Some aspects of large sample covariance matrices

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Sample covariance matrix and problem of high-dimensionality

Random matrix theory for large sample covariance matrix
  Marčenko-Pastur distributions
  CLT’s for linear spectral statistics

Problem 1: testing on high-dimensional covariance matrices

Problem 2: testing in high-dimensional regressions

An example where Marčenko-Pastur law does not hold
  High-dimensional theory fo eigenvalues of $S_n$ from mixtures
Sample covariance matrix and problem of high-dimensionality
Sample variance/covariances from a multivariate population

- Let \( x, \ldots, x_1, \ldots, x_n, \ldots \) an i.i.d. sequence of \( \mathbb{R}^p \)-valued random vectors with common distribution \( \mu \) (population);

- Sample variance/covariance matrix: (assuming \( \mathbb{E}(x) = 0 \))

\[
S_n = \frac{1}{n} \sum_{k=1}^{n} x_k x_k^T.
\]

That is, if we write \( x_k = (\xi_{1k}, \ldots, \xi_{pk})^T \),

\[
S_n(i, j) = \frac{1}{n} \sum_{k=1}^{n} \xi_{ik} \xi_{jk}, \quad 1 \leq i, j \leq p.
\]

[sample cross-moments between dimensions/variables \( i \) and \( j \).]

- The population variance/covariance matrix is

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

Both \( S_n \) and \( \Sigma \) are nonnegative definite and trivially,

\[
\mathbb{E}S_n = \Sigma.
\]
Is $S_n$ a “good enough” estimator of $\Sigma$?

**Large sample theory**

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

1. **Law of large numbers:** $S_n \xrightarrow{a.s.} \Sigma = \mathbb{E}[xx^T]$, \quad [once $\mathbb{E}[\|x\|^2] < \infty$]

2. **Central limit theorem:** $\sqrt{n} [S_n - \Sigma] \Rightarrow \mathcal{N}(0, \Lambda)$, \quad \[ \text{with some asymptotic variance/covariance matrix } \Lambda. \]

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

**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:

<table>
<thead>
<tr>
<th>Data Source</th>
<th># variables</th>
<th>sample size</th>
<th>ratio $p/n$</th>
<th>Small / Big</th>
</tr>
</thead>
<tbody>
<tr>
<td>Portfolio</td>
<td>$\sim 100$</td>
<td>500</td>
<td>0.2</td>
<td>S</td>
</tr>
<tr>
<td>Climate survey</td>
<td>320</td>
<td>600</td>
<td>0.21</td>
<td>S</td>
</tr>
<tr>
<td>Speech analysis</td>
<td>$\sim 10^3$</td>
<td>$\sim 10^3$</td>
<td>$\sim 1$</td>
<td>S</td>
</tr>
<tr>
<td>ORL Face database</td>
<td>1440</td>
<td>320</td>
<td>4.5</td>
<td>B</td>
</tr>
<tr>
<td>Micro-arrays</td>
<td>10000</td>
<td>1000</td>
<td>10</td>
<td>B</td>
</tr>
</tbody>
</table>
Consider

- a “white”/unit Gaussian population \( x \sim \mathcal{N}(0, I_p) \), that is,

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

- given a sample \( x_1, \ldots, x_n \) from \( x \), the sample covariance matrix is,

\[
S_n = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T = \frac{1}{n} W_n,
\]

Here

\[
W_n = \sum_{i=1}^{n} x_i x_i^T = (x_1, \ldots, x_n)(x_1, \ldots, x_n)^T \sim \text{Wishart}(n, I_p)
\]

- let \( \lambda_1 \geq \cdots \geq \lambda_p \geq 0 \) be eigenvalues of \( S_n \).
Example (cont.)

Large sample limits: \( p \) fixed while \( n \to \infty \)

1. LLN: \( S_n \xrightarrow{a.s.} I_p \);
   by continuity, \( (\lambda_1, \ldots, \lambda_p) \xrightarrow{a.s.} 1 \).

2. CLT:

\[
\sqrt{n} (S_n - I_p) \Rightarrow \mathcal{N}(0, *) ,
\]

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: \( S_n \not\sim I_p \);
   \[
   \frac{1}{p} \sum_{k=1}^{p} \delta_{\lambda_k} \Rightarrow \text{Marčenko-Pastur law}
   \]

2. CLT:

\[
(\lambda_1^2 + \cdots + \lambda_p^2) - p - p^2/n \Rightarrow \mathcal{N}(m, *).
\]
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 $\sim 1$
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

\[
\text{RMT Marčenko-Pastur limit} \gg \text{classical large sample limit}
\]
Empirical performance of the Marčenko-Pastur limiting scheme

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Sample size</th>
<th>$p/n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ultra-dim</td>
<td>50</td>
<td>10</td>
</tr>
<tr>
<td>Low-dim</td>
<td>50</td>
<td>1</td>
</tr>
<tr>
<td>Low-dim</td>
<td>50</td>
<td>0.1</td>
</tr>
</tbody>
</table>

$p/n$ values: 10, 1, 0.1
Random matrix theory for large sample covariance matrix
The Marčenko-Pastur distribution

**Theorem.** Assume:

- Population $\mathbf{x} = (\xi_1, \ldots, \xi_p)^T$ has i.i.d. components with mean 0 and variance 1; (so $\Sigma = I_p$);
- $\mathbf{x}_1, \ldots, \mathbf{x}_n$ 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

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

where

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

\[ f(x) = \frac{1}{2\pi y x} \sqrt{(x - a)(b - x)}, \quad (1 - \sqrt{y})^2 = a \leq x \leq b = (1 + \sqrt{y})^2. \]

<table>
<thead>
<tr>
<th>( y \sim p/n )</th>
<th>a</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/8</td>
<td>0.42</td>
<td>1.83</td>
</tr>
<tr>
<td>1/4</td>
<td>0.25</td>
<td>2.25</td>
</tr>
<tr>
<td>1/2</td>
<td>0.09</td>
<td>2.91</td>
</tr>
</tbody>
</table>
The generalized Marčenko-Pastur distribution

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

- \( X = p \times n \) 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 \( S_n = \frac{1}{n} T_p^{1/2} X X^T T_p^{1/2} \) 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 \( T_p = \text{diag}\{1, \ldots, 1, 4, \ldots, 4, 10, \ldots, 10\}. \)

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 \( r_t(i) = \log \frac{p_t(i)}{p_{t-1}(i)} \) from 2007-09-24 to 2011-09-12;
The sample correlation matrix

Let the SCM $(488 \times 488)$

\[ S_n = \frac{1}{n} \sum_{t=1}^{n} (r_t - \bar{r})(r_t - \bar{r})^T. \]

We consider the sample correlation matrix $R_n$ with

\[ R_n(i, j) = \frac{S_n(i, j)}{[S_n(i, i)S_n(j, j)]^{1/2}}. \]

The 10 largest and 10 smallest eigenvalues of $R_n$ are:

\[
\begin{array}{cccccc}
237.95801 & 4.8568703 & \ldots & 0.0212137 & 0.0178129 \\
17.762811 & 4.394394 & \ldots & 0.0205001 & 0.0173591 \\
14.002838 & 3.4999069 & \ldots & 0.0198287 & 0.0164425 \\
8.7633113 & 3.0880089 & \ldots & 0.0194216 & 0.0154849 \\
5.2995321 & 2.7146658 & \ldots & 0.0190959 & 0.0147696 \\
\end{array}
\]
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 $F_n = \frac{1}{p} \sum_{j=1}^{p} \delta_{\lambda_j}$, 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.

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

for some asymptotic mean $m$ and variance $V$. 
Consider a sequence of sample covariance matrices $S_n$ s.t $F^{S_n} \Rightarrow F_y$, 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 $U$ of $\mathbb{C}$ including the support $[a, b] = [(1 - \sqrt{y})^2, (1 + \sqrt{y})^2]$ of the LSD

- for any $g$ analytic on $U$: $G_n(g) = p[F_n(g) - \mu^{y_n}(g)]$

where $\mu^{y_n}$ is the MP distribution of index $y_n \in (0, 1)$. 
Theorem

Assume that

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

Then,

\[
(G_n(g_1), \ldots, G_n(g_k)) \Rightarrow \mathcal{N}_k(m, V),
\]

with a given mean vector \( m = m(g_1, \ldots, g_k) \) and asymptotic covariance matrix 
\( V = V(g_1, \ldots, g_k) \).
two independent samples:

\[ x_1, \ldots, x_{n_1} \sim (0, I_p), \quad y_1, \ldots, y_{n_2} \sim (0, I_p) \]

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

Associated sample covariance matrices:

\[ S_1 = \frac{1}{n_1} \sum_{i=1}^{n_1} x_i x_i^T, \quad S_2 = \frac{1}{n_2} \sum_{j=1}^{n_2} y_j y_j^T. \]

Fisher matrix:

\[ V_n = S_1 S_2^{-1} \text{ where } n_2 > p. \]
LSD of random Fisher matrices

Assume

\[ y_{n_1} = \frac{p}{n_1} \rightarrow y_1 \in (0, 1), \quad y_{n_2} = \frac{p}{n_2} \rightarrow y_2 \in (0, 1). \]

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

\[
\ell(x) = \begin{cases} 
\frac{(1 - y_2) \sqrt{(b - x)(x - a)}}{2\pi x(y_1 + y_2 x)}, & a \leq x \leq b, \\
0, & \text{otherwise}
\end{cases}
\]

where

\[
a = (1 - y_2)^{-2} \left(1 - \sqrt{y_1 + y_2 - y_1 y_2}\right)^2, \quad b = (1 - y_2)^{-2} \left(1 + \sqrt{y_1 + y_2 - y_1 y_2}\right)^2.
\]
let $\tilde{U} \subset \mathbb{C}$ be an open set including the interval

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

for an analytic function $f$ on $\tilde{U}$, define

$$\tilde{G}_n(f) = p \left[ F_n^\vee(g) - F_{y_1,y_2}(g) \right],$$

where $F_{y_1,y_2}$ is the LSD with indexes $y_{nk}, k = 1, 2.$
Theorem

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

$$\left[ \tilde{G}_n(f_1), \cdots, \tilde{G}_n(f_k) \right] \Rightarrow \mathcal{N}_k(m, \nu) .$$
Limiting mean function $m$

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

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

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

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

where

\[
z(\zeta) = (1 - y_2)^{-2} \left[ 1 + h^2 + 2hR(\zeta) \right], \quad h = \sqrt{y_1 + y_2 - y_1y_2}.
\]
Limiting covariance function $\nu$

$$\nu(f_j, f_\ell) = \lim_{1 < r_1 < r_2 \to 1^+} \left[ (2.5) + (2.6) \right]$$

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

$$-\beta \cdot (y_1 + y_2)(1 - y_2)^2 \frac{1}{4\pi^2 h^2} \oint_{|\zeta_1|=1} \frac{f_j(z(\zeta_1))}{(\zeta_1 + \frac{y_2}{h_1})^2} d\zeta_1 \oint_{|\zeta_2|=1} \frac{f_\ell(z(\zeta_2))}{(\zeta_2 + \frac{y_2}{h_2})^2} d\zeta_2 \quad (2.6)$$

$$j, \ell \in \{1, \cdots, k\}.$$
Problem 1: testing on high-dimensional covariance matrices
Testing structure of a large covariance matrix

- a sample $\mathbf{x}_1, \ldots, \mathbf{x}_n \sim \mathcal{N}_p(\mu, \Sigma)$
- want to test hypothesis about structure of $\Sigma$:
  - $\Sigma = \mathbf{I}_p$ (identity test)
  - $\Sigma = c \times \mathbf{I}_p$, $c$ unknown (sphericity test)
  - $\Sigma$ 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 $H_0 : \Sigma = \mathbf{I}_p$

- LR statistic:
  \[
  T_n = n \left[ \text{tr} S_n - \log |S_n| - p \right], \quad S_n = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})',
  \]

Classical LRT - large sample limit:

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

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

where \( F_{y_n}^n \) is the Marčenko-Pastur law of index \( y_n \) and

\[
m(g) = -\frac{\log (1 - y)}{2},
\]

\[
\nu(g) = -2 \log (1 - y) - 2y.
\]
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 $H_1:$
  $\Sigma = \text{diag}(1, 0.05, 0.05, 0.05, \ldots, 0.05)$.

<table>
<thead>
<tr>
<th>$(p, \ n)$</th>
<th>CLRT</th>
<th>LRT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Size</td>
<td>Difference with 5%</td>
</tr>
<tr>
<td>(5, 500)</td>
<td>0.0803</td>
<td>0.0303</td>
</tr>
<tr>
<td>(10, 500)</td>
<td>0.0690</td>
<td>0.0190</td>
</tr>
<tr>
<td>(50, 500)</td>
<td>0.0594</td>
<td>0.0094</td>
</tr>
<tr>
<td>(100, 500)</td>
<td>0.0537</td>
<td>0.0037</td>
</tr>
<tr>
<td>(300, 500)</td>
<td>0.0515</td>
<td>0.0015</td>
</tr>
</tbody>
</table>
Problem 2: testing in high-dimensional regressions
A general linear hypothesis in a multivariate regression

A \( p \)-th dimensional regression model:

\[
x_i = Bz_i + \varepsilon_i, \quad i = 1, \ldots, n
\]

where

\[
\varepsilon_i \sim \mathcal{N}_p(0, \Sigma), \quad x_i \in \mathbb{R}^p, \quad z_i \in \mathbb{R}^q, \quad n \geq p + q.
\]

A general linear hypothesis:

- Write a bloc decomposition \( B = (B_1, B_2) \) with \( q_1 \) and \( q_2 \) columns \( (q = q_1 + q_2) \)

- To test

\[
H_0 : B_1 = M,
\]

with a given \( M \).
Let $\hat{\Sigma}_0$ and $\hat{\Sigma}_1$ be the likelihood “estimator” of $\Sigma$ under $H_0$ and the alternative, respectively.

LRT statistic equals

$$\frac{L_0}{L_1} = (\Lambda_n)^{n/2}, \quad \Lambda_n = \frac{|\Sigma|}{|\hat{\Sigma}_0|},$$

where $\Lambda_n$ is the celebrated Wilk’s $\Lambda$: Wilks ’32, ’34; Bartlett ’34.

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

$$U_n = -n \log \Lambda_n \Rightarrow \chi^2_{pq1}.$$ 

Less biased Bartlett’s correction:

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

Let \( p \to \infty, \ q_1 \to \infty, \ n-q \to \infty \) and

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

Then, under \( H_0 \),

\[
T_n = \nu(f)^{-\frac{1}{2}} \left[ - \log \Lambda_n - p \cdot F_{\gamma_{n_1},\gamma_{n_2}}(f) - m(f) \right] \Rightarrow \mathcal{N}(0,1),
\]

where \( m(f), \nu(f) \) and \( F_{\gamma_{n_1},\gamma_{n_2}}(f) \) are suitable constants computed from

\[
f(x) = \log(1 + \frac{y_{n_2}}{y_{n_1}}x).
\]
The centering term:

\[F_{y_{n1}, y_{n2}}(f) = \frac{y_{n2} - 1}{y_{n2}} \log c_n + \frac{y_{n1} - 1}{y_{n1}} \log (c_n - d_n h_n)\]

\[= \frac{y_{n1} + y_{n2}}{y_{n1} y_{n2}} \log \left(\frac{c_n h_n - d_n y_{n2}}{h_n}\right),\]

where

\[h_n = \sqrt{y_{n1} + y_{n2} - y_{n1} y_{n2}}\]

\[a_n, b_n = \frac{(1 \mp h_n)^2}{(1 - y_{n2})^2}\]

\[c_n, d_n = \frac{1}{2} \left[\sqrt{1 + \frac{y_{n2}}{y_{n1}}} b_n \pm \sqrt{1 + \frac{y_{n2}}{y_{n1}}} a_n\right], c_n > d_n,\]
The limiting parameters:

\[ m(f) = \frac{1}{2} \log \left( \frac{(c^2 - d^2)h^2}{(ch - y_2 d)^2} \right), \]
\[ v(f) = 2 \log \left( \frac{c^2}{c^2 - d^2} \right), \]

where

\[ h = \sqrt{y_1 + y_2 - y_1 y_2} \]
\[ a_0, b_0 = \frac{(1 \mp h)^2}{(1 - y_2)^2} \]
\[ c, d = \frac{1}{2} \left[ \sqrt{1 + \frac{y_2}{y_1} b_0} \pm \sqrt{1 + \frac{y_2}{y_1} a_0} \right], c > d. \]
A simulation experiment

- Gaussian entries,

- non central parameter $c_0 \sim d(H, H_0)$. 
An example where Marčenko-Pastur law does not hold
$p$-dimensional multivariate normal mixture (MNM):

$$f(x) = \sum_{j=1}^{K} \alpha_j \phi(x; \mu_j, \Sigma_j),$$

where

- $(\alpha_j)$: $K$ mixing weights
- $(\mu_j, \Sigma_j)$: parameters of the $j$th Gaussian component ($\phi$ is the multivariate Gaussian density function)

- high-dimensional situations: $p$ is large compared to the sample size $n$. 
Test for the covariance matrix in the MNM model

\[ f(x) = \sum_{j=1}^{K} \alpha_j \phi(x; \mu_j, \sigma_j^2 T_p^2) \quad \text{with} \quad \mu_j = 0 \quad (5.2) \]

in high-dimensional situations.

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

\[ x = w T_p z, \quad (5.3) \]

where

- \( z = (z_1, \ldots, z_p)' \) are i.i.d. \( E(z_i) = 0, E(z_i^2) = 1; \)
- \( w > 0 \) is a random scale, independent of \( z; \)
- \( T_p \in \mathbb{R}^{p \times p}, \ T_p > 0, \ \text{tr}(T_p^2)/p = 1; \)

Indeed: \( (5.3) \implies (5.2) \) if \( z \sim N(0, I_p), \ T_p = I_p \) and \( P(w^2 = \sigma_j^2) = \alpha_j. \)

Terminology: distribution of \( w^2 \), denoted \( G \), referred as *Population Mixing Distribution* (PMD).
Let $x_1, \ldots, x_n$ be a sample from the mixture $x$, with population covariance matrix $\Sigma = \mathbb{E}[x_1x_1^T]$

Sample covariance matrix: $S_n = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T$.

Random matrix theory: for $p, n$ large,

$$\text{eigenvalues of } \Sigma \sim \text{eigenvalues of } S_n$$

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

$$\mu_A = \frac{1}{p} \sum_{j=1}^{p} \delta_{\lambda_j},$$

where $(\lambda_j)_{1 \leq j \leq p}$ are the eigenvalues of $A$, $(\delta_b$: the Dirac mass at $b$).
Existing random matrix theory

population eigenvalues  sample eigenvalues

\( \mu_\Sigma : \text{ESD of } \Sigma \quad \rightsquigarrow \quad \mu_{S_n} : \text{ESD } S_n \)

Findings

Mixtures are not a usual high-dimensional population:

- normal population with \( \Sigma = I_p \): \( \mu_{S_n} \sim \) Marčenko-Pastur law
- mixture of normals with \( \Sigma = I_p \): \( \mu_{S_n} \neq \) Marčenko-Pastur law

(Both populations have uncorrelated components!)
Case of uncorrelated population I

- Consider the simplest case of \( x = z \): \( \mathbb{E}(x) = 0, \text{cov}(x) = I_p \).
- 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
  \[
  \mu S_n \xrightarrow{a.s.} \nu \quad (\text{MP law}).
  \]
- \( \nu(dx) = f(x)dx + (1 - 1/c)\delta_0(dx)1\{c>1\} \)
  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 \( x = wz \) where \( E(w^2) = 1 \); we have \( E(x) = 0, \text{cov}(x) = I_p \).

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

- We have that
  \[
  \mu S_n \xrightarrow{a.s.} \frac{1}{w} F^{c,G} \neq \text{MP law}.
  \]

- Example: The MNM is
  \[
  f(x) = 0.25\phi(x; 0, 2.5I_p) + 0.75\phi(x; 0, 0.5I_p)
  \]
  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 populations: \( x = z \) versus \( x = wz \)

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.
Why mixtures are different?

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

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

- **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

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

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

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

such that for each $p$ and $n$ the observation vectors can be represented as $x_i = w_i T_p z_i$ with $z_i = (z_{i1}, \ldots, z_{ip})'$, $i = 1, \ldots, n$.

Assumption (c). The spectral distribution $H_p$ of the matrix $T_p^2$ 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 $0 < a < b < \infty$. 
Suppose that Assumptions (a)-(c) hold. Then, almost surely, the empirical spectral distribution \( \mu_n := \mu_S_n \) converges in distribution to a probability distribution \( F_{c,G,H} \) whose Stieltjes transform \( m = m_{Fc,G,H}(z) \) is a solution to the following system of equations, defined on the upper complex plane \( \mathbb{C}^+ \),

\[
\begin{align*}
zm(z) &= -1 + \int \frac{p(z) t}{1 + cp(z) t} dG(t), \\
zm(z) &= -\int \frac{1}{1 + q(z) t} dH(t), \\
zm(z) &= -1 - zp(z) q(z),
\end{align*}
\]

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

\[ \{ m(z) : - (1 - c)/z + cm(z) \in \mathbb{C}^+, \ zp(z) \in \mathbb{C}^+, \ q(z) \in \mathbb{C}^+, \ z \in \mathbb{C}^+ \}. \]
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.
We study the fluctuation of linear spectral statistics (LSS) of $S_n$ under the simplest spherical mixture model:

$$x = wz,$$

that is $T_p = I_p$ and the PSD $H = \delta_1$.

By the previous theorem, $\mu_n := \mu_{S_n} \xrightarrow{D} F^{c,G}$.

Linear spectral statistics (LSS) are of the form

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

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 \( x_j = w_j z_j, \; j = 1, \ldots, n \), and let

\[
G_n = \frac{1}{n} \sum_{j=1}^{n} \delta_{w_j^2}, \quad \text{ESD} \; \mu_n \approx \left\{ \begin{array}{ll}
F_{c,G} & c_n \to c, \; G_n \xrightarrow{w} G, \\
F_{cn,G} & c \text{ is replaced with } c_n, \\
F_{cn,G_n} & (c, G) \text{ is replaced with } (c_n, G_n)
\end{array} \right.
\]

- The aim here is to study the fluctuation of

\[
\frac{1}{p} \sum_{j=1}^{p} f(\lambda_j) - \int f(x) dF_{cn,G}(x) = \int f \cdot d(\mu_n - F_{cn,G})
\]

through the decomposition

\[
\int f \cdot d(\mu_n - F_{cn,G}) = \int f \cdot d(\mu_n - F_{cn,G_n}) + \int f \cdot d(F_{cn,G_n} - F_{cn,G})
\]

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 \( f_1, \ldots, f_k \) be functions on \( \mathbb{R} \) analytic on an open interval containing
\[
\left[ a(0,1)(1/c)(1 - \sqrt{1/c})^2, b(1 + \sqrt{1/c})^2 \right].
\]
Write \( \Delta = E(z_{11}^4) - 3 \), then the random vectors
\[
n \left( \int f_1 \cdot d\mathcal{F}_{n1}, \ldots, \int f_k \cdot d\mathcal{F}_{n1} \right) \xrightarrow{D} N_k(\mu, \Gamma_1),
\]
\[
\sqrt{n} \left( \int f_1 \cdot d\mathcal{F}_{n2}, \ldots, \int f_k \cdot d\mathcal{F}_{n2} \right) \xrightarrow{D} N_k(0, \Gamma_2).
\]

Li and Y. (2017)

- Notice that
  \( \mathcal{F}_{n1} = F_n - F_{cn, G_n} \) is “asymptotically independent” of \( \mathcal{F}_{n2} = F_{cn, G_n} - F_{cn, G} \),
  which leads to a finite-sample corrected CLT
  \[
  \sqrt{n} \left( \int f_1 \cdot d\mathcal{F}_n, \ldots, \int f_k \cdot d\mathcal{F}_n \right) \sim N_k(\mu/\sqrt{n}, \Gamma_1/n + \Gamma_2). \tag{5.7}
  \]
Example: For $\hat{\beta}_n^2 = \sum_{j=1}^{p} \chi_j^2 / p$,

$$\sqrt{n} (\hat{\beta}_n^2 - \beta_2) \sim N \left( \frac{v_2}{\sqrt{n}}, \frac{\psi_{122}}{n} + \psi_{222} \right) \quad (5.8)$$

where the parameters are respectively

$$\beta_2 = c_n \gamma_2 + \gamma_1^2, \quad v_2 = (1 + \Delta) \gamma_2,$$

$$\psi_{122} = 4((2 + \Delta) \gamma_1^2 \gamma_2 / c + 8(2 + \Delta) \gamma_1 \gamma_2 + 4(\gamma_2^2 + c(2 + \Delta) \gamma_4)),$$

$$\psi_{222} = c^2(\gamma_4 - \gamma_2^2) + 4c \gamma_1 \gamma_3 + 4(1 - c) \gamma_1 \gamma_2 - 4 \gamma_1^4.$$  

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

<table>
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<td>(200,400)</td>
<td>$N(0, 39.32)$</td>
<td>$N(3.48, 48.88)$</td>
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