1. *Phase transition in PCA "spike" model:* Consider a finite sample of n i.i.d vectors $x_1, x_2, \ldots, x_n$ drawn from the p-dimensional Gaussian distribution $\mathcal{N}(0, \sigma^2 I_{p\times p} + \lambda_0 uu^T)$, where λ_0/σ^2 is the signal-to-noise ratio (SNR) and $u \in \mathbb{R}^p$. In class we showed that the largest eigenvalue λ of the sample covariance matrix S_n

$$S_n = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T$$

(a) Find λ given SNR > T

Suppose $t = \alpha u$ $\quad \alpha \sim N(0, \lambda_0)$ $\quad u$ is a direction s.t. $u^T u = 1$

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

$x = t + \varepsilon$ then $x \sim N(0, \underbrace{\sigma^2 I_p + \lambda_0 u u^T}_{\triangleq \Sigma})$ where Σ is $p \times p$

$x_i \sim N(0, \Sigma) \in \mathbb{R}^p$

$X = [x_1 | x_2 | \cdots x_n] \in \mathbb{R}^{p\times n}$

Assign $\dfrac{\text{signal of data}}{\text{signal of noise}} = \dfrac{\lambda_0}{\sigma^2} = SNR$

$S_n \triangleq \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T = \frac{1}{n} X X^T$

Then. the eigenvalue λ and corresponding eigenvector v satisfies

$S_n v = \lambda v$

In order to use MP distribution

$y_i \triangleq \Sigma^{-\frac{1}{2}} x_i$

then $Y = [y_1 | y_2 | \cdots y_n] = \Sigma^{-\frac{1}{2}} X \sim N(0, I_p)$

$T_n = \frac{1}{n} \cdot \sum_{i=1}^{n} y_i y_i^T = \frac{1}{n} \cdot Y Y^T$ is a Wishart Matrix

So the limit distribution of T_n's eigenvalues follow a MP distribution.

Connect T_n and S_n now

$T_n = \frac{1}{n} Y Y^T = \frac{1}{n} (\Sigma^{-\frac{1}{2}} X)(\Sigma^{-\frac{1}{2}} X)^T$ $\quad \Sigma^{-\frac{1}{2}}$ is symmetric

$= \Sigma^{-\frac{1}{2}} S_n \Sigma^{-\frac{1}{2}}$

thus $\quad S_n = \Sigma^{\frac{1}{2}} T_n \Sigma^{\frac{1}{2}}$

Since $\quad S_n v = \Sigma^{\frac{1}{2}} T_n \Sigma^{\frac{1}{2}} v = \lambda v$

$$\Sigma^{\frac{1}{2}} T_n (\Sigma \Sigma^{-\frac{1}{2}}) v = \lambda v$$

$$T_n \Sigma (\Sigma^{-\frac{1}{2}} v) = \Sigma^{-\frac{1}{2}} \lambda v = \lambda (\Sigma^{-\frac{1}{2}} v)$$

So λ, $(\Sigma^{-\frac{1}{2}} v)$ is the eigenvalue and corresponding eigenvector of $(T_n \Sigma)$

Suppose $\quad v^* = c(\Sigma^{-\frac{1}{2}} v)$ s.t. $v^{*T} v^* = 1$

$$c^2 (\Sigma^{-\frac{1}{2}} v)^T (\Sigma^{-\frac{1}{2}} v) = 1$$

$$c^2 v^T \Sigma^{-1} v = 1$$

$$c^2 v^T \Sigma^{-1} = v^T$$

$$c^2 v^T = v^T \cdot \Sigma$$

$$c^2 v = \Sigma v$$

$$c^2 = v^T \Sigma v$$

$$c^2 = \lambda_0 (u^T v)^2 + 6^2$$

$$= 6^2 \left(\frac{\lambda_0}{6^2} (u^T v)^2 + 1 \right)$$

$$= (R (u^T v)^2 + 1) 6^2$$

we use $v^* = c \cdot (\Sigma^{-\frac{1}{2}} v)$ a normalized eigenvector of (ΣT_n) from now on.

$T_n \Sigma v^* = \lambda v^*$

$$T_n (6^2 I_p + \lambda_0 u u^T) v^* = \lambda v^*$$

$$T_n 6^2 I_p v^* + \lambda_0 T_n u u^T v^* = \lambda v^*$$

$$\lambda_0 T_n u u^T v^* = (\lambda I_p - T_n 6^2 I_p) v^*$$

$$v^* = (\lambda I_p - T_n 6^2 I_p)^{-1} \lambda_0 T_n u u^T v^*$$

$$u^T v^* = u^T (\lambda I_p - T_n 6^2 I_p)^{-1} \lambda_0 T_n u u^T v^*$$

Suppose $\quad u^T v^* \neq 0$

$$1 = u^T (\lambda - T_n 6^2 I_p)^{-1} \lambda_0 T_n u \qquad (**)$$

Suppose $\quad T_n = W \Lambda W^T \qquad W W^T = I_p \qquad \Lambda = \mathrm{diag}\{\lambda_1 \cdots \lambda_p\}$

$$1 = \lambda_0 \cdot \sum_{i=1}^{p} u_i^2 \frac{\lambda_i}{\lambda - 6^2 \lambda_i} \qquad (*)$$

For $\Sigma u_i^2 = 1$ regard (a_i^2) as a probability measure

when $p, n \to \infty$ $\lim_{p,n\to\infty} \frac{p}{n} = \gamma$

we have $\lambda_i \sim MP$ distribution

for $(*)$

$$1 = \lambda_0 \cdot \sum_{i=1}^{p} u_i^2 \frac{\lambda_i}{\lambda - \sigma^2 \lambda_i} = \lambda_0 \int_a^b \frac{t}{\lambda - \sigma^2 t} \, d\mu^{MP}(t)$$

According to Stieltjes transform

$$1 = \frac{\lambda_0}{4\gamma} [2\lambda - (a+b) - 2\sqrt{|(\lambda-a)(b-\lambda)|}]$$

for $\lambda > (1+\sqrt{\gamma})^2 \triangleq b$ and $SNR > \sqrt{\gamma}$

Suppose $\sigma_\varepsilon^2 = 1$

for $SNR > \sqrt{\gamma}$ aka $\sigma_x^2 > \sqrt{\gamma}$

$$\lambda = \lambda_0 + \frac{\gamma}{\lambda_0} + 1 + \gamma = (1+\lambda_0)(1+\frac{\gamma}{\lambda_0})$$

So given $SNR > \sqrt{\gamma}$ $\lambda = \lambda_0 + \frac{\gamma}{\lambda_0} + 1 + \gamma = (1+\lambda_0)(1+\frac{\gamma}{\lambda_0})$

Actually
$$\lambda_{max}(S_n) = \begin{cases} (1+\sqrt{\gamma})^2 = b & \sigma_x^2 \le \sqrt{\gamma} \\ (1+\sigma_x^2)(1+\frac{\gamma}{\sigma_x^2}) & \sigma_x^2 > \sqrt{\gamma} \end{cases}$$

(b) we can estimate the $SNR = \frac{\sigma_x^2}{\sigma_\varepsilon^2}$ W.O.L.G $\sigma_\varepsilon^2 = 1$

by comparing the $\lambda_{max}(S_n)$ where $S_n = \frac{1}{n} X X^T$

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

If $\lambda_{max}(S_n) = b$ then we know $SNR \le \sqrt{\gamma}$

If $\lambda_{max}(S_n) = (1+\sigma_x^2)(1+\frac{\gamma}{\sigma_x^2})$ we know $SNR > \sqrt{\gamma}$

(c) According to $(**)$

$$1 = u^T (\lambda I_p - T_n \sigma^2 I_p)^{-1} \lambda_0 T_n u$$

$$u^T v^* = u^T (\lambda I_p - T_n \sigma^2 I_p)^{-1} \lambda_0 T_n u u^T v^*$$

$$1 = v^{*T} v^* = v^{*T} u u^T v^* = (u^T v^*)^T (u^T v^*)$$

$$(u^T v^*)^T (u^T v^*) = v^{*T} u u^T T_n \lambda_0 (\lambda I_p - T_n \cdot \sigma^2 I_p)^{-1} \cdot \underbrace{u u^T}_{=1} (\lambda I_p - T_n \sigma^2 I_p)^{-1} \lambda_0 T_n u u^T v^*$$

$$= \lambda_0^2 (u^T v^*)^T u^T T_n (\lambda I_p - T_n \cdot \sigma^2 I_p)^{-2} T_n u (u^T v^*)$$

Thus

$$|u^T v^*|^{-2} = \lambda_0^2 \, \tau \, u^T T_n (\lambda I_p - \sigma^2 T_n)^{-2} T_n u$$ By Monte Carlo

$$\sim \lambda_0^2 \int_a^b \frac{t^2}{(\lambda - \sigma^2 t)^2} \, d\mu^{MP}(t)$$ Integration

$$= \frac{\lambda_0^2}{4\gamma} \left(-4\gamma + (a+b) + 2\sqrt{(\lambda-a)(\lambda-b)} + \frac{\lambda(2\lambda-(a+b))}{\sqrt{(\lambda-a)(\lambda-b)}} \right)$$

Since $R = SNR = \frac{\sigma x^2}{\sigma_\varepsilon^2} = \frac{\lambda_0}{\sigma^2} > b = (1+\sqrt{\gamma})^2$

we proved that $\hat{\lambda} = \lambda_{max} \to (1+R)(1+\frac{\gamma}{R})$

Thus.

$$|u^T v^*|^2 = \frac{1-\frac{\gamma}{R}}{1+\gamma+\frac{2\gamma}{R}}$$

Now, we translate $|u^T v^*|^{-2}$ to $|u^T v|^{-2}$

$$|u^T v|^2 = \left(\frac{1}{c} u^T \Sigma^{\frac{1}{2}} v^*\right)^2$$

$$= \frac{1}{c}\left(((R u u^T + I_p)^{\frac{1}{2}} u)^T v^*\right)^2$$

$$= \frac{1}{c^2}\left((\sqrt{(1+R)} u)^T v^*\right)^2$$

$$= \frac{(1+R)(u^T v^*)^2}{R(u^T v)^2 + 1} = \frac{1+R-\frac{\gamma}{R}-\frac{\gamma}{R^2}}{1+R+\gamma+\frac{\gamma}{R}}$$

$$= \frac{1-\frac{\gamma}{R^2}}{1+\frac{\gamma}{R}}$$ where $\gamma = \lim_{p,n\to\infty} \frac{p}{n}$

$R = SNR = \frac{\sigma x^2}{\sigma_\varepsilon^2} = \frac{\lambda_0}{\sigma^2}$

(d) See the Code in PhaseTransition.ipynb attached in the homework email.