Some aspects of large sample covariance matrices

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Sample covariance matrix and problem of high-dimensionality

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- Marčenko-Pastur distributions
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An example where Marčenko-Pastur law does not hold

- High-dimensional theory fo eigenvalues of $\mathbf{S}_n$ from mixtures

Sample covariance matrix and problem of high-dimensionality

Sample variance/covariances from a multivariate population

- Let $\mathbf{x}, \ldots, \mathbf{x}_1, \ldots, \mathbf{x}_n, \ldots$ an i.i.d. sequence of $\mathbb{R}^p$-valued random vectors with common distribution μ (population);
- Sample variance/covariance matrix: (assuming $\mathbb{E}(\mathbf{x}) = \mathbf{0}$)

$$\mathbf{S}_n = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \mathbf{x}_k^T .$$

  That is, if we write $\mathbf{x}_k = (\xi_{1k}, \ldots, \xi_{pk})^T$,

$$\mathbf{S}_n(i,j) = \frac{1}{n}\sum_{k=1}^{n} \xi_{ik}\xi_{jk}, \quad 1 \le i,j \le p.$$

  [sample cross-moments between dimensions/variables i and j.]
- The population variance/covariance matrix is

$$\mathbf{\Sigma} = \mathbb{E}[\mathbf{x}\mathbf{x}^T], \quad (p \times p).$$

  Both $\mathbf{S}_n$ and $\mathbf{\Sigma}$ are nonnegative definite and trivially,

$$\mathbb{E}\mathbf{S}_n = \mathbf{\Sigma}.$$

Is $\mathbf{S}_n$ a "good enough" estimator of Σ ?

Large sample theory

Holding the dimension p while letting the sample size $n \to \infty$:

1. Law of large numbers: $\mathbf{S}_n \overset{\text{a.s.}}{\to} \mathbf{\Sigma} = \mathbb{E}[\mathbf{x}\mathbf{x}^T]$, [once $\mathbb{E}[\|\mathbf{x}\|^2] < \infty$]
2. Central limit theorem: $\sqrt{n}\,[\mathbf{S}_n - \mathbf{\Sigma}] \Rightarrow \mathcal{N}(\mathbf{0}, \mathbf{\Lambda})$,

   with some asymptotic variance/covariance matrix $\mathbf{\Lambda}$.

[once $\mathbb{E}[\|x\|^4] < \infty$]

- **A fundamental issue in statistics:**

  When analyzing a real "high-dimensional" data set with given (p, n)

  such that $p/n \gg 0$, *for example* $(p = 100, n = 500)$,

  approximation from this classical large sample theory becomes

  biased and inefficient!

(a). High-dimensional data is now common

- Many sources to high-dimensional data: electronic trading in finance; genomics;
- typical data dimensions and sample sizes:

	# variables p	sample size n	**ratio** p/n	**Small / Big**
portfolio	$\sim$ **100**	**500**	**0.2**	S
climate survey	320	600	0.21	S
speech analysis	$\sim 10^3$	$\sim 10^3$	~ 1	S
ORL face data base	1440	320	4.5	B
micro-arrays	10000	1000	10	B

(b). Example illustrating inefficiency of classical large sample limits

Consider

- a "white"/unit Gaussian populaiton $\mathbf{x} \sim \mathcal{N}(0, \mathbf{I}_p)$, that is,

$$\mathbf{x} = (\xi_1, \ldots, \xi_p)^T, \quad \xi_\ell \text{ are i.i.d. } \mathcal{N}(0, 1).$$

- given a sample $\mathbf{x}_1, \ldots, \mathbf{x}_n$ from $\mathbf{x}$, the sample covariance matrix is,

$$\mathbf{S}_n = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T = \frac{1}{n} \mathbf{W}_n,$$

  Here

$$\mathbf{W}_n = \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T = (\mathbf{x}_1, \ldots, \mathbf{x}_n)(\mathbf{x}_1, \ldots, \mathbf{x}_n)^T \quad \sim \quad \text{Wishart}(n, \mathbf{I}_p)$$

- let $\lambda_1 \geq \cdots \geq \lambda_p \geq 0$ be eigenvalues of $\mathbf{S}_n$.

Example (cont.)

Large sample limits: p **fixed while** $n \to \infty$

1. LLN: $\mathbf{S}_n \overset{a.s.}{\to} \mathbf{I}_p$; by continuity, $(\lambda_1, \ldots, \lambda_p) \overset{a.s.}{\to} 1$.
2. CLT:

$$\sqrt{n}\,(\mathbf{S}_n - \mathbf{I}_p) \;\Rightarrow\; \mathcal{N}(0, *),$$

   By delta method,

$$\sqrt{n}\,\left\{(\lambda_1^2 + \cdots + \lambda_p^2) - p\right\} \Rightarrow \mathcal{N}(0, *).$$

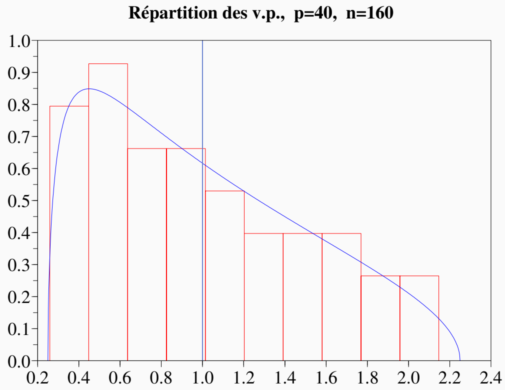
Random-matrix-theory (RMT) limits:

$n \to \infty$, $p = p_n \to \infty$ **such that** $p_n/n \to c > 0$

1. LLN: $\mathbf{S}_n \not\to \mathbf{I}_p$; $\frac{1}{p}\sum_{k=1}^{p} \delta_{\lambda_k} \;\Rightarrow$ Marčenko-Pastur law
2. CLT:

$$(\lambda_1^2 + \cdots, +\lambda_p^2) - p - p^2/n \Rightarrow \mathcal{N}(m, *).$$

Example (cont.)



1. Histogram of 40 eigenvalues of S_n simulated with $p = 40$ and $n = 160$
2. blue curve = RMT limit: Marčenko-Pastur law with index $\frac{p}{n} = \frac{1}{4}$

$$f(x) = \frac{1}{2\pi c x}\sqrt{(b-x)(x-a)}, \quad x \in [a,b] = [0.25, 2.25]$$

3. large sample limit: sample eigenvalues $\simeq 1$

(c) Marčenko-Pastur paradigm for high-dimensional statistics

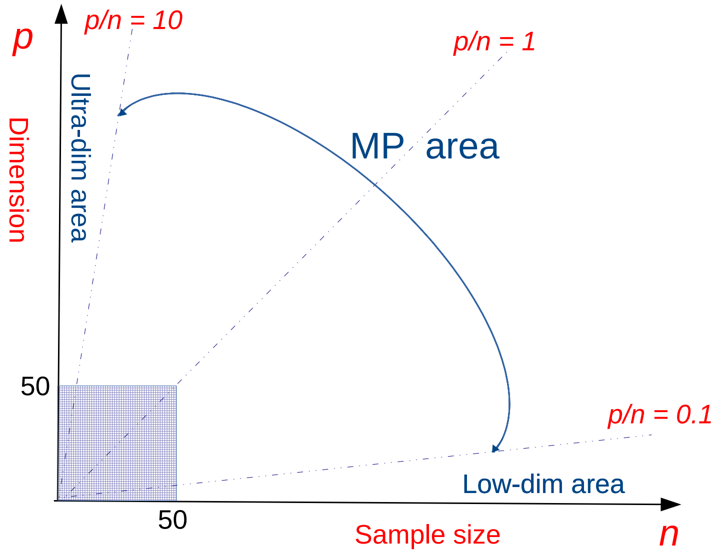
- Both the large sample limits and random matrix theory limits are mathematical theorems, are thus theoretically correct;
- But the question from a responsible statistician (now "data scientist") would be:

  Which theory to follow if data table has $(p, n) = (40, 160)$?

- Previous simulation shows clearly that

  RMT Marčenko-Pastur limit $\gg$ classical large sample limit !

Empirical performance of the Marčenko-Pastur limiting scheme



Random matrix theory for large sample covariance matrix

The Marčenko-Pastur distribution

Theorem. Assume : Marčenko & Pastur, 1967

- Population $\mathbf{x} = (\xi_1, \ldots, \xi_p)^T$ has i.i.d. components with mean 0 and variance 1; (so $\mathbf{\Sigma} = \mathbf{I}_p$);
- $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is an i.i.d. sample of $\mathbf{x}$;
- $n \to \infty$, $p = p(n) \to \infty$ and $p/n \to y \in (0, 1]$;

Then, the eigenvalue distribution of

$$S_n = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k \mathbf{x}_k^T = \frac{1}{n} \mathbf{X}\mathbf{X}^T = \frac{1}{n} (\mathbf{x}_1, \ldots, \mathbf{x}_n)(\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$$

converges to the distribution with density function

$$f(x) = \frac{1}{2\pi y x} \sqrt{(x-a)(b-x)}, \quad a \le x \le b,$$

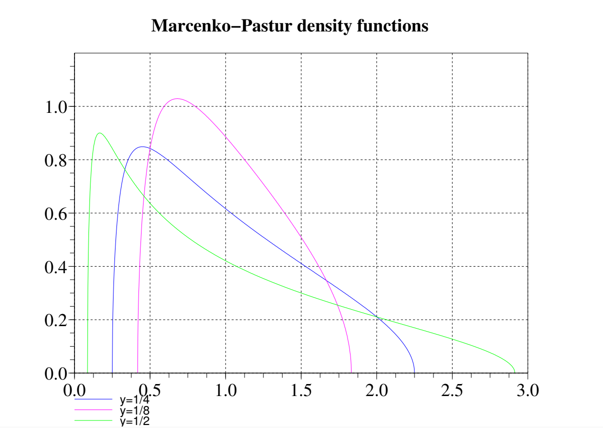
where

$$a = (1 - \sqrt{y})^2, \quad b = (1 + \sqrt{y})^2 .$$

The Marčenko-Pastur distribution

$$f(x) = \frac{1}{2\pi y x}\sqrt{(x-a)(b-x)}, \qquad (1-\sqrt{y})^2 = a \le x \le b = (1+\sqrt{y})^2.$$

$y \sim p/n$	a	b
1/8	0.42	1.83
1/4	0.25	2.25
1/2	0.09	2.91



The generalized Marčenko-Pastur distribution

Theorem. Assume : Marčenko & Pastur, (1967); Silverstein (1995)

- $\mathbf{X} = p \times n$ i.i.d. variables $(0, 1)$;
- $n \to \infty$, $p = p(n) \to \infty$ and $p/n \to y \in (0, 1]$;
- $(T_p)_{p \geq 1}$ is a sequence of non-negative Hermitian matrices whose eigenvalue distributions $(H_p)_p$ tend to a deterministic probability distribution H;

Then, the eigenvalue distribution of $S_n = \frac{1}{n} T_p^{1/2} \mathbf{X}\mathbf{X}^T T_p^{1/2}$ converges to a deterministic distribution $F_{y,H}$ characterized by its Stieltjes transform m which solves the following Marčenko-Pastur equation

$$m = \int \frac{1}{t(1 - y - yzm) - z} dH(t).$$

This solution is unique in the set $\{m \in \mathbb{C}^+ : -(1 - y)/z + ym \in \mathbb{C}^+\}$.

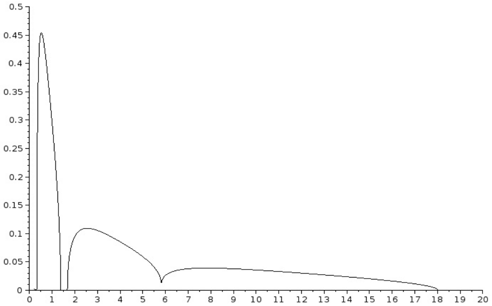
An example of generalized Marčenko-Pastur distribution

Assuming that $T_p = \mathrm{diag}\{\underbrace{1,\ldots,1}_{1/3},\underbrace{4,\ldots,4}_{1/3},\underbrace{10,\ldots,10}_{1/3}\}.$

Then the limiting Stieltjes transform m solves:

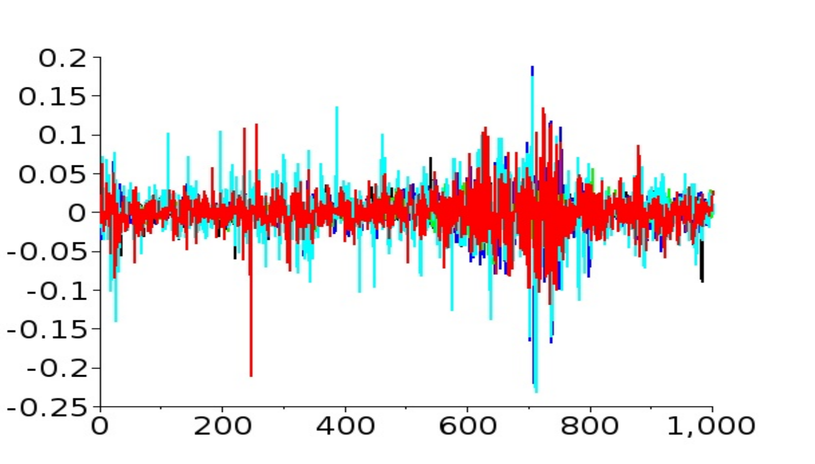
$$m = \frac{1/3}{1-y-yzm-z} + \frac{1/3}{4(1-y-yzm)-z} + \frac{1/3}{10(1-y-yzm)-z} \; .$$

By inversion of Stieltjes transform, density function is:



Example of stock data

- SP 500 daily stock prices ; $p = 488$ stocks;
- $n = 1000$ daily returns $\mathbf{r}_t(i) = \log p_t(i)/p_{t-1}(i)$ from 2007-09-24 to 2011-09-12;



- Let the SCM (488× 488)

$$\mathbf{S}_n = \frac{1}{n}\sum_{t=1}^{n}(\mathbf{r}_t - \bar{\mathbf{r}})(\mathbf{r}_t - \bar{\mathbf{r}})^T \ .$$

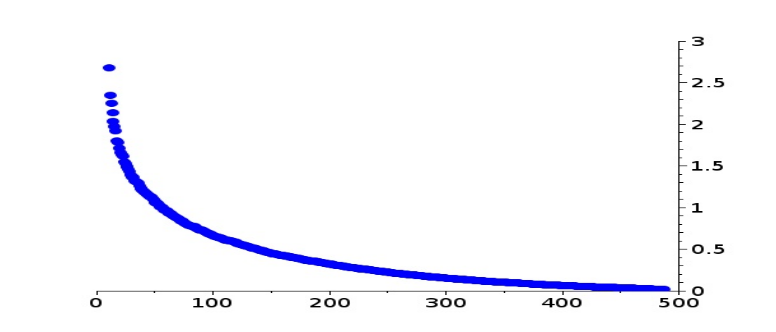
- We consider the sample correlation matrix $\mathbf{R}_n$ with

$$\mathbf{R}_n(i,j) = \frac{S_n(i,j)}{[S_n(i,i)S_n(j,j)]^{1/2}}.$$

- The 10 largest and 10 smallest eigenvalues of $\mathbf{R}_n$ are:

237.95801	4.8568703	...	0.0212137	0.0178129
17.762811	4.394394	...	0.0205001	0.0173591
14.002838	3.4999069	...	0.0198287	0.0164425
8.7633113	3.0880089	...	0.0194216	0.0154849
5.2995321	2.7146658	...	0.0190959	0.0147696

Sample eigenvalues of stock returns



[excluding the 10 largest: $\lambda_{11}, \ldots, \lambda_{488}$]

- Two important questions:
  - Explanation the largest sample eigenvalues (spikes, perturbation);
  - Provide a model for bulk correlation structure between the 488 returns.
- Both successfully analysed using

  Genelized Marčenko-Pastur distribution + spiked outliers

General issue:

- Assume that for a sequence of E.S.D F_n $\quad F_n = \frac{1}{p}\sum_{j=1}^{p} \delta_{\lambda_j}$, we have proved the existence of a limiting distribution F;
- Given a "smooth" function g, e.g. $g(x) = x - 1 - \log x$, consider the linear spectral statistic (LSS):

$$F_n(g) = \frac{1}{p}\sum_{j=1}^{p} g(\lambda_j)$$

- Problem: find a_n, b_n s.t.

$$a_n\left[F_n(g) - b_n\right] \Longrightarrow \mathcal{N}(m, V)$$

for some asymptotic mean m and variance V.

CLT for LSS of sample covariance matrices

- Consider a sequence of sample covariance matrices S_n s.t $F^{S_n} \Longrightarrow F_y$, the Marcčenko-Pastur distribution of index y;
- CLT's for regular functions g have a long history

  Arharov (1971); Jonsson (1982) ; Johnsson (1998); Sinai & Soshnikov (1998);
  Bai & Silverstein (2004); Bai and Y. (2005); Lytova & Pastur (2009)

Following Bai & Silverstein '04, let

- an open set $\mathcal{U}$ of $\mathbb{C}$ including the support $[a, b] = [(1-\sqrt{y})^2, (1+\sqrt{y})^2]$ of the LSD
- for any g analytic on $\mathcal{U}$: $G_n(g) = p\,[F_n(g) - \mu^{y_n}(g)]$
  where μ^{y_n} is the MP distribution of index $y_n \in (0, 1)$.

Bai and Silverstein (2004)

Theorem

Assume that

- $g_1, \cdots, g_k$ *are* k *analytic functions on* $\mathcal{U}$;
- *the matrix entries* x_{ij} *are i.i.d. real-valued random variables such that* $Ex_{ij} = 0,\ Ex_{ij}^2 = 1,\ E{x_{ij}}^4 = 3.$
- *as* $n, p \to \infty$, $y_n = \frac{p}{n} \to y \in (0, 1)$;

Then,

$$(G_n(g_1), \cdots, G_n(g_k)) \Rightarrow \mathcal{N}_k(m, V),$$

with a given mean vector $m = m(g_1, \ldots, g_k)$ *and asymptotic covariance matrix* $V = V(g_1, \ldots, g_k)$.

CLT for LSS of random Fisher matrices

- two independent samples:

$$\mathbf{x}_1, \ldots, \mathbf{x}_{n_1} \sim (0, I_p), \qquad \mathbf{y}_1, \ldots, \mathbf{y}_{n_2} \sim (0, I_p)$$

  with i.i.d coordinates of mean 0 and variance 1

- Associated sample covariance matrices:

$$S_1 = \frac{1}{n_1} \sum_{i=1}^{n_1} \mathbf{x}_i \mathbf{x}_i^T, \qquad S_2 = \frac{1}{n_2} \sum_{j=1}^{n_2} \mathbf{y}_j \mathbf{y}_j^T.$$

- Fisher matrix: $V_n = S_1 S_2^{-1}$ where $n_2 > p$.

- Assume

$$y_{n_1} = \frac{p}{n_1} \to y_1 \in (0,1), \qquad y_{n_2} = \frac{p}{n_2} \to y_2 \in (0,1) \ .$$

- Under mild moment conditions, the ESD $F_n^{V_n}$ of V_n has a LSD F_{y_1,y_2} with density (Wachter distribution):

$$\ell(x) = \begin{cases} \dfrac{(1-y_2)\sqrt{(b-x)(x-a)}}{2\pi x(y_1+y_2x)}, & a \le x \le b, \\ 0, & \text{otherwise} \end{cases}$$

where

$$a = (1-y_2)^{-2}\left(1-\sqrt{y_1+y_2-y_1y_2}\right)^2, \quad b = (1-y_2)^{-2}\left(1+\sqrt{y_1+y_2-y_1y_2}\right)^2.$$

CLT for LSS of random Fisher matrices

- let $\widetilde{\mathcal{U}} \subset \mathbb{C}$ be an open set including the interval

$$\left[I_{(0,1)}(y_1)\frac{(1-\sqrt{y_1})^2}{(1+\sqrt{y_2})^2}, \quad \frac{(1+\sqrt{y_1})^2}{(1-\sqrt{y_2})^2} \right],$$

- for an analytic function f on $\widetilde{\mathcal{U}}$, define

$$\widetilde{G_n}(f) = p\left[F_n^{V_n}(g) - F_{y_{n_1}, y_{n_2}}(g) \right] ,$$

where $F_{y_{n_1}, y_{n_2}}$ is the LSD with indexes y_{n_k}, $k = 1, 2$.

Zheng (2008)

Theorem

Assume $E\mathbf{x}_{11}^4 = E\mathbf{y}_{11}^4 < \infty$ *and let* $\beta = E|\mathbf{x}_{11}|^4 - 3$. *Then for any analytic functions* $f_1, \cdots, f_k$ *defined on* $\widetilde{\mathcal{U}}$,

$$\left[\widetilde{G}_n(f_1), \cdots, \widetilde{G}_n(f_k)\right] \Longrightarrow \mathcal{N}_k(m, \upsilon) \ .$$

Zheng (2008)

Limiting mean function m

$$m(f_j) = \lim_{r \to 1_+} [(2.1) + (2.2) + (2.3)]$$

$$\frac{1}{4\pi i} \oint_{|\zeta|=1} f_j(z(\zeta)) \left[\frac{1}{\zeta - \frac{1}{r}} + \frac{1}{\zeta + \frac{1}{r}} - \frac{2}{\zeta + \frac{y_2}{hr}} \right] d\zeta \quad (2.1)$$

$$+ \frac{\beta \cdot y_1 (1 - y_2)^2}{2\pi i \cdot h^2} \oint_{|\zeta|=1} f_j(z(\zeta)) \frac{1}{(\zeta + \frac{y_2}{hr})^3} d\zeta \quad (2.2)$$

$$+ \frac{\beta \cdot y_2 (1 - y_2)}{2\pi i \cdot h} \oint_{|\zeta|=1} f_j(z(\zeta)) \frac{\zeta + \frac{1}{hr}}{(\zeta + \frac{y_2}{hr})^3} d\zeta, \quad (2.3)$$

where

$$z(\zeta) = (1 - y_2)^{-2} \left[1 + h^2 + 2h\mathcal{R}(\zeta) \right], \qquad h = \sqrt{y_1 + y_2 - y_1 y_2}. \quad (2.4)$$

Zheng (2008)

Limiting covariance function υ

$$\upsilon(f_j, f_\ell) = \lim_{1<r_1<r_2\to 1_+} [(2.5) + (2.6)]$$

$$-\frac{1}{2\pi^2}\oint_{|\zeta_2|=1}\oint_{|\zeta_1|=1}\frac{f_j(z(r_1\zeta_1))f_\ell(z(r_2\zeta_2))r_1r_2}{(r_2\zeta_2 - r_1\zeta_1)^2}d\zeta_1 d\zeta_2, \tag{2.5}$$

$$-\frac{\beta\cdot(y_1+y_2)(1-y_2)^2}{4\pi^2h^2}\oint_{|\zeta_1|=1}\frac{f_j\left(z(\zeta_1)\right)}{(\zeta_1+\frac{y_2}{hr_1})^2}d\zeta_1\oint_{|\zeta_2|=1}\frac{f_\ell\left(z(\zeta_2)\right)}{(\zeta_2+\frac{y_2}{hr_2})^2}d\zeta_2 \tag{2.6}$$

$j, \ell \in \{1, \cdots, k\}.$

Problem 1: testing on high-dimensional covariance matrices

Testing structure of a large covariance matrix

- a sample $\mathbf{x}_1, \ldots, \mathbf{x}_n \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- want to test hypothesis about structure of $\boldsymbol{\Sigma}$:
  - $\boldsymbol{\Sigma} = \mathbf{I}_p$ (identity test)
  - $\boldsymbol{\Sigma} = c \times \mathbf{I}_p$, c unknown (sphericity test)
  - $\boldsymbol{\Sigma}$ is diagonal, block diagonal, Toeplitz, band, etc.
- in high-dimensional case, several previous work exist:
  Ledoit & Wolf '02; Schott '07; Srivastava '05 ...
- we focus on the simplest case of identity test $H_0 : \quad \boldsymbol{\Sigma} = \mathbf{I}_p$
- LR statistic:

$$T_n = n\left[trS_n - \log|S_n| - p\right], \quad S_n = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \overline{\mathbf{x}})(\mathbf{x}_i - \overline{\mathbf{x}})',$$

Classical LRT -large sample limit:

- when $n \to \infty$, $T_n \Longrightarrow \chi^2_{p(p+1)/2}$ (data dimension p is fixed)
- Procedure based on this limit is rapidly deficient when p is not "small".

RMT Corrected LRT:

Bai, Jiang, Y. and Zheng (2009)

Theorem

Assume $p/n \to y \in (0,1)$ *and let* $g(x) = x - \log x - 1$. *Then, under* H_0 *and when* $n \to \infty$

$$\left[\frac{T_n}{n} - p \cdot F^{y_n}(g)\right] \Rightarrow \mathcal{N}(m(g), \upsilon(g)),$$

where F^{y_n} *is the Marčenko-Pastur law of index* y_n *and*

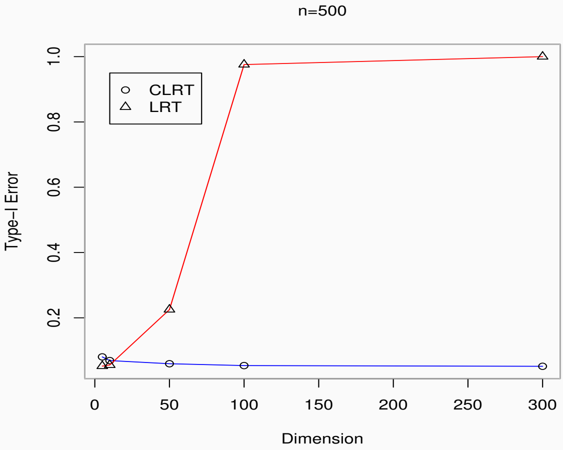
$$\begin{aligned} m(g) &= -\frac{\log(1-y)}{2}, \\ \upsilon(g) &= -2\log(1-y) - 2y. \end{aligned}$$

Comparison of LRT and Corrected LRT by simulation

- nominal test level $\alpha = 0.05$;
- for each (p, n), 10,000 independent replications with real Gaussian variables.
- Powers are estimated under the alternative H_1:
  $\Sigma = \mathrm{diag}(1, 0.05, 0.05, 0.05, \ldots, 0.05)$.

	CLRT			LRT	
(p, n)	Size	Difference with 5%	Power	Size	Power
(5, 500)	0.0803	0.0303	0.6013	0.0521	0.5233
(10, 500)	0.0690	0.0190	0.9517	0.0555	0.9417
(50, 500)	0.0594	0.0094	1	0.2252	1
(100, 500)	0.0537	0.0037	1	0.9757	1
(300, 500)	0.0515	0.0015	1	1	1

On a plot


n=500
CLRT
LRT
Type–I Error
1.0
0.8
0.6
0.4
0.2
0
50
100
150
200
250
300
Dimension

Problem 2: testing in high-dimensional regressions

A general linear hypothesis in a multivariate regression

A p-th dimensional regression model:

$$\mathbf{x}_i = \mathbf{B}\mathbf{z}_i + \varepsilon_i, \quad i = 1, \ldots, n$$

where

$$\varepsilon_i \sim \mathcal{N}_p(0, \boldsymbol{\Sigma}), \quad \mathbf{x}_i \in \mathbb{R}^p, \quad \mathbf{z}_i \in \mathbb{R}^q, \quad n \geq p + q.$$

A general linear hypothesis:

- Write a bloc decomposition $\mathbf{B} = (\mathbf{B}_1, \mathbf{B}_2)$ with q_1 and q_2 columns ($q = q_1 + q_2$)
- To test

$$H_0 : \ \mathbf{B}_1 = \mathbf{M} \ ,$$

  with a given $\mathbf{M}$.

Wilk's $\boldsymbol{\Lambda}$

- Let $\widehat{\boldsymbol{\Sigma}}_0$ and $\widehat{\boldsymbol{\Sigma}}_1$ be the likelihood "estimator" of $\boldsymbol{\Sigma}$ under H_0 and the alternative, respectively
- LRT statistic equals

$$\mathscr{L}_0/\mathscr{L}_1 = (\boldsymbol{\Lambda}_n)^{n/2}, \quad \boldsymbol{\Lambda}_n = \frac{|\widehat{\boldsymbol{\Sigma}}|}{|\widehat{\boldsymbol{\Sigma}}_0|} ,$$

where $\boldsymbol{\Lambda}_n$ is the celebrated Wilk's $\boldsymbol{\Lambda}$: Wilks '32, '34 ; Bartlett '34.

- Classic (low dimensional) approximation of LRT: for fixed p and q, $n \to \infty$ and under H_0:

$$U_n = -n \log \boldsymbol{\Lambda}_n \Rightarrow \chi^2_{pq_1} .$$

- Less biased Bartlett's correction:

$$\tilde{U}_n = -k \log \boldsymbol{\Lambda}_n, \quad k = n - q - \frac{1}{2}(p - q_1 + 1) .$$

Bai, Jiang, Y. and Zheng (2010)

Theorem

Let $p \to \infty,\ q_1 \to \infty,\ n-q \to \infty$ and

$$y_{n_1} = \frac{p}{q_1} \to y_1 \in (0,1), \quad y_{n_2} = \frac{p}{n-q} \to y_2 \in (0,1).$$

Then, under H_0,

$$T_n = \upsilon(f)^{-\frac{1}{2}} \left[-\log \boldsymbol{\Lambda}_n - p \cdot F_{y_{n_1}, y_{n_2}}(f) - m(f)\right] \Rightarrow \mathscr{N}(0,1),$$

where $m(f), \upsilon(f)$ and $F_{y_{n_1}, y_{n_2}}(f)$ are suitable constants computed from

$$f(x) = \log(1 + \frac{y_{n_2}}{y_{n_1}} x) \ .$$

The centering term:

$$F_{y_{n_1},y_{n_2}}(f) = \frac{y_{n_2}-1}{y_{n_2}}\log c_n + \frac{y_{n_1}-1}{y_{n_1}}\log(c_n - d_n h_n)$$
$$= +\frac{y_{n_1}+y_{n_2}}{y_{n_1}y_{n_2}}\log\left(\frac{c_n h_n - d_n y_{n_2}}{h_n}\right),$$

where

$$h_n = \sqrt{y_{n_1}+y_{n_2}-y_{n_1}y_{n_2}}$$
$$a_n, b_n = \frac{(1\mp h_n)^2}{(1-y_{n_2})^2}$$
$$c_n, d_n = \frac{1}{2}\left[\sqrt{1+\frac{y_{n_2}}{y_{n_1}}b_n} \pm \sqrt{1+\frac{y_{n_2}}{y_{n_1}}a_n}\right], c_n > d_n,$$

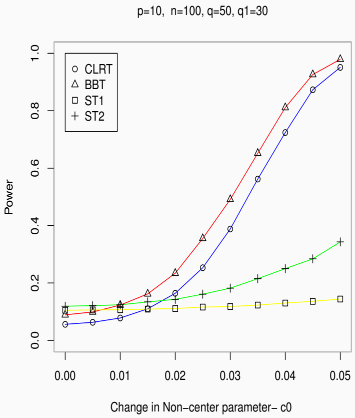
The limiting parameters:

$$
\begin{aligned}
m(f) &= \frac{1}{2}\log\frac{(c^2-d^2)h^2}{(ch-y_2d)^2}\,,\\
\upsilon(f) &= 2\log\left(\frac{c^2}{c^2-d^2}\right)\,,
\end{aligned}
$$

where

$$
\begin{aligned}
h &= \sqrt{y_1+y_2-y_1y_2}\\
a_0, b_0 &= \frac{(1\mp h)^2}{(1-y_2)^2}\\
c, d &= \frac{1}{2}\left[\sqrt{1+\frac{y_2}{y_1}b_0} \pm \sqrt{1+\frac{y_2}{y_1}a_0}\right], c > d.
\end{aligned}
$$

A simulation experiment



- Gaussian entries,
- non central parameter $c_0 \sim d(H, H_0)$.

An example where Marčenko-Pastur law does not hold

Multivariate normal mixture

- p-dimensional *multivariate normal mixture* (MNM):

$$f(\mathbf{x}) = \sum_{j=1}^{K} \alpha_j \phi(\mathbf{x};\, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j), \tag{5.1}$$

  where

  - (α_j): K mixing weights
  - $(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$: parameters of the jth Gaussian component (ϕ is the multivariate Gaussian density function)

- high-dimensional situations: p is large compared to the sample size n.

Statistical testing problem

- Test for the covariance matrix in the MNM model

$$f(\mathbf{x}) = \sum_{j=1}^{K} \alpha_j \phi(\mathbf{x};\, \boldsymbol{\mu}_j, \sigma_j^2 \mathbf{T}_p^2) \quad \text{with} \quad \boldsymbol{\mu}_j = 0 \tag{5.2}$$

in high-dimensional situations.

- This model is a special case of a p-dimensional *scale mixture*,

$$\mathbf{x} = w \mathbf{T}_p \mathbf{z}, \tag{5.3}$$

where

  - $\mathbf{z} = (z_1, \ldots, z_p)'$ are i.i.d. $E(z_i) = 0$, $E(z_i^2) = 1$;
  - $w > 0$ is a random scale, independent of $\mathbf{z}$;
  - $\mathbf{T}_p \in \mathbb{R}^{p \times p}$, $\mathbf{T}_p > 0$, $\mathrm{tr}(\mathbf{T}_p^2)/p = 1$;

Indeed: (5.3) $\Longrightarrow$ (5.2) if $\mathbf{z} \sim N(0, \mathbf{I}_p)$, $\mathbf{T}_p = \mathbf{I}_p$ and $P(w^2 = \sigma_j^2) = \alpha_j$.

- Terminology: distribution of w^2, denoted G, referred as *Population Mixing Distribution* (PMD).

- Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be a sample from the mixture $\mathbf{x}$, with population covariance matrix $\mathbf{\Sigma} = \mathbb{E}[\mathbf{x}_1 \mathbf{x}_1^T]$
- Sample covariance matrix: $\mathbf{S}_n = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i'.$
- Random matrix theory: for p, n large,

$$\text{eigenvalues of } \mathbf{\Sigma} \quad \rightsquigarrow \quad \text{eigenvalues of } \mathbf{S}_n$$

Terminology. *Empirical spectral distribution* (ESD) of a $p \times p$ symmetric matrix $\mathbf{A}$:

$$\mu_{\mathbf{A}} = \frac{1}{p} \sum_{j=1}^{p} \delta_{\lambda_j},$$

where $(\lambda_j)_{1 \le j \le p}$ are the eigenvalues of $\mathbf{A}$, (δ_b: the Dirac mass at b).

Existing random matrix theory

population eigenvalues sample eigenvalues

$\mu_{\boldsymbol{\Sigma}}$: ESD of $\boldsymbol{\Sigma}$ $\rightsquigarrow$ $\mu_{\mathbf{S}_n}$: ESD $\mathbf{S}_n$

Findings

Mixtures are not a usual high-dimensional population:

normal population with $\boldsymbol{\Sigma} = \mathbf{I}_p$: $\mu_{\mathbf{S}_n} \sim$ Marčenko-Pastur law

mixture of normals with $\boldsymbol{\Sigma} = \mathbf{I}_p$: $\mu_{\mathbf{S}_n} \neq$ Marčenko-Pastur law

(Both populations have uncorrelated components!)

Case of uncorrelated population I

- Consider the simplest case of $\mathbf{x} = \mathbf{z}$: $E(\mathbf{x}) = 0$, $\text{cov}(\mathbf{x}) = I_p$.
- Assume the Marčenko-Pastur regime:

$$p = p_n, \quad \text{and} \quad p_n/n \to c > 0 \quad \text{as} \quad n \to \infty.$$

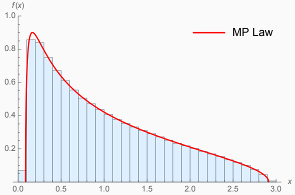
- We have that

$$\mu_{\mathbf{S}_n} \xrightarrow[w]{a.s.} \nu \text{ (MP law).}$$

- $\nu(dx) = f(x)dx + (1-1/c)\delta_0(dx)1_{\{c>1\}}$ where

$$f(x) = \frac{\sqrt{(b-x)(x-a)}}{2\pi cx} 1_{[a,b]}(x),$$

where $a = (1-\sqrt{c})^2$ and $b = (1+\sqrt{c})^2$.



The Marčenko-Pastur law (red line). The dimensions are $(p, n, c) = (500, 1000, 0.5)$ and $rep = 100$.

Case of uncorrelated population II

- Consider a simple mixture $\mathbf{x} = w\mathbf{z}$ where $E(w^2) = 1$;

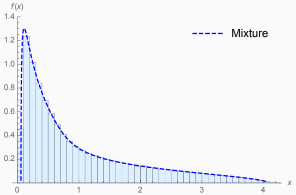
  we have $E(\mathbf{x}) = 0$, $\text{cov}(\mathbf{x}) = \mathbf{I}_p$.

- Assume again the Marčenko-Pastur regime: $p_n/n \to c > 0$.

- We have that

$$\mu_{\mathbf{S}_n} \xrightarrow[w]{a.s.} F^{c,G} \neq \text{MP law}.$$

- Example: The MNM is $f(\mathbf{x}) = 0.25\phi(\mathbf{x};\, 0, 2.5I_p) + 0.75\phi(\mathbf{x};\, 0, 0.5I_p)$ with $c = 1/2$.



The LSD (blue line) from the MNM. The dimensions are $(p, n, c) = (500, 1000, 0.5)$ and $rep = 100$. The support interval is $[0.0576, 4.0674]$.

Comparison between the two cases

Uncorrelated populaitons: $\mathbf{x} = \mathbf{z}$ versus $\mathbf{x} = w\ \mathbf{z}$

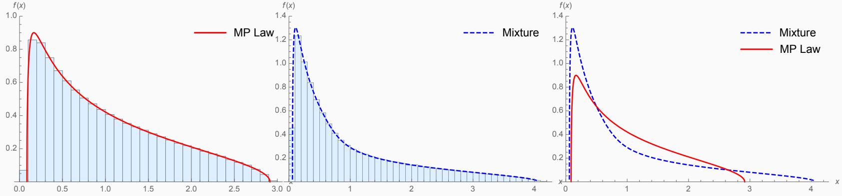


Figure 1: The Marčenko-Pastur law (red line) v.s. the LSD (blue line) from an MNM with identity covariance. The dimensions are $(p, n, c) = (500, 1000, 0.5)$ and $rep = 100$. The support intervals are $[0.0858, 2.9142]$ and $[0.0576, 4.0674]$, respectively.

High-dimensional mixtures needs new random matrix theory

Why mixtures are different?

- Main reason: coordinates of $\mathbf{x}$ could be uncorrelated but strongly dependent in the sense that:

$$\mathrm{var}(\|\mathbf{x}\|^2) \propto p^2, \quad p \to \infty.$$

- Consequence: much we have done so far for high-dimensional covariance matrices do not apply to high-dimensional mixtures.

- **Remark**
  - It is known that if for any bounded sequence (in spectral norm) $(\mathbf{A}_p)$, we have

$$\mathrm{var}\mathbf{x}^T\mathbf{A}_p\mathbf{x} = o(p^2),$$

then the corresponding sample covariance $\mathbf{S}_n$ satisfies the Marčenko-Pastur law. Bai and Zhou (2008)

Also called "good vector" by Pastur and Pajor (2009)

Setting of a general scale mixture

Assumption (a). The sample and population sizes n, p both tend to infinity with their ratio $c_n = p/n \to c \in (0, \infty)$.

Assumption (b). There are two independent arrays of i.i.d. random variables $(z_{ij})_{i,j\geq 1}$ and $(w_i)_{i\geq 1}$, satisfying

$$\mathbb{E}(z_{11}) = 0, \quad \mathbb{E}(z_{11}^2) = 1, \quad \mathbb{E}(z_{11}^4) < \infty, \tag{5.4}$$

such that for each p and n the observation vectors can be represented as $\mathbf{x}_i = w_i \mathbf{T}_p \mathbf{z}_i$ with $\mathbf{z}_i = (z_{i1}, \ldots, z_{ip})'$, $i = 1, \ldots, n$.

Assumption (c). The spectral distribution H_p of the matrix $\mathbf{T}_p^2$ weakly converges to a probability distribution H, as $p \to \infty$, referred as *Population Spectral Distribution* (PSD).

Assumption (d). The support set S_G of the MD G is bounded above and from below, that is $S_G \subset [a, b]$ for some $0 < a < b < \infty$.

Theorem

Suppose that Assumptions (a)-(c) hold. Then, almost surely, the empirical spectral distribution $\mu_n := \mu_{\mathbf{S}_n}$ *converges in distribution to a probability distribution* $F^{c,G,H}$ *whose Stieltjes transform* $m = m_{F^{c,G,H}}(z)$ *is a solution to the following system of equations, defined on the upper complex plane* $\mathbb{C}^+$*,*

$$\begin{cases} zm(z) = -1 + \int \frac{p(z)t}{1+cp(z)t} dG(t), \\ zm(z) = -\int \frac{1}{1+q(z)t} dH(t), \\ zm(z) = -1 - zp(z)q(z), \end{cases} \tag{5.5}$$

where $p(z)$ *and* $q(z)$ *are two auxiliary analytic functions. The solution is also unique in the set*

$$\{m(z) : -(1-c)/z + cm(z) \in \mathbb{C}^+,\ zp(z) \in \mathbb{C}^+,\ q(z) \in \mathbb{C}^+,\ z \in \mathbb{C}^+\}.$$

Li and Y. (2017)

Some special cases of limiting spectral distributions

- When the distributions H and/or G degenerate to some Dirac mass, the system (5.5) simplifies to a single equation leading to several well-known LSDs.
  - Case 1. If $H = G = \delta_1$, then the equations become
    $$z = -\frac{1}{m} + \frac{1}{1 + cm},$$
    which defines the standard MP law (Marčenko-Pastur, 1969).
  - Case 2. If $G = \delta_1$, then the equations turn into
    $$m = \int \frac{1}{t(1 - c - cmz) - z} dH(t) \ ,$$
    which defines the generalized MP law (Silverstein 1995).
  - Case 3. If $H = \delta_1$, then the equations reduce to
    $$z = -\frac{1}{m} + \int \frac{t}{1 + ctm} dG(t) \ , \tag{5.6}$$
    which defines an LSD corresponding to a scale-mixture population with spherical covariance matrix.

Fluctuations of eigenvalue statistics

- We study the fluctuation of linear spectral statistics (LSS) of $\mathbf{S}_n$ under the simplest spherical mixture model:

$$\mathbf{x} = w\mathbf{z},$$

  that is $\mathbf{T}_p = \mathbf{I}_p$ and the PSD $H = \delta_1$.

- By the previous theorem, $\mu_n := \mu_{\mathbf{S}_n} \xrightarrow{\mathscr{D}} F^{c,G}$.

- Linear spectral statistics (LSS) are of the form

$$\frac{1}{p}\sum_{j=1}^{p} f(\lambda_j) = \int f(x) d\mu_{\mathbf{S}_n}(x) = \int f d\mu_{\mathbf{S}_n}$$

  where f is a function on $[0, \infty)$.

- In Bai and Silverstein (2004), the LSS under their settings are proved to be asymptotically normal distributions:

$$\sum_{j=1}^{p} f(\lambda_j) - p \cdot \kappa(n, p) \xrightarrow{D} N(a, s^2)$$

  However, we show that this CLT does not apply to the present model of scale mixtures.

Fluctuations of eigenvalue statistics

- Express the sample as $\mathbf{x}_j = w_j \mathbf{z}_j$, $j = 1, \ldots, n$, and let

$$G_n = \frac{1}{n}\sum_{j=1}^{n} \delta_{w_j^2}, \quad \text{ESD } \mu_n \approx \begin{cases} F^{c,G} & c_n \to c,\, G_n \xrightarrow{w} G, \\ F^{c_n,G} & c \text{ is replaced with } c_n, \\ F^{c_n,G_n} & (c, G) \text{ is replaced with } (c_n, G_n) \end{cases}$$

- The aim here is to study the fluctuation of

$$\boxed{\frac{1}{p}\sum_{j=1}^{p} f(\lambda_j) - \int f(x) dF^{c_n,G}(x) = \int f \cdot d(\mu_n - F^{c_n,G})}$$

through the decomposition

$$\int f \cdot d(\mu_n - F^{c_n,G}) = \int f \cdot d(\mu_n - F^{c_n,G_n}) + \int f \cdot d(F^{c_n,G_n} - F^{c_n,G})$$

Write it as:

$$\int f \cdot d\mathcal{F}_n = \int f \cdot d\mathcal{F}_{n1} + \int f \cdot d\mathcal{F}_{n2}.$$

A central limit theorem

Theorem

Suppose that Assumptions (a)-(d) hold. Let $f_1, \dots, f_k$ *be functions on* $\mathbb{R}$ *analytic on an open interval containing* $\left[aI_{(0,1)}(1/c)(1-\sqrt{1/c})^2, b(1+\sqrt{1/c})^2\right]$. *Write* $\Delta = E(z_{11}^4) - 3$, *then the random vectors*

$$n\left(\int f_1 \cdot d\mathcal{F}_{n1}, \ \dots, \int f_k \cdot d\mathcal{F}_{n1}\right) \xrightarrow{D} N_k(\mu, \Gamma_1),$$

$$\sqrt{n}\left(\int f_1 \cdot d\mathcal{F}_{n2}, \ \dots, \int f_k \cdot d\mathcal{F}_{n2}\right) \xrightarrow{D} N_k(0, \Gamma_2).$$

Li and Y. (2017)

- Notice that

  $\mathcal{F}_{n1} = F_n - F^{c_n, G_n}$ is "asymptotically independent" of $\mathcal{F}_{n2} = F^{c_n, G_n} - F^{c_n, G}$,

  which leads to a finite-sample corrected CLT

$$\sqrt{n}\left(\int f_1 \cdot d\mathcal{F}_n, \ \dots, \int f_k \cdot d\mathcal{F}_n\right) \dot{\sim} N_k(\mu/\sqrt{n}, \Gamma_1/n + \Gamma_2). \qquad (5.7)$$

Applications to empirical moments

- Example: For $\widehat{\beta}_{n2} = \sum_{j=1}^{p} \lambda_j^2/p$,

$$\sqrt{n}\left(\widehat{\beta}_{n2} - \beta_2\right) \dot{\sim} N\left(v_2/\sqrt{n}, \psi_{122}/n + \psi_{222}\right) \tag{5.8}$$

where the parameters are respectively

$$\beta_2 = c_n\gamma_2 + \gamma_1^2, \quad v_2 = (1+\Delta)\gamma_2,$$
$$\psi_{122} = 4((2+\Delta)\gamma_1^2\gamma_2/c + 8(2+\Delta)\gamma_1\gamma_2 + 4(\gamma_2^2 + c(2+\Delta)\gamma_4)),$$
$$\psi_{222} = c^2(\gamma_4 - \gamma_2^2) + 4c\gamma_1\gamma_3 + 4(1-c)\gamma_1^2\gamma_2 - 4\gamma_1^4.$$

Here, $\gamma_j = \int t^j dG(t)$ are the moments of the limiting mixing distribution G (not observed in a mixture !)

- Numerical results: PMD $G = 0.4\delta_1 + 0.6\delta_3$, $z_{ij} \sim \sqrt{1/6} \cdot (\chi_3^2 - 3)$.

Statistic	(p, n)	limiting distribution	correction
$\sqrt{n}(\widehat{\beta}_{n2} - \tilde{\beta}_2)$	(200,400)	$N(0, 39.32)$	$N(3.48, 48.88)$