# Eigen-Structure of Sample Covariance

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#### Material

- EL KAROUI, N. Spectrum estimation for large dimensional covariance matrices using random matrix theory.
   The Annals of Statistics 36, 6 (2008), 2757–2790 [1]
- PAUL, D. Asymptotics of sample eigenstructure for a large dimensional spiked covariance model.
   Statistica Sinica (2007), 1617–1642 [3]
- LEDOIT, O., AND WOLF, M. A well-conditioned estimator for large-dimensional covariance matrices.
   Journal of multivariate analysis 88, 2 (2004), 365–411 [2]

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## Eigenvalue of Covariance

- Principal component analysis (PCA)
- Low-dimensional approximation to the data by projecting the data on the "best" possible k-dimensional subspace.

## Setting

- We observed iid random vectors  $X_1, \ldots, X_n$  in  $\mathbb{R}^p$ .
- Assume that covariance of  $X_i$  is  $\Sigma_p$
- Sample covariance :  $S_p = \frac{1}{n-1}(X-\bar{X})^T(X-\bar{X})$



### Fixed p, large n

- It is well known that eigenvalues of  $S_p$  are good estimators of that of  $\Sigma_p$ .
- Let  $l_i$  be the ordered eigenvalues of  $S_p$   $(l_1 > l_2 > \cdots)$  and  $\lambda_i$  be the ordered that of  $\Sigma_p$   $(\lambda_1 > \lambda_2 > \cdots)$ .

$$\sqrt{n}(I_i - \lambda_i) \stackrel{d}{\rightarrow} N(0, \lambda_i^2)$$

where  $X_i$  are normally distributed.

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## Large n, large p

- Let us consider the simplest case where  $\Sigma_p = I_p$ .
- If  $X_i$  are iid and have a fourth moment, and if  $\frac{p}{n} \to \gamma$ , then

$$\mathit{I}_1 
ightarrow (1+\sqrt{\gamma})^2$$
 a.s.

• Note that if n = p, then  $l_1$  goes to 4.



## Large n, large p

- [3] focuses on Eigenvector of Sample Covariance.
- $\Sigma_p = diag(I_1, I_2, \dots, I_M, 1, \dots, 1)$
- If  $p/n \to \gamma \in (0,1)$ , then the sample eigenvectors can be inconsistency according to true eigenvalues.
  - If  $I_{\rm v}>1+\sqrt{\gamma}$ ,

$$|<
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m v},e_{
m v}>|
ightarrow\sqrt{\left(1-rac{\gamma}{(\it l_{
m v}-1)^2}
ight)\Big/\left(1+rac{\gamma}{\it l_{
m v}-1}
ight)}.$$

• If 
$$I_{
u} \leq 1 + \sqrt{\gamma}$$
,

$$|< p_v, e_v >| \rightarrow 0.$$



#### Recent work on covariance estimation

- There is some work on shrinkage of eigenvalues to improve covariance estimation.
- [2] proposed to estimate  $\Sigma_p$  by  $(1-\rho)S_p + \rho I_p$ .
- The estimator can be viewed as maintaining eigenvector and linearly shrinkaging the eigenvalues.

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#### From vectors to measures

- There are some issues that arise when estimating vectors (set of eigenvalues) of high dimension.
- Propose to associate high-dimensional vectors probability measures.
  - Allow us to look into the structure of the population eigenvectors.
  - Practical benefits of the measure estimation approach.

#### From vectors to measures

- Suppose we have a eigenvalue  $(\lambda_1, \ldots, \lambda_p)$  of  $\Sigma_p$ .
- Define a measure with p point mass with equal weight, and denote  $H_p$  as the **population spectral distribution**.

$$dH_p(x) = \frac{1}{p} \sum_{i=1}^p \delta_{\lambda_i}(x).$$

ullet Equivalently, define **empirical spectral distribution**  $F_p$  as

$$dF_p(x) = \frac{1}{p} \sum_{i=1}^p \delta_{l_i}(x).$$

# Example of spectral distribution

- Suppose  $dH_p = (1 \frac{1}{p})\delta_1 + \frac{1}{p}\delta_2$ .
  - $\implies$  It means that the  $\Sigma_p$  has one eigenvalue that is equal to 1, and (p-1) that are equal to 2.
- Clearly,  $H_p$  weakly converges to  $H_{\infty}$ , with  $dH_{\infty} = \delta_1$ .

- $H_p$ : Population spectral distribution,  $F_p$ : Empirical spectral distribution,
- $F_p \to F_{\infty}$ .
- $H_p \to H_\infty$ .
- Some theorem connects  $F_{\infty}$  and  $H_{\infty}$ .
- Our goal is estimating  $H_p$  by  $F_p$ .



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## Stieltjes transform of measures

ullet Stieltjes transform of a measure G on  $\mathbb R$  is defined as

$$m_G(z) = \int \frac{dG(x)}{x-z}$$
 for  $z \in \mathbb{C}^+$ ,

where  $\mathbb{C}^+ = \mathbb{C} \cup \{z : \mathit{Im}(z) > 0\}.$ 

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# Properties of Stieltjes transforms on $\mathbb R$

#### **Properties**

- If G is a probability measure,  $m_G(z) \in \mathbb{C}^+$  if  $z \in \mathbb{C}^+$  and  $\lim_{v \to \infty} (-iy) \cdot m_G(iy) = 1$ .
- If F and G are two measures, and if  $m_F(z)=m_G(z)$ , for all  $z\in\mathbb{C}^+$ , then G=F, a.s.
- And so on....

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# Stieltjes transform of the spectral distribution

• Stieltjes transform of the spectral distribution  $\Gamma_p$  of a  $p \times p$  matrix  $A_p$  is

$$m_{\Gamma_p}(z) = \frac{1}{p} trace((A_p - zI_p)^{-1}).$$

#### **Definition**

We will call  $v_{F_n}$  the function defined by

$$v_{F_p}(z) = (1 - \frac{p}{n}) \frac{-1}{z} + \frac{p}{n} m_{F_p}(z).$$

#### Theorem

#### **Theorem**

Suppose the data matrix X can be written  $X=Y\Sigma_p$ , where  $\Sigma_p$  is a  $p\times p$  positive definite matrix and Y is an  $n\times p$  matrix whose entries are i.i.d. (real or complex), with  $E(Y_{ij})=0$ ,  $E(|Y_{ij}|^2)=1$  and  $E(|Y_{ij}|^4)<\infty$ . Assume that  $H_p$  converges weakly to a limit denoted  $H_\infty$ . Then, when  $p,n\to\infty$ , and  $p/n\to\gamma$ ,  $\gamma\in(0,\infty)$ :

- $v_{F_p}(z) o v_{\infty}(z)$  a.s., where  $v_{\infty}(z)$  is a deterministic function.
- ullet  $v_{\infty}(z)$  satisfies the Marcenko-Pastur equation

$$-\frac{1}{v_{\infty}(z)} = z - \gamma \int \frac{\lambda dH_{\infty}(\lambda)}{1 + \lambda v_{\infty}(z)} \quad \forall z \in \mathbb{C}^+.$$

 The previous equation has one and only one solution which is the Stieltjes transform of a measure.

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## Strategy

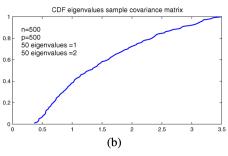
- **1** Estimating the measure  $H_{\infty}$  appearing in the Marcenko-Pastur equation.
- **②** Estimating  $\lambda_i$  as the ith quantile of  $\hat{H}_{\infty}$ .
- **3** Since we are considering fixed distribution asymptotics  $(H_p = H_\infty)$ ,  $\hat{H}_\infty$  will serve as estimate of  $H_p$

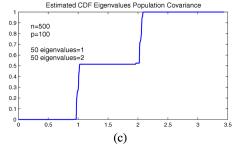
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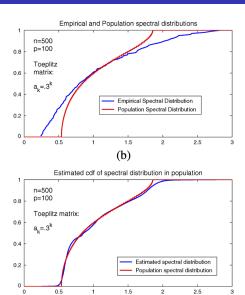
### **Examples**

- n = 500, p = 100
- CASE1 : Consider the  $\Sigma_p$  which has 50% of its eigenvalues equal to 1 and 50% equal to 2.
- CASE2 : Consider the Toeplitz matrix  $\Sigma_p$  with entries  $0.3^{|i-j|}$ .









(c)

#### References I

- EL KAROUI, N. Spectrum estimation for large dimensional covariance matrices using random matrix theory. The Annals of Statistics 36, 6 (2008), 2757–2790.
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- [3] PAUL, D. Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica* (2007), 1617–1642.