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

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 TW₁ is the Tracy-Widom distribution

• under $H_1: \Sigma = \mathbf{I}_p + \theta \nu \nu', \theta > 0$, 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 $(0 \le \theta < \sqrt{\gamma})$, 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

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

¹Hypergeometric functions are:

| | | Statistical method | $n_1\mathbf{H}$ | $n_2\mathbf{E}$ | Univariate Analog |
|-------------------|---------|---|---|--------------------|----------------------|
| $_0\mathcal{F}_0$ | PCA | Principal components analysis | $W_p(n_1, \Sigma + \Phi)$ | $n_2\Sigma$ | χ^2 |
| $_1\mathcal{F}_0$ | SigD | Signal detection | $W_p(n_1, \Sigma + \Phi)$ | $W_p(n_2, \Sigma)$ | non-central χ^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, Σ 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 Σ 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 $\theta > 0$, ϕ are unknown, and ϕ 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 θ , we have

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

where θ_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*₁**H** equal to the sample covariance matrix
- $\mathbf{E} = \mathbf{\Sigma}$

SigD Now consider testing the **equality** of covariance matrices Ω and Σ , 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.

REG₀ Next, consider a linear regression with multivariate response

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

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 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 REG₀ 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 Σ of rows of ϵ . 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 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

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

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)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 $\boldsymbol{\phi} \in \mathbb{R}^p$ 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, REG₀: random H and deterministic E
- PCA and SigD are parallel to REG₀
- 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 $i > j$

²**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 Φ , Λ 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, 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 | $_{ m p}\mathcal{F}_{ m q}$ | $\alpha(\theta)$ | 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**₀
 - 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

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

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

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 φ 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.³

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 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 $\theta \leq \overline{\theta}$ (in Tab.18.3), the top eigenvalue $\lambda_1 \to \beta_+$, the upper boundary of support of F_{γ} almost surely
- when $\theta > \overline{\theta}$, λ_1 **separates** from *he bulk* of the other eigenvalues and a.s. converges to a point strictly above β_+

Hence,

- under the *super-critical* cases where $\theta > \overline{\theta}$, 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 \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 Λ under the null and under the <u>sub-critical</u> alternatives are mutually <u>contiguous</u>.

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 $p \le \min\{n_1, n_2\}$, 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 $\alpha(\theta)$, Φ_{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.18.4⁴

· 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)

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

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

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

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

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

$$f_{h}(z) \begin{cases} \frac{1-c_{1}}{c_{1}} \varphi_{0}(t_{0}) & \text{REG}_{0} \\ \frac{1-c_{1}}{c_{1}} \left(\varphi_{j}(t_{j}) + \kappa \ln \kappa - (\kappa - 1) \ln(\kappa - 1) \right) & \text{REG,CCA} \end{cases}$$

$$g_{h}(z) \begin{cases} (1+4\eta_{0})^{-1/4} (1+o(1)) & \text{REG}_{0} \\ \sqrt{\frac{c_{1}}{r^{2}}} e^{-iw_{j}/2} \left| \varphi_{j}''(t_{j}) \right|^{-1/2} \varphi_{j}(t_{j}) (1+o(1)) & \text{REG,CCA} \end{cases}$$

$$(18.19)$$

Together, we have

Lemma 18.2.2: Saddle Points

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

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

for $\theta \in (0, \overline{\theta}_c)$, $z_0 > b_+$ where $\overline{\theta}_c$ 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)

$$\mathcal{K}_1 = \{z_0 + it : 0 \le t \le 2z_0\}$$
 $\mathcal{K}_2 = \{x + i2z_0 : -\infty < x \le z_0\}$

• **REG**₀, **CCA** (as in Fig.18.4)

$$\mathcal{K}_{1} = \left\{ z_{1} + |z_{0} - z_{1}| \exp\left\{i\gamma\right\} : \gamma \in [0, \pi/2] \right\} \qquad \mathcal{K}_{2} = \left\{ z_{1} - x + |z_{0} - z_{1}| \exp\left\{i\pi/2\right\} : x \geq 0 \right\}$$

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.



 \mathcal{K}_2 \mathcal{K}_1 \mathcal{K}_2 \mathcal{K}_2 \mathcal{K}_2

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 , -Re f(z) is **strictly decreasing**.

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

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

first, consider a general integral

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

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, ω , s.t. $\forall \omega \in \Omega$ for sufficiently large p

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

$$\sup_{z \in (z_0, b)_{\mathcal{K}}} |z - z_0| > C_1 \qquad \sup_{z \in C_0} |z - z_0| < C_1$$

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

A2 ϕ_2 satisfies that $C_2 \leq |\phi_2| \leq C_3$

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

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

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.

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

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 $p \to \infty$, 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 $p \to \infty$, 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 $\phi_2^{1/2} = \exp\left\{(\log\left|\phi_2\right| + i\arg\phi_2)/2\right\}$ with the branch of $\arg\phi_2$ chosen s.t. $\left|\arg\phi_2 + 2/\beta\right| \leq \pi/2$

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 $d^2f(z_0)/dz^2$:

- for all 6 cases, $f(z_0) = 0$
- for all 6 cases, $d^2 f(z_0)/dz^2 < 0$, its explicit form $D_2 \equiv \theta^2 \left(-d^2 f(z_0)/dz^2\right)^{-1}$ is given in Tab.18.5 then, we can have the Laplace appoximation as

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

| Case | Value of D_2 | Case | Value of D_2 |
|---------|------------------------------------|------|--|
| SMD | $1-\theta^2$ | PCA | $c_1\left(c_1-\theta^2\right)(1+\theta)^2$ |
| REG_0 | $c_1(1+c_1+2\theta)(c_1-\theta^2)$ | REG | $c_1h(c_1 + \theta + (1 + \theta)l)/l^4$ |
| SigD | $r^2h(1+\theta)^2/l^4$ | CCA | $c_1^2 \left(2(c_1 + \theta) + l(1 - c_1) \right) / (l^3(c_1 + c_2))$ |

Theorem 18.2.5: Laplace Approximation

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

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

where $O_p(p^{-1})$ is uniform in $\theta \in (0, \overline{\theta} - \epsilon]$ 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 $\overline{\theta}$ be the threshold corresponding to F_{γ} as in Tab.18.3, let ϵ be an arbitrarily small fixed positive number, then $\forall \theta \in (0, \overline{\theta} - \epsilon]$, as $\mathbf{n}, p \xrightarrow{\gamma} \infty$, we have

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

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 $\theta \in (0, \overline{\theta} - \epsilon]$.

Here, statistic $\Delta_p(\theta)$ is a linear spectral statistic, weakly converging to a Gaussian process indexed by $\theta \in (0, \overline{\theta} - \epsilon]$. Next, we derive the asymptotic expectation and covariances of $\mathcal{L}(\theta, \Lambda)$:

Theorem 18.2.7: Asymptotic Moments of LR

Suppose that the null hypothesis holds, $\theta_0=0$. Let $\overline{\theta}$ be the threshold corresponding to F_{γ} as in Tab.18.3, let ϵ be an arbitrarily small fixed positive number and $C[0,\overline{\theta}-\epsilon]$ be the space of continuous functions on $[0,\overline{\theta}-\epsilon]$ equipped with the supremum norm. Then $\ln \mathcal{L}(\theta;\Lambda)$ viewed as random

elements of $C[0,\overline{\theta}-\epsilon]$ converge weakly to $\mathcal{L}(\theta)$ with Gaussian finite dimensional distributions such that

$$\mathbb{E}\mathcal{L}(\theta) = \frac{1}{4}\ln(1 - \delta^2(\theta))$$
$$Cov\left(\mathcal{L}(\theta_1), \mathcal{L}(\theta_2)\right) = -\frac{1}{2}\ln\left(1 - \delta(\theta_1)\delta(\theta_2)\right)$$

with

$$\delta(\theta) = \begin{cases} \theta, & \text{SMD} \\ \theta/\sqrt{\gamma_1}, & \text{PCA,REG}_0 \\ \theta\rho/(\gamma_1 + \gamma_2 + \theta\gamma_2), & \text{SigD,REG,CCA} \end{cases}$$

here, ρ , γ_1 , γ_2 are the limits of r, c_1 , c_2 as \mathbf{n} , $p \xrightarrow{\gamma} \infty$

References

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