

## 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 **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<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

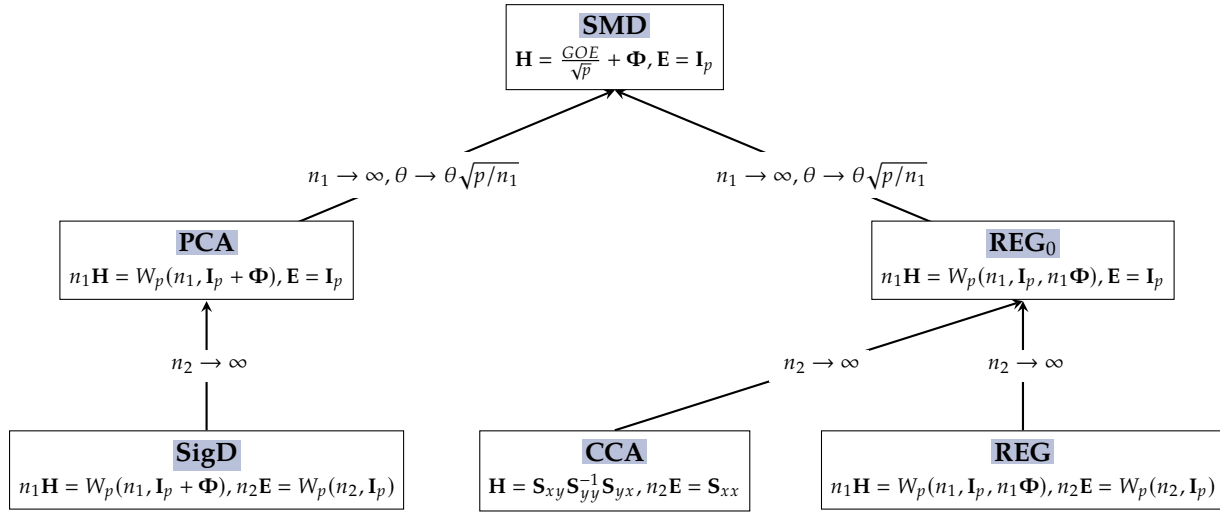
$$\Lambda = \text{diag} \{ \lambda_1, \dots, \lambda_p \}$$

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

## References

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