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

$$\boldsymbol{\Sigma} = \mathrm{Cov}(\mathbf{X}_i) = \mathbf{I} + \sum_{k=1}^{M} \theta_k \nu_k \nu_k' = \boldsymbol{\Sigma}_0 + \boldsymbol{\Phi}$$

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 $\boldsymbol{\Phi} = \mathbf{0}$, 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 ν_k
- How to test θ_k

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

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

against the null

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

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 $\mathbf{X} = \left(\mathbf{X}_1' \quad \cdots \quad \mathbf{X}_n'\right)'$, $\mathbf{X}'\mathbf{X}$ 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

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

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 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

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

  where TW_1 is the Tracy-Widom distribution

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

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

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:

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

with $p \times p$ matrices

$$n_1 \mathbf{H} = \sum_{k=1}^{n_1} \mathbf{x}_k \mathbf{x}_k' \qquad\qquad \text{\textit{hypothesis} SS}$$

$$n_1 \mathbf{E} = \sum_{k=1}^{n_1} \mathbf{z}_k \mathbf{z}_k' \qquad\qquad \text{\textit{error} SS}$$

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[1] $_p\mathcal{F}_q$

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[1]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, $_0\mathcal{F}_0(\mathbf{S}) = e^{\mathrm{tr}(\mathbf{S})}$, $_1\mathcal{F}_0(a, \mathbf{S}) = |\mathbf{I} - \mathbf{S}|^{-a}$
- two matrix inputs, where $\mathbf{S}, \mathbf{T}$ are both symmetric

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

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 disppears, 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 hull hypothesis that the population covariance $\mathbf{\Omega} = \mathbf{\Sigma}$, with the alternative of interest being

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

where $\theta > 0$, ϕ are unknown, and ϕ is normalized s.t. $\left\|\mathbf{\Sigma}^{-1/2}\phi\right\| = 1$. 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

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

where θ_0 is the true value of the *spike*. A **maximal invariant statistic** consists of the solutions $\lambda_1 \geq \cdots \geq \lambda_p$ 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

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

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

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

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

REG$_0$ Next, consider a linear regression with multivariate response

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

with known covariance matrix Σ of the i.i.d. Gaussian rows of the error matrix $\boldsymbol{\epsilon}$. Here, to test linear restrictions on the matrix of coefficients $\boldsymbol{\beta}$, 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 $\boldsymbol{\beta}$), 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 $\theta > 0$, $\left\|\Sigma^{-1/2}\boldsymbol{\phi}\right\| = 1$ and $\|\boldsymbol{\psi}\| = 1$
- $\mathbf{Y}_2$ 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 $\lambda_1, \cdots, \lambda_p$ to

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

where $\mathbf{H} = \mathbf{Y}_1'\mathbf{Y}_1/n_1$ and $\mathbf{E} = \Sigma$. 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 $W_p(n_1, \Sigma)$. Here,

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

Again, W.L.O.G, assume $\Sigma = I_p$. This **canonical form** of REG$_0$ is essentially equivalent to the setting of **matrix denoising**

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

REG   Again, consider the linear regression

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

but **NOT** knowing the covariance matrix Σ of rows of $\boldsymbol{\epsilon}$. Here, the solutions again solve $\det\left(\mathbf{H} - \lambda\mathbf{E}\right) = \mathbf{0}$ with

$$\mathbf{H} = \mathbf{Y}_1'\mathbf{Y}_1/n_1, \ \ \mathbf{E} = \mathbf{Y}_3'\mathbf{Y}_3/n_2$$

this represents a multivariate analog of the F ratio: the difference between the sum of squared residuals in the restricted and unrestricted regressions to the sum of squared residuals in the restricted regression. Again, as $n_2 \to \infty$, REG reduces to REG$_0$.

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 $t = 1, \cdots, n_1 + n_2$. Partition the population and sample covariance matrices of the observations $(x_t', y_t')'$ into

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

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

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

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

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

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

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

with

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

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 $\lambda_1, \cdots, \lambda_p$ to $\det(\mathbf{H} - \lambda \mathbf{E}) = \mathbf{0}$ 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$_0$**: random $\mathbf{H}$ and deterministic $\mathbf{E}$
- **PCA** and **SigD** are *parallel* to **REG$_0$**
- **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

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

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[2] $\mathbf{Z}$ is from the GOE that it is **symmetric** and

$$\mathbf{Z}_{ii} \sim \mathcal{N}(0, 2) \qquad\qquad\qquad\qquad \mathbf{Z}_{ij} \sim \mathcal{N}(0, 1) \text{ if } i > j$$

Figure 18.2: SMD and 5 Classes of Statistical Problems

SMD
$\mathbf{H} = \frac{GOE}{\sqrt{p}} + \mathbf{\Phi}, \mathbf{E} = \mathbf{I}_p$

$n_1 \to \infty, \theta \to \theta\sqrt{p/n_1}$ $n_1 \to \infty, \theta \to \theta\sqrt{p/n_1}$

PCA
$n_1\mathbf{H} = W_p(n_1, \mathbf{I}_p + \mathbf{\Phi}), \mathbf{E} = \mathbf{I}_p$

REG$_0$
$n_1\mathbf{H} = W_p(n_1, \mathbf{I}_p, n_1\mathbf{\Phi}), \mathbf{E} = \mathbf{I}_p$

$n_2 \to \infty$ $n_2 \to \infty$ $n_2 \to \infty$

SigD
$n_1\mathbf{H} = W_p(n_1, \mathbf{I}_p + \mathbf{\Phi}), n_2\mathbf{E} = W_p(n_2, \mathbf{I}_p)$

CCA
$\mathbf{H} = \mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}, n_2\mathbf{E} = \mathbf{S}_{xx}$

REG
$n_1\mathbf{H} = W_p(n_1, \mathbf{I}_p, n_1\mathbf{\Phi}), n_2\mathbf{E} = W_p(n_2, \mathbf{I}_p)$

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

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

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

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

where $\mathbf{a} = (a_1, \cdots, a_p)$ and $\mathbf{b} = (b_1, \cdots, b_q)$ 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	$\mathbf{\Phi}_{11}$
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

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

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 $\theta_0 = 0$), $\lambda_1, \cdots, \lambda_p$ 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 $\lambda_1, \cdots, \lambda_p$ follows

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

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

$$F_\gamma^{W}(\lambda) \to F_{\gamma_1}^{MP}(\lambda) \qquad\qquad \gamma_2 \to 0$$
$$F_{\gamma_1}^{MP}(\sqrt{\gamma_1}\lambda + 1) \to F^{SC}(\lambda) \qquad\qquad \gamma_1 \to 0$$

If φ is a *well-behaved* function, the centered **linear spectral statistic**

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

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	$F_\gamma^{\lim}$	Density, $\lambda \in [\beta_-, \beta_+]$	$\beta_\pm$	Threshold $\overline{\theta}$
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	$\frac{(\gamma_1+\gamma_2)R(\lambda)}{2\pi\gamma_1\lambda(\gamma_1-\gamma_2\lambda)}$	$\gamma_1\left(\frac{\rho\pm1}{\rho\pm\gamma_2}\right)^2$	$\frac{\rho+\gamma_2}{1-\gamma_2}$
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 *sub-critical* 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 *sub-critical* alternatives are mutually contiguous.

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[3]The centering constant is defined in terms of $F_{\mathbf{c}} = \{c_1, c_2\}$, 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 $\lambda_1, \cdots, \lambda_p$ counter-clockwise, returning to $-\infty$, then

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

where $s = p/2 - 1$, the values of $\alpha(\theta), \Phi_{11}, a, b, \mathrm{p}, \mathrm{q}$ 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,

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

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

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

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

$$f(z) = f_c + f_e(z) + f_h(z)$$
$$g(z) = g_c \times g_e(z) \times g_h(z)$$

where f_c and g_c do not depend on z.

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

- first

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

  where g_c remains bounded as $\mathbf{n}, p \xrightarrow{\gamma} \infty$, and the values of f_c and g_c are given as Tab.18.4[4]
- second, consider

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

  where

$$f_e(z) \int \ln(z - \lambda) dF_{\mathbf{c}}(\lambda) \tag{18.13}$$

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

---

[4]In 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	$1 + \theta^2/2 + \log\theta$	θ
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

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

where

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

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

- 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

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

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 $m \to \infty$, we have

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

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

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

where

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

and

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

the relevant saddle points are given as

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

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

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

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

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

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

Together, we have

> **Lemma 18.2.2: Saddle Points**
>
> The saddle points $z_0(\theta, \mathbf{c})$ of $f(z)$ satisfies
>
> $$z_0(\theta, \mathbf{c}) = \begin{cases} \theta + 1/\theta & \text{SMD} \\ (1+\theta)(\theta + c_1)/\theta & \text{PCA, REG}_0 \\ (1+\theta)(\theta + c_1)/(\theta l(\theta)) & \text{SigD, REG, CCA} \end{cases} \tag{18.21}$$
>
> for $\theta \in (0, \overline{\theta}_{\mathbf{c}})$, $z_0 > b_+$ where $\overline{\theta}_{\mathbf{c}}$ is the threshold corresponding to $F_{\mathbf{c}}$.

As $c_2 \to 0$, 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 $c_1 \to 0$. 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 $c_1 \to 0$ 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)

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

- **REG$_0$, CCA** (as in Fig.18.4)

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

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 $\mathcal{C}$ 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.
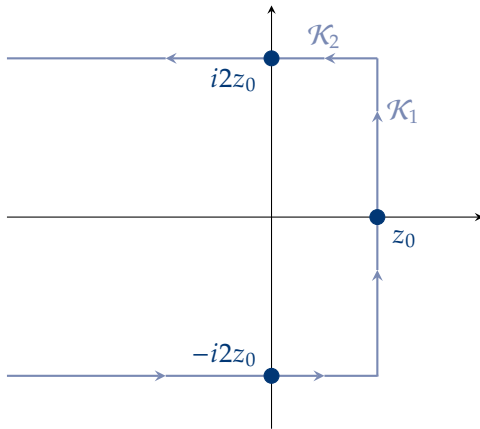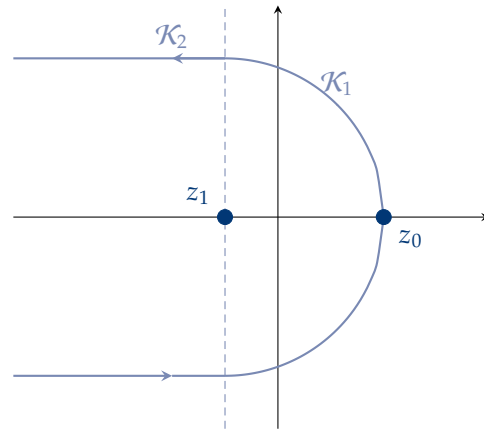

Figure 18.3: $\mathcal{K}$ for SMD, PCA, SigD

Figure 18.4: $\mathcal{K}$ for REG$_0$, CCA

Together, we have that for all 6 cases (SMD, PCA, SigD, REG$_0$, REG and CCA), we have

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

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

References

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