \|} + \frac{\langle v_d, y_2 - y_1\rangle}{\| y_2 - y_1 \|} < 0\right). \end{aligned} \tag{3.38}$$

From [19], when d tends to infinity $z_1,\ y_1,\ y_2$ tend to form an equilateral triangle where each edge has length approximately $(2d)^{1/2}$. Therefore, the projection of the vector $z_1 - y_1$ onto the vector $y_2 - y_1$, given by $\langle z_1 - y_1, y_2 - y_1\rangle / \| y_2 - y_1 \|$, is approximately $(2d)^{1/2}/2 = (d/2)^{1/2}$. Thus, when d is large enough (3.38) is approximately

$$\begin{aligned} &P\left((d/2)^{1/2} + \frac{\langle v_d, y_2 - y_1\rangle}{(2d)^{1/2}} < 0\right) = P\left((d/2)^{1/2} < \frac{2^{1/2} \| v_d \| N_1}{(2d)^{1/2}}\right) \\ &= P\left(N_1 > \frac{d}{2^{1/2} \| v_d \|}\right) = P\left(N_1 > \frac{d^{1-\delta}}{2^{1/2}}\right) = 1 - \Phi\left(\frac{d^{1-\delta}}{2^{1/2}}\right), \end{aligned}$$

where $N_1 = \langle v_d, y_1 - y_2\rangle / (2^{1/2} \| v_d \|)$ is a r.v. with standard normal distribution and $\Phi(\cdot)$ is its distribution function. Hence

$$P(\langle x_1 - y_1, y_2 - y_1\rangle < 0) \longrightarrow \begin{cases} 0, & \text{if } \delta < 1; \\ 1 - \Phi(2^{-1/2}), & \text{if } \delta = 1; \\ 1/2, & \text{if } \delta > 1, \end{cases} \tag{3.39}$$

as $d \to \infty$, and from (3.37) we have the result. □

We now consider $m = 1$ and $n = 2$, which is a simple but very illustrative case. Let $\mathbf{p}$ be the orthogonal projection of x_1 onto the line passing through y_1 and y_2. If $\mathbf{p}$ is outside the segment joining y_1 and y_2, define $\mathbf{p}_0$ as y_1 or y_2 depending on whether x_1 is closer to y_1 or closer to y_2, respectively. Recall that the SVM orthogonal vector is the difference between the two closest points of the convex hulls of the classes. In this case the convex hulls are the point x_1 and the segment joining y_1 and y_2. From Lemma 3.3.1 we have that when $d \to \infty$ the SVM orthogonal vector tends to be $v_{SVM} = x_1 - \mathbf{p}$, if $0 < \delta < 1$; $v_{SVM} = x_1 - \mathbf{p}_0$, if $\delta > 1$; $v_{SVM} = x_1 - \mathbf{p}$ with probability $2\Phi(2^{-1/2}) - 1 \approx 0.52$ and $v_{SVM} = x_1 - \mathbf{p}_0$ with probability $2 - 2\Phi(2^{-1/2}) \approx 0.48$, if $\delta = 1$.

Now we will compare the SVM method with the MD method under the cases when $0 < \delta < 1$ and when $\delta > 1$, in the setting $m = 1$ and $n = 2$. We find that when $\| v_d \| = d^\delta$

with $1/2 < \delta < 1$, i.e. when the distance between classes, $\| v_d \|$, is bigger than the distance within classes, the MD classification is better than SVM, in the sense of having an asymptotically smaller angle between the orthogonal vector and the optimal direction. This is because the difference between the squares of Angle(v_{SVM}, v_d) and Angle(v_{MD}, v_d) tends to be positive since this difference is approximately a multiple of a chi-square r.v. when d is large. Note that this case corresponds to the setting $\| v_d \| d^{-1/2} \to \infty$.

Theorem 3.3.1 (Case $m = 1$, $n = 2$) *Suppose $\| v_d \| = d^{\delta}$ with $1/2 < \delta < 1$. Let v_{SVM} and v_{MD} be the corresponding vector $\widetilde{v}$ given in Lemma 3.2.1 for the SVM and MD method, respectively. Let $A_{SVM} = \text{Angle}(v_{SVM}, v_d)$ and $A_{MD} = \text{Angle}(v_{MD}, v_d)$, then*

$$A^2_{SVM} - A^2_{MD} = 2\frac{\mathcal{X}^2_1}{d} + O_p(d^{-(1+\epsilon)}) \qquad \text{as } d \to \infty,$$

for some $\epsilon > 0$ and where $\mathcal{X}^2_1$ is a r.v. with the chi-square distribution with one degree of freedom.

Proof. Let z_1, $\overline{y}$, y_i, for $i = 1, 2$, be as in the proof of Theorem 3.2.1. Since $1/2 < \delta < 1$, by Lemma 3.3.1 when d is sufficiently large the orthogonal projection of x_1 onto the line passing through y_1 and y_2 is on the segment joining these vectors with probability approximately one. Therefore, when d is large enough, if $\mathbf{p}$ is this projection we can consider that

$$\mathbf{p} = a_1 y_1 + a_2 y_2, \quad \text{with } a_1, a_2 \geq 0,\ a_1 + a_2 = 1. \tag{3.40}$$

It can be seen that

$$a_1 = \frac{\langle x_1 - \overline{y}, y_1 - y_2 \rangle}{\| y_1 - y_2 \|^2} + \frac{1}{2}, \quad a_2 = \frac{\langle x_1 - \overline{y}, y_2 - y_1 \rangle}{\| y_1 - y_2 \|^2} + \frac{1}{2}. \tag{3.41}$$

From Hall, *et al.* [19] we have that

$$\| y_1 - y_2 \|^2 = 2d + O_P(1), \qquad \text{as } d \to \infty.$$

Therefore, we use this asymptotic result to express a_1 and a_2 as

$$a_1 = \frac{\langle x_1 - \overline{y}, y_1 - y_2 \rangle}{2d} + \frac{1}{2}, \quad a_2 = \frac{\langle x_1 - \overline{y}, y_2 - y_1 \rangle}{2d} + \frac{1}{2}$$

for d sufficiently large. Thus,

$$\begin{aligned} \mathbf{p} = a_1 y_1 + a_2 y_2 &= \left(\frac{\langle x_1 - \overline{y}, y_1 - y_2 \rangle}{2d} + \frac{1}{2} \right) y_1 + \left(- \frac{\langle x_1 - \overline{y}, y_1 - y_2 \rangle}{2d} + \frac{1}{2} \right) y_2 \\ &= \frac{\langle x_1 - \overline{y}, y_1 - y_2 \rangle}{2d} (y_1 - y_2) + \overline{y} \\ &= \frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle}{2d} (y_1 - y_2) + \frac{\langle v_d, y_1 - y_2 \rangle}{2d} (y_1 - y_2) + \overline{y}. \end{aligned} \tag{3.42}$$

Note that in this case $v_{SVM} = x_1 - \mathbf{p} = x_1 - (a_1 y_1 + a_2 y_2)$ because x_1 and $\mathbf{p}$ are the closest points of the convex hulls. Therefore, (3.42) gives

$$\begin{aligned} \langle v_{SVM}, v_d \rangle &= \langle x_1 - \mathbf{p}, v_d \rangle = \langle z_1 - \mathbf{p}, v_d \rangle + \langle v_d, v_d \rangle \\ &= \langle z_1 - \overline{y}, v_d \rangle - \frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle \langle y_1 - y_2, v_d \rangle}{2d} \\ &\quad - \frac{\langle y_1 - y_2, v_d \rangle^2}{2d} + \langle v_d, v_d \rangle . \end{aligned} \tag{3.43}$$

By (3.32) we have $\| v_{SVM} \|^2 / \| v_d \|^2 \xrightarrow{w} 1$ as $d \to \infty$, so we can consider $\| v_{SVM} \| / \| v_d \| = 1$ when d is large enough. Hence for large d we have that

$$\cos(A_{SVM}) = \frac{\langle v_{SVM}, v_d \rangle}{\| v_{SVM} \| \| v_d \|} = \frac{\langle v_{SVM}, v_d \rangle}{\| v_d \|^2}$$

and substituting (3.43) into the last expression we have

$$\begin{aligned} \cos(A_{SVM}) &= \frac{\langle z_1 - \overline{y}, v_d \rangle}{\| v_d \|^2} - \frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle \langle y_1 - y_2, v_d \rangle}{2d \| v_d \|^2} \\ &\quad - \frac{\langle y_1 - y_2, v_d \rangle^2}{2d \| v_d \|^2} + 1. \end{aligned} \tag{3.44}$$

Similarly we can see that

$$\cos(A_{MD}) = \frac{\langle z_1 - \overline{y}, v_d \rangle}{\| v_d \|^2} + 1. \tag{3.45}$$

Therefore, from (3.44) and (3.45) we have

$$\cos(A_{MD}) - \cos(A_{SVM}) = \frac{\langle y_1 - y_2, v_d \rangle^2}{2d \| v_d \|^2} + \frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle \langle y_1 - y_2, v_d \rangle}{2d \| v_d \|^2}. \tag{3.46}$$

We observe that for the first term on the right side of (3.46)

$$\frac{\langle y_1 - y_2, v_d \rangle^2}{2d \| v_d \|^2} = \frac{N_1^2}{d} = \frac{\mathcal{X}_1^2}{d}, \tag{3.47}$$

where $N_1 = \langle y_1 - y_2, v_d \rangle / (\sqrt{2} \| v_d \|)$ is a r.v. with standard normal distribution and $\mathcal{X}_1^2$ is a r.v. with chi-square distribution with one degree of freedom. For the second term on the right side of (3.46), observe that $z_1 - \overline{y}$ and $y_1 - y_2$ are independent with distribution $N_d(0, \gamma I_d)$ and $N_d(0, 2I_d)$ respectively, where $\gamma = 3/2$. Thus, the terms in the sum of the inner product $\langle z_1 - \overline{y}, y_1 - y_2 \rangle = \sum_{k=1}^{d} (z_1^{(k)} - \overline{y}^{(k)})(y_1^{(k)} - y_2^{(k)})$ are independent identically distributed r.v.'s with mean 0 and variance 2γ. Then by the Central Limit Theorem (see [36, pp. 313])

$$\frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle}{(2\gamma d)^{1/2}} \xrightarrow{w} N_2, \tag{3.48}$$

where N_2 is a r.v. with standard normal distribution. By hypothesis we have $\| v_d \| = d^\delta$ with $1/2 < \delta < 1$, so let $2\epsilon = \delta - 1/2 > 0$ and note that

$$\frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle \langle y_1 - y_2, v_d\rangle}{2d \| v_d \|^2} = \frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle}{2^{1/2} d \| v_d \|} \frac{\langle y_1 - y_2, v_d\rangle}{2^{1/2} \| v_d \|}$$
$$\frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle}{2^{1/2} d^{\delta+1}} N_1 = \frac{\gamma^{1/2}}{d^{\epsilon+1}} \frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle}{(2\gamma d)^{1/2}} \frac{N_1}{d^\epsilon} \tag{3.49}$$

where N_1 is as before. Using (3.48) and the fact that $N_1/d^\epsilon \stackrel{w}{\to} 0$ as $d \to \infty$ we have

$$\gamma^{1/2} \frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle}{(2\gamma d)^{1/2}} \frac{N_1}{d^\epsilon} \stackrel{w}{\longrightarrow} 0.$$

Thus, from (3.49)

$$\frac{\langle z_1 - \overline{y}, y_1 - y_2\rangle \langle y_1 - y_2, v_d\rangle}{2d \| v_d \|^2} = O_P(d^{-(1+\epsilon)}), \tag{3.50}$$

as $d \to \infty$.

The Taylor expansion of the cosine is given by $\cos(x) = 1 - x^2/2 + O(x^4)$ in the limit as x tends to 0. So we can use this result and the fact that A_{SVM} and A_{MD} converge to 0 in probability as $d \to \infty$ by Theorem 3.2.1, to approximate the left side of (3.46) by

$$\frac{A^2_{SVM}}{2} - \frac{A^2_{MD}}{2}$$

when d is large. Therefore, from (3.46), (3.47) and (3.50)

$$A^2_{SVM} - A^2_{MD} = 2\frac{\mathcal{X}^2_1}{d} + O_P(d^{-(1+\epsilon)}),$$

as $d \to \infty$. □

The next theorem considers the case $0 < \delta < 1/2$, that is when the distance between classes is lower than the distance within classes and $\| v_d \| d^{-1/2} \to 0$. In this case we have that the MD method tends to be a little better than the SVM method when d is large because the difference between Angle(v_{SVM}, v_d) and Angle(v_{MD}, v_d) tends to be a multiple of a product-normal distribution (which is symmetric around zero) plus a multiple of a chi-square distribution. However, when d grows the two methods are indistinguishable because the multiple of the chi-square r.v. converges to zero faster than the multiple of the product-normal distribution. This provides a theoretical proof of the conjecture suggested by the simulation results shown in Figure 2a of [28], where the proportion of wrong classification of new data for the SVM method is always bigger than that for the MD method, and these proportions tend to the same value as the dimension increases, considering a Gaussian assumption for the data.

Theorem 3.3.2 (Case $m = 1$, $n = 2$) *Suppose $v_d = (d^\delta, 0, \ldots, 0)^\top$ with $0 < \delta < 1/2$. Let A_{SVM} and A_{MD} be as in Theorem 3.3.1, then*

$$A_{SVM} - A_{MD} = \frac{N_0}{d} + \frac{\mathcal{X}_1^2}{\gamma^{1/2} d^{3/2-\delta}} + O(d^{-(3/2-\delta+\epsilon')})$$
$$= \frac{N_0}{d} + O_p(d^{-(1+\epsilon)})$$

as $d \to \infty$ for some $\epsilon', \epsilon > 0$, where N_0 converges in distribution to the product of two independent standard normal random variables as $d \to \infty$ and $\mathcal{X}_1^2$ is a r.v. with the chi-square distribution with one degree of freedom.

Proof. Let z_1, $\overline{y}$, y_i, for $i = 1, 2$, be as in the proof of Theorem 3.2.1. Since $0 < \delta < 1/2$, by Lemma 3.3.1 when d is sufficiently large the orthogonal projection of x_1 onto the line passing through y_1 and y_2 is on the segment joining these vectors with probability approximately one. Therefore, for d sufficiently large we can consider this projection $\mathbf{p}$ as in (3.40) with a_1 and a_2 as in (3.41). Thus, when d is large enough $v_{SVM} = x_1 - \mathbf{p}$. As in the proof of Theorem 3.3.1, using (3.43) and the fact that by (3.33) $\| v_{SVM} \|^2 / d \xrightarrow{w} \gamma$ as $d \to \infty$, we have that for d sufficiently large

$$\cos(A_{MD}) - \cos(A_{SVM}) = \frac{\langle z_1 - \overline{y}, y_1 - y_2 \rangle \langle y_1 - y_2, v_d \rangle}{2\gamma^{1/2} d^{3/2} \| v_d \|} + \frac{\langle y_1 - y_2, v_d \rangle^2}{2\gamma^{1/2} d^{3/2} \| v_d \|}. \quad (3.51)$$

Since $\cos(\theta) = \sin(\frac{\pi}{2} - \theta)\ \forall \theta \in \mathbb{R}$, we have $\cos(A_{SVM}) = \sin(\frac{\pi}{2} - A_{SVM})$ and $\cos(A_{MD}) = \sin(\frac{\pi}{2} - A_{MD})$. By the Taylor expansion of the sine around zero, $\sin(x) = x + O(x^3)$ in the limit as x tends to 0, and the fact that $A_{SVM} \xrightarrow{w} \pi/2$, $A_{MD} \xrightarrow{w} \pi/2$ as $d \to \infty$ (by Theorem 3.2.1), we can approximate the left side of (3.51) by $A_{SVM} - A_{MD}$ when d is sufficiently large. The right side of (3.51) is equal to

$$\frac{(z_1^{(1)} - \overline{y}^{(1)})(y_1^{(1)} - y_2^{(1)})^2 + \sum_{k=2}^d (z_1^{(k)} - \overline{y}^{(k)})(y_1^{(k)} - y_2^{(k)})(y_1^{(1)} - y_2^{(1)})}{2\gamma^{1/2} d^{3/2}} + \frac{(y_1^{(1)} - y_2^{(1)})^2}{2\gamma^{1/2} d^{3/2-\delta}}$$
$$= R + K,$$

where

$$R = \frac{\sum_{k=2}^d (z_1^{(k)} - \overline{y}^{(k)})(y_1^{(k)} - y_2^{(k)})(y_1^{(1)} - y_2^{(1)})}{2\gamma^{1/2} d^{3/2}} = \frac{1}{d} \left(\frac{d-1}{d} \right)^2 N_1 \sum_{k=2}^d \frac{w_k}{(2\gamma)^{1/2} (d-1)^{1/2}}, \quad (3.52)$$

with $N_1 = (y_1^{(1)} - y_2^{(1)})/2^{1/2}$ a r.v. with standard normal distribution, $w_k = (z_1^{(k)} - \overline{y}^{(k)})(y_1^{(k)} - y_2^{(k)})$, for $k = 2, \ldots, d$, and

$$K = \frac{(y_1^{(1)} - y_2^{(1)})^2}{(2\gamma)^{1/2} d^{3/2-\delta}} + \frac{(z_1^{(1)} - \overline{y}^{(1)})(y_1^{(1)} - y_2^{(1)})^2}{2\gamma^{1/2} d^{3/2}}. \quad (3.53)$$

Note that w_k, $k = 2, 3, \ldots, d$, are i.i.d. random variables with $E(w_k) = 0$ and $\text{Var}(w_k) = 2\gamma$, then by the Central Limit Theorem the sum of the right side of (3.52) converges in distribution to a r.v. N_2 with standard normal distribution independent of N_1. Therefore, for d large enough we have that R is approximately equal to N_0/d, where N_0 is a random variable which converges in distribution to $N_1 N_2$ as $d \to \infty$. Thus we have

$$A_{SVM} - A_{MD} = \frac{N_0}{d} + K \qquad \text{as } d \to \infty. \tag{3.54}$$

Writing $\epsilon' = \delta/2 > 0$, we have

$$d^{3/2-\delta+\epsilon'} \frac{(z_1^{(1)} - \overline{y}^{(1)})(y_1^{(1)} - y_2^{(1)})^2}{2\gamma^{1/2} d^{3/2}} \xrightarrow{w} 0 \qquad \text{as } d \to \infty.$$

Therefore, the second term of K in (3.53) is $O_p(d^{-(3/2-\delta+\epsilon')})$ and

$$K = \frac{\mathcal{X}_1^2}{\gamma^{1/2} d^{3/2-\delta}} + O_p(d^{-(3/2-\delta+\epsilon')}), \tag{3.55}$$

where $\mathcal{X}_1^2 = (y_1^{(1)} - y_2^{(1)})^2/2$ has a chi-square distribution with one degree of freedom. Now, let $2\epsilon = 1/2 - \delta > 0$ and note that $d^{1+\epsilon} K \xrightarrow{w} 0$ as $d \to \infty$. Thus we also have

$$K = O_p(d^{-(1+\epsilon)}) \qquad \text{as } d \to \infty. \tag{3.56}$$

Therefore, from (3.54), (3.55) and (3.56)

$$\begin{aligned} A_{SVM} - A_{MD} &= \frac{N_0}{d} + \frac{\mathcal{X}_1^2}{\gamma^{1/2} d^{3/2-\delta}} + O_p(d^{-(3/2-\delta+\epsilon')}) \\ &= \frac{N_0}{d} + O_p(d^{-(1+\epsilon)}) \end{aligned}$$

$d \to \infty$. □

Finally for the case when $\delta > 1$, which is in the setting $\| v_d \| d^{-1/2} \to \infty$, we also have that the MD method tends to be better than the SVM method when d is large as we can see in the next theorem.

Theorem 3.3.3 (Case $m = 1$, $n = 2$) *Suppose $\| v_d \| = d^\delta$ with $\delta > 1$. Let A_{SVM} and A_{MD} be as in Theorem 3.3.1, then*

$$P(A_{SVM} > A_{MD}) \longrightarrow 1 \qquad \text{as } d \to \infty. \tag{3.57}$$

Proof. Let z_1, $\overline{y}$, y_i, for $i = 1, 2$, be as in the proof of Theorem 3.2.1. By Lemma 3.3.1, since $\delta > 1$ we have that the orthogonal projection of x_1 onto the line joining y_1 and y_2 tends to be outside the segment joining these vectors when $d \to \infty$, thus the closest point to x_1 in the segment joining y_1 and y_2 is y_1 or y_2. Let $\mathbf{p}_0$ be this point, note that $\mathbf{p}_0 = y_1$ if $\text{Angle}(x_1 - y_1, y_2 - y_1) > \pi/2$, that is if $\langle x_1 - y_1, y_2 - y_1 \rangle < 0$. Analogously, $\mathbf{p}_0 = y_2$ if $\langle x_1 - y_2, y_1 - y_2 \rangle < 0$. Let $\mathbf{I}_A$ be the indicator function of the set A. Then

$$\mathbf{p}_0 = y_1 \mathbf{I}_{[\langle x_1 - y_1, y_2 - y_1 \rangle < 0]} + y_2 \mathbf{I}_{[\langle x_1 - y_2, y_1 - y_2 \rangle < 0]}$$

and by (3.39) $P(\mathbf{p}_0 = y_1) = P(\langle x_1 - y_1, y_2 - y_1 \rangle < 0) \to 1/2$ as $d \to \infty$, analogously for y_2. Because the orthogonal vector of the SVM hyperplane is the difference between the two closest points of the convex hulls of the classes we have $v_{SVM} = x_1 - \mathbf{p}_0$.

As in the proof of Theorem 3.3.2 we can approximate $\cos(A_{MD}) - \cos(A_{SVM})$ by $A_{SVM} - A_{MD}$ as $d \to \infty$. Therefore, for d sufficiently large $P(A_{SVM} > A_{MD}) = P(A_{SVM} - A_{MD} > 0)$ is approximately

$$P(\cos(A_{MD}) - \cos(A_{SVM}) > 0) = P\left(\frac{\langle v_{MD}, v_d \rangle}{\| v_{MD} \| \| v_d \|} - \frac{\langle v_{SVM}, v_d \rangle}{\| v_{SVM} \| \| v_d \|} > 0 \right).$$

Since $\| v_{SVM} \|^2 / \| v_d \|^2 \xrightarrow{w} 1$, $\| v_{MD} \|^2 / \| v_d \|^2 \xrightarrow{w} 1$ as $d \to \infty$ by (3.32), we have that the last probability is approximately

$$\begin{aligned} P\left(\frac{\langle v_{MD}, v_d \rangle}{\| v_d \|^2} - \frac{\langle v_{SVM}, v_d \rangle}{\| v_d \|^2} > 0 \right) &= P(\langle x_1 - \overline{y}, v_d \rangle - \langle x_1 - \mathbf{p}_0, v_d \rangle > 0) \\ &= P(\langle \mathbf{p}_0 - \overline{y} \rangle > 0). \end{aligned}$$

Recall that from [19] the vectors z_1, y_1, y_2 tend to form an equilateral triangle as $d \to \infty$ because they are independent vectors with multivariate standard normal distribution. Thus $\text{Angle}(z_1 - y_i, \overline{y} - y_i) = \text{Angle}(z_1 - y_i, y_j - y_i)$ tends to be less than $\pi/2$ as $d \to \infty$ and therefore

$$P(\langle z_1 - y_i, \overline{y} - y_i \rangle > 0) \longrightarrow 1 \qquad \text{as } d \to \infty, \tag{3.58}$$

for $i, j \in \{1, 2\}$ and $i \neq j$.

Suppose $\mathbf{p}_0 = y_i$ for $i \in \{1, 2\}$, then $\langle x_1 - y_i, y_j - y_i \rangle < 0$ and $\langle x_1 - y_i, \overline{y} - y_i \rangle < 0$ but

$$\langle x_1 - y_i, \overline{y} - y_i \rangle = \langle z_1 - y_i, \overline{y} - y_i \rangle + \langle v_d, \overline{y} - y_i \rangle,$$

then

$$\langle \mathbf{p}_0 - \overline{y}, v_d \rangle = \langle y_i - \overline{y}, v_d \rangle \ > \ \langle z_1 - y_i, \overline{y} - y_i \rangle$$

and (3.58) implies that

$$P(\langle \mathbf{p}_0 - \overline{y}, v_d \rangle > 0) \longrightarrow 1 \qquad \text{as } d \to \infty.$$

Thus we have

$$P(A_{SVM} > A_{MD}) \longrightarrow 1$$

as $d \to \infty$. □

As a conclusion we have that the MD method seems to be better than the SVM method under the settings of the last three theorems. We conjecture that these results can be extended for the general case $m, n \geq 2$.

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