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# Topic 18: Eigenvalue and Spike Models

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Key points: .

**Disclaimer**: The note is built on Prof. Jinchi Lv's lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.

#### 18.1 Motivation

Consider n independent observations  $\mathbf{X}_i \in \mathbb{R}^p$  drawn from a  $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ , then the covariance can be decomposed into 2 parts, white noise and low rank

$$\Sigma = \text{Cov}(\mathbf{X}_i) = \mathbf{I} + \sum_{k=1}^{M} \theta_k \nu_k \nu_k' = \Sigma_0 + \mathbf{\Phi}$$

where M denotes the **number of spikes** in the distribution of eigenvalues. The idea is: spikes deviate from a reference model along a <u>small fixed number</u> of unknown directions. If  $\Phi = 0$ , then none of the sample eigenvalues is separated from the bulk.

**Why a spike model is interesting?** A spike model can help determine the latent dimension of the data, some examples being

- Principal component analysis (PCA): spikes are related to the directions of the most variations of the data, i.e., the principal components
- Clustering model: M spikes is equivalent to M+1 clusters
- Economic significance: *M* is related to the number of factor loadings

Then the question is threefold:

- How to determine *M*
- How to estimate  $v_k$
- How to test  $\theta_k$

Under rank one alternative, we would like to test the hypothesis

$$H_1: \mathbf{\Sigma} = \mathbf{I}_p + \theta \mathbf{\nu} \mathbf{\nu}', \theta > 0$$

against the null

$$H_0: \mathbf{\Sigma} = \mathbf{I}_p$$

with the key assumptions:

A1 Gaussian error

A2 large  $p: p \le n$  but allows  $p/n \to \gamma \in (0,1)$ 

Under these assumptions, for the  $n \times p$  data matrix  $\mathbf{X} = (\mathbf{X}'_1 \cdots \mathbf{X}'_n)'$ ,  $\mathbf{X}'\mathbf{X}$  has a p-dimensional **Wishart** distribution  $W_p(n, \Sigma)$  with the degree of freedom n and covariance matrix  $\Sigma$ , which is a *random matrix*.

If  $\mathbf{Y} = \mathbf{M} + \mathbf{X}$ , that is, the sum of the *random matrix*  $\mathbf{X}$  and a *deterministic matrix*  $\mathbf{M}$  (also  $n \times p$ ), then  $\mathbf{Y}'\mathbf{Y}$  has a p-dimensional Wishart distribution  $W_p(n, \Sigma, \Psi)$  with n degrees of freedom, covariance matrix  $\Sigma$  and non-centrality matrix  $\mathbf{\Psi} = \Sigma^{-1}\mathbf{M}'\mathbf{M}$ .

## Definition 18.1.1: Density of Wishart Distribution

The PDF of Wishart distribution is defined as

$$f(\mathbf{X}) = \frac{1}{2^{np/2} \Gamma_p\left(\frac{n}{2}\right) |\mathbf{\Sigma}|^{n/2}} |\mathbf{X}|^{(n-p-1)/2} \exp\left(-\frac{1}{2} \operatorname{tr}\left(\mathbf{\Sigma}^{-1} \mathbf{X}\right)\right)$$

where **X** is a symmetric positive semidefinite and  $\Gamma_p\left(\frac{n}{2}\right)$  is a multivariate gamma function such that

$$\Gamma_p\left(\frac{n}{2}\right) = \pi^{\frac{p(p-1)}{4}} \prod_{j=1}^p \Gamma\left(\frac{n}{2} - \frac{j-1}{2}\right)$$

Notice that the sample covariance matrix  $S = \frac{1}{n}X'X$  is just a scaled version of Wishart distribution

$$n\mathbf{S} = \mathbf{X}'\mathbf{X} \sim W_n(n, \mathbf{\Sigma})$$

For  $\Sigma = \mathbf{I}_p$ , the empirical distribution fo eigenvalues converges to Marcenko-Pastur distribution

$$f^{\text{MP}}(x) = \frac{1}{2\pi\gamma x} \sqrt{(b_+ - x)(x - b_-)}$$

where  $b_{\pm} = (1 \pm \sqrt{\gamma})^2$ . Then:

• under  $H_0: \Sigma = \mathbf{I}_p$ , we have

$$n^{2/3} \left( \frac{\lambda_1 - \mu(\gamma)}{\sigma(\gamma)} \right) \stackrel{d}{\to} TW_1$$

where TW<sub>1</sub> is the Tracy-Widom distribution

• under  $H_1: \Sigma = \mathbf{I}_p + \theta \nu \nu', \theta > 0$ , if  $\theta$  is strong  $(\theta \gg \sqrt{\gamma})$ , then

$$n^{1/2}\left(\frac{\lambda_1-\rho(\theta,\gamma)}{\tau(\theta,\gamma)}\right) \xrightarrow{d} \mathcal{N}(0,1)$$

Here, the largest eigenvalue test is the best test. **But** when the signal is weak  $(0 \le \theta < \sqrt{\gamma})$ , the largest eigenvalue under the alternative converges to the same distribution as null:

$$n^{2/3} \left( \frac{\lambda_1 - \rho(\theta, \gamma)}{\tau(\theta, \gamma)} \right) \xrightarrow{d} TW_1$$

which means that the largest eigenvalue test *fails*. On top of this, **resampling** also fails when p is large. Next, we develop another test to cope with these problems.



Figure 18.1: Failure of Resampling Test (n = p = 100)

# 18.2 Johnstone and Onatski (2020)

Consider the basic equation of classical multivariate statistics:

$$\det\left(\mathbf{H} - \mathbf{x}\mathbf{E}\right) = 0\tag{18.1}$$

with  $p \times p$  matrices

$$n_1\mathbf{H} = \sum_{k=1}^{n_1} \mathbf{x}_k \mathbf{x}'_k$$
 hypothesis SS
$$n_1\mathbf{E} = \sum_{k=1}^{n_1} \mathbf{z}_k \mathbf{z}'_k$$
 error SS

The solution  $\mathbf{x}$  is generalized eigenvalues  $\{\lambda_i\}_{i=1}^p$ , which are the eigenvalue of  $\mathbf{F}$ -ratio  $\mathbf{E}^{-1}\mathbf{H}$ . Johnstone and Onatski (2020) summarized 5 topics using  $\mathbf{E}^{-1}\mathbf{H}$  relying on the five most common hypergeometric functions  $\mathbf{E}^{-1}\mathbf{H}$  relying on the five most common hypergeometric functions  $\mathbf{E}^{-1}\mathbf{H}$  relying on the five most common hypergeometric functions  $\mathbf{E}^{-1}\mathbf{H}$ 

• scalar inputs

$${}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;x) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_p)_k} \frac{x^k}{k!}$$

where  $(a_i)_k$  are generalized Pochhammer symbols

- single matrix inputs, where  $\boldsymbol{S}$  is symmetric and usually diagonal

$${}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{S}) = \sum_{k=0}^{\infty} \sum_{\kappa} \frac{(a_1)_{\kappa} \cdots (a_p)_{\kappa}}{(b_1)_{\kappa} \cdots (b_p)_{\kappa}} \frac{C_{\kappa}(\mathbf{S})}{k!}$$

where  $C_k$  are the zonal polynomials. Easily,  $_0\mathcal{F}_0(\mathbf{S}) = e^{\operatorname{tr}(\mathbf{S})}, _1\mathcal{F}_0(a,\mathbf{S}) = |\mathbf{I} - \mathbf{S}|^{-a}$ 

- two matrix inputs, where  $\boldsymbol{S},\boldsymbol{T}$  are both symmetric

$$_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{S},\mathbf{T}) = \int_{O(p)} {}_{\mathbf{p}}\mathcal{F}_{\mathbf{q}}(a,b;\mathbf{SUTU'})(d)\mathbf{U}$$

<sup>&</sup>lt;sup>1</sup>Hypergeometric functions are:

		Statistical method	$n_1\mathbf{H}$	$n_2\mathbf{E}$	Univariate Analog
$_0\mathcal{F}_0$	PCA	Principal components analysis	$W_p(n_1, \Sigma + \Phi)$	$n_2\Sigma$	$\chi^2$
$_1\mathcal{F}_0$	SigD	Signal detection	$W_p(n_1, \Sigma + \Phi)$	$W_p(n_2, \Sigma)$	non-central $\chi^2$
$_0\mathcal{F}_1$	$REG_0$	Multivariate regression, with known error	$W_p(n_1, \Sigma, n_1\mathbf{\Phi})$	$n_2\Sigma$	F
$_1\mathcal{F}_1$	REG	Multivariate regression, with unknown error	$W_p(n_1, \mathbf{\Sigma}, n_1\mathbf{\Phi})$	$W_p(n_2, \Sigma)$	non-central F
$_2\mathcal{F}_1$	CCA	Canonical correlation analysis	$W_p(n_1, \Sigma, \Phi(\mathbf{Y}))$	$W_p(n_2, \Sigma)$	$\frac{r^2}{1-r^2}$

Table 18.1: 5 Statistical Methods

For  $_0\mathcal{F}_0$  and  $_0\mathcal{F}_1$ , **E** is deterministic,  $\Sigma$  is known,  $n_2$  disppears, otherwise **E** is independent of **H**.

## 18.2.1 Definitions and global assumptions

Let **Z** be an  $n \times p$  data matrix with rows (observations) drawn **i.i.d.** from  $\mathcal{N}_p(\mathbf{0}, \Sigma)$ , and a deterministic matrix **M** of  $n \times p$ , then for  $\mathbf{Y} = \mathbf{M} + \mathbf{Z}$ ,

- $\mathbf{H} = \mathbf{Y'Y}$  has a p dimensional Wishart distribution  $W_p(n, \Sigma, \Psi)$  with n degrees of freedom, covariance matrix  $\Sigma$  and non-centrality matrix  $\Psi = \Sigma^{-1}\mathbf{M'M}$
- the corresponding central Wishart distribution with  $\mathbf{M} = \mathbf{0}$  is  $W_p(n, \Sigma)$

Johnstone and Onatski (2020) assume a relative low dimensionality  $p \le \min\{n_1, n_2\}$  where  $n_1, n_2$  are the degrees of freedom as in Table 18.1, where

- $p \le n_2$  ensures almost sure invertibility of matrix **E** in Equation 18.1
- $p \le n_1$  is not essential, but reduces the number of various situations of consideration.

#### 18.2.2 5 classes of problems

With these assumptions, they established a unified statistical problem **symmetric matrix denoising (SMD)** that can be linked to the 5 classes of problems:

**PCA**  $n_1$  i.i.d. observations drawn from  $\mathcal{N}_p(\mathbf{0}, \mathbf{\Omega})$  to test the hull hypothesis that the population covariance  $\mathbf{\Omega} = \mathbf{\Sigma}$ , with the alternative of interest being

$$\Omega = \Sigma + \Phi$$
, with  $\Phi = \theta \phi \phi'$ 

where  $\theta > 0$ ,  $\phi$  are unknown, and  $\phi$  is normalized s.t.  $\|\Sigma^{-1/2}\phi\| = 1$ . W.L.O.G., assume  $\Sigma = \mathbf{I}_p$ , then under the alternative, the first principal component explains a larger portion of the variation than the other principal components. Re-formulate the hypotheses in terms of the spectral *spike* parameter  $\theta$ , we have

$$H_0: \theta_0 = 0$$
  $H_1: \theta_0 = \theta > 0$  (18.2)

where  $\theta_0$  is the true value of the *spike*. A **maximal invariant statistic** consists of the solutions  $\lambda_1 \ge \cdots \ge \lambda_p$  of Equation 18.1 with

- *n*<sub>1</sub>**H** equal to the sample covariance matrix
- $\mathbf{E} = \mathbf{\Sigma}$

**SigD** Now consider testing the **equality** of covariance matrices  $\Omega$  and  $\Sigma$ , corresponding to 2 independent p-dimensional mean-zero Gaussian samples of size  $n_1$  and  $n_2$ , with the alternative still

$$\Omega = \Sigma + \Phi$$
, with  $\Phi = \theta \phi \phi'$ 

and again, assume  $\Sigma = I_v$  (but NOT necessarily known), here, instead of Equation 18.1, consider

$$\det\left(\mathbf{H} - \lambda \left(\mathbf{E} + \frac{n_1}{n_2}\mathbf{H}\right)\right) = 0 \tag{18.3}$$

naturally, SigD reduces to PCA as  $n_2 \rightarrow \infty$  while  $n_1$  and p held constant.

**REG**<sub>0</sub> Next, consider a linear regression with multivariate response

$$Y = X\beta + \epsilon$$

with known covariance matrix  $\Sigma$  of the i.i.d. Gaussian rows of the error matrix  $\epsilon$ . Here, to test linear restrictions on the matrix of coefficients  $\beta$ , we can split the matrix of transformed response variables Y into 3 parts  $Y_1$ ,  $Y_2$ ,  $Y_3$ , where

•  $\mathbf{Y}_1$  is  $n_1 \times p$  where p is the number of response variables,  $n_1$  is the number of linear restrictions (per each of the p columns of matrix  $\boldsymbol{\beta}$ ), under the null  $H_0$ :  $\mathbb{E}\mathbf{Y}_1 = 0$ , versus the alternative

$$\mathbb{E}\mathbf{Y}_1 = \sqrt{n_1 \theta} \boldsymbol{\psi} \boldsymbol{\phi}' \tag{18.4}$$

where  $\theta > 0$ ,  $\left\| \mathbf{\Sigma}^{-1/2} \boldsymbol{\phi} \right\| = 1$  and  $\left\| \boldsymbol{\psi} \right\| = 1$ 

- $\mathbf{Y}_2$  is  $(q n_1) \times p$ , where q is the number of regressors
- $\mathbf{Y}_3$  is  $(T q) \times p$ , where T is the number of observations

In this case, tests can be based on the solutions  $\lambda_1, \dots, \lambda_p$  to

$$\det(\mathbf{H} - \lambda \mathbf{E}) = \mathbf{0}$$

where  $\mathbf{H} = \mathbf{Y}_1'\mathbf{Y}_1/n_1$  and  $\mathbf{E} = \mathbf{\Sigma}$ . The solutions represent a multivaraite analog of the difference between the sum of squared residuals in the restircted and unrestricted regressions. Under the null,  $n_1\mathbf{H}$  is distributed as  $W_p(n_1, \mathbf{\Sigma})$ . Here,

$$n_1 \mathbf{H} \sim W_p(n_1, \Sigma)$$
 under  $H_0$   
 $n_1 \mathbf{H} \sim W_p(n_1, \Sigma, n_1 \Phi)$ , where  $\Phi = \theta \Sigma^{-1} \phi \phi'$  under  $H_1$ 

Again, W.L.O.G, assume  $\Sigma = \mathbf{I}_p$ . This **canonical form** of REG<sub>0</sub> is essentially equivalent to the setting of **matrix denoising** 

$$Y_1 = M + Z$$

**REG** Again, consider the linear regression

$$Y = X\beta + \epsilon$$

but NOT knowing the covariance matrix  $\Sigma$  of rows of  $\epsilon$ . Here, the solutions again solve  $\det(H - \lambda E) = 0$  with

$$\mathbf{H} = \mathbf{Y}_{1}'\mathbf{Y}_{1}/n_{1}, \ \mathbf{E} = \mathbf{Y}_{3}'\mathbf{Y}_{3}/n_{2}$$

this represents a multivariate analog of the F ratio: the difference between the sum of squared residuals in the restricted and unrestricted regressions to the sum of squared residuals in the restricted regression. Again, as  $n_2 \to \infty$ , REG reduces to REG<sub>0</sub>.

**CCA** Consider testing for independence between Gaussian vectors  $x_t \in \mathbb{R}^p$  and  $y_t \in \mathbb{R}^{n_1}$ , given zero-mean observations with  $t = 1, \dots, n_1 + n_2$ . Partition the population and sample covariance matrices of the observations  $(x'_t, y'_t)'$  into

$$\begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix} \qquad \begin{pmatrix} \mathbf{S}_{xx} & \mathbf{S}_{xy} \\ \mathbf{S}_{yx} & \mathbf{S}_{yy} \end{pmatrix}$$

respsectively. Under  $H_0: \Sigma_{xy} = \mathbf{0}$ , while the alternative is

$$\Sigma_{xy} = \sqrt{\frac{n_1 \theta}{n_1 \theta + n_1 + n_2}} \phi \psi' \tag{18.5}$$

where the nuisance parameters  $\phi \in \mathbb{R}^p$  and  $\psi \in \mathbb{R}^{n_1}$  are normalized s.t.

$$\left\|\boldsymbol{\Sigma}_{xx}^{-1/2}\boldsymbol{\phi}\right\| = \left\|\boldsymbol{\Sigma}_{yy}^{-1/2}\boldsymbol{\psi}\right\| = 1$$

And the test can be based on the squared sample canonical correlations  $\lambda_1, \cdots, \lambda_p$  that solves

$$\det\left(\mathbf{H} - \lambda \mathbf{E}\right) = \mathbf{0}$$

with

$$\mathbf{H} = \mathbf{S}_{xy} \mathbf{S}_{yy}^{-1} \mathbf{S}_{yx}$$
 
$$\mathbf{E} \mathbf{S}_{xx}$$

#### 18.2.3 SMD

For a  $\mathbf{X} = \mathbf{\Phi} + \mathbf{Z}/\sqrt{p}$  where  $\mathbf{Z}$  is a noise matrix from the **Gaussian Orthogonal Ensemble** (GOE)<sup>2</sup> We seek to make inference about a symmetric rank-one *signal* matrix  $\mathbf{\Phi} = \theta \phi \phi'$ . The null and the alternative is again as in 18.2. The nuisance vector  $\boldsymbol{\phi} \in \mathbb{R}^p$  is normalized s.t.  $\|\boldsymbol{\phi}\| = 1$ .

The problem remains **invariant** under the multiplication of X from the left by an orthogonal matrix, and from the right by its transpose. A maximal invariant statistic consists of the solutions  $\lambda_1, \dots, \lambda_p$  to  $\det(H - \lambda E) = 0$  with H = X and  $E = I_p$ .

SMD can be viewed as a degenerate version of the 5 classes of problems, as shown in Figure 18.2:

- SMD, PCA, REG<sub>0</sub>: random H and deterministic E
- PCA and SigD are parallel to REG<sub>0</sub>
- CCA has a different structure of H and E

#### 18.2.4 The likelihood ratios

The goal is to study the asymptotic behavior of likelihood ratios based on the observed eigenvalues

$$\Lambda = \operatorname{diag}\left\{\lambda_1, \cdots, \lambda_p\right\}$$

$$\mathbf{Z}_{ii} \sim \mathcal{N}(0,2)$$

$$\mathbf{Z}_{ij} \sim \mathcal{N}(0,1)$$
 if  $i > j$ 

<sup>&</sup>lt;sup>2</sup>**Z** is from the GOE that it is **symmetric** and



Figure 18.2: SMD and 5 Classes of Statistical Problems

then the likelihood of the alternative versus the null is given by

$$\mathcal{L}(\theta, \Lambda) = \frac{p(\Lambda; \theta)}{p(\Lambda; 0)} = \alpha(\theta)_{p} \mathcal{D}_{q}(\mathbf{a}, \mathbf{b}; \mathbf{\Phi}, \Lambda)$$
(18.6)

where  $\Phi = \Phi(\theta)$  is a *p*-dimensional matrix diag  $\{\Phi_{11}, 0, \dots, 0\}$ . Consider the hypergeometric functions of 2 matrix arguments  $\Phi$ ,  $\Lambda$  are defined as

$${}_{p}\mathcal{F}_{q}(\mathbf{a},\mathbf{b};\mathbf{\Phi},\mathbf{\Lambda}) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\kappa-k} \frac{(a_{1})_{\kappa} \cdots (a_{p})_{\kappa}}{(b_{1})_{\kappa} \cdots (b_{1})_{\kappa}} \frac{C_{\kappa}(\mathbf{\Phi})C_{\kappa}(\mathbf{\Lambda})}{C_{\kappa}(\mathbf{I}_{p})}$$

where  $\mathbf{a} = (a_1, \dots, a_p)$  and  $\mathbf{b} = (b_1, \dots, b_q)$  are parameters,  $\kappa$  are partitions of the integer k,  $(a_j)_{\kappa}$  and  $(b_i)_{\kappa}$  are the generalized Pochhammer symbols,  $C_{\kappa}$  are the zonal polynomials. For each of the 6 classes of problems, we have the parameters as in Table where  $n = n_1 + n_2$ .

Table 18.2: Parameters of the Likelihood Ratios in Eq.18.6

Classes	$_{ m p}\mathcal{F}_{ m q}$	$\alpha(\theta)$	а	b	$\mathbf{\Phi}_{11}$
SMD	$_0\mathcal{F}_0$	$\exp(-p\theta^2/4)$	-	-	$\theta p/2$
PCA	$_0\mathcal{F}_0$	$(1+\theta)^{-n_1/2}$	-	-	$\theta n_1/(2(1+\theta))$
SigD	$_1\mathcal{F}_0$	$(1+\theta)^{-n_1/2}$	-	-	$\theta n_1/(n_2(1+\theta))$
$REG_0$	$_0\mathcal{F}_1$	$\exp(-n_1\theta/2)$	-	$n_1/2$	$\theta n_1^2/4$
REG	$_1\mathcal{F}_1$	$\exp(-n_1\theta/2)$	n/2	$n_1/2$	$\theta n_1^2/(2n_2)$
CCA	$_2\mathcal{F}_1$	$(1+n_1\theta/n)^{-n/2}$	(n/2, n/2)	$n_1/2$	$\theta n_1^2/(n_2^2 + n_2 n_1(1+\theta))$

Some links in Fig.18.2 can also be established via asymptotic relations between hypergeometric functions.

**Asymptotic behavior of the likelihood ratios** consider that as  $n_1, n_2, p$  go to infinity so that

$$c_1 \equiv \frac{p}{n_1} \to \gamma_1 \in (0, 1)$$
  $c_2 \equiv \frac{p}{n_2} \to \gamma_2 \in (0, 1]$  (18.7)

which can be denoted as  $\mathbf{n}$ ,  $p \to_{\gamma} \infty$  where  $\mathbf{n} = \{n_1, n_2\}$  and  $\gamma = \{\gamma_1, \gamma_2\}$ .

- **Under the null** (the true value of the spike  $\theta_0 = 0$ ),  $\lambda_1, \dots, \lambda_p$  are the eigenvalues of
  - $GOE/\sqrt{p}$ , for **SMD**
  - $W_p(n_1, \mathbf{I}_p)/n_1$ , for **PCA** and **REG**<sub>0</sub>
  - a p-dimensional multivariate beta matrix with parameters  $n_1/2$  and  $n_2/2$  (here scaled by a factor of  $n_2/n_1$ ), for **SigD**, **REG**, **CCA**

and the empirical distribution of  $\lambda_1, \dots, \lambda_p$  follows

$$\hat{F} = \frac{1}{p} \sum_{j=1}^{p} I \left\{ \lambda_{j} \leq \lambda \right\} \xrightarrow{a.s.} F_{\gamma} = \begin{cases} F^{SC} & \text{semi-circle distribution, for SMD} \\ F^{MP} & \text{Marchenko-Pastur distribution, for PCA, REG}_{0} \end{cases}$$

$$F^{W} & \text{Wachter distribution, for SigD, REG, CCA}$$

A summary of the 3 classes of distributions is shown in Table 18.3. And the cumulative distribution functions  $F_{\nu}^{\text{lim}}(\lambda)$  are linked in the sense that

$$F_{\gamma}^{W}(\lambda) \to F_{\gamma_{1}}^{MP}(\lambda) \qquad \qquad \gamma_{2} \to 0$$
$$F_{\gamma_{1}}^{MP}(\sqrt{\gamma_{1}}\lambda + 1) \to F^{SC}(\lambda) \qquad \qquad \gamma_{1} \to 0$$

If  $\varphi$  is a *well-behaved* function, the centered **linear spectral statistic** 

$$\sum_{j=1}^{p} \varphi(\lambda_j) - p \int \varphi(\lambda)(d) F_{\mathbf{c}}^{\lim}(\lambda)$$
(18.8)

converges in distribtuion to a Gaussian random variable in each of the semicircle, Marchenko-Pastur and Wachter cases.<sup>3</sup>

Table 18.3: Semi-circle, Marchenko-Pastur, scaled Wachter distributions

Case	$F_{\gamma}^{\mathrm{lim}}$	Density, $\lambda \in [\beta, \beta_+]$	$eta_\pm$	Threshold $\overline{\theta}$		
SMD	SC	$rac{R(\lambda)}{2\pi} \ R(\lambda)$	±2	1		
PCA, REG <sub>0</sub>	MP	$\frac{R(\lambda)}{2\pi\gamma_1\lambda}$	$(1 \pm \sqrt{\gamma_1})^2$	$\sqrt{\gamma_1}$		
SigD, REG, CCA	W	$\frac{(\gamma_1 + \gamma_2)R(\lambda)}{2\pi\gamma_1\lambda(\gamma_1 - \gamma_2\lambda)}$	$\gamma_1 \left( \frac{\rho \pm 1}{\rho \pm \gamma_2} \right)^2$	$\frac{\rho + \gamma_2}{1 - \gamma_2}$		
where $R(\lambda) = \sqrt{(\beta_+ - \lambda)(\lambda - \beta)}$ , $\rho = \sqrt{\gamma_1 + \gamma_2 - \gamma_1 \gamma_2}$						

#### • Under the alternative

- when  $\theta \leq \overline{\theta}$  (in Tab.18.3), the top eigenvalue  $\lambda_1 \to \beta_+$ , the upper boundary of support of  $F_{\gamma}$  almost surely
- when  $\theta > \overline{\theta}$ ,  $\lambda_1$  **separates** from *he bulk* of the other eigenvalues and a.s. converges to a point strictly above  $\beta_+$

#### Hence,

- under the *super-critical* cases where  $\theta > \overline{\theta}$ , the likelihood ratio degenerates, the sequences of measures corresponding to the distributions of  $\Lambda$  under the null and under the *super-critical* alternatives are asymptotically mutually singular as  $\mathbf{n}$ ,  $p \xrightarrow{\gamma} \infty$  for SMD and PCA.
- under the <u>sub-critical</u> cases where  $\theta < \overline{\theta}$ , the likelihood ratio converges to a Guassian process, the sequences of measures corresponding to the distribution of  $\Lambda$  under the null and under the <u>sub-critical</u> alternatives are mutually <u>contiguous</u>.

<sup>&</sup>lt;sup>3</sup>The centering constant is defined in terms of  $F_c = \{c_1, c_2\}$ , that is, the *correct centering* can be computed using the densities in Tab.18.3, where  $\gamma_1, \gamma_2$  are replaced by  $c_1 \equiv p/n_1, c_2 \equiv p/n_2$  respectively.

**Contour integral representation** The asymptotic behavioral of the likelihood ratios (Eq.18.6) depends on that of  ${}_p\mathcal{F}_q(a,b;\Psi,\Lambda)$ , of which the asymptotics are well established when the dimension of the matrix arguments remain **fixed**. Now consider the case where  $\Phi$ ,  $\Lambda$  diverge to infinity. In single-spiked models,  $\Phi$  has rank one, then  ${}_p\mathcal{F}_q(a,b;\Psi,\Lambda)$  can be represented in the form of a **contour integral** of a hypergeometric function of a single scalar argument:

### Lemma 18.2.1: Contour Integral Representations for Likelihood Ratios

Assume  $p \le \min\{n_1, n_2\}$ , let  $\mathcal{K}$  be a contour in the complex plan  $\mathbb{C}$  taht starts at  $-\infty$ , encircles 0 and  $\lambda_1, \dots, \lambda_p$  counter-clockwise, returning to  $-\infty$ , then

$$\mathcal{L}(\theta; \mathbf{\Lambda}) = \frac{\Gamma(s+1)\alpha(\theta)q_s}{\mathbf{\Phi}_{11}^s 2\pi i} \int_{\mathcal{K}} {}_{\mathbf{p}} \mathcal{F}_{\mathbf{q}}(a-s, b-s; \mathbf{\Psi}_{11}z) \prod_{j=1}^p (z-\lambda_j)^{-1/2} dz$$
 (18.9)

where s = p/2 - 1, the values of  $\alpha(\theta)$ ,  $\Phi_{11}$ , a, b, p, q for difference cases are given in Tab.18.2, and a - s, b - s are vectors with elements  $a_i - s$ ,  $b_j - s$  respectively,

$$q_s = \prod_{j=1}^{p} \frac{\Gamma(a_j - s)}{\Gamma(a_j)} \prod_{i=1}^{q} \frac{\Gamma(b_i)}{\Gamma(b_i - s)}$$

next, we want to approximate 18.9 in a Laplace form, that is, to make the right-hand side looks like

$$\mathcal{L}(\theta; \mathbf{\Lambda}) = \sqrt{\pi p} \frac{1}{2\pi i} \int_{\mathcal{K}} \exp\left\{-\left(\frac{p}{2}\right) f(z; \theta)\right\} g(z; \theta) dz$$
 (18.10)

The goal of the transformation is to have the function  $f(\cdot)$ ,  $g(\cdot)$  will have the forms of a sum and a product:

$$f(z) = f_c + f_e(z) + f_h(z)$$
  

$$g(z) = g_c \times g_e(z) \times g_h(z)$$

where  $f_c$  and  $g_c$  do not depend on z.

The transformation from Eq.18.9 to Eq.18.10 is done in 3 steps:

• first

$$\frac{\Gamma(s+1)\alpha(\theta)q_s}{\Phi_{11}^s 2\pi i} = \exp\left\{-\frac{p}{2}f_c\right\}g_c \tag{18.11}$$

where  $g_c$  remains bounded as  $\mathbf{n}, p \xrightarrow{\gamma} \infty$ , and the values of  $f_c$  and  $g_c$  are given as Tab.18.4<sup>4</sup>

· second, consider

$$\prod_{j=1}^{p} (z - \lambda_j)^{-1/2} = \exp\left\{-\frac{p}{2} f_e(z)\right\} g_e(z)$$
 (18.12)

where

$$f_e(z) \int \ln(z - \lambda) dF_c(\lambda)$$
 (18.13)

$$g_e(z) \exp\left\{-\frac{p}{2} \int \ln(z-\lambda) d\left(\hat{F}(\lambda) - F_c(\lambda)\right)\right\} \qquad \xrightarrow{\mathbf{n}, p \xrightarrow{\gamma} \infty} \text{Gaussian random variable}$$
 (18.14)

<sup>4</sup>In Tab.18.4 the terms o(1) do **not** depend on  $\theta$ .  $l(\theta) = 1 + \frac{(1+\theta)c_2}{c_1}$ ,  $r^2 = c_1 + c_2 - c_1c_2$ ,  $f_{10} = -1 - \frac{r^2}{c_1c_2}\log\frac{r^2}{c_1+c_2} + \log\frac{c_1+c_2}{c_1}$ ,  $\check{g}_{10} = c_1^{-1}r(c_1+c_2)^{1/2}$ ,  $f_{21} = -1 - \frac{\theta}{c_1} - \frac{r^2}{c_1c_2}\log\frac{r^2}{c_1l(\theta)}$ .

Table 18.4: Values of  $f_c$  and  $\check{g}_c = \frac{g_c}{1+o(1)}$ 

for  $f_e(z)$  and  $g_e(z)$  to be well-defined,  $z \notin \text{supp}(F_c)$  and  $z \notin \text{supp}(\hat{F})$ .

• third, consider

$$_{p}\mathcal{F}_{q}(a-s,b-s,\mathbf{\Phi}_{11}z) = \exp\left\{-\frac{p}{2}f_{h}(z)\right\}g_{h}(z)$$
 (18.15)

where

$$f_h(z) = \begin{cases} -z\theta & \text{SMD} \\ -z\frac{\theta}{c_1(1+\theta)} & \text{PCA} \\ \ln\left[1 - \frac{c_2z\theta}{c_1(1+\theta)}\right]\frac{r^2}{c_1c_2} & \text{SigD} \end{cases}$$

$$g_h(z) = \begin{cases} 1 & \text{SMD, PCA} \\ \left[1 - \frac{c_2z\theta}{c_1(1+\theta)}\right]^{-1} & \text{SigD} \end{cases}$$

$$(18.16)$$

$$g_h(z) = \begin{cases} 1 & \text{SMD, PCA} \\ \left[1 - \frac{c_2 z \theta}{c_1 (1 + \theta)}\right]^{-1} & \text{SigD} \end{cases}$$
 (18.17)

- when q=0,  $_p\mathcal{F}_q$  can be expressed in terms of elementary functions:  $_0\mathcal{F}_0(z)=e^z$ ,  $_1\mathcal{F}_0(a;z)=(1-z)^{-a}$
- when q = 1,  $p\hat{\mathcal{F}}_q$  can **NOT** be represented exactly in terms of elementary functions. Hence, consider the asymptotic approximations

$${}_{p}\mathcal{F}_{q} = \begin{cases} {}_{0}\mathcal{F}_{1}(m+1; m^{2}\eta_{0}) \equiv F_{0} & \text{REG}_{0} \\ {}_{1}\mathcal{F}_{1}(m\kappa+1; m+1; m\eta_{1}) \equiv F_{1} & \text{REG} \\ {}_{2}\mathcal{F}_{1}(m\kappa+1; m\kappa+1; m+1; \eta_{2}) \equiv F_{2} & \text{CCA} \end{cases}$$
(18.18)

where  $m = \frac{n_1 - p}{2}$ ,  $\kappa = \frac{n - p}{n_1 - p}$ , and

$$\eta_{j} \begin{cases} \frac{z\theta}{(1-c_{1})^{2}} & j = 0\\ \frac{z\theta c_{2}}{c_{1}(1-c_{1})} & j = 1\\ \frac{z\theta c_{2}^{2}}{c_{1}^{2}l(\theta)} & j = 2, l(\theta) = 1 + \frac{(1+\theta)c_{2}}{c_{1}} \end{cases}$$

Johnstone and Onatski (2020) outlined the asymptotics of  $F_i$ , j = 0, 1, 2 as

\* j=0: Let  $\varphi_0(t) = \ln t - t - \eta_0/t + 1$  and  $t_0 = (1 + \sqrt{1 + t\eta_0})/2$ , and  $\forall \delta > 0$ , let  $\Omega_{0\delta}$  be the set of  $\eta_0 \in \mathbb{C}$ s.t.  $|\arg \eta_0| \le \pi - \delta$ , then as  $m \to \infty$ , we have

$$F_0 = (1 + 4\eta_0)^{-1/4} \exp\{-m\varphi_0(t_0)\} (1 + o(1))$$

\* j=1,2: consider the contour integral representations

$$F_j = \frac{C_m}{2\pi i} \int_0^{(1+)} \exp\left\{-m\varphi_j(t)\right\} \psi_j(t) dt$$

where

$$C_m = \frac{\Gamma(m+1)\Gamma(m(\kappa-1)+1)}{\Gamma(m\kappa+1)}$$

and

$$\varphi_j(t) = \begin{cases} -\eta_j t - \kappa \ln t + (\kappa - 1) \ln(t - 1), & j = 1 \\ -\kappa \ln(t/(1 - \eta_j t)) + (\kappa - 1) \ln(t - 1), & j = 2 \end{cases} \qquad \psi_j(t) = \begin{cases} (t - 1)^{-1}, & j = 1 \\ (t - 1)^{-1}(1 - \eta_j t)^{-1}, & j = 2 \end{cases}$$

the relevant saddle points are given as

$$t_{j} = \begin{cases} \frac{1}{2\eta_{j}} \left\{ \eta_{j} - 1 + \sqrt{(\eta_{j} - 1)^{2} + 4\kappa\eta_{j}} \right\}, & j = 1\\ \frac{1}{2\eta_{j}(\kappa - 1)} \left\{ -1 + \sqrt{1 + 4\kappa(\kappa - 1)\eta_{j}} \right\}, & j = 2 \end{cases}$$

then as  $m \to \infty$ , for j = 1, 2

$$F_{j} = C_{m} \psi_{j}(t_{j}) e^{-iw_{j}/2} \left| 2\pi m \varphi_{j}''(t_{j}) \right|^{-1/2} \exp \left\{ -m \varphi_{j}(t_{j}) \right\} (1 + o(1))$$

# References

Iain M Johnstone and Alexei Onatski. Testing in high-dimensional spiked models. *The Annals of Statistics*, 48(3), 2020.