

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 θ_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 Σ , 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 Σ 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 of 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 TW_1 is the Tracy-Widom distribution

- under $H_1 : \Sigma = \mathbf{I}_p + \theta \mathbf{v}\mathbf{v}'$, $\theta > 0$, if θ 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 functions¹

${}_p\mathcal{F}_q$

¹Hypergeometric 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 | $W_p(n_1, \mathbf{\Sigma} + \mathbf{\Phi})$ | $n_2 \mathbf{\Sigma}$ | χ^2 |
| ${}_1\mathcal{F}_0$ | SigD | Signal detection | $W_p(n_1, \mathbf{\Sigma} + \mathbf{\Phi})$ | $W_p(n_2, \mathbf{\Sigma})$ | non-central χ^2 |
| ${}_0\mathcal{F}_1$ | REG ₀ | 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 $\theta > 0$, ϕ are unknown, and ϕ 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 θ , we have

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

where θ_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.

REG₀ Next, consider a linear regression with multivariate response

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

with known covariance matrix Σ of the i.i.d. Gaussian rows of the error matrix ϵ . Here, to test linear restrictions on the matrix of coefficients β , 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 β), 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 REG₀ 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 Σ of rows of ϵ . 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 REG₀.

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)**² 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**, **REG₀**: random \mathbf{H} and deterministic \mathbf{E}
- **PCA** and **SigD** are *parallel* to **REG₀**
- **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

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

² \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 diag $\{\Phi_{11}, 0, \dots, 0\}$. Consider the hypergeometric functions of 2 matrix arguments Φ, Λ 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, κ are partitions of the integer k , $(a_j)_{\kappa}$ and $(b_i)_{\kappa}$ are the generalized Pochhammer symbols, C_{κ} 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 | Φ_{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

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

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 **REG₀**
 - 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

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

A summary of the 3 classes of distributions is shown in Table 18.3. And the cumulative distribution functions $F_\gamma^{\lim}(\lambda)$ 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 φ is a *well-behaved* function, the centered **linear spectral statistic**

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

converges in distribution to a Gaussian random variable in each of the semicircle, Marchenko-Pastur and Wachter cases.³

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

| Case | F_γ^{\lim} | Density, $\lambda \in [\beta_-, \beta_+]$ | β_\pm | Threshold $\bar{\theta}$ |
|---|-------------------|---|--|--|
| SMD | SC | $\frac{R(\lambda)}{2\pi}$ | ± 2 | 1 |
| PCA, REG ₀ | 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_γ almost surely
 - when $\theta > \bar{\theta}$, λ_1 **separates** from the bulk of the other eigenvalues and a.s. converges to a point strictly above β_+

Hence,

- under the *super-critical* cases where $\theta > \bar{\theta}$, the likelihood ratio degenerates, the sequences of measures corresponding to the distributions of Λ 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 Λ under the null and under the *sub-critical* alternatives are mutually **contiguous**.

³The 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 γ_1, γ_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 Φ, Λ diverge to infinity. In single-spiked models, Φ 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} taht 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 $\mathbf{n}, p \xrightarrow{y} \infty$, and the values of f_c and g_c are given as Tab.18.4⁴

- 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

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

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

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

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 ₀ | $1 + \frac{\theta+c_1}{c_1} + \log \frac{\theta}{c_1} + \frac{1-c_1}{c_1} \log(1-c_1)$ | $\theta c_1^{-1} (1-c_1)^{-1/2}$ |
| 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**₀, 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)

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

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

- **REG₀, 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 τ -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 REG₀, CCA

Together, we have that for all 6 cases (SMD, PCA, SigD, REG₀, 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,ω are omitted hereafter)

Assuming that $\exists C_1, \dots, C_4 > 0$ that do not depend on p, ω , 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 ϕ_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, ω), 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 ϕ_s and χ_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

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

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 in Tab. 18.5

then, we can have the Laplace approximation as

Table 18.5: Values of $D_2 \equiv \theta^2 (-d^2 f(z_0)/dz^2)^{-1}$

| Case | Value of D_2 | Case | Value of D_2 |
|------------------|--|------|---|
| SMD | $1 - \theta^2$ | PCA | $c_1 (c_1 - \theta^2) (1 + \theta)^2$ |
| REG ₀ | $c_1(1 + c_1 + 2\theta)(c_1 - \theta^2)$ | REG | $c_1 h(c_1 + \theta + (1 + \theta)l)/l^4$ |
| SigD | $r^2 h(1 + \theta)^2/l^4$ | CCA | $c_1^2 (2(c_1 + \theta) + l(1 - c_1)) / (l^3(c_1 + c_2))$ |

Theorem 18.2.5: Laplace Approximation

Suppose that the null hypothesis holds, i.e., $\theta_0 = 0$. Let $\bar{\theta}$ be the threshold corresponding to F_γ as given in Tab.18.3, and let ϵ be an arbitrarily small fixed positive number, then $\forall \theta \in (0, \bar{\theta} - \epsilon]$, as $\mathbf{n}, p \xrightarrow{\gamma} \infty$, we have

$$\mathcal{L}(\theta; \Lambda) = \frac{g(z)}{\sqrt{-d^2 f(z_0)/dz^2}} + O_p(p^{-1}) \quad (18.22)$$

where $O_p(p^{-1})$ is uniform in $\theta \in (0, \bar{\theta} - \epsilon]$ and the principal branch of the square root is taken.

Asymptotics of LR from Theorem 18.2.5, let

$$\Delta_p(\theta) = p \int \ln(z_0(\theta) - \lambda) d(\hat{F}(\lambda) - F_c(\lambda))$$

where $\Delta_p(\theta)$ is defined as zero in the event of asymptotically negligible probability that $z_0 \leq \lambda_1$.

Theorem 18.2.6: Asymptotics of LR

Suppose that the null hypothesis holds, $\theta_0 = 0$. Let $\bar{\theta}$ be the threshold corresponding to F_γ as in Tab.18.3, let ϵ be an arbitrarily small fixed positive number, then $\forall \theta \in (0, \bar{\theta} - \epsilon]$, as $\mathbf{n}, p \xrightarrow{\gamma} \infty$, we have

$$\mathcal{L}(\theta, \Lambda) = \exp \left\{ -\frac{1}{2} \Delta_p(\theta) + \frac{1}{2} \ln (1 - [\delta_p(\theta)]^2) \right\} (1 + o_p(1))$$

where

$$\delta_p(\theta) = \begin{cases} \theta, & \text{SMD} \\ \theta/\sqrt{c_1}, & \text{PCA, REG}_0 \\ \theta r/(c_1 l(\theta)), & \text{SigD, REG, CCA} \end{cases}$$

and $r^2 = c_1 + c_2 - c_1 c_2$ and $o_p(1)$ is uniform in $\theta \in (0, \bar{\theta} - \epsilon]$.

Here, statistic $\Delta_p(\theta)$ is a linear spectral statistic, weakly converging to a Gaussian process indexed by $\theta \in (0, \bar{\theta} - \epsilon]$.

References

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