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Spectrum estimation for large dimensional covariance matrices using random matrix theory

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Abstract

Estimating the eigenvalues of a population covariance matrix from a sample covariance matrix is a problem of fundamental importance in multivariate statistics; the eigenvalues of covariance matrices play a key role in many widely techniques, in particular in Principal Component Analysis (PCA). In many modern data analysis problems, statisticians are faced with large datasets where the sample size, n, is of the same order of magnitude as the number of variables p. Random matrix theory predicts that in this context, the eigenvalues of the sample covariance matrix are not good estimators of the eigenvalues of the population covariance.

We propose to use a fundamental result in random matrix theory, the Marčenko-Pastur equation, to better estimate the eigenvalues of large dimensional covariance matrices. The Marčenko-Pastur equation holds in very wide generality and under weak assumptions. The estimator we obtain can be thought of as "shrinking" in a non linear fashion the eigenvalues of the sample covariance matrix to estimate the population eigenvalue. Inspired by ideas of random matrix theory, we also suggest a change of point of view when thinking about estimation of high-dimensional vectors: we do not try to estimate directly the vectors but rather a probability measure that describes them. We think this is a theoretically more fruitful way to think about these problems.

Our estimator gives fast and good or very good results in extended simulations. Our algorithmic approach is based on convex optimization. We also show that the proposed estimator is consistent.

1 Introduction

With data acquisition and storage now easy, today's statisticians often encounter datasets for which the sample size, n and the number of variables p, are both large: in the order of hundreds, thousands, millions, or even billions in situations such as web search problems.

The analysis of these datasets using classical methods of multivariate statistical analysis requires some care. While the ideas are still relevant, the intuition for the estimators that are used and the interpretation of the results are often - implicitly - justified by assuming an asymptotic framework of p fixed and n growing infinitely large. This assumption was consistent with the practice of statistics when these ideas were developed, since investigation of datasets with a large number of variables was very difficult. A better theoretical framework for modern - i.e large p - datasets, however is the assumption of the so-called "large n, large p" asymptotics. In other words, one should consider that both n and p go to infinity, perhaps with the restriction that their ratio goes to a finite limit γ, and draw practical insights from the theoretical results obtained in this setting.

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We will turn our attention to an object of central interest in multivariate statistics: the eigenvalues of covariance matrices. A key application is Principal Components Analysis (PCA), where one searches for a good low dimensional approximation to the data by projecting the data on the "best" possible k dimensional subspace: here "best" means that the projected data explain as much variance in the original data as possible. This amount of variance explained is measured by the eigenvalues of the population covariance matrix, Σ_p, and hence we need to find a way to estimate those eigenvalues. We will discuss in the course of the paper other problems where the eigenvalues of Σ_p play a key role.

We take a moment here to give a few examples that illustrate the differences that occur under the different asymptotic settings. To pose the problem more formally, let us say that we observe iid random vectors $X_1, \ldots, X_n$ in $\mathbb{R}^p$, and that the covariance of X_i is Σ_p. We call X the data matrix whose rows are the X_i's. In the classical context, where p is fixed and n goes to ∞, a fundamental result of (Anderson, 1963) says that the eigenvalues of the sample covariance matrix $S_p = (X - \bar{X})'(X - \bar{X})/(n-1)$ are good estimators of the population eigenvalues (i.e the eigenvalues of Σ_p). More precisely, calling l_i the ordered eigenvalues of S_p ($l_1 \geq l_2 \ldots$) and λ_i the ordered eigenvalues of Σ_p ($\lambda_1 \geq \lambda_2 \ldots$), it was shown in (Anderson, 1963) that

$$\sqrt{n}(l_i - \lambda_i) \Rightarrow \mathcal{N}(0, 2\lambda_i^2) \ ,$$

when the X_i are normally distributed and all the λ_i's are distinct. This result provided rigorous grounds for estimating the eigenvalues of the population covariance matrix, Σ_p, with the eigenvalues of the sample covariance matrix, S_p, when p is small compared to n. (For more details on Anderson's theorem, we refer the reader to (Anderson, 2003) Theorem 13.5.1.)

Shifting assumptions to "large n, large p" asymptotics induces fundamental differences in the behavior of multivariate statistics, some of which we will highlight in the course of the paper. As a first example, let us consider the case where $\Sigma_p = \mathrm{Id}_p$, so all the population eigenvalues are equal to 1. A result first shown in (Geman, 1980) under some moment growth assumptions, and later refined in (Yin et al., 1988), states that if the entries of the X_i's are i.i.d and have a fourth moment, and if $p/n \to \gamma$, then

$$l_1 \to (1 + \sqrt{\gamma})^2 \ \text{ a.s.}$$

In particular, l_1 is not a consistent estimator of λ_1. Note that by picking $n = p$, l_1 tends to 4 whereas $\lambda_1 = 1$. (For more general Σ_p, see (El Karoui, To Appear) Section 4.3 for numerically explicit results about the limit of l_1.)

As the case of $\Sigma_p = \mathrm{Id}_p$ illustrated, when n and p are both large, the largest sample eigenvalue is biased, sometime dramatically so. Hence, we should correct this bias in the largest sample eigenvalue(s) if we want to use them in data analysis. Theoretical results predict that the behavior of extreme sample eigenvalues can be quite subtle; in particular, depending on how far an isolated population eigenvalue is from the bulk of the population spectrum, the corresponding sample eigenvalue can either be isolated, and far away from the bulk of the sample eigenvalues, or be absorbed by the bulk of the sample eigenvalues (see (Baik et al., 2005), (El Karoui, To Appear), (Baik and Silverstein, 2004), (Paul, To Appear)). One thing is however clear from the most recent theoretical results : if we wish to de-bias extreme sample eigenvalues, we need an accurate estimate of the so-called population spectral distribution, a probability measure that characterizes the population eigenvalues (see (El Karoui, To Appear)). This is what our algorithm will deliver.

We have so far mostly discussed extreme sample eigenvalues. However, much is also known about the behavior of the whole vector of sample eigenvalues $(l_1, l_2, \ldots, l_p)$ and its asymptotic behavior. In particular, theory predicts that in the "large n, large p" case, the scree plot (i.e the plot of the sample eigenvalues vs. their rank; see (Mardia et al., 1979)) becomes uninformative and deceptive. What we propose in this paper is to use random matrix theory to develop practically useful tools to remedy the flaws appearing in some widely used tools in multivariate statistics.

Before we discuss how we will go about it, let us briefly discuss some issues that arise when estimating vectors of large dimension, since working in an asymptotic setting where $p \to \infty$ is not without additional difficulties. Since we will try to estimate vectors of increasingly larger and larger size, an appropriate notion of convergence is needed if we want to quantify the quality of our estimators. Standard norms in high-dimensions not necessarily a very good choice: for instance, if we are in $\mathbb{R}^{100}$, and make an error of

size 1/100 in all coordinates, the resulting l_1 error is 1, even though, at least intuitively, it would seem like we are doing well. Also, if we made a large error (say size 1) in one direction, the l_2 norm would be large (larger than 1 at least), even though we may have gotten the structural information about this vector (and almost all its coordinates) "right". Inspired by ideas of random matrix theory, we propose to associate to high-dimensional vectors probability measures that describe them. We will explain this in more detail in Section 2.1. After this change of point of view, our focus becomes trying to estimate these measures. Why choosing to estimate measures? The reasons are many. Chief among them is that this approach will allow us to look into the structure of the population eigenvalues. For instance, we would like to be able to say whether all population eigenvalues are equal, or whether they are clustered around say two values, or if they are uniformly spread out on an interval. Because the ratio p/n can make the scree plot appear smooth (and hence in some sense uninformative) regardless of the true population eigenvalue structure, this structural information is not well estimated by currently existing methods. We discuss other practical benefits (like scalability with p) of the measure estimation approach in 3.3.7. In the context of PCA, where usually the concern is not to estimate each population eigenvalues with very high precision, but rather to have an idea of the structure of the population spectrum to guide the choice of lower-dimensional subspaces on which to project the data, this measure approach is particularly appealing. Examples to come later in the paper will illustrate this point.

Random matrix theory plays a key role in our approach to this measure estimation problem. A main ingredient of our method is a fundamental result, which we call the Marčenko-Pastur equation (see Theorem 1), which relates the asymptotic behavior of the sample eigenvalues to the population eigenvalues. The assumptions under which the theorem holds are very weak (a fourth moment condition) and hence it is very widely applicable. Until now, this theorem has not been used to do inference on population eigenvalues. Partly this is because in its general form it has not received much attention in statistics, and partly because the inverse problem that needs to be considered is very hard to solve if it is not posed the right way. We propose an original way to approach inverting the Marčenko-Pastur equation. In particular, we will be able to estimate given the eigenvalues of the sample covariance matrix S_p the probability measure, H_p, that describes the population eigenvalues. We use the standard names *empirical spectral distribution* for F_p and *population spectral distribution* for H_p. It is important to state clearly what asymptotic framework we place ourselves in. We will consider that when p and n go to infinity, H_p stays fixed. In particular, it has a limit, denoted H_∞. We call this framework "asymptotics at fixed spectral distribution". Of course, fixing H_p does not imply that we fix p. For instance, sometime we will have $H_p = \delta_1$, for all p. Since the parameter of interest in our problems is really the measure H_p, the fixed spectral distribution asymptotics corresponds to classical assumptions for parameter estimation in statistics, where the parameter does not change with the number of variables observed. We refer the reader to 3.3.6 for a more detailed discussion.

To solve the inverse problem posed by the Marčenko-Pastur equation, we propose to discretize the Marčenko-Pastur equation and then use convex optimization methods to solve the discretized version of the problem. In doing so, we obtain a fast and provably accurate algorithm to estimate the population parameter of interest, H_p, from the sample eigenvalues. The approach is non-parametric since no assumptions are made *a priori* on the structure of the population eigenvalues. One outcome of the algorithm is an efficient graphical method to look at the structure of the population eigenvalues. Another outcome is that since we have an estimate of the measure that describes the population eigenvalues, standard statistical ideas then allow us to get estimates of the individual population eigenvalues λ_i. Some subtle problems may arise when doing so and we address them in 3.3.6. The final result of the algorithm can be thought of as performing non-linear shrinkage of the sample eigenvalues to estimate the population eigenvalues.

We want to highlight two contributions of our paper. First, we propose to estimate measures associated with high-dimensional vectors rather than estimating the vectors. This gives rise to natural notions of consistency and accuracy of our estimates which are reasonable theoretical requirements for any estimator to achieve. And second, we make use, for the first time, of a fundamental result of random matrix theory to solve an important practical problem in multivariate statistics.

The rest of the paper is divided into four parts. In Section 2, we give some background on results in Random Matrix Theory that will be needed. We do not assume that the reader has any familiarity with the topic. In Section 3, we present our algorithm to estimate H_p, the population spectral distribution, and also the population eigenvalues. In Section 4, we present the results of some simulations. We give in

Section 5 a proof of consistency of our algorithm. The Appendix contains some details on implementation of the algorithm.

A note on notation is needed before we start: in the rest of the paper, p will always be a function of n, with the property that $p(n)/n \to \gamma$ and $\gamma \in (0, \infty)$. To avoid cumbersome notations, we will usually write p and not $p(n)$.

2 Background: Random matrix theory of sample covariance matrices

There is a large body of work concerned with the limiting behavior of the eigenvalues of a sample covariance matrix when p and n both go to ∞; it constitutes an important subset of what is commonly known as Random Matrix Theory, to which we now turn. This is a wide area of research, of which we will only give a very quick and self-contained overview. Our eventual aim in this section is to introduce a fundamental result, the Marčenko-Pastur equation, that relates the asymptotic behavior of the eigenvalues of the sample covariance matrix to that of the population covariance in the "large n, large p" asymptotic setting. The formulation of the result requires that we introduce some concepts and notations.

2.1 Changing point of views: from vectors to measures

One of the first problems to tackle is to find a mathematically efficient way to express the limit of a vector whose size grows to ∞. (Recall that there are p eigenvalues to estimate in our problem and p goes to ∞.) A fairly natural way to do so is to associate to any vector a probability measure. More explicitly, suppose we have a vector $(y_1, \ldots, y_p)$ in $\mathbb{R}^p$. We can associate to it the following measure:

$$dG_p(x) = \frac{1}{p} \sum_{i=1}^{p} \delta_{y_i}(x) \ .$$

G_p is thus a measure with p point masses of equal weight, one at each of the coordinates of the vector.

In the rest of the paper, we will denote by H_p the spectral distribution of the population covariance matrix Σ_p, i.e the measure associated with the vector of eigenvalues of Σ_p. We will refer to H_p as *the population spectral distribution.* We can write this measure as

$$dH_p(x) = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i}(x) \ ,$$

where δ_{λ_i} is a point mass, of mass 1, at λ_i. We also call δ_{λ_i} a "dirac" at λ_i. The simplest example of population spectral distribution is found when $\Sigma_p = \mathrm{Id}_p$. In this case, for all i, $\lambda_i = 1$, and $dH_p = \delta_1$. So the population spectral distribution is a point mass at 1 when $\Sigma_p = \mathrm{Id}_p$.

Similarly, we will denote by F_p the measure associated with the eigenvalues of the sample covariance matrix S_p. We refer to F_p as the *empirical spectral distribution.* Equivalently, we define

$$dF_p(x) = \frac{1}{p} \sum_{i=1}^{p} \delta_{l_i}(x) \ .$$

The change of focus from vector to measure implies a change of focus in the notion of convergence we will consider adequate. In particular, for consistency issues, the notion of convergence we will use is weak convergence of probability measures. While this is the natural way to pose the problem mathematically, we may ask if it will allow us to gather the statistical information we are looking for. An example of the difficulties that arise is the following. Suppose $dH_p = (1 - 1/p)\, \delta_1 + 1/p\, \delta_2$. In other words, the population covariance has one eigenvalue that is equal to 2 and $(p-1)$ that are equal to 1. Clearly, when $p \to \infty$, H_p weakly converges to H_∞, with $dH_\infty = \delta_1$. So all information about the large and isolated eigenvalue 2, which is present in H_p for all p and is naturally of great interest in PCA, seems lost in the limit. This is not the case when one does asymptotic at fixed spectral distribution and consider that we are following a sequence of models which are going to infinity with $H_p = H_{p_0} = H_\infty$, where p_0 is the p which is given

by the data set. Fixed distribution asymptotics is more akin to what is done in classical statistics and we place ourselves in this framework. We refer the reader to 3.3.6 for a more detailed justification of our point.

In other respects, associating a measure to a vector in the way we described is meaningful mostly when one wants to have information about the whole set of values taken by the coordinates of the vector, and not about each coordinate. In particular, when going from vector to measure as described above we are losing all coordinate information: permuting the coordinates would drastically change the vector but yield the same measure. However, in the case of vectors of eigenvalues, since there is a canonical way to represent the vector (the i-th largest eigenvalue occupying the i-th coordinate), the information contained in the measure is sufficient. This measure approach is especially good when we are not focused on getting all the fine details of the vectors right, but rather when we are looking for structural information concerning the values taken by the coordinates.

An important area of random matrix theory for sample covariance matrices is concerned with understanding the properties of F_p as p (and n) go to ∞. A key theorem , which we review later (see Theorem 1), states that for a wide class of sample covariance matrices, F_∞, the limit of F_p, is asymptotically non-random. Furthermore, the theorem connects F_∞ to H_∞, the limit of H_p: given H_∞, we can theoretically compute F_∞, by solving a complicated equation. In data analysis, we observe the empirical spectral distribution, F_p. Our goal, of course, as far as eigenvalues are concerned, is to estimate the population spectral distribution, H_p. Our method will "invert" the relation between F_∞ and H_∞, so that we can go from F_p to $\widehat{H}_p$, an estimate of H_p. The method does not work directly with F_p but with a tool that is similar in flavor to the characteristic function of a distribution: the Stieltjes transform of a measure. We introduce this tool in the next subsection. As we will see later, it will also play a key role in our algorithm.

2.2 The Stieltjes transform of measures

A large number of results concerning the asymptotic properties of the eigenvalues of large dimensional random matrices are formulated in terms of limiting behavior of the Stieltjes transform of their empirical spectral distributions. The Stieltjes transform is a convenient and very powerful tool in the study of the convergence of spectral distribution of matrices (or operators), just as the characteristic function of a probability distribution is a powerful tool for central limit theorems. Most importantly, there is a simple connection between the Stieltjes transform of the spectral distribution of a matrix and its eigenvalues.

By definition, the Stieltjes transform of a measure G on $\mathbb{R}$ is defined as

$$m_G(z) = \int \frac{dG(x)}{x - z}\ , \text{ for } z \in \mathbb{C}^+,$$

where $\mathbb{C}^+ \triangleq \mathbb{C} \bigcap \{z : \operatorname{Im}(z) > 0\}$ is the set of complex numbers with strictly positive imaginary part. The Stieltjes transform appears to be known under several names in different areas of mathematics. It is sometimes referred to as Cauchy or Abel-Stieltjes transform. Good references about Stieltjes transforms include (Akhiezer, 1965, Sections 3.1-2), (Lax, 2002, Chapter 32), (Hiai and Petz, 2000, Chapter 3) and (Geronimo and Hill, 2003).

For the purpose of this paper, where will consider only compactly supported measures, the following results will be needed:

Fact. *Important properties of Stieltjes transforms of measures on $\mathbb{R}$:*

1. *If G is a probability measure, $m_G(z) \in \mathbb{C}^+$ if $z \in \mathbb{C}^+$ and $\lim_{y\to\infty} -iym_G(iy) = 1$.*
2. *If F and G are two measures, and if $m_F(z) = m_G(z)$, for all $z \in \mathbb{C}^+$, then $G = F$, a.e.*
3. *(Geronimo and Hill, 2003, Theorem 1): If G_n is a sequence of probability measures and $m_{G_n}(z)$ has a (pointwise) limit $m(z)$ for all $z \in \mathbb{C}^+$, then there exists a probability measure G with Stieltjes transform $m_G = m$ if and only if $\lim_{y\to\infty} -iym(iy) = 1$. If it is the case, G_n converges weakly to G.*
4. *(Geronimo and Hill, 2003, Theorem 2): The same is true if the convergence happens only for an infinite sequence $\{z_i\}_{i=1}^\infty$ in $\mathbb{C}^+$ with a limit point in $\mathbb{C}^+$.*

5. *If t is a continuity point of the cdf of G, $dG(t)/dt = \lim_{\epsilon\to 0} \frac{1}{\pi} Im\left(m_G(t+i\epsilon)\right)$*

For proofs, we refer the reader to (Geronimo and Hill, 2003).

Note that the Stieltjes transform of the spectral distribution Γ_p of a $p \times p$ matrix A_p is just

$$m_{\Gamma_p}(z) = \frac{1}{p}\text{trace}\left((A_p - z\text{Id}_p)^{-1}\right) .$$

Finally, it is clear that points 3 and 4 above can be used to show convergence of probability measures if one can control the corresponding Stieltjes transforms.

2.3 A fundamental result: the Marčenko-Pastur equation

In the study of covariance matrices, a remarkable result exists that describes the limiting behavior of the empirical spectral distribution, F_∞, in terms of the limiting behavior of the population spectral distribution, H_∞. The connection between these two measures is made through an equation that links the Stieltjes transform of the empirical spectral distribution to an integral against the population spectral distribution. We call this equation the Marčenko-Pastur equation because it first appeared in the landmark paper of (Marčenko and Pastur, 1967). The result was independently re-discovered in (Wachter, 1978) and then refined in (Silverstein and Bai, 1995) and (Silverstein, 1995). In particular, (Silverstein, 1995) is the only paper where the case of a non-diagonal population covariance is tackled.

In what follows, we will be working with an $n \times p$ data matrix X. We call $S_p = X^*X/n$ and denote m_{F_p} the Stieltjes transform of the spectral distribution, F_p, of S_p. We will call v_{F_p} the function defined by $v_{F_p}(z) = (1-p/n)\frac{-1}{z} + \frac{p}{n} m_{F_p}(z)$. v_{F_p} is the Stieltjes transform of the spectral distribution of XX^*/n.

Currently, the most general version of the result is found in (Silverstein, 1995) and states the following:

Theorem 1. *Suppose the data matrix X can be written $X = Y\Sigma_p^{1/2}$, where Σ_p is a $p \times p$ positive definite matrix and Y is an $n \times p$ matrix whose entries are i.i.d (real or complex), with $E(Y_{i,j}) = 0$, $E(|Y_{i,j}|^2) = 1$ and $E(|Y_{i,j}|^4) < \infty$.*

Call H_p the population spectral distribution, i.e the distribution that puts mass $1/p$ at each of the eigenvalues of the population covariance matrix, Σ_p. Assume that H_p converges weakly to a limit denoted H_∞. (We write this convergence $H_p \Rightarrow H_\infty$.) Then, when $p, n \to \infty$, and $p/n \to \gamma$, $\gamma \in (0, \infty)$,

1. *$v_{F_p}(z) \to v_\infty(z)$, a.s, where $v_\infty(z)$ is a deterministic function*

2. *$v_\infty(z)$ satisfies the equation*

$$-\frac{1}{v_\infty(z)} = z - \gamma \int \frac{\lambda dH_\infty(\lambda)}{1+\lambda v_\infty(z)} , \forall z \in \mathbb{C}^+ \tag{M-P}$$

3. *The previous equation has one and only one solution which is the Stieltjes transform of a measure.*

In plain English, under the assumptions put forth in Theorem 1, the spectral distribution of the sample covariance matrix is asymptotically non-random. Furthermore, it is fully characterized by the true population spectral distribution, through the equation (M-P).

A particular case of equation (M-P) is often of interest: the situation when all the population eigenvalues are equal to 1. Then of course, $H_p = H_\infty = \delta_1$. A little bit of elementary work leads to the well-known fact in random matrix theory that the empirical spectral distribution, F_p, converges (a.s) to the Marčenko-Pastur law, whose density is given by, if $\gamma \leq 1$,

$$f_\gamma(x) = \sqrt{(b-x)(x-a)}/(2\pi x\gamma) , \quad \text{with } a = (1-\gamma^{1/2})^2 , b = (1+\gamma^{1/2})^2 .$$

We refer the reader to (Marčenko and Pastur, 1967), (Bai, 1999) and (Johnstone, 2001) for more details and explanations concerning the case $\gamma > 1$. One point of statistical interest is that even though the true population eigenvalues are all equal to 1, the empirical ones are now spread on the interval $[(1-\gamma^{1/2})^2, (1+\gamma^{1/2})^2]$. Plotting the density also shows that its shape vary with γ in a non-trivial way. These two remarks illustrate some of the difficulties that need to be overcome when working under "large n, large p" asymptotics.

3 Algorithm and Statistical considerations

3.1 Formulation of the estimation problem

A remarkable feature of the equation (M-P) is that the knowledge of the limiting distribution of the eigenvalues in the population given by H_∞ fully characterizes the limiting behavior of the eigenvalues of the sample covariance matrix. However, the relationship between the two is hard to disentangle. As is common in statistics, the question is how to invert this relationship to estimate H_p. The question thus becomes, given $l_1, \ldots, l_p$, the eigenvalues of a sample covariance matrix, can we estimate the population eigenvalues, $\lambda_1, \ldots, \lambda_p$, using Equation (M-P)? Or in terms of spectral distribution, can we estimate H_p from F_p?

Our strategy is the following: 1) the first aim is to estimate the measure H_∞ appearing in the Marčenko-Pastur equation. 2) Given an estimator, $\widehat{H}_\infty$, of this measure, we will estimate λ_i as the i-th quantile of our estimated distribution. It is common in statistical practice to get these estimates by using the $i/(p+1)$ percentile and this is what we do. (We come back to possible difficulties getting from $\widehat{H}_p$ to $\hat{\lambda}_i$ in 3.3.6.) 3) An important point is that since we are considering fixed distribution asymptotics, our estimate of H_∞ will serve as our estimate of H_p, so $\widehat{H}_p = \widehat{H}_\infty$.

The main question, then, is how to approach step 1: estimating H_∞ based only on F_p. Of course, since we can compute the eigenvalues of S_p, we can compute $v_{F_p}(z)$ for any z we choose. By evaluating v_{F_p} at a grid of values $\{z_j\}_{j=1}^{J_n}$, we have a set of values $\{v_{F_p}(z_j)\}_{j=1}^{J_n}$ for which equation (M-P) should (approximately) hold. We want to find $\widehat{H}_\infty$ that will "best" satisfy equation (M-P) across the set of values of $v_{F_p}(z_j)$. In other words, we will pick

$$\widehat{H}_p = \widehat{H}_\infty = \underset{H}{\operatorname{argmin}}\ L\left(\left\{\frac{1}{v_{F_p}(z_j)} + z_j - \frac{p}{n}\int \frac{\lambda dH(\lambda)}{1+\lambda v_{F_p}(z_j)}\right\}_{j=1}^{J_n}\right) ,$$

where the optimization is over probability measures H, and L is a loss function to be chosen later. In this way we are "inverting" the equation (M-P), going from F_p, an estimate of F_∞, to an estimate of H_∞.

We will solve this inverse problem in two steps: discretization and convex optimization. We give a high-level overview of our method and postpone implementation details to the Appendix.

To summarize, we face the following interpolation problem: given J an integer and $(z_j, v_{F_p}(z_j))_{j=1}^{J}$ we want to find an estimate of H_∞ that approximately satisfies equation (M-P). In Section 5, we show that doing so for L_∞ loss function leads to a consistent estimator of H_∞, under the reasonable assumption that all spectra are bounded.

3.2 The algorithm

In order to alleviate the notations, we will replace the notation H_∞ by H when it does not cause any confusion.

3.2.1 Discretization

Naturally, dH can be simply approximated by a weighted sum of point masses:

$$dH(x) \simeq \sum_{k=1}^{K} w_k \delta_{t_k}(x) ,$$

where $\{t_k\}_{k=1}^{K}$ is a grid of points, chosen by us, and w_k's are weights. The fact that we are looking for a probability measure imposes the constraints

$$\sum_{k=1}^{K} w_k = 1 , \text{ and } w_k \geq 0 .$$

This approximation turns the optimization over measures problem into searching for a vector of weights in $\mathbb{R}_+^K$. After discretization, the integral in equation (M-P) can be approximated by

$$\int \frac{\lambda dH(\lambda)}{1+\lambda v} \simeq \sum_{k=1}^{K} w_k \frac{t_k}{1+t_k v} \ .$$

Hence finding a measure that approximately satisfies Equation (M-P) is equivalent to finding a set of weights $\{w_k\}_{k=1}^K$, for which we have

$$-\frac{1}{v_\infty(z_j)} \simeq z_j - \frac{p}{n}\sum_{k=1}^{K} w_k \frac{t_k}{1+t_k v_\infty(z_j)} \ , \forall j \ .$$

Naturally, we do not get to observe v_∞, and so we make a further approximation and replace v_∞ by v_{F_p}. Our problem is thus to find $\{w_k\}_{k=1}^K$ such that

$$-\frac{1}{v_{F_p}(z_j)} \simeq z_j - \frac{p}{n}\sum_{k=1}^{K} w_k \frac{t_k}{1+t_k v_{F_p}(z_j)} \ , \forall j \ .$$

One good thing about this approach is that the problem we now face is linear in the weights, which are the only unknowns here. We will demonstrate that this allows us to cast the problem as a relatively simple convex optimization problem.

3.2.2 Convex Optimization formulation

To show that we can formulate our inverse problem as a convex problem, let us call the approximation errors we make

$$e_j = \frac{1}{v_{F_p}(z_j)} + z_j - \frac{p}{n}\sum_{k=1}^{K} w_k \frac{t_k}{1+v_{F_p}(z_j)t_k} \ .$$

As explained above, there are two sources of error in e_j: one comes from the discretization of the integral involving H_∞. The other one comes from the substitution of v_∞, a non-random and asymptotic quantity, by v_{F_p}, a (random) quantity computable from the data. e_j is of course a complex number in general.

We can now state several convex problems as approximation of the inversion of the Marčenko-Pastur equation problem. We show in Section 5 consistency of the solution of the "L_∞" version of the problem described below. Here are a few examples of convex formulations for our inverse problem. In all these problems, the w_k's are constrained to sum to 1 and to be non-negative.

1. "L_∞" version: Find w_k's to

$$\text{Minimize} \max_{j=1,\ldots,J_n} \max\left\{|\mathrm{Re}\,(e_j)|\,, |\mathrm{Im}\,(e_j)|\right\}$$

2. "L_2" version: Find w_k's to

$$\text{Minimize} \sum_{j=1}^{J_n} |e_j| \ .$$

3. "L_2-squared" version: Find w_k's to

$$\text{Minimize} \sum_{j=1}^{J_n} |e_j|^2 \ .$$

The advantages of formulating our problem as a convex optimization problem are many. We will come back to the more statistical issues later. From a purely numerical point of view, we are guaranteed that an optimum exists, and fast algorithms are available. In practice, we used the optimization package MOSEK (see (MOSEK, 2006)), within Matlab, for solving our problems.

Because the rest of the article focuses particularly on the "L_∞" version of the problem described above, we want to give a bit more details about it. The "translation" of the problem into a convex optimization problem is

$$\begin{gathered}\min_{(w_1,\ldots,w_K,u)} u \\ \forall j,\ -u \leq \mathrm{Re}\,(e_j) \leq u \\ \forall j,\ -u \leq \mathrm{Im}\,(e_j) \leq u \\ \text{subject to } \sum_{i=1}^{K} w_k = 1 \\ \text{and } w_k \geq 0, \forall k\end{gathered}$$

This is a linear program (LP) with unknowns $(w_1, \ldots, w_K)$ and u (see (Boyd and Vandenberghe, 2004) for standard manipulations to make it a standard form LP).

The simulations we present in Section 4 were made using this version of this algorithm. The proof in Section 5 applies to this version of the algorithm.

3.3 Statistical considerations

The formulation we proposed is quite flexible and has several important qualities. For instance, regularization constraints can be easily handled through our proposal. We also can view the algorithm as a form of "basis pursuit" in measure space, from which we can draw some practical conclusions.

3.3.1 Regularization and constraints

Methods to invert the Marčenko-Pastur equation should be flexible enough to accommodate reasonable constraints that could provide additional improvement to our estimate of H_p. The fact that we essentially just optimize over the weights w_k's mean that we can easily regularize and add constraints. For instance, we might want to regularize our estimator and make it smoother by adding a total variation penalty (on the w_k's) to our objective function. In terms of constraints, we might want to specify that the first moment of our estimate $\widehat{H}_p$ match the trace of S_p/p, since we know that the trace of S_p/p is a good estimate of the trace of Σ_p/p (see e.g (Jonsson, 1982)), and that the trace of Σ_p/p is equal to the first moment of H_p. Note that constraints on the moments of our estimator are linear in the w_k's and so such constraints would still lead to a convex problem. The framework we provide can very easily incorporate these two examples of penalty and constraints, as well as many others.

3.3.2 A "basis pursuit" point of view

A semantic point is needed before we start our discussion. We use the term "basis pursuit" in a loose sense: we are not referring to the algorithm proposed in (Chen et al., 1998) but rather use this expression as a generic term for describing techniques that aim to optimize the representations of functional objects in overcomplete dictionaries. We refer the reader to (Hastie et al., 2001, Chapter 5) for some of the core statistical ideas of these so-called basis expansion methods.

The algorithm we propose can be viewed as a relaxation of a measure estimation problem. We want to estimate a measure H_∞ and instead of searching among all possible probability measures, we restrict our search space to mixtures of certain class of probability measures. In 3.2.1 for instance, we restricted the choice to mixture of point masses. In that sense, we can view it as a type of "basis pursuit" in probability measure space. We first choose a "dictionary" of probability measures on the real line, and we then decompose our estimator on this dictionary, searching for the best coefficients. Hence our problem can be formulated as

$$\text{find the best possible weights } \{w_1, \ldots, w_N\} \text{ with } d\widehat{H} = \sum_{i=1}^{N} w_i dM_i$$

where the M_i's are the measures in our dictionary.

In the preceding discussion on discretization, we restricted ourselves to M_i's being point masses at chosen "grid points". Of course, we can enlarge our dictionary to include, for instance:

1. Probability measures that are uniform on an interval: $dM_i(x) = 1_{x\in[a_i,b_i]}dx/(b_i - a_i)$.
2. Probability measures that have a linearly increasing density on an interval $[a_i, b_i]$ and density 0 elsewhere. So $dM_i(x) = 1_{[a_i,b_i]}2(x - a_i)/(b_i - a_i)^2dx$, and density 0 elsewhere.
3. Probability measures that have a linearly decreasing density on an interval $[a_i, b_i]$, and density 0 elsewhere. So $dM_i(x) = 1_{[a_i,b_i]}2(b_i - x)/(b_i - a_i)^2dx$.

If we decide to include a probability measure M in our dictionary, the only requirement is that we be able to compute the integral

$$\int \frac{\lambda dM(\lambda)}{1 + \lambda v}$$

for any v in $\mathbb{C}^+$.

Choosing a larger dictionary increases the size of the convex optimization problems we try to solve, and hence is at first glance computationally harder. However, statistically, enlarging the dictionary may lead to sparser representations of the measure we are estimating, and hence, at least intuitively, lead to better estimates of H_∞. The most favorable case is of course when H_∞ is a mixture of a small number of measures present in our dictionary. For instance, if H_∞ has a density whose graph is a triangle, having measures as described in points 2 and 3 above would most likely lead to sparser and maybe more accurate estimates. In the presence of a priori information on H_∞, the choice of dictionary should be adapted so that H_∞ has a sparse representation in the dictionary.

3.3.3 Useful properties of the algorithm

One important advantage of choosing to estimate measures instead of choosing to estimate a high-dimensional vector is that the algorithm's complexity does not increase with the size of the answer required by the user. Hence given a p dimensional vector of eigenvalues, once the values $v_{F_p}(z_j)$ are computed, the computational cost of the algorithm is the same irrespective of p. This means that for large p problems, only one difficult computation is required: that of the eigenvalues of the empirical covariance matrix. Our algorithm is hence, in some sense, "dimension-free", i.e, except for the computation of the eigenvalues, it is insensitive to the dimensionality of our original problem. This scaling property is important for high-dimensional problems.

Another good property of our method is that it is independent of the basis in which the data is represented. Because our method requires only as input the eigenvalues of the sample covariance matrix - quantities obviously independent of the original basis of the data - our method is basis independent.

In other respects, Theorem 1 holds for random variables that have a 4-th moment; we are not limited to Gaussian random variables. Complex random variables are also possible. Hence, the theorem is well-suited for wide applicability. Elementary properties of Gaussian random variables show that Theorem 1 covers all possible Gaussian problems. This will not be true for all distributions, but the scope of the theorem is still very wide. Note also that the Equation (M-P) holds in greater generality than mentioned in Theorem 1. We refer the reader to the original paper (Marčenko and Pastur, 1967) for further examples, in particular when the data is distributed on spheres or ellipsoids. (The original formulation of the theorem allows for dependence between the entries of the matrix Y, but the convergence is not shown to be almost sure.)

3.3.4 The case $p > n$ and how large is large?

Another advantage of the proposed method is that it is insensitive to whether p is larger than n or n is larger than p. The only requirement is that they both be quite large. We had reasonable to good results in simulation as soon as $p > 30$ or so. As a matter of fact, it is quite clear that to have reasonably accurate estimates of the eigenvalues, we need to "populate" the interval $[\lambda_p, \lambda_1]$ with enough points, for otherwise quantile methods may be somewhat inaccurate.

3.3.5 On covariance estimation, linear and non-linear shrinkage of eigenvalues

There is some classical and more recent statistical work on shrinkage of eigenvalues to improve covariance estimation. We refer the reader to Section 4.1 in (Ledoit and Wolf, 2004) for some examples due to Charles Stein and Leonard Haff, unfortunately in unpublished manuscripts. More recently, in the interesting paper by (Ledoit and Wolf, 2004), what was proposed is to linearly shrink the eigenvalues of S_p toward the identity : i.e l_i's become $\tilde{l}_i = (1-\rho)l_i + \rho$'s, for some ρ, independent of i, chosen using the data and the Marčenko-Pastur law. Then the authors of (Ledoit and Wolf, 2004) proposed to estimate Σ_p by $(1-\rho)S_p + \rho Id_p$. Since this latter matrix and S_p have the same eigenvectors, their method of covariance estimation can be viewed as linearly shrinking the sample eigenvalues and keeping the eigenvectors of S_p as estimates of the eigenvectors of Σ_p.

Our method of estimation of the population eigenvalues can be viewed as doing a non-linear shrinkage of the sample eigenvalues. While we could propose to just keep the eigenvectors of S_p as estimates of the eigenvectors of Σ_p, and hence get an estimate of the population covariance matrix, we think one should be able to do better by using the eigenvalue information to drive the eigenvector estimation. It is known that in "large n, large p" asymptotics, the eigenvectors of the sample covariance matrix are not consistent estimators of the population eigenvectors (see (Paul, To Appear)), even in the most favorable cases. However, having a good idea of the structure of the population eigenvalues should help us estimate the eigenvectors of the population covariance matrix, or at least formulate the right questions for the problem at hand. For instance, the inferred structure of the covariance matrix could help us decide how many subspaces we need to identify: if, for example, it turned out that the population eigenvalues were clustered around two values, we would have to identify two subspaces, the dimensions of these subspaces being the number of eigenvalues clustered around each value. Also, having estimates of the eigenvalues tell us how much variance our "eigenvectors" will have to explain. In other words, our hope is that taking advantage of the crucial eigenvalue information we are now able to gather will lead to better estimation of Σ_p by doing a "reasoned" spectral decomposition. Work in this direction is in progress.

3.3.6 Asymptotics at fixed spectral distribution and isolated eigenvalues

Our algorithm actually uses asymptotics assuming a fixed spectral distribution: we are essentially fixing $H_p = H_\infty$ when solving our optimization problem. Naturally, this does not mean that p is fixed. Note that this is what is classically done is statistics: for the simple problem of estimating the mean of a population from a sample $Z_1, \ldots, Z_K$, it is common to assume that the Z_k's have the same mean μ, and that μ does not depend on K. However, when studying the asymptotic properties of this simple estimator, we could require to actually have $\mu(K)$, with $\mu(K) \to \mu$. (All we would have to do is have a triangular array of data, and getting to observe just one row of this array at a time.) Hence our fixed spectral distribution "assumption" is very natural and similar to classical assumptions made in estimation problems.

Let us go back now to the problem of isolated eigenvalues. Suppose we get to see data in $\mathbb{R}^{p_0}$ for some p_0. Then, any isolated eigenvalue that may be present is numerically treated as if the mass that is attached to it is held fixed at $1/p_0$ when $p \to \infty$. So a point mass at the corresponding population eigenvalue would appear in $\widehat{H}_p$. This has been verified numerically. If the estimator were perfect, this mass should be equal to $1/p_0$. However, because of variability it may not be exactly of mass $1/p_0$. Then, estimating the population eigenvalues by the quantiles of the estimated population spectral distribution, we may "miss" this isolated eigenvalue. In the case of the largest eigenvalue, that would happen if the mass found numerically at this isolated eigenvalue is less than $1/(p_0+1)$. So isolated eigenvalues will require special care and caution, particularly in going from $\widehat{H}_p$ to $\hat{\lambda}_i$. While the method focuses on identifying the structure of the population eigenvalues and hence may have problems when it comes to estimating isolated eigenvalues, we have found in practice that it still provided a good tool for this task but that some care was required.

3.3.7 Existing related work

As far as we know, there has been no work on non-parametric estimation of H_p or H_∞ using the Marčenko-Pastur equation. However, some work exists in the Physics' literature ((Burda et al., 2004,

2005)), that takes advantage of the Marčenko-Pastur law to estimate some moments of H_∞. H_∞ is then assumed to a be a mixture of a finite and pre-specified number of point masses (see (Burda et al., 2004, p. 303)) and the moments are then matched with possible point masses and weights. While these methods might be of some use sometimes, we think they require too many assumptions to be practically acceptable for a broad class of problems. It might be tempting to try to develop an non-parametric estimator from moments, but we think that without the strong assumptions made in (Burda et al., 2004), those estimators will suffer drastically from: 1) the number of moments needed a priori may be large, and large moments are very unreliable estimators; 2) moments estimated indirectly may not constitute a genuine family of moments: certain Hankel matrices need to be positive semi-definite and will not necessarily be so. Semi-definite programming type corrections will then be necessary, but hard to implement. 3) Even if one has a genuine moment sequence, there are usually many distributions with the same moments. Choosing between them is clearly going to be a difficult task.

4 Simulations

We now present some simulations to illustrate the practical capabilities of the method. The objectives of eigenvalues estimation are many-folds and depend of the area of applications. We review some of those that inspired our work.

In settings like PCA, one basically wishes to discover some form of structure in the covariance matrix by looking at the eigenvalues of the sample covariance matrix. In particular, a situation where the population eigenvalues are different from each other indicates that projecting the data in some projections will be more "informative" that projecting it in other directions; while in the case where all the population eigenvalues are equal, all projections are equally informative or uninformative. As our brief discussion of the Marčenko-Pastur law illustrated, in the "large n, large p" setting, it is difficult to know from the sample eigenvalues whether all population eigenvalues are equal to each other or not, or even if there is any kind of structure in them. When p and n are both large, standard graphical methods like the scree plot tend to look similar whether or not there is structure in the data. We will see that our approach is able to differentiate between the situations. Among other things, our method can thus be thought as a alternative to the scree plot for high-dimensional problems.

In other applications, one focuses more on trying to estimate the value of the largest or smallest eigenvalues. In PCA, the largest population eigenvalues measure how much variance we can explain through a low dimensional projection and is hence important. In financial applications, like the Markovitz' portfolio optimization problem, the small population eigenvalues are important. They essentially measure what is the minimum risk one can take by investing in a portfolio of certain stocks (see (Laloux et al., 1999) and (Campbell et al., 1996, Chapter 5)). However, as explained in the Appendix, the largest eigenvalue of the sample covariance matrix tends to overestimate the largest eigenvalue of the population covariance. And similarly, the smallest eigenvalue of the sample covariance matrix tends to underestimate its population counterpart. What that means is that using these measures of "information" and "risk", we will tend to overestimate the amount of information there is in our data and tend to underestimate the amount of risk there is in our portfolios. So it is important to have tools to correct this bias. Our estimator provides a way to do so.

4.1 Details of the simulations

We illustrate the performance of our method on three cases, each with very different covariance structure. We will give more details on each individual case in the following subsections.

We now describe more precisely these examples. The first case is that of $\Sigma_p = \mathrm{Id}_p$, in other words, there is no "information" in the data. However standard graphical statistical methods like the "scree plot" will tend to show a pattern in the eigenvalues. We will show that our method is generally able to inform us that all the eigenvalues are equal.

The second case is one where Σ_p has 50% of its eigenvalues equal to 1 and 50% equal to 2. While it should be easy to discern that there are two very distinct clusters of eigenvalues in the population, in

high-dimension the sample eigenvalues will often blur the clusters together. We show that our method generally recovers these two clusters well.

Finally, the third example is one where Σ_p is a Toeplitz matrix. More details on Toeplitz matrices are given in 4.1.3. This situation poses a harder estimation problem. While the asymptotic behavior of the eigenvalues of such matrices is well understood, there are generally no easy and explicit formulas to represent the limit. We present the results to show that even in this difficult setting, our method performs quite well.

To measure the performance of our estimators, we compare the Lévy distances between our estimator, $\widehat{H}_p$, and the true distribution of the population eigenvalues, H_p, to that of the empirical spectral distribution, F_p, to H_p. Our choice is motivated by the fact that the Lévy distance can be used as a metric for weak convergence of distributions on $\mathbb{R}$. Recall (see e.g (Durrett, 1996)) that the Lévy distance between two distributions F and G on the real line is defined as

$$d_L(F,G) = \inf\{\epsilon > 0 : F(x-\epsilon) - \epsilon \leq G(x) \leq F(x+\epsilon) + \epsilon \ , \forall x\} \ .$$

In the plots we will depict the cumulative distribution function (cdf) of our estimated measures. Recall that the estimates of the population eigenvalues λ_i's are obtained by taking appropriate percentiles of these measures.

4.1.1 The case $\Sigma_p = \mathrm{Id}_p$

In this situation, the Marčenko-Pastur law predicts that instead of being concentrated at 1 like the population eigenvalues, the sample eigenvalues will be spread on the interval $[(1-\sqrt{p/n})^2, (1+\sqrt{p/n})^2]$. This is problematic, since by looking at the scree plot of just the sample eigenvalues, one might think that some population eigenvalues are (much) larger than others and hence some projections of the data are more informative than others. This is vividly illustrated on Figure 1a. However, as we see on Figure 1c, the method we propose finds that the population spectral distribution is very close to a point mass at 1, and all eigenvalues are thus close to 1. Statistically, this of course means that there is no preferred direction to project the data. All directions are equally informative, or uninformative.

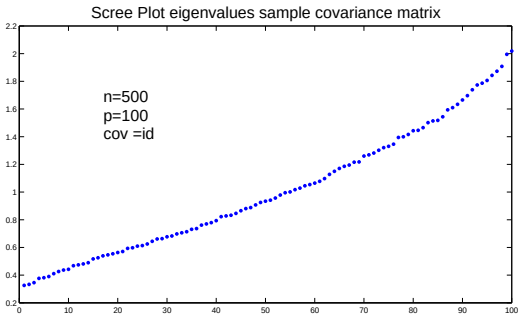
The figures presented in Figure 1 were chosen at random among 1000 Monte-Carlo simulations and are very encouraging. To further our empirical investigation of the performance of our method, we repeated the estimation process 1000 times. Another advantage is that on further investigation (manually checking the graphs of many of the estimators we obtained) we saw that the estimator consistently gets the structure "right", namely a huge spike in the vicinity of 1. This is of course very important for applications such as PCA, where the structure of the spectrum of the covariance matrix is of fundamental importance. For each repetition, we estimated the distribution of the eigenvalues in the population, and computed the Lévy distance of our estimator, $\widehat{H}_p$, to the true distribution, H_p, in this case a point mass at 1. We did the same for the empirical spectral distribution F_p. Figure 2 shows the ratio $d_L(\widehat{H}_p, H_p)/d_L(F_p, H_p)$ for these simulations. Our estimator clearly outperforms the one derived from the sample covariance matrix, often by a dramatic factor.

4.1.2 The case $H_p = .5\delta_1 + .5\delta_2$

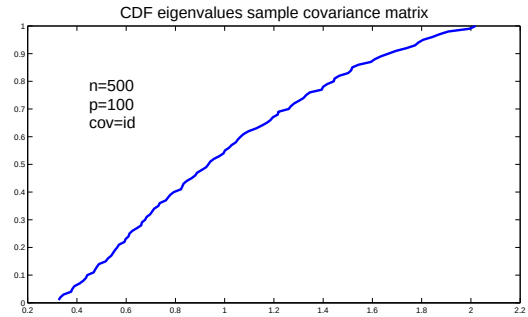
In this case the eigenvalues of the population covariance matrix are split into two clusters of equal size. For the specific example we investigate, 50% of the eigenvalues are equal to 1 and 50% are equal to 2.

While it should be easy to discern that there are two very distinct clusters of population eigenvalues, when p is sufficiently close to n the two clusters merge together and the scree plot of the sample eigenvalues does not show a clear separation between the two regions. The Marčenko-Pastur law predicts (in the case of identity covariance) that the sample eigenvalues spread over larger and larger intervals as p gets closer to n. Therefore, it is intuitively not surprising that when we have two not too distant clusters of population eigenvalues, the corresponding sample eigenvalues would start to overlap if p is close enough to n.

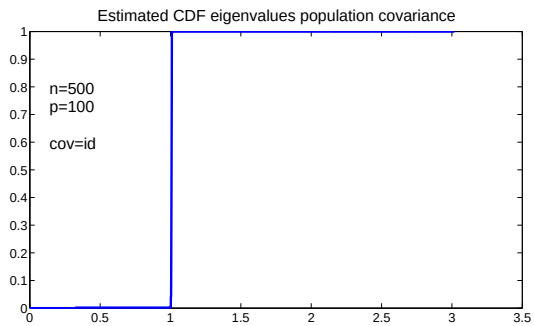
We did a Monte Carlo analysis (similar to the one done in the case of Id_p covariance) of our estimator and did comparisons to the empirical spectral distribution. As in the case of Id_p, we present a figure showing the ratio of the Lévy distance of the two estimates to the true distribution. Figure 4 shows that



(a) Eigenvalues (scree plot) of the sample covariance matrix



(b) CDF eigenvalues, sample covariance matrix (F_p)



(c) CDF eigenvalues, estimated population covariance matrix ($\widehat{H}_p$)

Figure 1: case $\mathbf{\Sigma_p = Id_p}$. The three figures above compare the performance of our estimator to the one derived from the sample covariance matrix on one realization of the data. The data matrix X is 500×100. All its entries are iid $\mathcal{N}(0,1)$. The population covariance is $\Sigma_p = \mathrm{Id}_{100}$, so the distribution of the eigenvalues is a point mass at 1. This is what our estimator (Figure (c)) recovers. Average computation time (over 1000 repetitions) was 13.33 seconds, according to `Matlab` tic and toc functions. Implementation details are in the Appendix.

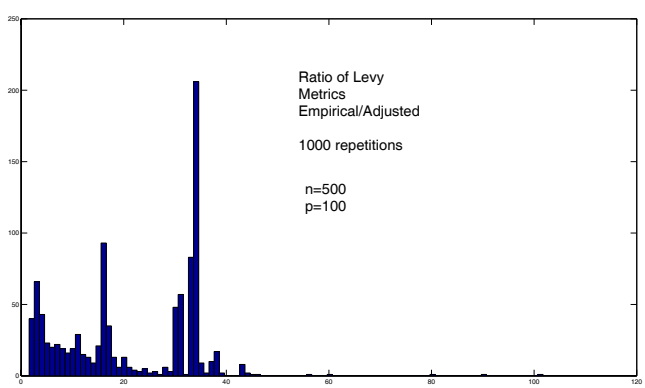
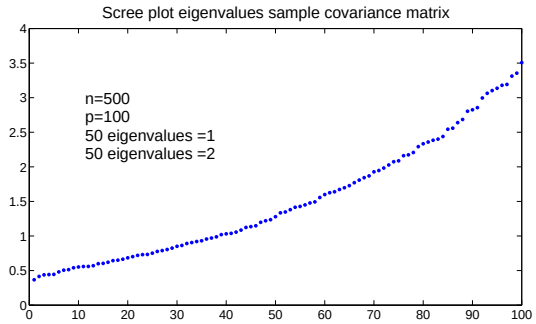
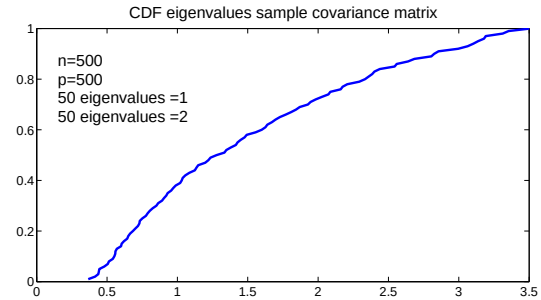


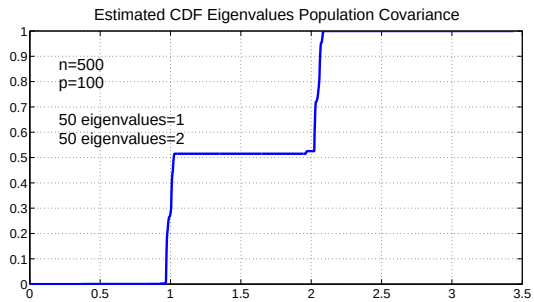
Figure 2: case $\mathbf{\Sigma_p = Id_p}$: Ratios $d_L(\widehat{H}_p, H_p)/d_L(F_p, H_p)$ over 1,000 repetitions. Dictionary consisted of only point masses. Large values indicate better performance of our algorithm. All ratios were found to be larger than 1.



(a) Scree plot of eigenvalues, sample covariance matrix: no clear separation around the 50th eigenvalue



(b) CDF eigenvalues sample covariance matrix (F_p)



(c) Estimated CDF of eigenvalues of population covariance matrix ($\widehat{H}_p$)

Figure 3: case $\boldsymbol{H_p = .5\delta_1 + .5\delta_2}$: the three figures above compare the performance of our estimator on one realization of the data. The data matrix Y is 500×100. All its entries are iid $\mathcal{N}(0,1)$. The covariance is diagonal and has spectral distribution $H_p = .5\delta_1 + .5\delta_2$. In other words, 50 eigenvalues are equal to 1 and fifty eigenvalues are equal to 2. This is essentially what our estimator (Figure (c)) recovers. Average computation time (over 1000 repetitions) was 15.71 seconds, according to `Matlab` tic and toc functions.

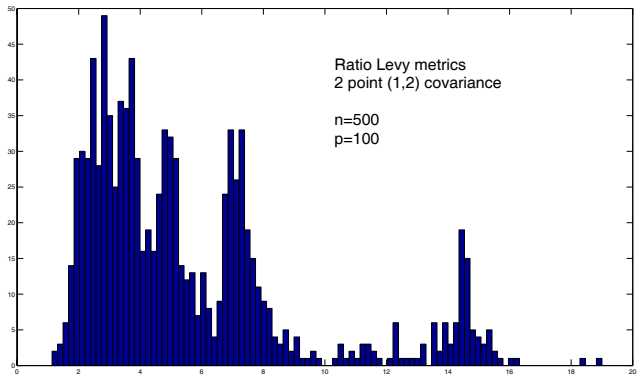
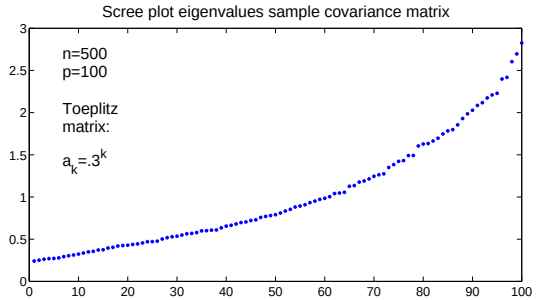
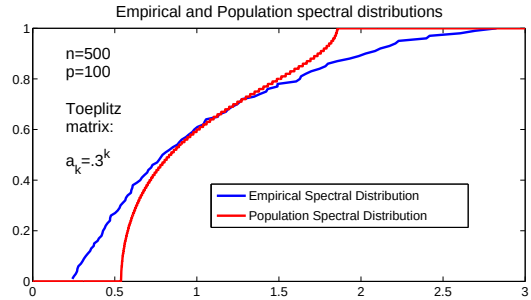


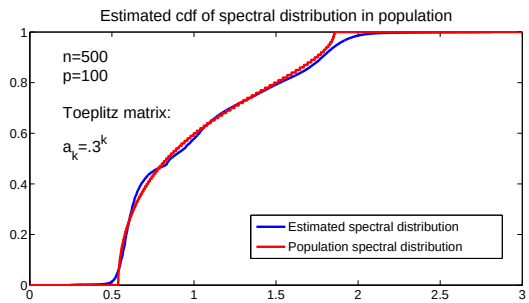
Figure 4: case $\boldsymbol{H_p = .5\delta_1 + .5\delta_2}$: Ratios $d_L(\widehat{H}_p, H_p)/d_L(F_p, H_p)$ over 1,000 repetitions. Dictionary consisted of only point masses. Large values indicate better performance of our algorithm. All ratios were found to be larger than 1.



(a) Scree plot, Eigenvalues sample covariance matrix



(b) CDF eigenvalues sample covariance matrix (F_p)



(c) Estimated CDF of eigenvalues of population covariance matrix ($\widehat{H}_p$)

Figure 5: case $\boldsymbol{\Sigma_p}$ **Toeplitz with entries.3**$^{|i-j|}$: the three figures above show the performance of our estimator on one realization of the data. The data matrix Y is 500×100. All its entries are iid $\mathcal{N}(0,1)$. The covariance is Toeplitz, with $t(|i-j|) = .3^{|i-j|}$. In Figure (c), we superimpose our estimator (blue curve) and the true distribution of eigenvalues (red curve). Average computation time (over 1000 repetitions) was 16.61 seconds, according to `Matlab` tic and toc functions.

once again our estimator clearly outperforms the one derived from the sample covariance matrix, by a large factor. Again, upon further investigation, the estimator generally gets the correct structure of the distribution of the population eigenvalues: in this case two spikes at 1 and 2.

4.1.3 The case of a Toeplitz covariance matrix

Finally, we performed the same type of analysis on a Toeplitz matrix, to show that the method we propose works quite well on more complicated types of covariance structures. Note that generally this is inherently a quite difficult problem, if we do not assume a priori that we know that the matrix is Toeplitz.

We recall that a Toeplitz matrix T is a matrix whose entries satisfy $T_{i,j} = t(i-j)$, for a certain function t. Since covariance matrices are symmetric, the Toeplitz matrices at hand will satisfy $T_{i,j} = t(|i-j|)$. The limiting spectral distribution of these objects are very well understood: see (Böttcher and Silbermann, 1999), (Gray, 2002) or (Grenander and Szegö, 1958).

Approaches exist that take advantage of the particular structure of a Toeplitz matrix. See for instance, the interesting papers (Bickel and Levina, 2004) and for even more generality - beyond Toeplitz matrices - (Bickel and Levina, 2006). However, these approaches are very basis dependent; they assume that the variables are measured in the appropriate basis. In data analysis, this may sometimes be justified and sometimes not. In particular, if the order of the variables is permuted, the resulting estimators might change. Since we want to be able to avoid this type of behavior, we feel that a "basis independent" method is needed and should be available. Finding such a method was one of the original motivations of our investigations.

Once again, the results displayed in Figure 5 are quite encouraging. Note that this time, the population spectral distribution could only be approximated by a large number of elements of our dictionary. So there was no sparse representation of H_∞ in our chosen dictionary of measures. However, computation time was

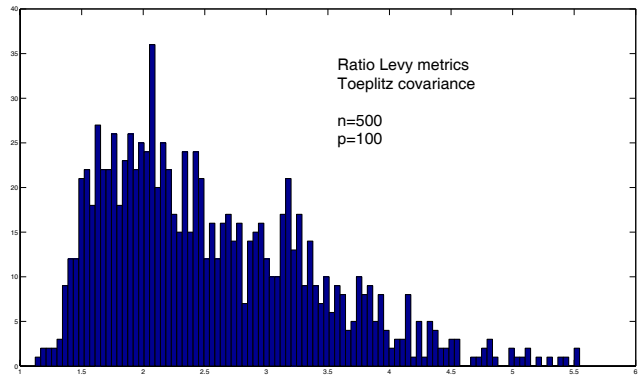


Figure 6: **Case Σ_p Toeplitz with entries ($.3^{|i-j|}$)**: Ratios $d_L(\widehat{H}_p, H_p)/d_L(F_p, H_p)$ over 1,000 repetitions. Dictionary consisted of only point masses. Large values indicate better performance of our algorithm. All ratios were found to be larger than 1.

not severely affected and the results are still quite good. To give a more detailed comparison, we present in Figure 6 a histogram of ratios $d_L(\widehat{H}_p, H_p)/d_L(F_p, H_p)$.

5 Consistency

In this section, we prove that the algorithm we propose leads to a consistent (in the sense of weak convergence of probability measures) estimator of the spectral distribution of the covariance matrices of interest.

More precisely, we focus on the "L_∞" version of the algorithm proposed in 3.2.2. In short, the theoretical results we prove state that as our computational resources grow (both in terms of size of available data and grid points on which to evaluate functions), the estimator $\widehat{H}_p$ converges to H_∞. The meaning of Theorem 2, which follows, is the following. We first choose a family of points $\{z_j\}$ in the upper-half of the complex plane, with a limit point in the upper-half of the complex plane. We assume that the population spectral distribution H_p has a limit, in the sense of weak convergence of distributions, when $p \to \infty$. We call this limit H_∞. This assumption of weak convergence allows us to vary H_p, as p grows, and to not be limited to $H_p = H_\infty$ for the theory; this provides maximal generality. We then solve the "L_∞" version of our optimization problem, by including more and more of the z_j's in the optimization problem as $n \to \infty$. We assume in Theorem 2 that we can solve this problem by optimizing over all probability measures. Then Theorem 2 shows that the solution of the optimization problem, $\widehat{H}_p$, converges in distribution to the limiting population spectral distribution, H_∞. In Corollary 1, we show that the same conclusion holds if the optimization is now made over probability measures that are mixture of point masses, whose locations are on a grid whose step size goes to 0 with p and n. Actually, the requirement is that the dictionary of measures we use contain these diracs. It can of course be larger. Hence, Corollary 1 proves consistency of the estimators specifically obtained through our algorithm. Beside the assumptions of Theorem 1, we assume that all the spectra of the population covariances are (uniformly) bounded. That translates into the mild requirement that the support of all H_p's be contained in a same compact set. Note that in the context of asymptotics at fixed spectral distribution, this is automatically satisfied.

We now turn to a more formal statement of the theorem. The notation $B(z_0, r)$ denotes the closed ball of center z_0 and radius r. Our main theorem is the following.

Theorem 2. *Suppose we are under the setup of Theorem 1, $H_p \Rightarrow H_\infty$ and $p/n \to \gamma$, with $0 < \gamma < \infty$. Assume that the spectra of the Σ_p's are uniformly bounded. Let $J_1, J_2, \ldots,$ be a sequence of integers tending to ∞. Let $z_0 \in \mathbb{C}^+$ and $r \in \mathbb{R}^+$ be such that $B(z_0, r) \subset \mathbb{C}^+$. Let $z_1, z_2, \ldots$ be a sequence of complex variables*

with an accumulation point, all contained in $B(z_0, r)$. Let $\widehat{H}_p$ be the solution of

$$\widehat{H}_p = \underset{H}{\operatorname{argmin}} \max_{j \le J_n} \left| \frac{1}{v_{F_p}(z_j)} + z_j - \frac{p}{n} \int \frac{\lambda dH(\lambda)}{1 + \lambda v_{F_p}(z_j)} \right| , \tag{1}$$

where H is a probability measure. Then we have

$$\widehat{H}_p \Rightarrow H_\infty \, , a.s \, .$$

Before we turn to proving the theorem, we need a few intermediate results. An important step in the proof is the following analytic lemma.

Lemma 1. *Suppose we have a family $\{z_i\}_{i=1}^\infty$ of complex numbers in $\mathbb{C}^+$, with an accumulation point in $\mathbb{C}^+$. Suppose there exist a sequence $\{J_i\}_{i=1}^\infty$ of integers tending to ∞, a sequence $\{\epsilon_i\}_{i=1}^\infty$ of positive reals tending to 0, a sequence $\{p(n)\}_{n=1}^\infty$ of integers, with $p(n)/n \to \gamma \in \mathbb{R}_+^*$, and a sequence of probability measures $\{\widehat{H}_p\}_{p=1}^\infty$ such that*

$$\forall j \le J_n \, , \left| \frac{1}{v_{F_p}(z_j)} + z_j - \frac{p}{n} \int \frac{\lambda d\widehat{H}_p(\lambda)}{1 + \lambda v_{F_p}(z_j)} \right| < \epsilon_n \, . \tag{2}$$

Assume that v_∞ satisfies

$$-\frac{1}{v_\infty(z_j)} = z_j - \gamma \int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_\infty(z_j)} \, , \tag{3}$$

for some probability measure H_∞. Assume that $v_{F_p}(z_j) \to v_\infty(z_j)$, and both are analytic in $\mathbb{C}^+$ and from $\mathbb{C}^+$ to $\mathbb{C}^+$. Further, assume that $|v_\infty(z_j)| < C$ for some $C \in \mathbb{R}$, and $|Im\left(v_{F_p}(z_j)\right)| > \delta$, as well as $|Im\left(v_\infty(z_j)\right)| > \delta$, for some $\delta > 0$. Then

$$\widehat{H}_p \Rightarrow H_\infty \, .$$

Proof. Since v_∞ satisfies

$$\frac{1}{v_\infty(z_j)} + z_j - \gamma \int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_\infty(z_j)} = 0 \, ,$$

equation (2) reads

$$\left| \frac{1}{v_{F_p}(z_j)} - \frac{1}{v_\infty(z_j)} + \left(\gamma - \frac{p}{n}\right) \int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_\infty(z_j)} + \frac{p}{n} \left(\int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_\infty(z_j)} - \int \frac{\lambda d\widehat{H}_p(\lambda)}{1 + \lambda v_{F_p}(z_j)} \right) \right| < \epsilon_n \, .$$

Note that since $|\mathrm{Im}\left(v_{F_p}\right)| > \delta$ and $|\mathrm{Im}\left(v_\infty\right)| > \delta$, and given that

$$\left| \frac{1}{v_{F_p}} - \frac{1}{v_\infty} \right| \le \frac{|v_{F_p} - v_\infty|}{|\mathrm{Im}\left(v_{F_p}\right)| |\mathrm{Im}\left(v_\infty\right)|} \, ,$$

we have $|1/v_{F_p} - 1/v_\infty| \to 0$.

Also, because $p/n \to \gamma$, the previous equation implies that

$$\int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_\infty(z_j)} - \int \frac{\lambda d\widehat{H}_p(\lambda)}{1 + \lambda v_{F_p}(z_j)} \to 0 \, .$$

Now because $v_{F_p}(z_j) \to v_\infty(z_j)$, we have

$$\begin{aligned} \left| \int \frac{\lambda d\widehat{H}_p(\lambda)}{1 + \lambda v_{F_p}(z_j)} - \int \frac{\lambda d\widehat{H}_p(\lambda)}{1 + \lambda v_\infty(z_j)} \right| &= \left| \int \frac{\lambda^2 (v_\infty(z_j) - v_{F_p}(z_j)) d\widehat{H}_p(\lambda)}{(1 + \lambda v_\infty(z_j))(1 + \lambda v_{F_p}(z_j))} \right| \\ &\le \frac{\left|v_{F_p}(z_j) - v_\infty(z_j)\right|}{|\mathrm{Im}\left(v_{F_p}(z_j)\right)| |\mathrm{Im}\left(v_\infty(z_j)\right)|} \to 0 \, . \end{aligned}$$

So we have

$$\int \frac{\lambda d\widehat{H}_p(\lambda)}{1+\lambda v_\infty(z_j)} \to \int \frac{\lambda dH_\infty(\lambda)}{1+\lambda v_\infty(z_j)} \ .$$

We remark that for $m \in \mathbb{C}^+$, and G a probability measure on $\mathbb{R}$, whose Stieltjes transform is denoted by S_G,

$$\int \frac{\lambda dG(\lambda)}{1+\lambda m} = \frac{1}{m} - \frac{1}{m}\int \frac{dG(\lambda)}{1+\lambda m} = \frac{1}{m} - \frac{1}{m^2}\int \frac{dG(\lambda)}{1/m+\lambda} = \frac{1}{m} - \frac{1}{m^2} S_G\left(-\frac{1}{m}\right) \ .$$

Hence, when the assumptions of the lemma are satisfied, we have

$$S_{\widehat{H}_p}\left(-\frac{1}{v_\infty(z_j)}\right) \to S_{H_\infty}\left(-\frac{1}{v_\infty(z_j)}\right) \ .$$

Now since $v_\infty(z_j)$ satisfies Equation (3), we see that if $v_\infty(z_j) = v_\infty(z_k)$, then $z_j = z_k$. Hence, $\{-1/v_\infty(z_j)\}_{j=1}^\infty$ is an infinite sequence of complex numbers in $\mathbb{C}^+$. Moreover, because v_∞ is analytic in $\mathbb{C}^+$, it is continuous, and so $\{-1/v_\infty(z_j)\}_{j=1}^\infty$ has an accumulation point. Further, because $|v_\infty(z_j)| < \infty$ and $\mathrm{Im}\,(v_\infty(z_j)) > \delta$, this accumulation point is in $\mathbb{C}^+$.

So under the assumptions of the lemma, we have shown that there exist an infinite sequence $\{y_j\}_{j=1}^\infty$ of complex numbers in $\mathbb{C}^+$, with an accumulation point in $\mathbb{C}^+$, such that

$$S_{\widehat{H}_p}(y_j) \to S_{H_\infty}(y_j) \ , \forall j \ .$$

According to (Geronimo and Hill, 2003), Theorem 2, this implies that

$$\widehat{H}_p \Rightarrow H_\infty \ .$$

□

In the context of spectrum estimation, the intuitive meaning of the previous lemma is that if for a sequence of complex numbers $\{z_j\}_{j=1}^\infty$ with an accumulation point in $\mathbb{C}^+$, we can find a sequence of $\widehat{H}_p$'s approximately satisfying the Marčenko-Pastur equation at more and more of the z_j's when n grows, then this sequence of measures will converge to H_∞.

We now state and prove a few results that will be needed in the proof of Theorem 2. The first one is a remark concerning Stieltjes transforms.

Proposition 1. *The Stieltjes transform, S_H, of any probability measure H on $\mathbb{R}$, is Lipschitz $1/u_{\min}^2$ on $\mathbb{C}^+ \cap \{Im\,(z) > u_{\min}\}$.*

Hence, if $S_{H_n}(z) \to S_{H_\infty}(z)$ pointwise, where all the measures considered are probability measures, the convergence is uniform on compact subsets of $\mathbb{C}^+ \cap \{Im\,(z) > u_{\min}\}$.

Proof. We first show the Lipschitz character of S_H. We have

$$S_H(z_1) - S_H(z_2) = \int \left(\frac{1}{\lambda - z_1} - \frac{1}{\lambda - z_2}\right) dH(\lambda) = (z_1 - z_2)\int \frac{dH(\lambda)}{(\lambda - z_1)(\lambda - z_2)} \ .$$

Now $|\lambda - z_1| > |\mathrm{Im}\,(\lambda - z_1)\,| > u_{\min}$. So

$$|S_H(z_1) - S_H(z_2)| \le \frac{|z_1 - z_2|}{u_{\min}^2} \ .$$

So we have shown that S_H is uniformly Lipschitz $1/u_{\min}^2$ on $\mathbb{C}^+ \bigcap \{\mathrm{Im}\,(z) > u_{\min}\}$.

Now, it is an elementary and standard fact of analysis that if a sequence of K-Lipschitz functions converge pointwise to a K-Lipschitz function, then the convergence is uniform on compact sets. This shows the uniform convergence part of our statement. □

In the proof of the Theorem, we will need the result of the following proposition.

Proposition 2. *Assume the assumptions underlying Theorem 1 are satisfied. Recall that v_{F_p} is the Stieltjes transform of $\widetilde{F}_p$, the spectral distribution of $XX^*/n = Y\Sigma_p Y^*/n$. Assume that the population spectral distribution H_p has a limit H_∞ and that all the spectra are uniformly bounded. Let $z \in B(z_0, r)$, with $B(z_0, r) \subset \mathbb{C}^+$. Then, almost surely,*

$$\exists N, n > N \Rightarrow \inf_{n, z \in B(z_0,r)} Im\left(v_{F_p}(z)\right) = \delta > 0 \ .$$

Proof. Since we assume that all spectra are bounded, we can assume that the population eigenvalues are all uniformly bounded by K. Because the spectral norm is a matrix norm and $X = Y\Sigma_p^{1/2}$, we have

$$\lambda_{\max}(X^*X/n) \leq \lambda_{\max}(\Sigma_p)\lambda_{\max}(Y^*Y/n) \ .$$

Now it is a standard result in random matrix theory that, $\lambda_{\max}(Y^*Y/n) \to (1+\gamma)^2$, a.s, so for n large enough,

$$\lambda_{\max}(Y^*Y/n) \leq 2(1+\gamma)^2 \text{ a.s} \ .$$

Calling $z = u + iv$, we have

$$\mathrm{Im}\left(v_{F_p}(z)\right) = \int \frac{v d\widetilde{F}_p(\lambda)}{(\lambda - u)^2 + v^2} \geq \int \frac{v d\widetilde{F}_p(\lambda)}{2(\lambda^2 + u^2) + v^2} \ ,$$

because $v \geq 0$. Now, the remark we made concerning the eigenvalues of X^*X/n implies that almost surely, for n large enough, $\widetilde{F}_p$ puts all its mass within $[0, C]$, for some C. Therefore,

$$\mathrm{Im}\left(v_{F_p}(z)\right) \geq \frac{v}{C^2 + v^2 + 2u^2} \ ,$$

and hence $\mathrm{Im}\left(v_{F_p}(z)\right)$ is a.s bounded away from 0, for n large enough. □

To show that we can find "good" probability measures when solving our optimization problem, we will need to exhibit a sequence of measures that approximately satisfy the Marčenko-Pastur equation. The next proposition is a step in this direction.

Proposition 3. *Let $r \in \mathbb{R}^+$ and $z_0 \in \mathbb{C}^+$ be given and satisfying $B(z_0, r) \subset \mathbb{C}^+$. Suppose $p/n \to \gamma$ when $n \to \infty$, and $\forall \epsilon \, \exists N : n > N \Rightarrow \forall z \in B(z_0, r), \ |v_{F_p}(z) - v_\infty(z)| < \epsilon$, where v_∞ satisfies equation (3). Suppose further that $|Im\,(v_\infty(z))\,| > u_{\min}$ on $B(z_0, r)$. Then, if $\epsilon < u_{\min}/2$,*

$$\exists N' \in \mathbb{N}, \ \forall z \in B(z_0, r), \ \forall n > N', \ \left| \frac{1}{v_{F_p}(z)} + z - \frac{p}{n} \int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_{F_p}(z)} \right| < 2\epsilon \frac{1 + 2\gamma}{u_{\min}^2}$$

Proof. Using equation (3) we find that

$$\begin{aligned}
\Delta_n(z) &= \frac{1}{v_{F_p}(z)} + z - \frac{p}{n} \int \frac{\lambda dH_\infty(\lambda)}{1 + \lambda v_{F_p}(z)} \\
&= \frac{1}{v_{F_p}(z)} - \frac{1}{v_\infty(z)} + \frac{p}{n} \int \left(\frac{\lambda}{1 + \lambda v_\infty(z)} - \frac{\lambda}{1 + \lambda v_{F_p}(z)} \right) dH_\infty(\lambda) \\
&+ \left(\gamma - \frac{p}{n}\right) \int \frac{\lambda}{1 + \lambda v_\infty(z)} dH_\infty(\lambda) \\
&\triangleq \Delta_n^I(z) + \left(\gamma - \frac{p}{n}\right) \int \frac{\lambda}{1 + \lambda v_\infty(z)} dH_\infty(\lambda)
\end{aligned}$$

Because $\gamma - p/n \to 0$, and $|\lambda/(1 + \lambda v_\infty(z))| \leq 1/|\mathrm{Im}\,(v_\infty(z))\,| \leq 1/u_{\min}$, we have

$$\left(\gamma - \frac{p}{n}\right) \int \frac{\lambda}{1 + \lambda v_\infty(z)} dH_\infty(\lambda) \to 0 \ \text{ uniformly on } B(z_0, r) \ .$$

Now, of course,

$$\Delta_n^I(z) = \frac{v_\infty(z) - v_{F_p}(z)}{v_{F_p}(z)v_\infty(z)} - \frac{p}{n}(v_{F_p}(z) - v_\infty(z)) \int \frac{\lambda^2}{(1+\lambda v_{F_p}(z))(1+\lambda v_\infty(z))} dH_\infty(\lambda) \ .$$

We remark that $|v_{F_p}(z)| > |\mathrm{Im}\left(v_{F_p}(z)\right)| > u_{\min} - \epsilon > u_{\min}/2$. Hence, if n is large enough,

$$\left|\Delta_n^I(z)\right| \leq 2\frac{|v_\infty(z) - v_{F_p}(z)|}{u_{\min}^2} + 2\frac{p}{n}\frac{|v_{F_p}(z) - v_\infty(z)|}{u_{\min}^2} \leq \epsilon \frac{2}{u_{\min}^2}\left(1 + 2\gamma\right) \ .$$

□

We now turn to proving Theorem 2

Proof of Theorem 2. According to Propositions 1 and 2, the assumptions put forth in Proposition 3 are a.s satisfied for v_{F_p} and v_∞ is the Stieltjes as in Theorem 1. Note also that Theorem 1 states that a.s, $v_{F_p}(z) \to v_\infty(z)$, and that all these functions are analytic in $\mathbb{C}^+$. In other words, they have the properties needed for Lemma 1 to apply.

In particular, Proposition 3 implies that if $\{z_j\}$ is a family of complex numbers included in $B(z_0, r)$, and if $\widehat{H}_p$ is the solution of equation (1), equation (2) will be satisfied almost surely, with a family $\{\epsilon_j\}$ of positive real numbers that converge to 0. According to Lemma 1, this implies that,

$$\widehat{H}_p \Rightarrow H_\infty \ , \text{almost surely.}$$

□

As a corollary of Theorem 2, we are now ready to prove consistency of our algorithm.

Corollary 1 (Consistency of proposed algorithm). *Assume the same assumptions as in Theorem 2. Call $\widehat{H}_p$ the solution of equation (1), where the optimization is now over measures which are sums of atoms, the location of which are restricted to belong to a grid (depending on n) whose step size is going to 0 as $n \to \infty$. Then*

$$\widehat{H}_p \Rightarrow H_\infty \ a.s \ .$$

Proof. All that is needed is to show that a discretized version of H_∞ furnishes a good sequence of measures in the sense that Proposition 3 holds for this sequence of discretized version of H_∞.

We call H_{M_n} a discretization of H_∞ on a regular discrete grid of size $1/M_n$. For instance, we can choose $H_{M_n}(x)$ to be a step function, with $H_{M_n}(x) = H_\infty(x)$ is $x = l/M_n$, $l \in \mathbb{N}$, and H_{M_n} is constant on $[l/M_n, (l+1)/M_n)$. Recall also that H_∞ is compactly supported.

In light of the proof of Proposition 3, for the corollary to hold, it is sufficient to show that uniformly in $z \in B(z_0, r)$,

$$\left|\int \frac{\lambda}{1+\lambda v_{F_p}(z)} dH_{M_n}(\lambda) - \int \frac{\lambda}{1+\lambda v_{F_p}(z)} dH_\infty(\lambda)\right| \to 0 \ .$$

Now calling $d_W\left(H_{M_n}, H_\infty\right)$ the Wasserstein distance between H_{M_n} and H_∞, we have

$$d_W\left(H_{M_n}, H_\infty\right) = \int_0^\infty \left|H_{M_n}(x) - H_\infty(x)\right| dx \to 0 \text{ as } n \to \infty \ .$$

(H_{M_n} and H_∞ put mass only on $\mathbb{R}^+$, so the previous integral is restricted to $\mathbb{R}^+$. We refer the reader to the survey (Gibbs and Su, 2001) for properties of different metrics on probability measures.)

In other respects, it is easy to see that under the assumptions of Proposition 3, there exists N such that, $\sup_{n>N, z\in B(z_0,r)} |v_{F_p}(z)| \leq K$, for some $K < \infty$. Recall also that under the same assumptions, $\inf_{n>N, z\in B(z_0,r)} \mathrm{Im}\left(v_{F_p}(z)\right) \geq \delta$, for some $\delta > 0$.

For two probability measures G and H, we also have

$$d_W\left(G, H\right) = \sup_f \left\{\left|\int f dG - \int f dH\right| ; \ f \text{ a 1-Lipschitz function}\right\} \ .$$

Hence, because H_∞ and H_{M_n} are supported on a compact set that is independent of n, to have the result we want, it will be enough to show that

$$f_{v_{F_p}(z)}(\lambda) = \frac{\lambda}{1 + \lambda v_{F_p}(z)}$$

is uniformly Lipschitz (as a function of λ) when $z \in B(z_0, r)$ and $n > N$.

Now note that

$$f_{v_{F_p}(z)}(\lambda_1) - f_{v_{F_p}(z)}(\lambda_2) = \frac{\lambda_1 - \lambda_2}{(1 + \lambda_1 v_{F_p}(z))(1 + \lambda_2 v_{F_p}(z))} .$$

If $\lambda \leq 1/(2K)$, then $|\lambda v_{F_p}(z)| \leq 1/2$, so $|1 + \lambda v_{F_p}(z)| \geq 1/2$. If $\lambda \geq 1/(2K)$, then $|1 + \lambda v_{F_p}(z)| \geq \lambda \mathrm{Im}\left(v_{F_p}(z)\right) \geq \delta/(2K)$. So $|1 + \lambda v_{F_p}(z)| \geq \min(1/2, \delta/(2K)) = C$. Hence $f_{v_{F_p}(z)}$ is $1/C^2$-Lipschitz, and C is uniform in n and z, as needed.

Having thus extended Proposition 3 to discretized versions of H_∞, the proof of the corollary is the same as that of Theorem 2. □

The proof of the corollary makes clear that when solving the optimization problem over any dictionary of probability measures containing point masses (but also possibly other measures) at grid points on a grid whose step size goes to 0, the algorithm will lead to a consistent estimator.

Finally, as explained in the Appendix, the algorithm we implemented start with $v_{F_p}(z_j)$ sequences, as opposed to simply z_j sequences. It can be straightforwardly adapted to handle the z_j's as a starting point, too, but we got slightly better numerical results when starting with $v_{F_p}(z_j)$. The proof we just gave could be adapted to handle the situation where the $v_{F_p}(z_j)$'s are used as starting point. However, a few other technical issues would have to be addressed that we felt would make the important ideas of the proof less clear. Hence we decided to show consistency in the setting of Corollary 1.

6 Conclusion

In this paper we have presented an original method to estimate the spectrum of large dimensional covariance matrices. We place ourselves in a "large n, large p" asymptotic framework, where both the number of observations and the number of variables is going to infinity, while their ratio goes to a finite, non-zero limit. Approaching problems in this framework is increasingly relevant as datasets of larger and larger size become more common.

Instead of estimating individually each eigenvalue, we propose to associate to each vector of eigenvalues a probability distribution and estimate this distribution. We then estimate the population eigenvalues as the appropriate quantiles of the estimated distribution. We use a fundamental result of random matrix theory, the Marčenko-Pastur equation, to formulate our estimation problem. We propose a practical method to solve this estimation problem, using tools from convex optimization.

The estimator has good practical properties: it is fast to compute on modern computers (we use the software (MOSEK, 2006) to solve our optimization problem) and scales well with the number of parameters to estimate. We show that our estimator of the distribution of interest is consistent, where the appropriate notion of convergence is weak convergence of distributions.

The estimator performs a non-linear shrinkage of the sample eigenvalues. It is basis independent and we hope will help in improving the estimation of eigenvectors of large dimensional covariance matrices. To the best of our knowledge, our method is the first that harnesses deep results of random matrix theory to practically solve estimation problems. We have seen in simulations that the improvement it leads to are often dramatic. In particular, it enables us to find structure in the data when it exists and to conclude to its absence where there is none, even when classical methods would point to different conclusions.

APPENDIX

A.1 Implementation details

We plan to release the software we used to create the figures appearing in the simulation and data analysis section in the near future. However, we want to mention here the choices of parameters we made to implement our algorithm. The justifications for them is based on intuitions coming from studying the equation (M-P).

Scaling of the eigenvalues If all the entries of the data matrix are multiplied by a constant a, then the eigenvalues of Σ_p are multiplied by a^2, and so are the eigenvalues of S_p. Hence, if the eigenvalues of S_p are divided by a factor a, Equation (M-P) remains valid if we change $H_\infty(x)$ into $H_\infty(ax)$. In practice, we scale the empirical eigenvalues by l_1 the largest eigenvalue of S_p. We solve our convex optimization problem with the scaled eigenvalues to obtain $H_\infty(l_1 x)$, from which we get $H_\infty(x)$ through easy manipulations. The subsequent details describe how we solve our convex optimization problem, after rescaling of the eigenvalues.

Choice of $(z_j, v(z_j))$ We have found that using 100 pairs $(z_j, v(z_j))$ was generally sufficient to obtain good and quick (10s-60s) results in simulations. More points is of course better. With 200 points, solving the problem took more time, but was still doable (40s-3mins). In the simulations and data analysis presented afterwards, we first chose the $v(z_j)$ and numerically found the corresponding z_j using `Matlab`'s optimization toolbox. We took $v(z_j)$ to have a real part equally spaced (every .02) on $[0, 1]$, and imaginary part of 10^{-2} or 10^{-3}. In other words, our $v(z_j)$'s consisted of two (discretized) segments in $\mathbb{C}^+$, the second one being obtained from the first one by a vertical translation of $9 * 10^{-3}$.

Choice of interval to focus on The largest (resp. smallest) eigenvalue of a $p \times p$ symmetric matrix S are convex (resp. concave) functions of the entries of the matrix. This is because $l_1(S) = \sup_{\|u\|_2=1} u'Su$, where u is a vector in $\mathbb{R}^p$. Hence $l_1(S)$ is the supremum of linear functionals of the entries of the matrix. Similarly, $l_p(S) = \inf_{\|u\|_2=1} u'Su$, so $l_p(S)$ is a concave function of the entries of S. Note that the sample covariance matrix S_p is an unbiased estimator of Σ_p. By Jensen's inequality, we therefore have $E(l_1(S_p)) \geq l_1(E(S_p)) = \lambda_1(\Sigma_p)$. In other words, $l_1(S_p)$ is a biased estimator of $\lambda_1(\Sigma_p)$, and tends to overestimate it. Similarly, $l_p(S_p)$ is a biased estimator of $\lambda_p(\Sigma_p)$ and tends to underestimate it. More detailed studies of l_1 and l_p indicate that they do not fluctuate too much around their mean. Practically, as $n \to \infty$, we will have with large probability, $l_p \leq \lambda_p$ and $l_1 \geq \lambda_1$. (In certain cases, concentration bounds can make the previous statement rigorous.) Hence, after rescaling of the eigenvalues, it will be enough to focus on probability measures supported on the interval $[l_p/l_1, 1]$ when decomposing $H_\infty(l_1 x)$.

Choice of dictionary In the "smallest" implementation, we limit ourselves to a dictionary consisting of point masses on the interval $[l_p/l_1, 1]$, with equal spacing of .005. We call ζ_p the length of this interval. In larger implementations, we split the interval $[l_p/l_1, 1]$ into dyadic intervals, getting at scale k, 2^k intervals: $[l_p/l_1 + j2^{-k}\zeta_p, l_p/l_1 + (j+1)2^{-k}\zeta_p]$, for $j = 0, \ldots, 2^k - 1$. We store the end points of all the intervals at all the scales from $k = 2$ to $k = 8$ for the coarsest implementation and up to 10 for the finest We implemented dictionaries containing:

1. Point masses every .005 on $[l_p/l_1, 1]$, and probability measures supported on the dyadic intervals described above that have constant density on these intervals.

2. Point masses every .005 on $[l_p/l_1, 1]$, and probability measures supported on the dyadic intervals described above that have constant density on these intervals, as well as probability measures on those dyadic intervals that have linearly increasing and linearly decreasing densities.

The simulations presented above were made with this latter choice of dictionary using scales up to 8.

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