Estimation of the population spectral distribution from a large dimensional sample covariance matrix

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Abstract: This paper introduces a new method to estimate the spectral distribution of a population covariance matrix from high-dimensional data. The method is founded on a meaningful generalization of the seminal Marčenko-Pastur equation, originally defined in the complex plane, to the real line. Beyond its easy implementation and the established asymptotic consistency, the new estimator outperforms two existing estimators from the literature in almost all the situations tested in a simulation experiment. An application to the analysis of the correlation matrix of S&P stocks data is also given.

Key words and phrases: Empirical spectral distribution, high-dimensional data, Marčenko-Pastur distribution, large sample covariance matrices, Stieltjes transform

1 Introduction

Let \( x_1, \ldots, x_n \) be a sequence of i.i.d. zero-mean random vectors in \( \mathbb{R}^p \) or \( \mathbb{C}^p \), with a common population covariance matrix \( \Sigma_p \). When the population size \( p \) is not negligible with respect to the sample size \( n \), modern random matrix theory indicates that the sample covariance matrix

\[
S_n = \frac{1}{n} \sum_{j=1}^{n} x_j x_j^*
\]

does not approach \( \Sigma_p \). For instance, in a simple case where \( \Sigma_p = I_p \) (identity matrix), the eigenvalues of \( S_n \) will spread over an interval approximately equal to \( (1 \mp \sqrt{p/n})^2 \) around the unique population eigenvalue 1 of \( \Sigma_p \) (Marčenko and Pastur (1967), Yin et al. (1988) and Bai and Yin (1993)). Therefore, classical statistical procedures based on an approximation of \( \Sigma_p \) by \( S_n \) become inconsistent in such high dimensional data situations.
To be precise, let us recall that the spectral distribution (SD) $G^A$ of an $m \times m$ Hermitian matrix (or real symmetric) $A$ is the measure generated by its eigenvalues $\{\lambda_i^A\}$,

$$G^A = \frac{1}{m} \sum_{i=1}^{m} \delta_{\lambda_i^A},$$

where $\delta_b$ denotes the Dirac point measure at $b$. Let $(\sigma_i)_{1 \leq i \leq p}$ be the $p$ eigenvalues of the population covariance matrix $\Sigma_p$. We are particularly interested in the following SD

$$H_p := G^{\Sigma_p} = \frac{1}{p} \sum_{i=1}^{p} \delta_{\sigma_i}.$$  

Following the random matrix theory, both sizes $p$ and $n$ will grow to infinity. It is then natural to assume that $H_p$ weakly converges to a limiting distribution $H$ when $p \to \infty$. We refer this limiting SD $H$ as the population spectral distribution (PSD) of the observation model.

The main observation is that under reasonable assumptions, when both dimensions $p$ and $n$ become large at a proportional rate say $c$, almost surely, the (random) SD $G^{S_n}$ of the sample covariance matrix $S_n$ will weakly converge to a deterministic distribution $F$, called limiting spectral distribution (LSD). Naturally this LSD $F$ depends on the PSD $H$, but in general this relationship is complex and has no explicit form. The only exception is the case where all the population eigenvalues $(\sigma_i)$ are unit, i.e. $\Sigma_p \equiv I_p$ ($H = \delta_1$); the LSD $F$ is then explicit known to be the Marčenko-Pastur distribution with an explicit density function. For a general PSD $H$, this relationship is expressed via an implicit equation, see Section 3, Eqs. (1) and (3).

An important question here is the recovering of the PSD $H$ (or $H_p$) from the sample covariance matrix $S_n$. This question has a central importance in several popular statistical methodologies like Principal Component Analysis (Johnstone (2001)), Kalman filtering or Independent Component Analysis which all rely on an efficient estimation of some population covariance matrices.

Recently, El Karoui (2008) has proposed a variational and nonparametric approach to this problem based on an appropriate distance function using the Marčenko-Pastur equation (1) below and a large dictionary made with base density functions and Dirac point masses. The proposed estimator is proved consistent in a nonparametric estimation sense assuming both the dictionary size and the number of observations $n$ tend to infinity. However, no result on the convergence rate of the estimator, e.g. a central limit theorem, is given.

In another important work Rao et al. (2008), the authors propose to use a suitable set of empirical moments, say the first $q$ moments: for $k = 1, \ldots, q$, $\hat{\alpha}_k = p^{-1} \text{tr} S_n^k = p^{-1} \sum_{m=1}^{p} \lambda_m^k$ where $(\lambda_m)$ are the eigenvalues of $S_n$ (assuming $p \leq n$). Here a pure parametric approach is adopted and the PSD depends on a set of real parameters $\theta$: $H = H(\theta)$. Therefore, when $n \to \infty$ and under appropriate normalization, the sample moments $(\hat{\alpha}_k)$ will have a Gaussian limiting distribution with asymptotic mean and variance $\{m_\theta, Q_\theta\}$ which are functions of the (unknown) parameters $\theta$. In Rao et al. (2008), the authors propose an estimator $\hat{\theta}_R$ of the parameters by maximizing the asymptotic Gaussian likelihood of $\hat{\alpha} = (\hat{\alpha}_j)_{1 \leq j \leq q}$, with distribution $N_q(m_\theta, Q_\theta)$. Intensive simulations illustrate the consistency and the asymptotic normality of this estimator. However, their simulation experiments are limited to simplest situations and no theoretic result are provided concerning the consistency of the estimator. An important difficulty in this approach is that the functions $m_\theta$ and $Q_\theta$ have no explicit form.

In a recent work Bai et al. (2010), a modification of the procedure in Rao et al. (2008) is proposed to get a direct moments estimator based on the sample moments $(\hat{\alpha}_j)$. Compared to El Karoui (2008) and Rao et al. (2008), this moment estimator is simpler and much easier
to implement. Moreover, the convergence rate of this estimator (asymptotic normality) is also established. A recent paper by the authors in Chen et al. (2010) has also analyzed the underlying order selection problem and proposed a solution based on the cross-validation principle.

However, despite all the above contributions, there is still a need for new methods of estimation. Actually, the general approach in El Karoui (2008) has several implementation issues that seem to be responsible for its relatively low performance as attested by the very simple nature of provided simulation results. This low efficiency is probably due to the use of a too general dictionary made with large number of discrete distributions and piece-wisely linear densities. Concerning the moment based methods in Rao et al. (2008) and Bai et al. (2010), we will see that their accuracy degrades drastically as the number of parameters to be estimated increases. Lastly, it is well known that the contour-integral based method in a related work Mestre (2008) is limited to a small class of discrete models where distinct population eigenvalues should generate non-overlapping clusters of sample eigenvalues.

The new approach developed in this paper can be viewed as a synthesis of the optimization approach in El Karoui (2008) and the parametric setup in Bai et al. (2010). On one hand, we adopt the optimization approach and will prove that it is in general preferable to the moment approaches. On the other hand, using a generic parametric approach for discrete PSDs as well as continuous PSDs, we are able to avoid the aforementioned implementation difficulties in El Karoui (2008). Another important contribution from the paper is that the optimization problem has been moved from the complex plan to the real line by considering a characteristic equation (Marčenko-Pastur equation) on the real line. The obtained optimization procedure is then much simpler than the original one in El Karoui (2008).

The rest of the paper is organized as follows. In the next section, we provide a Marčenko-Pastur equation defined on the real line which will be the cornerstone of our estimation method. This method is developed in Section 3 and we prove its strong consistency. Then, in Section 4, simulation experiments are carried out to compare the performance of three estimation methods under investigation. The last section collects proofs of main theorems.

2 Marčenko-Pastur equation on the real line

Throughout the paper, \( A^{1/2} \) stands for any Hermitian square root of a non-negative definite Hermitian matrix \( A \). Our model assumptions are as follows.

Assumption (a). The sample and population sizes \( n, p \) both tend to infinity, and in such a way that \( p/n \to c \in (0, \infty) \).

Assumption (b). There is a doubly infinite array of i.i.d. complex-valued random variables \( (w_{ij}), i, j \geq 1 \) satisfying

\[
E(w_{11}) = 0, \quad E(|w_{11}|^2) = 1,
\]

such that for each \( p, n \), letting \( W_n = (w_{ij})_{1 \leq i \leq p, 1 \leq j \leq n} \), the observation vectors can be represented as \( x_j = \Sigma_p^{1/2} w_{j} \) where \( w_{j} = (w_{ij})_{1 \leq i \leq p} \) denotes the \( j \)-th column of \( W_n \).

Assumption (c). The SD \( H_p \) of \( \Sigma_p \) weakly converges to a probability distribution \( H \) as \( n \to \infty \).

The assumptions (a)-(c) are classical conditions for the celebrated Marčenko-Pastur theorem (Marčenko and Pastur (1967); Silverstein (1995), see also Bai and Silverstein (2010)). More precisely, under these Assumptions, almost surely, as \( n \to \infty \), the empirical SD \( F_n := G^{\wedge n} \) of \( S_n \) weakly converges to a (nonrandom) generalized Marčenko-Pastur distribution \( F \).

Unfortunately, except the simplest case where \( H \equiv \delta_1 \), the LSD \( F \) has no explicit form and it is characterized as follows. Let \( \gamma(z) \) denote the Stieltjes transform of \( cF + (1 - c)\delta_0 \),
which is a one-to-one map defined on the upper half complex plane \( \mathbb{C}^+ = \{ z \in \mathbb{C} : \Im(z) > 0 \} \). This transform satisfies the following fundamental Marčenko-Pastur equation (MP):

\[
z = -\frac{1}{g(z)} + c \int \frac{t}{1 + t g(z)} dH(t), \quad z \in \mathbb{C}^+.
\]

The above MP equation excludes the real line from its domain of definition. As the first contribution of the paper, we fill this gap by an extension of the MP equation to the real line. The estimation method introduced in Section 3 will be entirely based on this extension.

The support of a distribution \( G \) is denoted by \( S_G \) and its complementary set by \( S_c G \), since the ESD \( F_n \) is observed, we will use \( s_n \), the Stieltjes transform of \( (p/n) F_n + (1 − p/n) \delta_0 \) to approximate \( s \) in the MP equation. More precisely, let for \( u \in \mathbb{R} \),

\[
s_n(u) = -\frac{1 − p/n}{u} + \frac{1}{n} \sum_{l=1}^n \frac{1}{\lambda_l - u}.
\]

It is clear that the domain of \( s_n(u) \) is \( S_c F_n \). Thus, \( s_n(u) \)'s are well defined on \( \hat{U} \) for all large \( n \), where \( \hat{U} \) is the interior of \( U = \lim \inf_{n \to \infty} S_c F_n \). \( \{0\} \).

**Theorem 2.1.** Assume that the assumptions (a)-(b)-(c) hold. Then

1. for any \( u \in \hat{U} \), \( s_n(u) \) converges to \( s(u) \),
2. for any \( u \in S_c F \), \( s = s(u) \) is a solution to equation

\[
u = -\frac{1}{s} + c \int \frac{t}{1 + t s} dH(t),
\]

3. the solution is also unique in the set \( B^+ = \{ s \in \mathbb{R} \{0\} : du/ds > 0, (−s)^{-1} \in S_c u \} \),
4. for any non-empty open interval \( (a, b) \subset B^+ \), \( s \) is uniquely determined by \( u(s) \), \( s \in (a, b) \).

The proof is given in the last section. Some remarks are in order.

1. Notice that since \( (-\infty, 0) \subset \hat{U} \subset S_c F \), there are infinitely many \( u \)-points such that \( s_n(u) \) almost surely converges to \( s(u) \).

2. The MP equation (3) can be inverted in the following sense: the knowledge of \( u(s) \) on any interval in \( B^+ \) (see Figure 1) will uniquely determine the PSD \( H \). The estimation method in Section 3 will be built on this property.

### 3 Estimation

#### 3.1 The method

We consider the estimation problem in a parametric setup. Suppose \( H = H(\theta) \) is the limit of \( H_p \) with unknown parameter vector \( \theta \in \Theta \subset \mathbb{R}^d \). The procedure of the estimation of \( H \) includes three steps:

1. Choose a \( u \)-net \( \{u_1, \ldots, u_m\} \) from \( \hat{U} \), where \( u_j \)'s are distinct and the size \( m \) is no less than \( q \).
Figure 1: The curve of $u = u(s)$ (solid thin), and the sets $B^+$ and $S_c^F$ (solid thick) for $H = 0.3\delta_2 + 0.4\delta_7 + 0.3\delta_{10}$ and $c = 0.1$. $u_i = u(s_i), s_i \in B^+, i = 1, 2, 3, 4$.

S2. For each $u_j$, calculate $\hat{u}_j(s_j)$ using (2) and plug the pair into the MP equation (3). Then, we obtain $m$ approximate equations

$$u_j \simeq \frac{1}{\Sigma(u_j)} + \frac{p}{n} \int \frac{tdH(t, \theta)}{1 + t \Sigma(u_j)}$$

$$:= \hat{u}_j(s_j, \theta) \quad (j = 1, \ldots, m).$$

S3. Find the least squares solution of $\theta$,

$$\hat{\theta}_n = \arg \min_{\theta \in \Theta} \sum_{j=1}^{m} \left(u_j - \hat{u}_j(s_j, \theta)\right)^2.$$ 

We name $\hat{\theta}_n$ as the least squares estimate (LSE) of $\theta$. Accordingly, $\hat{H} = H(\hat{\theta}_n)$ is called the LSE of $H$. A central issue here is the choice of the $u$-net $\{u_1, \ldots, u_m\}$. In Section 4, we will provide a robust method for this choice that can be used in practice with real data.

This procedure can also be applied to the MP equation (1) in complex field as in El Karoui (2008). Similarly to our first two steps, the author chose a $z$-net from $C^+$ and created a system of approximate equations by a discretisation $H$ as a weighted sum of a grid of pre-chosen mass points. The estimates of the weight parameters were then obtained by minimizing the approximation errors in terms of the $L_\infty$ norm. The author also suggested to use a $z$-net with $\Re(z) < 0$ and $\Im(z)$ near 0. This is almost equivalent to choosing a $u$-net with $u < 0$ in our procedure. But we strongly suggest to use more $u$-points from $U \cap R^+$ if possible, since these points are likely to carry some different information about $H$ comparing with negative $u$-points. For the optimization step, whatever the distance used ($L_2$-norm, $L_\infty$-norm, etc.) our method would be easier and faster than El Karoui’s one since the optimization is carried on the real domain.

### 3.2 Consistency

We establish the strong consistency of our estimator in two models that are widely used in the literature. The estimates will be further studied in the simulation section.
The first model is made with discrete PSDs with finite support on \( \mathbb{R}^+ \), i.e.

\[
H(\theta) = m_1 \delta_{a_1} + \cdots + m_k \delta_{a_k}, \quad \theta \in \Theta,
\]

where \( m_k = 1 - \sum_{i=1}^{k-1} m_i \), \( \theta = (a_1, \ldots, a_k, m_1, \ldots, m_{k-1}) \) are \((2k-1)\) unknown parameters and

\[
\Theta = \left\{ \theta \in \mathbb{R}^{2k-1} : m_i > 0, \sum_{i=1}^{k} m_i = 1; 0 < a_1 < \cdots < a_k < +\infty \right\}.
\]

Here, Equation (3) can be simplified to

\[
u = -\frac{1}{\xi} + c \sum_{i=1}^{k} \frac{a_i m_i}{1 + a_i \xi}.
\]

For the well-definition of the equation on \( \Theta \), we assume that the \( \nu \)-net satisfies

\[
\inf_{\theta \in \Theta} \min_{i,j} |1 + a_i \xi(u_j)| \geq \delta, \quad (4)
\]

where \( \delta \) is some positive constant. It is clearly satisfied if all the \( u_j \)'s are negative.

**Theorem 3.1.** In addition to the assumptions (a)-(b)-(c), suppose that the true value of the parameter \( \theta_0 \) is an inner point of \( \Theta \) and the condition (4) is fulfilled. Then, the LSE \( \hat{\theta}_n \) for the discrete model is strongly consistent, that is, almost surely, \( \hat{\theta}_n \to \theta_0 \).

Next we suppose that the PSD \( H(\theta) \) has a probability density \( h(t|\theta) \) with respect to Lebesgue measure. From Szegö (1959) (Chapters 2, 4), if \( h(t|\theta) \) has finite moments of all order, it can be expanded in terms of Laguerre polynomials:

\[
h(t|\theta) = \sum_{j \geq 0} c_j \psi_j(t) e^{-t},
\]

where

\[
c_j = \int \psi_j(t) h(t|\theta) dt.
\]

As discussed in Bai et al. (2010), we consider a family of \( h(t|\theta) \) with finite expansion

\[
h(t|\theta) = \sum_{j=0}^{q} c_j \psi_j(t) e^{-t} = \sum_{j=0}^{q} \alpha_j t^j e^{-t}, \quad t > 0, \quad \theta \in \Theta,
\]

where \( \alpha_0 = 1 - \alpha_1 - \cdots - q! \alpha_q \), \( \theta = (\alpha_1, \ldots, \alpha_q) \), and

\[
\Theta = \left\{ \theta \in \mathbb{R}^q : h(t|\theta) > 0, \ t \in \mathbb{R}^+ \right\}.
\]

For this model, Equation (3) becomes

\[
u = -\frac{1}{\xi} + c \sum_{j=0}^{q} \alpha_j \int \frac{t^{j+1} e^{-t}}{1 + \xi t} dt.
\]

It’s clear that the calculation of \( \hat{\theta}_n \) is here simple since the above equation is linear with respect to \( \theta \).

**Theorem 3.2.** In addition to the assumptions (a)-(b)-(c), suppose that the true value of the parameter \( \theta_0 \) is an inner point of \( \Theta \). Then, the LSE \( \hat{\theta}_n \) for the continuous model is strongly consistent.
Table 1: Wasserstein distances of estimates for $H = 0.5\delta_1 + 0.5\delta_2$.

|          | $p/n = 0.2$ | $p/n = 1$ | $p/n = 2$ |
|----------|-------------|-----------|-----------|
| LSE Mean | 0.0437      | 0.0601    | 0.0893    |
| S.D.     | 0.0573      | 0.0735    | 0.1077    |
| RMSE Mean| 0.0491      | 0.0689    | 0.0859    |
| S.D.     | 0.0320      | 0.0482    | 0.0629    |
| BCY Mean | 0.0500      | 0.0664    | 0.0871    |
| S.D.     | 0.0331      | 0.0466    | 0.0617    |

4 Simulation experiments

In this section, simulations are carried out to compare our LSE with the approximate quasi-likelihood estimate in Rao et al. (2008) (referred as RMSE) and the moment estimate in Bai et al. (2010) (referred as BCY). We do not include the estimator of El Karoui (2008) in this study since this estimator is nonparametric using a suitable approximation dictionary while the LSE is based on a parametric form of unknown PSDs.

We study five different PSDs: three of them are discrete and two continuous. Samples are drawn from mean-zero real normal population with the dimensions $n = 500$ and $p = 100, 500, 1000$. Statistics are computed from 1000 independent replications.

To evaluate the quality of an estimate $\hat{H} = H(\hat{\theta})$, instead of looking at individual values $(\hat{\theta}_i)$ of the parameters, we use a global distance, namely the Wasserstein distance

$$W = \int |Q_H(t) - Q_{\hat{H}}(t)|dt$$

where $Q_{\mu}(t)$ is the quantile function of distribution $\mu$. The use of Wasserstein distance is motivated by the fact that it applies to both discrete and continuous distributions (unlike other common distance like kullback-leibler or $L_2$ distance).

For the LSE, we need to choose a $u$-net from $S^+_{p,n} \cap S^+_p \setminus \{0\}$. When $H$ has finite support, the upper and lower bounds of $S_F \setminus \{0\}$ can be estimated respectively by $\lambda_{\text{max}} = \max\{\lambda_i\}$ and $\lambda_{\text{min}} = \min\{\lambda_i : \lambda_i > 0\}$ where $\lambda_i$'s are sample eigenvalues. As a consequence, we design a primary set:

$$U = \begin{cases} (-10, 0) \cup (0, 0.5\lambda_{\text{min}}) \cup (5\lambda_{\text{max}}, 10\lambda_{\text{max}}) & \text{(discrete model, } p \neq n), \\ (-10, 0) \cup (5\lambda_{\text{max}}, 10\lambda_{\text{max}}) & \text{(discrete model, } p = n), \\ (-10, 0) & \text{(continuous model).} \end{cases}$$

Next, we choose $l$ equally spaced $u$-points from each individual interval of $U$. We name this process as adaptive choice of $u$-net. Here we set $l = 20$ for all cases considered in simulation, that is, for example we take $\{-10 + 10t/21, t = 1, \ldots, 20\}$ from the first interval.

Case 1: $H = 0.5\delta_1 + 0.5\delta_2$. This is a simple case as $H$ has only two atoms with equal weights. Table 1 shows that all the three estimates are consistent, and their efficiency is very close.

Case 2: $H = 0.3\delta_1 + 0.4\delta_3 + 0.3\delta_5$. In this case, we increase the order of $H$. Analogous statistics are summarized in Table 2. The results show that LSE clearly outperforms RMSE and BCY in the light of the Wasserstein distance. Particularly, RMSE and BCY have not converged yet with dimensions $n = 500$ and $p = 500, 1000$, while LSE only contains a small bias in such situations. This exhibits the robustness of our method with respect to the increase of the order.

Case 3: $H = 0.3\delta_1 + 0.4\delta_5 + 0.3\delta_{15}$. In this case, we increase the variance of $H$. Table 3 collects the simulation results. Compared with Table 2, RMSE and BCY deteriorate significantly
Table 2: Wasserstein distances of estimates for $H = 0.3\delta_1 + 0.4\delta_3 + 0.3\delta_5$.

|        | $p/n = 0.2$ | $p/n = 1$ | $p/n = 2$ |
|--------|-------------|-----------|-----------|
| LSE    | Mean        | 0.1589    | 0.3566    | 0.4645    |
|        | S.D.        | 0.1836    | 0.4044    | 0.5156    |
| RMSE   | Mean        | 0.2893    | 0.7494    | 0.8153    |
|        | S.D.        | 0.0966    | 0.2188    | 0.1080    |
| BCY    | Mean        | 0.2824    | 0.5840    | 0.7217    |
|        | S.D.        | 0.1769    | 0.2494    | 0.2156    |

Table 3: Wasserstein distances of estimates for $H = 0.3\delta_1 + 0.4\delta_5 + 0.3\delta_{15}$.

|        | $p/n = 0.2$ | $p/n = 1$ | $p/n = 2$ |
|--------|-------------|-----------|-----------|
| LSE    | Mean        | 0.1756    | 0.2524    | 0.5369    |
|        | S.D.        | 0.2105    | 0.3013    | 0.6282    |
| RMSE   | Mean        | 0.7090    | 1.4020    | 1.9160    |
|        | S.D.        | 0.0524    | 0.6501    | 0.2973    |
| BCY    | Mean        | 0.9926    | 1.5379    | 1.8562    |
|        | S.D.        | 0.5618    | 0.6875    | 0.7526    |

while LSE remains stable. The average Wasserstein distances of LSE are (at least) a third less than those of RMSE and BCY for all $p$ and $n$ used. This demonstrates the robustness of our method with respect to the increase of the variance.

Case 4: $h(t) = (\alpha_0 + \alpha_1 t)e^{-t}, \alpha_1 = 1$. This is the simplest continuous model with only one parameter to be estimated. In this case, $H$ is a gamma distribution with shape parameter 2 and scale parameter 1. Statistics in Table 4 show that all the three estimates have similar efficiency.

Case 5: $h(t) = (\alpha_0 + \alpha_1 t + \alpha_2 t^2 + \alpha_3 t^3)e^{-t}, \alpha_1 = \alpha_2 = \alpha_3 = 1/9$. This model with three parameters becomes more difficult to estimate. RMSE and BCY have large bias and/or large standard deviations in all dimensions we used, see Table 5. In contrast, our LSE performs fairly well and again outperform these two moment based methods.

In summary, the LSE outperforms the RMSE and BCY estimators in all the tested situations. On the other hand, as expected, the performances of the RMSE and the BCY estimators
Table 5: Wasserstein distances of estimates for \( h(t) = (t + t^2 + t^3)e^{-t/9}. \)

|           | p/n = 0.2 | p/n = 1 | p/n = 2 |
|-----------|-----------|---------|---------|
| LSE Mean  | 0.1895    | 0.0902  | 0.0740  |
| S.D.      | 0.1103    | 0.0526  | 0.0378  |
| RMSE Mean | 0.3163    | 0.1515  | 0.1156  |
| S.D.      | 0.2062    | 0.0863  | 0.0670  |
| BCY Mean  | 0.3139    | 0.1554  | 0.1114  |
| S.D.      | 0.2007    | 0.0907  | 0.0624  |

are very close since they are all based on empirical moments (however, as explained in Bai et al. (2010), the BCY estimator is much easier to implement).

Finally, we analyze the relationship between the size of a \( u \)-net and the efficiency of LSE. The average of Wasserstein distances of LSE with respect to different \( l \) values (the number of \( u \)-points picked from each individual interval) is plotted for Case 3 and Case 5, see Figure 2. The results show that unless \( l \) is too small, the estimation efficiency remains remarkably stable with different values of \( l \).

![Figure 2: The average of Wasserstein distances of LSE with respect to \( l \) (\( l = 5, 10, \ldots, 30 \)) for Case 3 (left) and Case 5 (right) with \( p = 100, n = 500 \) (solid lines), \( p = 500, n = 500 \) (dashed lines), and \( p = 1000, n = 500 \) (dotted lines).](image)

5 Application to S&P 500 stocks data

In this section, we present a financial application of our estimation procedure in analysing an empirical correlation matrix of stock returns. We study a set of 488 U.S. stocks included in the S&P 500 index from September, 2007 to September 2011 (1001 trading days, 12 stocks have been removed because of missing values). Here, the data dimension is \( p = 488 \) and the number of observations is \( n = 1000 \).

Following Bouchaud and Potters (2009), we suppose that there is a PSD \( H(\alpha) \) for the stock returns with an inverse cubic density \( h(t|\alpha) \):

\[
h(t|\alpha) = c\frac{1}{(t - a)^3}I(t \geq \alpha), \quad 0 \leq \alpha < 1,
\]
where \( c = 2(1 - \alpha)^2 \) and \( a = 2\alpha - 1 \). Notice that when \( \alpha \to 1^- \), the inverse cubic model tends to the MP case (\( H = \delta_1 \)), so that this prior model is very flexible.

For the estimation procedure, we first remove the 6 largest sample eigenvalues which are deemed as spikes over the bulk of sample eigenvalues. As in Section 3, we use \( l = 20 \) equally spaced \( u \)-points in \((-10, 0)\). The LSE of \( \alpha \) turns out to be \( \hat{\alpha} = 0.4380 \). The RMSE and BCY don’t exist for this model for the reason that the moments of \( H \) don’t depend on the unknown parameter.

Limiting spectral densities corresponding to the LSE estimate \( h(t|0.4380) \) and \( H = \delta_1 \) are shown in Figure 3. We also plot the empirical spectral density of the correlation matrix, and the curve is smoothed by using a Gaussian kernel estimate with bandwidth \( h = 0.05 \).

Figure 3: The empirical density of the sample eigenvalues (plain black line), compared to the MP density (dashed line) and the limiting spectral density corresponding to the LSE estimate \( h(t|0.4380) \) (dashed-dotted line).

From Figure 3, we could see that the MP density is far away from the empirical density curve. This confirms a widely believed fact that the correlation matrix may have more structure than just several spikes on top of the identity matrix. By contrast, the cubic model with \( \alpha = 0.4380 \) yields a much more satisfying fit to the empirical density curve.

6 Proofs

We first recall useful results in three lemmas. The first one is provided in Silverstein (1995) and the two others in Silverstein and Choi (1995).

**Lemma 6.1.** Assume that the assumptions (a)-(b)-(c) hold. Then, almost surely, the empirical spectral distribution \( F_n \) converges in distribution, as \( n \to \infty \), to a non-random probability measure \( F \), whose Stieltjes transform \( s = s(z) \) is a solution to the equation

\[
 s = \int \frac{1}{t(1 - c - cs) - z} dH(t).
\]

The solution is also unique in the set \( \{ s \in \mathbb{C} : -(1 - c)/z + cs \in \mathbb{C}^+ \} \).

**Lemma 6.2.** If \( u \in S_F^c \setminus \{0\} \), then \( \bar{g} = \bar{g}(u) \) satisfies

1. \( \bar{g} \in \mathbb{R} \setminus \{0\} \)
2. \( (\bar{g})^{-1} \in S_H^c \)
3. \( du/\bar{g} > 0 \).

Conversely, if \( \bar{g} \) satisfies (1)-(3), then \( u = u(\bar{g}) \in S_F^c \setminus \{0\} \).
We are going to show \( H \) dominated convergence theorem, taking the limit as \( n \to \infty \). Then, for any \( \{s \} \) satisfying, for all \( n \),

\[
\left| s \right| > n,
\]

we may conclude that \( \left| s \right| \) is bounded on the set \( S \). Therefore, each side of (5) can be expressed as

\[
\int \frac{t}{1 + t_2} dH_1(t) = \int \frac{t}{1 + t_2} dH_2(t).
\]

We are going to show \( H_1 = H_2 \) almost everywhere with respect to Lebesgue measure on \( \mathbb{R} \).

For any \( s_0 \in (a, b) \), \(-1/2s_0\) is an inner point of \( S \), then there is \( \delta > 0 \) such that

\[
U(-1/2s_0, 0) \subset S
\]

which implies \( \left| 1 + t_2 \right| > \delta \) for all \( t \in S \). Choose \( \varepsilon_0 = \min\left\{ (2b_0/1 + \delta_0, b - b_0, s_0 - a) \right\} \).

Then, for any \( s \in U(s_0, \varepsilon_0) \), \( 1 + t_2 \) has the same sign as \( 1 + t_2 \). Define

\[
g(t, u) = \begin{cases} 
1 & (1 + t_2 > 0, u > 0), \\
-1 & (1 + t_2 < 0, u < 0), \\
0 & (u(1 + t_2)u \leq 0).
\end{cases}
\]

We have then

\[
\int \frac{t}{1 + t_2} dH_1(t) = \int \int_{-\infty}^{\infty} g(t, u)e^{-(1/2s_0)^u} du, \ s \in U(s_0, \varepsilon_0).
\]

Therefore, each side of (5) can be expressed as

\[
\int \frac{t}{1 + t_2} dH_1(t) = \int \int_{-\infty}^{\infty} g(t, u)e^{-(1/2s_0)^u} dH_2(t)e^{-(2s_0)^u} du.
\]
It is clear that the left hand side of (6) is the Laplace transform of
\[ \int_0^\infty g(t,u)e^{\frac{1}{4} + \omega \theta} dH_i(t). \]
By the uniqueness of Laplace transform, we have then
\[ \int_0^\infty g(t,u)e^{\frac{1}{4}} dH_1(t) = \int_0^\infty g(t,u)e^{\frac{1}{4}} dH_2(t), \]
and thus \( H_1 = H_2 \) almost everywhere.

### 6.2 Proof of Theorem 3.1

Define
\[ \varphi(\theta) = \sum_{j=1}^m \left( u_j - u(s_j, \theta) \right)^2, \]
where \( s_j = g(u_j) \) (\( j = 1, \ldots, m \)). We first state and prove the following proposition.

**Proposition 6.1.** If \( u_1, \ldots, u_m \) are distinct and \( m \geq q = 2k - 1 \), then \( \varphi(\theta) = 0 \) for the discrete model has a unique solution \( \theta_0 \) on \( \Theta \).

**Proof.** Since \( g(u) \) is a bijective function from \( S^p \) to \( B^+ \) and \( u_1, \ldots, u_m \) are distinct, \( s_1, \ldots, s_m \) are also distinct.

Suppose there is a \( \theta = (a_1, \ldots, a_k, m_1, \ldots, m_{k-1}) \) such that \( \varphi(\theta) = 0 \). Denote by \( \theta_0 = (a'_1, \ldots, a'_k, m'_1, \ldots, m'_{k-1}) \) the true value of the parameter. We will show that \( \theta = \theta_0 \). Denote \( b_i = 1/a_i \) and \( b'_i = 1/a'_i \) \( (i = 1, \ldots, k) \), we have then
\[ \sum_{i=1}^k \frac{m_i}{s_j + b_i} = \sum_{i=1}^k \frac{m'_i}{s_j + b'_i} \quad (j = 1, \ldots, m). \quad (7) \]

Now look \( s_j \) as a parameter \( s \) and reduction to common factors leads to
\[ (s + b'_1) \cdots (s + b'_k) \sum_{i=1}^k m_i \prod_{\ell \neq i} (s + b_\ell) = (s + b_1) \cdots (s + b_k) \sum_{i=1}^k m'_i \prod_{\ell \neq i} (s + b'_\ell). \]
These are polynomials of degree \( 2k - 1 \); they coincide at \( m \geq 2k - 1 \) different points \( s = s_j \); they are then equal. Back to (7), we have now for all \( s \neq -b_i, -b'_i \),
\[ \sum_{i=1}^k \frac{m_i}{s + b_i} = \sum_{i=1}^k \frac{m'_i}{s + b'_i}. \]

Now each \( b_i \) should match one \( b'_i \), because otherwise \( b_i \neq b'_i \) for all \( \ell \) and by letting \( s \to -b_i \) we get a contradiction. So there is one \( b'_i \) matches (then unique) for \( b_i \). This proves also that \( m_i = m'_i \). As the \( b_i \) are ordered, it is necessary that \( b'_i = b'_i \) and hence also \( m_i = m'_i \). \( \square \)

Now let’s begin the proof of Theorem 3.1. Recall that
\[ \hat{\theta}_n = \arg\min_{\theta \in \Theta} \frac{1}{n} \sum_{j=1}^m \left( u_j + \frac{1}{s_n(u_j)} - \frac{p}{n} \int \frac{t dH(t, \theta)}{1 + t s_n(u_j)} \right)^2 \]
\[ := \arg\min_{\theta \in \Theta} \varphi_n(\theta). \]
Under the assumption of the theorem, by the convergence of $z_j(u_j)$ ($j = 1, \ldots, m$), $\varphi_n(\theta)$ is well defined on $\Theta$ for all large $n$. Moreover, for any fixed $\theta \in \Theta$, we have

$$\varphi_n(\theta) \to \varphi(\theta),$$

almost surely. Proposition 6.1 guarantees that $\theta = \theta_0$ is the unique solution to $\varphi(\theta) = 0$ on $\Theta$.

We claim that for almost all $\omega$, there is a compact set $\overline{\Theta} = \overline{\Theta}(\omega) \subset \Theta$ which contains all $\hat{\theta}_n(\omega)$ for large $n$. It’s easy to see that for all large $n$, $\varphi_n(\theta)$ is uniformly bounded on $\overline{\Theta}$ and has continues partial derivatives with respect to $\theta$. By the Vitali’s convergence theorem, we get

$$\sup_{\theta \in \overline{\Theta}} |\varphi_n(\theta) - \varphi(\theta)| \to 0. \quad (8)$$

For any $\varepsilon > 0$, by the continuity of $\varphi(\theta)$, we have

$$\inf_{|\theta - \theta_0| > \varepsilon} \varphi(\theta) > \varphi(\theta_0) = 0.$$

From this and (8), when $n$ is large,

$$\inf_{\theta \in \overline{\Theta}} \varphi_n(\theta) > \varphi_n(\theta_0).$$

This proves that minimum point $\hat{\theta}_n$ of $\varphi_n(\theta)$ for $\theta \in \overline{\Theta}$ must be in the ball $\{||\theta - \theta_0|| \leq \varepsilon\}$. Hence the convergence $\hat{\theta}_n \to \theta_0$.

To complete the proof, it is sufficient to prove the claim, i.e. there is a compact set $\overline{\Theta} \subset \Theta$ such that for large $n$,

$$\inf_{\theta \in \overline{\Theta}} \varphi_n(\theta) > \varphi_n(\theta_0).$$

Suppose not. Then there exists a sequence $\{\theta_l, l = 1, 2, \ldots\}$ tending to the boundary $\partial \Theta$ of $\Theta$ such that $\lim_{n \to \infty} \varphi_n(\theta_l) = \varphi(\theta_l) = 0$. By a similar technique used in the proof of Proposition 6.1, we may get $\theta = \theta_0$, a contradiction.

The first is that $\{\theta_l\}$ has a convergent sub-sequence, i.e. $\theta_{l_k} \to \theta \in \partial \Theta$, as $k \to \infty$, then it follows that

$$0 \leq \varphi(\theta) = \lim_{n \to \infty} \lim_{k \to \infty} \varphi_n(\theta_{l_k}) \leq \lim_{n \to \infty} \varphi_n(\theta_0) = \varphi(\theta_0) = 0,$$

hence $\varphi(\theta) = 0$. By a similar technique used in the proof of Proposition 6.1, we may get $\theta = \theta_0$, a contradiction.

The second is that $|\theta_l| = \left(\sum_{i=1}^{k} a_i^2 + \sum_{i=1}^{k-1} m_i^2\right)^{1/2} \to \infty$. Then we immediately know there exists $a_{il}$ such that $a_{il} \to \infty$, as $l \to \infty$. Without loss of generality, suppose that

\[
\begin{align*}
& a_{il} \to \infty \quad (1 \leq i \leq k_1), \\
& \sum_{i=k_1}^{k} m_{il} \to m_0 \\
& a_{il} \to a_i < \infty \quad (k_1 + 1 \leq i \leq k), \\
& m_{il} \to m_i \quad (k_1 + 1 \leq i \leq k - 1).
\end{align*}
\]

We have then

$$0 \leq \lim_{n \to \infty} \lim_{l \to \infty} \varphi_n(\theta_l) \leq \lim_{n \to \infty} \varphi_n(\theta_0) = \varphi(\theta_0) = 0,$$

and thus

$$\lim_{n \to \infty} \lim_{l \to \infty} \varphi_n(\theta_l) = \sum_{j=1}^{m} \left( z_j - \frac{1 - cm_0}{s_j} + c \sum_{i=k_1+1}^{k} \frac{a_i m_i}{1 + a_i s_j} \right)^2 = 0.$$
If \( m_0 = 0 \) then the problem is similar to the first case. Assume \( m_0 \neq 0 \). Denote \( \theta_0 = (a_1', \ldots, a_k', m_1', \ldots, m_k') \), we have

\[
\frac{m_0}{s_j} + \sum_{i=k_1+1}^{k} \frac{a_im_i}{1 + a_is_j} = \sum_{i=1}^{k} \frac{a_im_i'}{1 + a_is_j},
\]

for \( j = 1, \ldots, m \). Now look \( s_j \) as a parameter \( s \) and multiplying common factors leads to

\[
s \prod_{i=k_1+1}^{k} (1 + a_is) \prod_{i=1}^{k} (1 + a_i's) \left( \frac{m_0}{s} + \sum_{i=k_1+1}^{k} \frac{a_im_i}{1 + a_is} \right) = \prod_{i=k_1+1}^{k} (1 + a_is) \prod_{i=1}^{k} (1 + a_i's) \left( \sum_{i=1}^{k} \frac{a_im_i'}{1 + a_is} \right).
\]

These are polynomials of degree \( 2k - k_1 \leq 2k - 1 \); they coincide at \( m \geq 2k - 1 \) different points \( s = s_j \); they are then equal. Comparing their constant terms comes into conflict.

The proof is then complete.

### 6.3 Proof of Theorem 3.2

The proof of this theorem is similar to the proof of Theorem 3.1. We only present the following proposition.

**Proposition 6.2.** If \( u_1, \ldots, u_m \) are distinct and \( m \geq q \), then \( \varphi(\theta) = 0 \) for the continues model has a unique solution \( \theta_0 \) on \( \Theta \).

**Proof.** Suppose there is a \( \theta = (\alpha_1, \ldots, \alpha_q) \) such that \( \varphi(\theta) = 0 \). Denote by \( \theta_0 = (\alpha_1', \ldots, \alpha_k') \) the true value of the parameter. We will show that \( \theta = \theta_0 \).

Define \( p(t, \beta) = \beta_0 + \beta_1 t + \cdots + \beta_q t^q \), where \( \beta = (\beta_1, \ldots, \beta_q) \) and \( \beta_0 = 1 - \sum_{j=1}^{q} j! \beta_j \). We have then

\[
\int \frac{t}{1 + ts_j} p(t, \theta^*) e^{-t} dt = 0 \quad (j = 1, \ldots, m),
\]

where \( \theta^* = \theta - \theta_0 \) and \( s_j = s(u_j) \).

Suppose \( p(t, \theta^*) = 0 \) has \( q_0 \) \((\leq q)\) positive real roots \( t_1 < \cdots < t_{q_0} \), and denote \( t_0 = 0, t_{q_0+1} = +\infty \), then \( p(t, \theta^*) \) maintains the sign in each interval \((t_{i-1}, t_i)\) \((i = 1, \ldots, q_0 + 1)\). By mean value theorem, we have

\[
0 = \int_0^{+\infty} \frac{t}{1 + ts_j} p(t, \theta^*) e^{-t} dt = \sum_{i=1}^{q_0+1} \frac{\xi_i}{1 + \xi_i s_j} \int_{t_{i-1}}^{t_i} p(t, \theta^*) e^{-t} dt \quad (j = 1, \ldots, m),
\]

where \( \xi_i \in (t_{i-1}, t_i) \) \((i = 1, \ldots, q_0 + 1)\).

Now look \( s_j \) as a parameter \( s \) and reduction to common factors leads to

\[
0 = \sum_{i=1}^{q_0+1} \prod_{j \neq i} (1 + \xi_i s_j) \int_{t_{i-1}}^{t_i} p(t, \theta^*) e^{-t} dt.
\]

The left hand side is a polynomial of degree \( q_0 - 1 \leq q - 1 \) \((\text{the coefficient of } s^{q_0} = \prod_{j=1}^{q_0+1} \xi_j \int_0^{+\infty} p(t, \theta^*) e^{-t} dt = 0\)\); the equation has \( m \geq q \) different roots \( s = s_j \); the polynomial is then zero. Let \( s = \frac{1}{\xi_i} (i = 1, \ldots, q_0 + 1) \), we get

\[
\int_{t_{i-1}}^{t_i} p(t, \theta^*) e^{-t} dt = 0 \quad (i = 1, \ldots, q_0 + 1),
\]

which is followed by \( p(t, \theta^*) = 0 \), and thus \( \theta^* = 0 \). \( \square \)
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