

## 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  $\mathcal{N}(\mathbf{0}, \Sigma)$ , then the covariance can be decomposed into 2 parts, white noise and low rank

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

where  $M$  denotes the **number of spikes** in the distribution of eigenvalues. The idea is: spikes deviate from a reference model along a **small fixed number** of unknown directions. If  $\Phi = \mathbf{0}$ , 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  $\mathbf{v}_k$
- How to test  $\theta_k$

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

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

against the null

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

with the key assumptions:

A1 Gaussian error

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

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  $\Psi = \Sigma^{-1}\mathbf{M}'\mathbf{M}$ .

#### Definition 18.1.1: Density of Wishart Distribution

The PDF of Wishart distribution is defined as

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

where  $\mathbf{X}$  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  $\mathbf{S} = \frac{1}{n}\mathbf{X}'\mathbf{X}$  is just a scaled version of Wishart distribution

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

For  $\Sigma = \mathbf{I}_p$ , the empirical distribution for 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

$$n^{2/3} \left( \frac{\lambda_1 - \mu(\gamma)}{\sigma(\gamma)} \right) \xrightarrow{d} \text{TW}_1$$

where  $\text{TW}_1$  is the Tracy-Widom distribution

- under  $H_1 : \Sigma = \mathbf{I}_p + \theta \mathbf{v}\mathbf{v}'$ ,  $\theta > 0$ , 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 ( $0 \leq \theta < \sqrt{\gamma}$ ), the largest eigenvalue under the alternative converges to the same distribution as null:

$$n^{2/3} \left( \frac{\lambda_1 - \rho(\theta, \gamma)}{\tau(\theta, \gamma)} \right) \xrightarrow{d} \text{TW}_1$$

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:

$$\det(\mathbf{H} - \mathbf{x}\mathbf{E}) = 0 \quad (18.1)$$

with  $p \times p$  matrices

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

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

${}_p\mathcal{F}_q$

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<sup>1</sup>Hypergeometric functions are:

- scalar inputs

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

where  $(a_j)_k$  are generalized Pochhammer symbols

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

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

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

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

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

Table 18.1: 5 Statistical Methods

		Statistical method	$n_1 \mathbf{H}$	$n_2 \mathbf{E}$	Univariate Analog
${}_0\mathcal{F}_0$	PCA	Principal components analysis	$W_p(n_1, \mathbf{\Sigma} + \mathbf{\Phi})$	$n_2 \mathbf{\Sigma}$	$\chi^2$
${}_1\mathcal{F}_0$	SigD	Signal detection	$W_p(n_1, \mathbf{\Sigma} + \mathbf{\Phi})$	$W_p(n_2, \mathbf{\Sigma})$	non-central $\chi^2$
${}_0\mathcal{F}_1$	REG <sub>0</sub>	Multivariate regression, with known error	$W_p(n_1, \mathbf{\Sigma}, n_1 \mathbf{\Phi})$	$n_2 \mathbf{\Sigma}$	$F$
${}_1\mathcal{F}_1$	REG	Multivariate regression, with unknown error	$W_p(n_1, \mathbf{\Sigma}, n_1 \mathbf{\Phi})$	$W_p(n_2, \mathbf{\Sigma})$	non-central $F$
${}_2\mathcal{F}_1$	CCA	Canonical correlation analysis	$W_p(n_1, \mathbf{\Sigma}, \mathbf{\Phi}(\mathbf{Y}))$	$W_p(n_2, \mathbf{\Sigma})$	$\frac{r^2}{1-r^2}$

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

### 18.2.1 Definitions and global assumptions

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

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

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

- $p \leq n_2$  ensures almost sure invertibility of matrix  $\mathbf{E}$  in Equation 18.1
- $p \leq n_1$  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 null hypothesis that the population covariance  $\mathbf{\Omega} = \mathbf{\Sigma}$ , with the alternative of interest being

$$\mathbf{\Omega} = \mathbf{\Sigma} + \mathbf{\Phi}, \text{ with } \mathbf{\Phi} = \theta \phi \phi'$$

where  $\theta > 0$ ,  $\phi$  are unknown, and  $\phi$  is normalized s.t.  $\|\mathbf{\Sigma}^{-1/2}\phi\| = 1$ . W.L.O.G., assume  $\mathbf{\Sigma} = \mathbf{I}_p$ , 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

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

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

- $n_1 \mathbf{H}$  equal to the sample covariance matrix
- $\mathbf{E} = \mathbf{\Sigma}$

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

$$\mathbf{\Omega} = \mathbf{\Sigma} + \mathbf{\Phi}, \text{ with } \mathbf{\Phi} = \theta \phi \phi'$$

and again, assume  $\Sigma = \mathbf{I}_p$  (but NOT necessarily known), here, instead of Equation 18.1, consider

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

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

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

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  $\mathbf{Y}$  into 3 parts  $\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3$ , 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  $\beta$ ), under the null  $H_0 : \mathbb{E}\mathbf{Y}_1 = 0$ , versus the alternative

$$\mathbb{E}\mathbf{Y}_1 = \sqrt{n_1}\theta\psi\phi' \quad (18.4)$$

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

- $\mathbf{Y}_2$  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

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

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

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

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**

$$\mathbf{Y}_1 = \mathbf{M} + \mathbf{Z}$$

**REG** Again, consider the linear regression

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

but **NOT** knowing the covariance matrix  $\Sigma$  of rows of  $\epsilon$ . Here, the solutions again solve  $\det(\mathbf{H} - \lambda\mathbf{E}) = 0$  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  $n_2 \rightarrow \infty$ , 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

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

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

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

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

$$\|\Sigma_{xx}^{-1/2} \phi\| = \|\Sigma_{yy}^{-1/2} \psi\| = 1$$

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

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

with

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

### 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  $\phi \in \mathbb{R}^p$  is normalized s.t.  $\|\phi\| = 1$ .

The problem remains **invariant** under the multiplication of  $\mathbf{X}$  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  $\det(\mathbf{H} - \lambda \mathbf{E}) = 0$  with  $\mathbf{H} = \mathbf{X}$  and  $\mathbf{E} = \mathbf{I}_p$ .

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  $\mathbf{H}$  and deterministic  $\mathbf{E}$
- **PCA** and **SigD** are *parallel* to **REG<sub>0</sub>**
- **CCA** has a different structure of  $\mathbf{H}$  and  $\mathbf{E}$

### 18.2.4 The likelihood ratios

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

$$\Lambda = \text{diag} \{ \lambda_1, \dots, \lambda_p \}$$

<sup>2</sup> $\mathbf{Z}$  is from the GOE that it is **symmetric** and

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

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

Figure 18.2: SMD and 5 Classes of Statistical Problems



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

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

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

$${}_p\mathcal{F}_q(\mathbf{a}, \mathbf{b}; \Phi, \Lambda) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\kappa \vdash k} \frac{(a_1)_{\kappa} \cdots (a_p)_{\kappa}}{(b_1)_{\kappa} \cdots (b_q)_{\kappa}} \frac{C_{\kappa}(\Phi) C_{\kappa}(\Lambda)}{C_{\kappa}(\mathbf{I}_p)}$$

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	${}_p\mathcal{F}_q$	$\alpha(\theta)$	$a$	$b$	$\Phi_{11}$
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 <sub>0</sub>	${}_0\mathcal{F}_1$	$\exp(-n_1\theta/2)$	-	$n_1/2$	$\theta n_1^2/4$
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

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

which can be denoted as  $\mathbf{n}, p \rightarrow_{\gamma} \infty$  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**
  - $W_p(n_1, I_p)/n_1$ , 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

$$\hat{F} = \frac{1}{p} \sum_{j=1}^p \mathbf{I}\{\lambda_j \leq \lambda\} \xrightarrow{a.s.} F_\gamma = \begin{cases} F^{SC} & \text{semi-circle distribution, for SMD} \\ F^{MP} & \text{Marchenko-Pastur distribution, for PCA, REG}_0 \\ F^W & \text{Wachter distribution, for SigD, REG, CCA} \end{cases}$$

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

$$\begin{aligned} F_\gamma^W(\lambda) &\rightarrow F_{\gamma_1}^{MP}(\lambda) & \gamma_2 &\rightarrow 0 \\ F_{\gamma_1}^{MP}(\sqrt{\gamma_1}\lambda + 1) &\rightarrow F^{SC}(\lambda) & \gamma_1 &\rightarrow 0 \end{aligned}$$

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

$$\sum_{j=1}^p \varphi(\lambda_j) - p \int \varphi(\lambda) dF_c^{\text{lim}}(\lambda) \quad (18.8)$$

converges in distribution 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	$F_\gamma^{\text{lim}}$	Density, $\lambda \in [\beta_-, \beta_+]$	$\beta_\pm$	Threshold $\bar{\theta}$
SMD	SC	$\frac{R(\lambda)}{2\pi}$	$\pm 2$	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  $\theta \leq \bar{\theta}$  (in Tab.18.3), the top eigenvalue  $\lambda_1 \rightarrow \beta_+$ , the upper boundary of support of  $F_\gamma$  almost surely
  - when  $\theta > \bar{\theta}$ ,  $\lambda_1$  **separates** from the bulk of the other eigenvalues and a.s. converges to a point strictly above  $\beta_+$

Hence,

- under the *super-critical* cases where  $\theta > \bar{\theta}$ , 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  $n, p \xrightarrow{\gamma} \infty$  for SMD and PCA.
- under the *sub-critical* cases where  $\theta < \bar{\theta}$ , the likelihood ratio converges to a Gaussian process, the sequences of measures corresponding to the distribution of  $\Lambda$  under the null and under the *sub-critical* alternatives are mutually **contiguous**.

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

$$\mathcal{L}(\theta; \Lambda) = \frac{\Gamma(s+1)\alpha(\theta)q_s}{\Phi_{11}^s 2\pi i} \int_{\mathcal{K}} {}_p\mathcal{F}_q(a-s, b-s; \Psi_{11}z) \prod_{j=1}^p (z - \lambda_j)^{-1/2} dz \quad (18.9)$$

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  $a_j-s, b_j-s$  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

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

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

$$\begin{aligned} f(z) &= f_c + f_e(z) + f_h(z) \\ g(z) &= g_c \times g_e(z) \times g_h(z) \end{aligned}$$

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

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

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

- second, consider

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

where

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

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

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

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

Case	$f_c$	$\check{g}_c = \frac{g_c}{1+o(1)}$
SMD	$1 + \theta^2/2 + \log \theta$	$\frac{\theta}{\theta}$
PCA	$1 + \frac{1-c_1}{c_1} \log(1+\theta) + \log \frac{\theta}{c_1}$	$\theta(1+\theta)^{-1} c_1^{-1}$
SigD	$f_c^{\text{PCA}} + f_{10}$	$\check{g}_c^{\text{PCA}} \check{g}_{10}$
REG <sub>0</sub>	$1 + \frac{\theta+c_1}{c_1} + \log \frac{\theta}{c_1} + \frac{1-c_1}{c_1} \log(1-c_1)$	$\theta c_1^{-1} (1-c_1)^{-1/2}$
REG	$f_c^{\text{REG}_0} + f_{10}$	$\check{g}_c^{\text{REG}_0} \check{g}_{10}$
CCA	$f_c^{\text{REG}} + f_{21}$	$\frac{\check{g}_c^{\text{REG}} \check{g}_{10}}{l(\theta)}$

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

$${}_p\mathcal{F}_q(a-s, b-s, \Phi_{11}z) = \exp\left\{-\frac{p}{2}f_h(z)\right\} g_h(z) \quad (18.15)$$

where

$$f_h(z) = \begin{cases} -z\theta & \text{SMD} \\ -z \frac{\theta}{c_1(1+\theta)} & \text{PCA} \\ \ln\left[1 - \frac{c_2 z \theta}{c_1(1+\theta)}\right] \frac{r^2}{c_1 c_2} & \text{SigD} \end{cases} \quad (18.16)$$

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

- 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  $q = 1$ ,  ${}_p\mathcal{F}_q$  can **NOT** be represented exactly in terms of elementary functions. Hence, consider the asymptotic approximations

$${}_p\mathcal{F}_q = \begin{cases} {}_0\mathcal{F}_1(m+1; m^2 \eta_0) \equiv F_0 & \text{REG}_0 \\ {}_1\mathcal{F}_1(m\kappa+1; m+1; m\eta_1) \equiv F_1 & \text{REG} \\ {}_2\mathcal{F}_1(m\kappa+1; m\kappa+1; m+1; \eta_2) \equiv F_2 & \text{CCA} \end{cases} \quad (18.18)$$

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  $F_j$ ,  $j = 0, 1, 2$  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.  $|\arg \eta_0| \leq \pi - \delta$ , then as  $m \rightarrow \infty$ , 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

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

where

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

and

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

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  $m \rightarrow \infty$ , for  $j=1, 2$

$$F_j = C_m \psi_j(t_j) e^{-i w_j/2} \left| 2\pi m \varphi_j''(t_j) \right|^{-1/2} \exp \{ -m \varphi_j(t_j) \} (1 + o(1))$$

now, we can set the components of the Laplace form of  ${}_p\mathcal{F}_q$  for  $q=1$  as

$$f_h(z) \begin{cases} \frac{1-c_1}{c_1} \varphi_0(t_0) & \text{REG}_0 \\ \frac{1-c_1}{c_1} (\varphi_j(t_j) + \kappa \ln \kappa - (\kappa-1) \ln(\kappa-1)) & \text{REG, CCA} \end{cases} \quad (18.19)$$

$$g_h(z) \begin{cases} (1 + 4\eta_0)^{-1/4} (1 + o(1)) & \text{REG}_0 \\ \sqrt{\frac{c_1}{r^2}} e^{-i w_j/2} \left| \varphi_j''(t_j) \right|^{-1/2} \varphi_j(t_j) (1 + o(1)) & \text{REG, CCA} \end{cases} \quad (18.20)$$

Together, we have

#### Lemma 18.2.2: Saddle Points

The saddle points  $z_0(\theta, \mathbf{c})$  of  $f(z)$  satisfies

$$z_0(\theta, \mathbf{c}) = \begin{cases} \theta + 1/\theta & \text{SMD} \\ (1+\theta)(\theta+c_1)/\theta & \text{PCA, REG}_0 \\ (1+\theta)(\theta+c_1)/(\theta l(\theta)) & \text{SigD, REG, CCA} \end{cases} \quad (18.21)$$

for  $\theta \in (0, \bar{\theta}_c)$ ,  $z_0 > b_+$  where  $\bar{\theta}_c$  is the threshold corresponding to  $F_c$ .

As  $c_2 \rightarrow 0$ , while  $c_1$  stays constant, the value of  $z_0$  for **SigD**, **REG**, **CCA** converges to **PCA** and **REG**<sub>0</sub>, which converges to **SMD** as  $c_1 \rightarrow 0$ . Precisely, solving equation

$$\sqrt{c_1} z_0 + 1 = (1 + \sqrt{c_1} \theta)(\sqrt{c_1} \theta + c_1)/(\sqrt{c_1} \theta)$$

for  $z_0$  and taking limit as  $c_1 \rightarrow 0$  yields  $z_0 = \theta + 1/\theta$ .

Then, we have the deformed contour as  $\mathcal{K} = \mathcal{K}_+ \cup \mathcal{K}_-$ , with  $\mathcal{K}_-$  is the complex conjugate of  $\mathcal{K}_+$ , and  $\mathcal{K}_+ = \mathcal{K}_1 \cup \mathcal{K}_2$ , where

- **SMD, PCA, SigD** (as in Fig.18.3)

$$\mathcal{K}_1 = \{z_0 + it : 0 \leq t \leq 2z_0\}$$

$$\mathcal{K}_2 = \{x + i2z_0 : -\infty < x \leq z_0\}$$

- **REG<sub>0</sub>, CCA** (as in Fig.18.4)

$$\mathcal{K}_1 = \{z_1 + |z_0 - z_1| \exp \{i\gamma\} : \gamma \in [0, \pi/2]\} \quad \mathcal{K}_2 = \{z_1 - x + |z_0 - z_1| \exp \{i\pi/2\} : x \geq 0\}$$

where

$$z_1 = \begin{cases} -(1 - c_1)^2/(4\theta) & \text{for REG}_0 \\ -c_1(1 - c_1)^2 l(\theta)/(4\theta r^2) & \text{for CCA} \end{cases}$$

- **REG**: it can be described as an image of a contour  $C$  in  $\tau$ -plane where  $\tau = \eta_1 t_1$  with  $\eta_1 = z\theta c_2/[c_1(1 - c_1)]$ , see [Johnstone and Onatski \(2020, P.20-21\)](#) for details.



Figure 18.3:  $\mathcal{K}$  for SMD, PCA, SigD



Figure 18.4:  $\mathcal{K}$  for REG<sub>0</sub>, CCA

Together, we have that for all 6 cases (SMD, PCA, SigD, REG<sub>0</sub>, REG and CCA), we have

**Lemma 18.2.3:**  $\mathcal{K}_1$  are of steep descent

As  $z$  moves along the corresponding  $\mathcal{K}_1$  away from  $z_0$ ,  $-\text{Re}f(z)$  is **strictly decreasing**.

**Laplace approximation** Next, we can derive Laplace approximations to the integral (18.9)

$$\mathcal{L}(\theta; \Lambda) = \frac{\Gamma(s+1)\alpha(\theta)q_s}{\Phi_{11}^s 2\pi i} \int_{\mathcal{K}} {}_p\mathcal{F}_q(a-s, b-s; \Psi_{11}z) \prod_{j=1}^p (z - \lambda_j)^{-1/2} dz$$

first, consider a general integral

$$I_{p,\omega} = \int_{\mathcal{K}_{p,\omega}} e^{-p\phi_{p,\omega}(z)} \chi_{p,\omega}(z) dz$$

where

- $p$  is large,  $\omega \in \Omega \subset \mathbb{R}^k$  is a  $k$ -dimensional parameter
- $\mathcal{K}_{p,\omega}$  is a path in  $\mathbb{C}$  that starts at  $a_{p,\omega}$  and ends at  $b_{p,\omega}$
- $\phi_{p,\omega}, \chi_{p,\omega}(z)$  are single-valued holomorphic functions of  $z$ , in the case of  $\chi_{p,\omega}$  with probability increasing to 1 (subscripts  $p,\omega$  are omitted hereafter)

Assuming that  $\exists C_1, \dots, C_4 > 0$  that do not depend on  $p, \omega$ , s.t.  $\forall \omega \in \Omega$  for sufficiently large  $p$

A0 The length of the path  $\mathcal{K}$  is bounded, uniformly over  $\omega \in \Omega$  and all sufficiently large  $p$ ,

$$\sup_{z \in (z_0, b)_{\mathcal{K}}} |z - z_0| > C_1 \quad \sup_{z \in \mathcal{K}}$$

A1  $\phi(z)$  and  $\chi(z)$  are holomorphic in the ball  $|z - z_0| \leq C_1$

A2  $\phi_2$  satisfies that  $C_2 \leq |\phi_2| \leq C_3$

A3 The third derivative of  $\phi(z)$  satisfies inequality

$$\sup_{|z - z_0| \leq C_1} |d^3 \phi(z)/dz^3| \leq C_4$$

A4  $\forall 0 < \epsilon < C_1$  (not depending on  $p, \omega$ ), and  $\forall z_i \in \mathcal{K}$  s.t.  $|z_1 - z_0| = \epsilon$ ,  $\exists C_5, C_6 > 0$  s.t.

$$\operatorname{Re}(\phi(z_1) - \phi_0) C_5 \quad |\operatorname{Im}(\phi(z_i) - \phi_0)| < C_6$$

A5 For  $\Theta \subset \mathbb{C}$  that consists of all points whose Euclidean distance from  $\mathcal{K}$  is no larger than  $C_1$

$$\sup_{z \in \Theta} |\chi(z)| = O_p(1)$$

as  $p \rightarrow \infty$ , where  $O_p(1)$  is uniform in  $\omega \in \Omega$

Under Assumption A0-A5, we have

#### Lemma 18.2.4: A General Integral and the Laplace Approximation

For any positive integer  $k$  as  $p \rightarrow \infty$ , we have

$$I_{p,\omega} = 2e^{-p\phi_0} \left[ \sum_{s=0}^{k-1} \Gamma\left(s + \frac{1}{2}\right) \frac{a_{2s}}{p^{s+1/2}} + \frac{O_p(1)}{p^{k+1/2}} \right]$$

where

- $O_p$  is uniform in  $\omega \in \Omega$
- the coefficients  $a_{2s}$  can be expressed through  $\phi_s$  and  $\chi_s$  defined above:
  - $a_0 = \phi/[2\phi_2^{1/2}]$  where  $\phi_2^{1/2} = \exp\{(\log|\phi_2| + i \arg \phi_2)/2\}$  with the branch of  $\arg \phi_2$  chosen s.t.  $|\arg \phi_2 + 2/\beta| \leq \pi/2$

We then use the lemma above to obtain the Laplace approximation to

$$\mathcal{L}_1(\theta, \Lambda) = \sqrt{\pi p} \frac{1}{2\pi i} \int_{\mathcal{K}_1 \cup \bar{\mathcal{K}}_1} e^{-(p/2)f(z)} g(z) dz$$

here, we must know the values of  $f(z_0)$  and  $d^2 f(z_0)/dz^2$ :

- for all 6 cases,  $f(z_0) = 0$
- for all 6 cases,  $d^2 f(z_0)/dz^2 < 0$ , its explicit form  $D_2 \equiv \theta^2 (-d^2 f(z_0)/dz^2)^{-1}$  is given as

## References

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