Random Matrix Theory: Sampled Covariance Matrix

$X_i \in \mathbb{R}^p \sim \mathcal{N}(\mu, \sigma^2 I_p)$

$\hat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$

$\hat{\Sigma}_n = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \hat{\mu}_n)(X_i - \hat{\mu}_n)^T$

M.L.E.
p fixed
$n \to \infty$

$p \nearrow \quad n \nearrow \qquad \frac{p}{n} \to \gamma \neq 0$ 高维

$\to \infty$

Stein's Phenomenon $\quad \hat{\mu}_n^{MLE}$ 不是最优的. inadmissible

$R(\hat{\mu}_n, \mu) \leq R(\hat{\mu}_n^{MLE}, \mu) \quad \forall \mu \in \mathbb{R}^p$

$\quad\ \ " \quad\ < \quad\ " \qquad \exists \mu$

$\hat{\mu}_n^{JS}, \quad \hat{\mu}_n^{ST}.$

Sampled Covariance Matrix $\hat{\Sigma}_n$? $\quad p$ 大

$\lim_{n\to\infty} \frac{p}{n} = \gamma \neq 0.$

Johnstone '2006 $\quad$ RMT & Statistics

$X_i \sim \mathcal{N}(0, I_p) \qquad X^{p\times n} = [X_1 \cdots X_n]$

$\hat{\Sigma}_n = \frac{1}{n} X X^T \xrightarrow{\lim_{n\to\infty} \frac{p}{n} = 0} I_p$

Wishart Matrix

$\lambda_i(\hat{\Sigma}_n)$ eigenvalue $\quad$ Marcenko-Pastur Dist.

$$\sim \quad \mu_0^{MP}(t) = \begin{cases} 0, & t \notin [a,b] \\ \frac{\sqrt{(b-t)(t-a)}}{\sqrt{2\pi\gamma t}}\,dt, & t \in [a,b] \end{cases}, \quad \gamma \leq 1 \quad \lim_{n\to\infty} \frac{p}{n} \leq 1$$

$a = (1-\sqrt{\gamma})^2 \overset{\gamma \to 0}{\Rightarrow} a = b = 1$

$b = (1+\sqrt{\gamma})^2$

$\mu^{MP}(t) = 1(\gamma > 1)\,\delta_0(t) + \mu_0^{MP}(t), \quad \int \delta_0(t)\,dt = 1 - \frac{1}{\gamma}$

PCA: $\hat{\Sigma}_n = \frac{1}{n}\tilde{X}\tilde{X}^T \longrightarrow U\Lambda U^T$ $\quad \Lambda = \mathrm{diag}(\lambda_i)$

$\lambda_1 \geq \lambda_2 \cdots \lambda_k \cdots$

gap $\lambda_i - \lambda_{i+1}$? heuristic

Phase Transition in PCA

$$Y = X + \varepsilon = \alpha u + \varepsilon \qquad \|u\|_2 = 1$$

$u \in \mathbb{R}^p$ fixed given. $\alpha \sim N(0, \sigma_x^2)$ signal

noise $\varepsilon \sim N(0, \sigma_\varepsilon^2 I_p)$

SNR: $R = \frac{\sigma_x^2}{\sigma_\varepsilon^2}$

rank-1 signal + noise $Y \sim N(0, \Sigma)$

$$\Sigma = \underset{\substack{\uparrow \\ \text{rank-1 matrix}}}{\sigma_x^2 uu^T} + \underset{\substack{\uparrow \\ \text{sparse matrix}}}{\sigma_\varepsilon^2 I_p}, \qquad \frac{\sigma_x^2}{\sigma_\varepsilon^2} = R$$

$$\begin{bmatrix} * & & 0 \\ & \ddots & \\ 0 & & * \end{bmatrix}$$

$\hat{\Sigma}_n = \frac{1}{n}\tilde{Y}\tilde{Y}^T \xrightarrow{PCA}$ primary $\begin{cases} \text{eigenvalue} & \hat{\lambda}_{max}(\hat{\Sigma}_n) \leq \sigma_x^2 \\ \text{eigenvector} & \hat{v}_{max}(\cdot): u \end{cases}$ uu^T

$\sigma_\varepsilon^2 = 1$ MP dist

$$\hat{\lambda}_{max} \to \begin{cases} b = (1+\sqrt{\gamma})^2 & R \leq \sqrt{\gamma} \quad \text{随机谱上界} \\ (1+\sigma_x^2)\left(1+\frac{\gamma}{\sigma_x^2}\right) \neq \sigma_x^2, & R > \sqrt{\gamma} \quad \text{信号谱 biased} \end{cases}$$

$$|\langle \hat{v}_{max}, u \rangle|^2 \to \begin{cases} 0, & R \leq \sqrt{\gamma}. \quad \text{PCA 随机} \\ \dfrac{1 - \frac{\gamma}{\sigma_x^4}}{1 + \frac{\gamma}{\sigma_x^2}} \neq 1 & R > \sqrt{\gamma}, \quad \text{锥域 cone (biased)} \end{cases}$$

PT in PCA: SNR 小 易随机谱 Johnstone 2006

Bnak ↑ SNR 大 biased 信号谱 Est.

MDS → Kernel (El Karoui, Cheng-Singer)