

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 $W_p(n, \mathbf{\Sigma})$ with the degree of freedom n and covariance matrix $\mathbf{\Sigma}$, which is a *random matrix*.

If $\mathbf{Y} = \mathbf{M} + \mathbf{X}$, that is, the sum of the *random matrix* \mathbf{X} and a *deterministic matrix* \mathbf{M} (also $n \times p$), then $\mathbf{Y}'\mathbf{Y}$ has a p -dimensional Wishart distribution $W_p(n, \mathbf{\Sigma}, \mathbf{\Psi})$ with n degrees of freedom, covariance matrix $\mathbf{\Sigma}$ and non-centrality matrix $\mathbf{\Psi} = \mathbf{\Sigma}^{-1}\mathbf{M}'\mathbf{M}$.

Definition 18.1.1: Density of Wishart Distribution

The PDF of Wishart distribution is defined as

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

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

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

For $\mathbf{\Sigma} = \mathbf{I}_p$, the empirical distribution for eigenvalues converges to Marcenko-Pastur distribution

$$f^{\text{MP}}(x) = \frac{1}{2\pi\gamma x} \sqrt{(b_+ - x)(x - b_-)}$$

where $b_{\pm} = (1 \pm \sqrt{\gamma})^2$. Then:

- under $H_0 : \mathbf{\Sigma} = \mathbf{I}_p$, 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 $H_1 : \mathbf{\Sigma} = \mathbf{I}_p + \theta \mathbf{v}\mathbf{v}'$, $\theta > 0$, 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.

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

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

References

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