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Spectral analysis of the Moore–Penrose inverse of a large dimensional sample covariance matrix

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ABSTRACT

For a sample of n independent identically distributed p-dimensional centered random vectors with covariance matrix Σ_n let $\tilde{\mathbf{S}}_n$ denote the usual sample covariance (centered by the mean) and $\mathbf{S}_n$ the non-centered sample covariance matrix (i.e. the matrix of second moment estimates), where $p > n$. In this paper, we provide the limiting spectral distribution and central limit theorem for linear spectral statistics of the Moore–Penrose inverse of $\mathbf{S}_n$ and $\tilde{\mathbf{S}}_n$. We consider the large dimensional asymptotics when the number of variables $p \to \infty$ and the sample size $n \to \infty$ such that $p/n \to c \in (1, +\infty)$. We present a Marchenko–Pastur law for both types of matrices, which shows that the limiting spectral distributions for both sample covariance matrices are the same. On the other hand, we demonstrate that the asymptotic distribution of linear spectral statistics of the Moore–Penrose inverse of $\tilde{\mathbf{S}}_n$ differs in the mean from that of $\mathbf{S}_n$.

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1. Introduction

Many statistical, financial and genetic problems require estimates of the inverse population covariance matrix which are often constructed by inverting the sample covariance matrix. Nowadays, the modern scientific data sets involve the large number of sample points which is often less than the dimension (number of features) and so the sample covariance matrix is not invertible. For example, stock markets include a large number of companies which is often larger than the number of available time points; or the DNA can contain a fairly large number of genes in comparison to a small number of patients. In such situations, the Moore–Penrose inverse or pseudoinverse of the sample covariance matrix can be used as an estimator for the precision matrix (see, e.g., Srivastava [15], Kubokawa and Srivastava [7], Hoyle [6], Bodnar et al. [4]).

In order to better understand the statistical properties of estimators and tests based on the Moore–Penrose inverse in high-dimensional settings, it is of interest to study the asymptotic spectral properties of the Moore–Penrose inverse, for example convergence of its linear spectral statistics (LSS). This information is of great interest for high-dimensional statistics because more efficient estimators and tests, which do not suffer from the "curse of dimensionality" and do not reduce the number of dimensions, may be constructed and applied in practice. Most of the classical multivariate procedures are based on the central limit theorems assuming that the dimension p is fixed and the sample size n increases. However, it has been

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pointed out by numerous authors that this assumption does not yield precise distributional approximations for commonly used statistics, and that better approximations can be obtained considering scenarios where the dimension tends to infinity as well (see, e.g., Bai and Silverstein [2] and references therein). More precisely, under the high-dimensional asymptotics we understand the case when the sample size n and the dimension p tend to infinity, such that their ratio p/n converges to some positive constant c. Under this condition the well-known Marchenko–Pastur equation as well as Marchenko–Pastur law were derived (see, Marčenko and Pastur [8], Silverstein [14]).

While most authors in random matrix theory investigate spectral properties of the sample covariance matrix $\mathbf{S}_n = 1/n \sum_{i=1}^n \mathbf{y}_i \mathbf{y}_i^\top$ (here $\mathbf{y}_1, \ldots, \mathbf{y}_n$ denotes a sample of i.i.d. p-dimensional random column vectors with mean vector $\mathbf{0}$ and covariance matrix $\mathbf{\Sigma}_n$), Pan [10] studies the differences occurring if $\mathbf{S}_n$ is replaced by its centered version $\tilde{\mathbf{S}}_n = 1/n \sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})^\top$ (here $\bar{\mathbf{y}}$ denotes the sample mean of $\mathbf{y}_1, \ldots, \mathbf{y}_n$). Very recently, Zheng et al. [17] have clarified this issue using a *substitution principle* but it is still not clear if the same method is applicable to the Moore–Penrose inverse of the centered sample covariance matrix. Corresponding (asymptotic) spectral properties for the inverse of $\mathbf{S}_n$ have also been recently derived by Zheng et al. [16] in the case $p < n$, which correspond to the case $c < 1$. The aim of the present paper is to close a gap in the literature and focussing on the case $c \in (1, \infty)$. We investigate the differences in the asymptotic spectral properties of Moore–Penrose inverses of centered and non-centered sample covariance matrices. In particular we provide the limiting spectral distribution and the central limit theorem (CLT) for linear spectral statistics of the Moore–Penrose inverse of the sample covariance matrix.

In Section 2 we present the Marchenko–Pastur equation together with a Marchenko–Pastur law for the Moore–Penrose inverse of the sample covariance matrix. Section 3 is divided into two parts: the first one is dedicated to the CLT for the LSS of the pseudoinverse of the non-centered sample covariance matrix while the second part covers the case when the sample covariance matrix is a centered one. While the limiting spectral distributions for both sample covariance matrices are the same, it is shown that the asymptotic distribution of LSS of the Moore–Penrose inverse of $\mathbf{S}_n$ and $\tilde{\mathbf{S}}_n$ differ. Finally, some technical details are given in the Appendix.

2. Preliminaries and the Marchenko–Pastur equation

Throughout this paper we use the following notations and assumptions:

- For a symmetric matrix $\mathbf{A}$ we denote by $\lambda_1(\mathbf{A}) \geq \cdots \geq \lambda_p(\mathbf{A})$ its ordered eigenvalues and by $F^{\mathbf{A}}(t)$ the corresponding empirical distribution function (e.d.f.), that is

$$F^{\mathbf{A}}(t) = \frac{1}{p} \sum_{i=1}^p \mathbb{1}\{\lambda_i(\mathbf{A}) \leq t\},$$

where $\mathbb{1}\{\cdot\}$ is the indicator function.
- (A1) Let $\mathbf{X}_n$ be a $p \times n$ matrix which consists of independent and identically distributed (i.i.d.) real random variables with zero mean and unit variance.
- (A2) For the latter matrix $\mathbf{X}_n = (X_{ij})_{i=1,\ldots,p}^{j=1,\ldots,n}$ we assume additionally that $E(X_{11}^{4+\delta}) < \infty$ for some $\delta > 0$.
- By

$$\mathbf{Y}_n = \mathbf{\Sigma}_n^{\frac{1}{2}} \mathbf{X}_n$$

we define a $p \times n$ observation matrix with independent columns with mean vector $\mathbf{0}$ and covariance matrix $\mathbf{\Sigma}_n$.[1] It is further assumed that neither $\mathbf{\Sigma}_n^{\frac{1}{2}}$ nor $\mathbf{X}_n$ are observable.
- The centered and non-centered sample covariance matrix are denoted by

$$\tilde{\mathbf{S}}_n = \frac{1}{n}(\mathbf{Y}_n - \bar{\mathbf{y}}\mathbf{1}^\top)(\mathbf{Y}_n - \bar{\mathbf{y}}\mathbf{1}^\top)^\top = \frac{1}{n}\mathbf{Y}_n\mathbf{Y}_n^\top - \bar{\mathbf{y}}\bar{\mathbf{y}}^\top$$

$$\mathbf{S}_n = \frac{1}{n}\mathbf{Y}_n\mathbf{Y}_n^\top = \frac{1}{n}\mathbf{\Sigma}_n^{\frac{1}{2}}\mathbf{X}_n\mathbf{X}_n^\top\mathbf{\Sigma}_n^{\frac{1}{2}},$$

where $\mathbf{1}$ denotes the n-dimensional column vector of ones and $\bar{\mathbf{y}} = 1/n \sum_{i=1}^n \mathbf{y}_i$. The corresponding e.d.f.'s are given by $F^{\tilde{\mathbf{S}}_n}$ and $F^{\mathbf{S}_n}$, respectively.
- The Moore–Penrose inverse of a $p \times n$ matrix $\mathbf{A}$ is denoted by $\mathbf{A}^+$ and by definition must satisfy the following four criteria (see, e.g., Horn and Johnsohn [5])
  - (i) $\mathbf{A}\mathbf{A}^+\mathbf{A} = \mathbf{A}$,
  - (ii) $\mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+$,
  - (iii) $\mathbf{A}\mathbf{A}^+$ is symmetric,
  - (iv) $\mathbf{A}^+\mathbf{A}$ is symmetric.

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[1] We could easily include the population mean vector into the model but it will only make the formulas for weak convergence more complex not the analysis itself.

It is worth pointing out that the generalized inverse considered recently by Bodnar et al. [4] does not satisfy the conditions (iii) and (iv) presented above. If the matrix $\mathbf{A}$ has a full column rank then the matrix $\mathbf{A}^\top \mathbf{A}$ is invertible and the Moore–Penrose inverse obeys a simple representation given by

$$\mathbf{A}^+ = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top. \tag{2.1}$$

• For a function $G : \mathbb{R} \to \mathbb{R}$ of bounded variation we introduce the Stieltjes transform

$$m_G(z) = \int_{-\infty}^{+\infty} \frac{1}{\lambda - z} dG(\lambda); \quad z \in \mathbb{C}^+ \equiv \{z \in \mathbb{C} : \Im z > 0\}.$$

Remark 1. Although assumption (A2) requires the existence of moments of order $4 + \delta$, we suspect that the results of this paper also hold under the existence of moments of order 4. For a proof one would have to use truncation techniques as provided by Bai et al. [1] for the matrix $1/n \mathbf{Y}_n^\top \mathbf{Y}_n$. These extremely technical details are omitted for the sake of brevity and transparency.

Below we introduce three important results from Bai and Silverstein [3], which are used as key lemmas throughout the paper.

Lemma 2.1 (*Rank Inequality. Theorem A.43 of Bai and Silverstein [3]*)**.** *Let $\mathbf{A}$ and $\mathbf{B}$ be two $k \times k$-dimensional symmetric matrices. Then,*

$$\|F^{\mathbf{A}} - F^{\mathbf{B}}\|_\infty \leq \frac{1}{k} rank(\mathbf{A} - \mathbf{B}), \tag{2.2}$$

where $\|f\|_\infty = \sup_x |f(x)|$ is the usual supremum norm of a function $f : \mathbb{R} \to \mathbb{R}$.

Lemma 2.2 (*Marčenko–Pastur and Silverstein's Equations. Theorem 4.3 of Bai and Silverstein [3]*)**.** *Assume that* (A1) *holds, $p/n \to c \in (0, +\infty)$ and that F^{Σ_n} converges weakly to a cumulative distribution function (c.d.f.) H. Then the e.d.f.s $F^{1/n \mathbf{Y}_n \mathbf{Y}_n^\top}$ and $F^{1/n \mathbf{Y}_n^\top \mathbf{Y}_n}$ converge weakly almost surely to some deterministic c.d.f.s F and $\underline{F}$, respectively, whose Stieltjes transformations satisfy the relation*

$$m_{\underline{F}}(z) = -\frac{1-c}{z} + c m_F(z), \tag{2.3}$$

where $m_F(z)$ is the unique solution of the following equation

$$m_F(z) = \int_{-\infty}^{+\infty} \frac{dH(\tau)}{\tau(1 - c - czm_F(z)) - z}. \tag{2.4}$$

Lemma 2.3 (*Weak Convergence of Stieltjes Transforms. Lemma 9.11 of Bai and Silverstein [3] or Lemma 1.1 of Bai and Silverstein [2]*)**.** *Assume that*

(i) (A1) *and* (A2) *hold.*
(ii) $p/n \to c \in (0, +\infty)$ *as $n \to \infty$.*
(iii) Σ_n *is nonrandom symmetric and positive definite with a bounded spectral norm and the e.d.f. $H_n = F^{\Sigma_n}$ converges weakly to a nonrandom distribution function H.*

Then the random process

$$M_n(z) = p(m_{F^{1/n \mathbf{Y}_n \mathbf{Y}_n^\top}}(z) - m_{F_n}(z)) = n(m_{F^{1/n \mathbf{Y}_n^\top \mathbf{Y}_n}}(z) - m_{\underline{F}_n}(z))$$

with F_n ($\underline{F}_n$) being a finite sample approximation of F ($\underline{F}$) (see, Section 3 for details) forms a tight sequence on any positively oriented contour $\mathcal{C}$, which contains support of F_n for n large enough, and converges weakly to a Gaussian process $M(\cdot)$ with mean and covariance functions given by

$$EM(z) = \frac{c \int_{-\infty}^{+\infty} \frac{t^2 (m_{\underline{F}}(z))^3}{(1 + t m_{\underline{F}}(z))^3} dH(t)}{\left(1 - c \int_{-\infty}^{+\infty} \frac{t^2 (m_{\underline{F}}(z))^2}{(1 + t m_{\underline{F}}(z))^2} dH(t)\right)^2} \quad \text{and} \quad \text{Cov}(M(z_1), M(z_2)) = 2 \frac{m'_{\underline{F}}(z_1) m'_{\underline{F}}(z_2)}{\left(m_{\underline{F}}(z_1) - m_{\underline{F}}(z_2)\right)^2} - \frac{2}{(z_1 - z_2)^2}.$$

In this paper we are interested in the asymptotic properties of the empirical distribution function and linear spectral statistics of the eigenvalues of the Moore–Penrose inverse of the matrices $\tilde{\mathbf{S}}_n$ and $\mathbf{S}_n$. Actually, the limiting spectral distributions of both matrices coincide because they differ only by a rank one perturbation. This is shown in the following Lemma 2.4.

Lemma 2.4. *Let $\tilde{\mathbf{S}}_n^+$ and $\mathbf{S}_n^+$ be the Moore–Penrose inverses of centered and non-centered sample covariance matrices, respectively, then*

$$\|F^{\tilde{\mathbf{S}}_n^+} - F^{\mathbf{S}_n^+}\|_\infty \le \frac{2}{p}. \tag{2.5}$$

Proof. We obtain for the rank one update of the Moore–Penrose inverse (see Meyer [9])

$$\tilde{\mathbf{S}}_n^+ = (\mathbf{S}_n - \bar{\mathbf{y}}\bar{\mathbf{y}}^\top)^+ = \mathbf{S}_n^+ - \frac{\mathbf{S}_n^+ \bar{\mathbf{y}}\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 + (\mathbf{S}_n^+)^2 \bar{\mathbf{y}}\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}}} + \frac{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}}{(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}})^2} \mathbf{S}_n^+ \bar{\mathbf{y}}\bar{\mathbf{y}}^\top \mathbf{S}_n^+. \tag{2.6}$$

With the notation $\mathbf{u} = \mathbf{S}_n^+ \bar{\mathbf{y}}$ and $\mathbf{v} = (\mathbf{S}_n^+)^2 \bar{\mathbf{y}}$ the difference of the Moore–Penrose inverses can therefore be rewritten as follows

$$\begin{aligned} \mathbf{S}_n^+ - \tilde{\mathbf{S}}_n^+ &= \frac{\mathbf{u}\mathbf{v}^\top + \mathbf{v}\mathbf{u}^\top}{\mathbf{u}^\top \mathbf{u}} - \frac{\mathbf{u}^\top \mathbf{v}}{(\mathbf{u}^\top \mathbf{u})^2} \mathbf{u}\mathbf{u}^\top \\ &= \frac{1}{\mathbf{u}^\top \mathbf{u}} \left[\frac{\mathbf{u}^\top \mathbf{u}}{\mathbf{u}^\top \mathbf{v}} \mathbf{v}\mathbf{v}^\top - \left\{ \left(\frac{\mathbf{u}^\top \mathbf{v}}{\mathbf{u}^\top \mathbf{u}}\right)^{1/2} \mathbf{u} - \mathbf{v}\left(\frac{\mathbf{u}^\top \mathbf{u}}{\mathbf{u}^\top \mathbf{v}}\right)^{1/2} \right\} \left\{ \left(\frac{\mathbf{u}^\top \mathbf{v}}{\mathbf{u}^\top \mathbf{u}}\right)^{1/2} \mathbf{u} - \mathbf{v}\left(\frac{\mathbf{u}^\top \mathbf{u}}{\mathbf{u}^\top \mathbf{v}}\right)^{1/2} \right\}^\top \right] \\ &= \frac{1}{\mathbf{u}^\top \mathbf{v}} \mathbf{v}\mathbf{v}^\top - \frac{1}{\mathbf{u}^\top \mathbf{u}} \mathbf{w}\mathbf{w}^\top, \end{aligned} \tag{2.7}$$

where

$$\mathbf{w} = \left(\frac{\mathbf{u}^\top \mathbf{v}}{\mathbf{u}^\top \mathbf{u}}\right)^{1/2} \mathbf{u} - \mathbf{v}\left(\frac{\mathbf{u}^\top \mathbf{u}}{\mathbf{u}^\top \mathbf{v}}\right)^{1/2}.$$

Thus, the difference $\mathbf{S}_n^+ - \tilde{\mathbf{S}}_n^+$ is a matrix at most of rank 2 and the rank inequality of Lemma 2.1 yields the estimate (2.5). □

We now study the asymptotic properties of the e.d.f. of the spectrum of the Moore–Penrose inverse of the sample covariance matrices $\tilde{\mathbf{S}}_n$ and $\mathbf{S}_n$. As a consequence of Lemma 2.4 and equality (2.1) the asymptotic properties of the e.d.f. of both Moore–Penrose inverses can be studied concentrating on the matrix

$$\mathbf{S}_n^+ = (1/n\mathbf{Y}_n\mathbf{Y}_n^\top)^+ = \left[(1/\sqrt{n}\mathbf{Y}_n)^+\right]^\top (1/\sqrt{n}\mathbf{Y}_n)^+ = 1/n\mathbf{Y}_n(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-2}\mathbf{Y}_n^\top$$

together with the corresponding e.d.f. $F^{\mathbf{S}_n^+}$. Indeed, because $m_{F^{1/n\mathbf{Y}_n^\top\mathbf{Y}_n}}(z)$ tends almost surely to the solution of the Marchenko–Pastur equation we obtain the following result.

Theorem 2.1. *Assume that* (A1) *holds, $p/n \to c \in (1, \infty)$ as $n \to \infty$ and that F^{Σ_n} converges weakly to a cumulative distribution function (c.d.f.) H. Then the e.d.f. $F^{\mathbf{S}_n^+}$ converges weakly almost surely to some deterministic c.d.f. P whose Stieltjes transformation m_P satisfies the following equation*

$$m_P(z) = -\frac{1}{z}\left(2 - c^{-1} + \int_{-\infty}^{+\infty} \frac{dH(\tau)}{z\tau c(zm_P(z) + 1) - 1}\right).$$

Proof. Let $\mathbf{S}_n = \mathbf{U}_n\mathbf{D}_n\mathbf{U}_n^\top$ be the eigenvalue decomposition of the matrix $\mathbf{S}_n$, then

$$\begin{aligned} m_{F^{\mathbf{S}_n^+}}(z) &= \frac{1}{p}\text{tr}\left[\left((\mathbf{U}_n\mathbf{D}_n\mathbf{U}_n^\top)^+ - z\mathbf{I}\right)^{-1}\right] = \frac{1}{p}\text{tr}\left[\left(\mathbf{D}_n^+ - z\mathbf{I}\right)^{-1}\right] \\ &= \frac{p-n}{p}\left(-\frac{1}{z}\right) + \frac{n}{p}\frac{1}{n}\sum_{i=1}^n \frac{1}{\lambda_i((1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}) - z} \\ &= \left(1 - \frac{n}{p}\right)\left(-\frac{1}{z}\right) + \frac{n}{p}m_{F^{(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}}}(z). \end{aligned} \tag{2.8}$$

The last two equalities follow from the fact that the spectrum of the matrix $\mathbf{S}_n^+$ differs from that of $(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}$ by exactly $p - n$ zero eigenvalues. For the Stieltjes transform $m_{F^{(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}}}(z)$ in this expression we get

$$\begin{aligned} m_{F^{(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}}}(z) &= \frac{1}{n}\sum_{i=1}^n \frac{1}{\lambda_i^{-1}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n) - z} \\ &= -\frac{1}{nz}\sum_{i=1}^n \frac{\lambda_i(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)}{\lambda_i(1/n\mathbf{Y}_n^\top\mathbf{Y}_n) - \frac{1}{z}} \end{aligned}$$

$$= -\frac{1}{z} - \frac{1}{z^2}\frac{1}{n}\sum_{i=1}^{n}\frac{1}{\lambda_i(1/n\mathbf{Y}_n^\top\mathbf{Y}_n) - \frac{1}{z}}$$

$$= -\frac{1}{z} - \frac{1}{z^2}m_{F^{1/n\mathbf{Y}_n^\top\mathbf{Y}_n}}\left(\frac{1}{z}\right). \tag{2.9}$$

Combining the identities (2.8) and (2.9) provides an equation which relates the Stieltjes transforms of $F^{\mathbf{S}_n^+}$ and $F^{1/n\mathbf{Y}_n^\top\mathbf{Y}_n}$, that is

$$m_{F^{\mathbf{S}_n^+}}(z) = -\frac{1}{z} - \frac{n}{p}\frac{1}{z^2}m_{F^{1/n\mathbf{Y}_n^\top\mathbf{Y}_n}}(1/z). \tag{2.10}$$

It now follows from Lemma 2.2 that as $p/n \to c > 1$ the e.d.f.'s $F^{1/n\mathbf{Y}_n^\top\mathbf{Y}_n}$ and $F^{1/n\mathbf{Y}_n\mathbf{Y}_n^\top}$ converge weakly almost surely to non-generate distribution functions $\underline{F}$ and F with corresponding Stieltjes transforms satisfying the equation

$$m_{\underline{F}}(z) = -\frac{1-c}{z} + cm_F(z).$$

Consequently, we have from (2.10) almost surely

$$m_{F^{\mathbf{S}_n^+}}(z) \longrightarrow m_P(z) := -\frac{1}{z} - c^{-1}\frac{1}{z^2}\left(z(c-1) + cm_F(1/z)\right)$$

$$= -\frac{2-c^{-1}}{z} - \frac{m_F(1/z)}{z^2}$$

as $n \to \infty$, where $m_F(1/z)$ is the Stieltjes transform of the limiting distribution F of the e.d.f. of $\mathbf{S}_n$, which satisfies Eq. (2.4), namely

$$m_F(1/z) = \int_{-\infty}^{+\infty}\frac{dH(\tau)}{\tau\left(1 - c - c\frac{m_F(1/z)}{z}\right) - \frac{1}{z}}. \tag{2.11}$$

Thus, $z(c^{-1} - 2 - zm_P(z)) = m_F(1/z)$ must satisfy the same Eq. (2.11) which implies

$$z(c^{-1} - 2 - zm_P(z)) = \int_{-\infty}^{+\infty}\frac{dH(\tau)}{\tau\left(1 - c - c\frac{z(c^{-1}-2-zm_P(z))}{z}\right) - \frac{1}{z}}.$$

After some simplification the result follows. □

Corollary 2.1. *If $\mathbf{\Sigma}_n = \sigma^2\mathbf{I}_n$ and the assumptions of Theorem 2.1 are satisfied, then the e.d.f. of $\mathbf{S}_n$ converges weakly almost surely to a deterministic distribution function P with Stieltjes transform*

$$m_P(z) = -\frac{1}{z}\left(1 + \frac{-1/z + (c-1)\sigma^2 + \sqrt{(1/z - c\sigma^2 + \sigma^2)^2 - 4/z\sigma^2}}{2\sigma^2 c}\right).$$

Moreover, the limiting distribution is given by

$$P = (1 - c^{-1})\delta_0 + v(x)dx$$

where δ_a denotes the Dirac measure at the point $a \in \mathbb{R}$ and

$$v(x) = \begin{cases} c^{-1}\dfrac{\sqrt{(\lambda_+^{-1} - 1/x)(1/x - \lambda_-^{-1})}}{2\pi\sigma^2 x}, & x \in [\lambda_+^{-1}, \lambda_-^{-1}] \\ 0, & otherwise, \end{cases}$$

with $\lambda_+ = \sigma^2(1 + \sqrt{c})^2$ and $\lambda_- = \sigma^2(1 - \sqrt{c})^2$.

3. CLT for linear spectral statistics

For a (random) symmetric matrix $\mathbf{A}$ with spectrum $\lambda_1(\mathbf{A}), \ldots, \lambda_p(\mathbf{A})$ we consider the linear spectral statistic

$$F^{\mathbf{A}}(g) = \int_{-\infty}^{+\infty} g(x)dF^{\mathbf{A}}(x) = \frac{1}{p}\sum_{i=1}^{p} g(\lambda_i(\mathbf{A}))$$

where $g : \mathbb{R} \to \mathbb{R}$ is a given test function. In the next two sections we will investigate the asymptotic properties of $F^{\mathbf{S}_n^+}$ and $F_n^{\mathbf{S}_n^+}$.

3.1. Linear spectral statistics of $\mathbf{S}_n^+$

In the following discussion we consider the random function

$$G_n(x) = p(F^{\mathbf{S}_n^+} - P_n^*)(x),$$

where P_n^* is a finite sample proxy of the limiting spectral distribution P of $\mathbf{S}_n^+$. Note that the function P_n^* is constructed simply by substituting p/n for c and $H_n = F^{\mathbf{\Sigma}_n}$ for H into the limiting distribution P.

Theorem 3.1. *Assume that*

(i) *(A1) and (A2) hold.*
(ii) $\frac{p}{n} \to c \in (1, \infty)$ *as* $n \to \infty$.
(iii) *The population covariance matrix $\mathbf{\Sigma}_n$ is nonrandom symmetric and positive definite with a bounded spectral norm and the e.d.f. $H_n = F^{\mathbf{\Sigma}_n}$ converges weakly to a nonrandom distribution function H with a support bounded away from zero.*
(iv) $g_1, \ldots, g_k$ *are functions on $\mathbb{R}$ analytic on an open region D of the complex plane, which contains the real interval*

$$\left[0, \limsup_{n \to \infty} \lambda_{\max}(\mathbf{\Sigma}_n^{-1})/(1 - \sqrt{c})^2 \right].$$

(v) *Let $\mathbf{e}_i$ denote a p-dimensional vector with the ith element 1 and others 0, and define*

$$\kappa_i(z) = \mathbf{e}_i^\top \mathbf{\Sigma}_n^{1/2} (m_{\underline{F}}(1/z) \mathbf{\Sigma}_n + \mathbf{I})^{-1} \mathbf{\Sigma}_n^{1/2} \mathbf{e}_i,$$
$$\chi_i(z) = \mathbf{e}_i^\top \mathbf{\Sigma}_n^{1/2} (m_{\underline{F}}(1/z) \mathbf{\Sigma}_n + \mathbf{I})^{-2} \mathbf{\Sigma}_n^{1/2} \mathbf{e}_i$$

as the ith diagonal elements of the matrices

$$\mathbf{\Sigma}_n^{1/2} (m_{\underline{F}}(1/z) \mathbf{\Sigma}_n + \mathbf{I})^{-1} \mathbf{\Sigma}_n^{1/2}, \qquad \mathbf{\Sigma}_n^{1/2} (m_{\underline{F}}(1/z) \mathbf{\Sigma}_n + \mathbf{I})^{-2} \mathbf{\Sigma}_n^{1/2},$$

respectively. The population covariance matrix $\mathbf{\Sigma}_n$ satisfies

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n \kappa_i(z_1) \kappa_i(z_2) = h_1(z_1, z_2)$$

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n \kappa_i(z) \chi_i(z) = h_2(z)$$

then

$$\left(\int_{-\infty}^{+\infty} g_1(x) dG_n(x), \ldots, \int_{-\infty}^{+\infty} g_k(x) dG_n(x) \right)^\top \xrightarrow{\mathcal{D}} \left(X_{g_1}, \ldots, X_{g_k} \right)^\top,$$

where $\left(X_{g_1}, \ldots, X_{g_k} \right)^\top$ is a Gaussian vector with mean

$$E(X_g) = \frac{1}{2\pi i} \oint \frac{g(z)}{z^2} \frac{c \int_{-\infty}^{+\infty} \frac{t^2 (m_{\underline{F}}(1/z))^3}{(1 + t m_{\underline{F}}(1/z))^3} dH(t)}{\left(1 - c \int_{-\infty}^{+\infty} \frac{t^2 (m_{\underline{F}}(1/z))^2}{(1 + t m_{\underline{F}}(1/z))^2} dH(t) \right)^2} dz$$

$$+ \frac{E(X_{11}^4) - 3}{2\pi i} \oint \frac{g(z)}{z^2} \frac{c (m_{\underline{F}}(1/z))^3 h_2(z)}{1 - c \int_{-\infty}^{+\infty} \frac{t^2 (m_{\underline{F}}(1/z))^2}{(1 + t m_{\underline{F}}(1/z))^2} dH(t)} dz \tag{3.1}$$

and covariance function

$$\text{Cov}(X_{g_1}, X_{g_2}) = -\frac{1}{2\pi^2} \oint \oint \frac{g(z_1) g(z_2)}{z_1^2 z_2^2} \frac{m_{\underline{F}}'(1/z_1) m_{\underline{F}}'(1/z_2)}{(m_{\underline{F}}(1/z_1) - m_{\underline{F}}(1/z_2))^2} dz_1 dz_2$$

$$- \frac{E(X_{11}^4) - 3}{4\pi^2} \oint \oint \frac{g(z_1) g(z_2)}{z_1^2 z_2^2} (m_{\underline{F}}(1/z_1) m_{\underline{F}}(1/z_2) h_1(z_1, z_2))'' dz_1 dz_2. \tag{3.2}$$

The contours in (3.1) and (3.2) are both contained in the analytic region for the functions $g_1, \ldots, g_k$ and both enclose the support of P_n^* for sufficiently large n. Moreover, the contours in (3.2) are disjoint.

Proof. The proof of this theorem follows combining arguments from the proof of Lemma 1.1 of Bai and Silverstein [2] and Theorem 1 of Pan [10]. To be precise, we note first that $m_{F^{1/n \mathbf{Y}_n^\top \mathbf{Y}_n}}(z)$ converges almost surely with limit, say $m_{\underline{F}}(z)$. We also observe that the CLT of $p(m_{F^{\mathbf{S}_n^+}}(z) - m_P(z))$ is the same as of $-n(m_{F^{1/n \mathbf{Y}_n^\top \mathbf{Y}_n}}(1/z) - m_{\underline{F}}(1/z))/z^2$ and proceed in two steps

(i) Assume first that $E(X_{11}^4) = 3$. By Lemma 2.3 we get that the process

$$-\frac{n}{z^2}\left(m_{F^{1/n}\mathbf{Y}_n^\top \mathbf{Y}_n}(1/z) - m_{\underline{F}}(1/z)\right)$$

defined on an arbitrary positively oriented contour $\mathcal{C}$ which contains the support of P_n^* for sufficiently larger n converges weakly to a Gaussian process with mean

$$-\frac{1}{z^2}\frac{c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^3}{(1+tm_{\underline{F}}(1/z))^3}dH(t)}{\left(1-c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^2}{(1+tm_{\underline{F}}(1/z))^2}dH(t)\right)^2}$$

and covariance

$$\frac{2}{z_1^2 z_2^2}\frac{m_{\underline{F}}'(1/z_1)m_{\underline{F}}'(1/z_2)}{\left(m_{\underline{F}}(1/z_1) - m_{\underline{F}}(1/z_2)\right)^2} - \frac{2}{(z_1 - z_2)^2}.$$

In order to obtain the assertion of Theorem 3.1 we use again the argument made at the beginning of the proof and the following identity

$$\int_{-\infty}^{+\infty} g(x)dG_n(x) = -\frac{1}{2\pi i}\oint g(z)m_{G_n}(z)dz, \tag{3.3}$$

which is valid with probability one for any analytic function g defined on an open set containing the support of G_n if n is sufficiently large. The complex integral on the right-hand side of (3.3) is over certain positively oriented contour enclosing G on which the function g is analytic (see the discussion in Bai and Silverstein [2] following Lemma 1.1). Further, following the proof of Theorem 1.1 in Bai and Silverstein [2] we obtain that $\left(\int g_1(x)dG_n(x), \ldots, \int g_k(x)dG_n(x)\right)^\top$ converges weakly to a Gaussian vector $\left(X_{g_1}, \ldots, X_{g_k}\right)^\top$.

(ii) In the case $E(X_{11}^4) \neq 3$ we will use a result proved in Pan and Zhou [11], more precisely Theorem 1.4 of this reference. Here we find out that in the case $E(X_{11}^4) \neq 3$ there appears an additional summand in the asymptotic mean and covariance which involve the limiting functions $h_1(z_1, z_2)$ and $h_2(z)$ from assumption (v), namely for the mean we obtain the additional term

$$\frac{E(X_{11}^4) - 3}{z^2}\frac{c(m_{\underline{F}}(1/z))^3 h_2(z)}{1 - c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^2}{(1+tm_{\underline{F}}(1/z))^2}dH(t)}$$

and for the covariance

$$\frac{E(X_{11}^4) - 3}{z_1^2 z_2^2}\left(m_{\underline{F}}(1/z_1)m_{\underline{F}}(1/z_2)h_1(z_1, z_2)\right)''.$$

These new summands arise by studying the limits of products of $E(X_{11}^4) - 3$ and the diagonal elements of the matrix $(\mathbf{S}_n - 1/z\mathbf{I})^{-1}$ (see, Pan and Zhou [11], proof of Theorem 1.4). Imposing the assumption (v) we basically assure that these limits are the same.

The assertion is now obtained by the same arguments as given in part (i) of this proof. □

A version of Theorem 3.1 has been proved in Zheng et al. [16] for the usual inverse of the sample covariance matrix $\mathbf{S}_n^{-1}$. It is also not hard to verify the CLT for linear spectral statistics of $\tilde{\mathbf{S}}_n^{-1}$ in the case $c < 1$ with the same limit distribution. Theorem 3.1 shows that in the case $c \geq 1$ there appear additional terms in the asymptotic mean and covariance of the linear spectral statistics corresponding to $\mathbf{S}_n^+$.

In general, as we can see, the results on the limiting spectral distribution as well as the CLT for linear spectral statistics of $\mathbf{S}_n^+$ follow more or less from the already known findings which correspond to the matrix $1/n\mathbf{Y}_n^\top \mathbf{Y}_n$. In the next section we will show that the general CLT for LSS of the random matrix $\tilde{\mathbf{S}}_n^+$ is different from that of $\mathbf{S}_n^+$.

3.2. CLT for linear spectral statistics of $\tilde{\mathbf{S}}_n^+$

The goal of this section is to show that the CLT for linear spectral statistics of the Moore–Penrose inverse $\tilde{\mathbf{S}}_n^+$ differs from that of $\mathbf{S}_n^+$. In order to show why these two CLTs are different consider again the identity (2.6), that is

$$\tilde{\mathbf{S}}_n^+ = (\mathbf{S}_n - \bar{\mathbf{y}}\bar{\mathbf{y}}^\top)^+ = \mathbf{S}_n^+ - \frac{\mathbf{S}_n^+\bar{\mathbf{y}}\bar{\mathbf{y}}^\top(\mathbf{S}_n^+)^2 + (\mathbf{S}_n^+)^2\bar{\mathbf{y}}\bar{\mathbf{y}}^\top(\mathbf{S}_n^+)}{\bar{\mathbf{y}}^\top(\mathbf{S}_n^+)^2\bar{\mathbf{y}}} + \frac{\bar{\mathbf{y}}^\top(\mathbf{S}_n^+)^3\bar{\mathbf{y}}}{(\bar{\mathbf{y}}^\top(\mathbf{S}_n^+)^2\bar{\mathbf{y}})^2}\mathbf{S}_n^+\bar{\mathbf{y}}\bar{\mathbf{y}}^\top\mathbf{S}_n^+.$$

We emphasize here the difference to the well known Sherman–Morrison identity for the inverse of a non-singular matrix $\tilde{\mathbf{S}}_n$, that is

$$\tilde{\mathbf{S}}_n^{-1} = (\mathbf{S}_n - \bar{\mathbf{y}}\bar{\mathbf{y}}^\top)^{-1} = \mathbf{S}_n^{-1} + \frac{\mathbf{S}_n^{-1}\bar{\mathbf{y}}\bar{\mathbf{y}}^\top\mathbf{S}_n^{-1}}{1 - \bar{\mathbf{y}}^\top\mathbf{S}_n^{-1}\bar{\mathbf{y}}} \tag{3.4}$$

(see, Sherman and Morrison [13]). Note that it follows from the identity

$$1 - \bar{\mathbf{y}}^\top\mathbf{S}_n^+\bar{\mathbf{y}} = 1 - \frac{1}{n^2}\mathbf{1}^\top\mathbf{Y}^\top(1/\sqrt{n})\mathbf{Y}(1/n\mathbf{Y}^\top\mathbf{Y})^{-2}(1/\sqrt{n})\mathbf{Y}^\top\mathbf{Y}\mathbf{1} = 1 - \frac{\mathbf{1}^\top\mathbf{1}}{n} = 0,$$

that the right-hand side of the formula (3.4) is not defined for the Moore–Penrose inverse in the case $p > n$.

Now consider the resolvent of $\tilde{\mathbf{S}}_n^+$, namely

$$\mathbf{R}(z) = \left(\tilde{\mathbf{S}}_n^+ - z\mathbf{I}\right)^{-1} = \left(\mathbf{S}_n^+ - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top + \frac{1}{\mathbf{u}^\top\mathbf{u}}\mathbf{w}\mathbf{w}^\top - z\mathbf{I}\right)^{-1} = \left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top + \frac{1}{\mathbf{u}^\top\mathbf{u}}\mathbf{w}\mathbf{w}^\top\right)^{-1},$$

where we use (2.7) and the notations $\mathbf{u} = \mathbf{S}_n^+\bar{\mathbf{y}}$, $\mathbf{v} = (\mathbf{S}_n^+)^2\bar{\mathbf{y}}$ and $\mathbf{A}(z) = \mathbf{S}_n^+ - z\mathbf{I}$ and

$$\mathbf{w} = \left(\frac{\mathbf{u}^\top\mathbf{v}}{\mathbf{u}^\top\mathbf{u}}\right)^{1/2}\mathbf{u} - \mathbf{v}\left(\frac{\mathbf{u}^\top\mathbf{u}}{\mathbf{u}^\top\mathbf{v}}\right)^{1/2}$$

to obtain the last identity. A twofold application of the Sherman–Morrison formula yields the representation

$$\mathbf{R}(z) = \left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1} - \frac{\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}\frac{\mathbf{w}\mathbf{w}^\top}{\mathbf{u}^\top\mathbf{u}}\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}}{1 + \frac{1}{\mathbf{u}^\top\mathbf{u}}\mathbf{w}^\top\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}\mathbf{w}}$$

$$= \mathbf{A}^{-1}(z) + \frac{\frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{A}^{-1}(z)\mathbf{v}\mathbf{v}^\top\mathbf{A}^{-1}(z)}{1 - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}^\top\mathbf{A}^{-1}(z)\mathbf{v}} - \frac{\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}\frac{\mathbf{w}\mathbf{w}^\top}{\mathbf{u}^\top\mathbf{u}}\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}}{1 + \frac{1}{\mathbf{u}^\top\mathbf{u}}\mathbf{w}^\top\left(\mathbf{A}(z) - \frac{1}{\mathbf{u}^\top\mathbf{v}}\mathbf{v}\mathbf{v}^\top\right)^{-1}\mathbf{w}}. \tag{3.5}$$

Taking the trace of both sides of (3.5) we obtain the identity

$$pm_{F^{\tilde{\mathbf{S}}_n^+}}(z) = \operatorname{tr}(\mathbf{R}(z)) = pm_{F^{\mathbf{S}_n^+}}(z) + \frac{\mathbf{v}^\top\mathbf{A}^{-2}(z)\mathbf{v}}{\mathbf{u}^\top\mathbf{v} - \mathbf{v}^\top\mathbf{A}^{-1}(z)\mathbf{v}} - \frac{\mathbf{w}^\top\left(\mathbf{A}^{-1}(z) + \frac{\mathbf{A}^{-1}(z)\mathbf{v}\mathbf{v}^\top\mathbf{A}^{-1}(z)}{\mathbf{u}^\top\mathbf{v} - \mathbf{v}^\top\mathbf{A}^{-1}(z)\mathbf{v}}\right)^2\mathbf{w}}{\mathbf{u}^\top\mathbf{u} + \mathbf{w}^\top\mathbf{A}^{-1}(z)\mathbf{w} + \frac{(\mathbf{w}^\top\mathbf{A}^{-1}(z)\mathbf{v})^2}{\mathbf{u}^\top\mathbf{v} - \mathbf{v}^\top\mathbf{A}^{-1}(z)\mathbf{v}}}, \tag{3.6}$$

which indicates that the CLTs for linear spectral statistics of Moore–Penrose sample covariance matrices of $\mathbf{S}_n^+$ and $\tilde{\mathbf{S}}_n^+$ might differ. In fact, the following result shows that the last two terms on the right-hand side of (3.6) are asymptotically not negligible.

Theorem 3.2. *Let $\tilde{G}_n(x) = p(F^{\tilde{\mathbf{S}}_n^+}(g) - P_n^*(g))$ and suppose that the assumptions of Theorem 3.1 are satisfied, then*

$$\left(\int_{-\infty}^{+\infty}g_1(x)d\tilde{G}_n(x), \ldots, \int_{-\infty}^{+\infty}g_k(x)d\tilde{G}_n(x)\right)^\top \xrightarrow{\mathcal{D}} \left(X_{g_1}, \ldots, X_{g_k}\right)^\top,$$

where $\left(X_{g_1}, \ldots, X_{g_k}\right)^\top$ is a Gaussian vector with mean

$$E(X_g) = -\frac{1}{2\pi i}\oint\frac{g(z)}{z^2}\frac{c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^3}{(1+tm_{\underline{F}}(1/z))^3}dH(t)}{\left(1 - c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^2}{(1+tm_{\underline{F}}(1/z))^2}dH(t)\right)^2}dz$$

$$-\frac{E(X_{11}^4) - 3}{2\pi i}\oint\frac{g(z)c(m_{\underline{F}}(1/z))^3h_2(z)}{1 - c\int_{-\infty}^{+\infty}\frac{t^2(m_{\underline{F}}(1/z))^2}{(1+tm_{\underline{F}}(1/z))^2}dH(t)}dz - \frac{1}{2\pi i}\oint\frac{g(z)}{z^2}\frac{m_{\underline{F}}'(1/z)}{m_{\underline{F}}(1/z)}dz \tag{3.7}$$

and covariance function

$$\operatorname{Cov}(X_{g_1}, X_{g_2}) = -\frac{1}{2\pi^2}\oint\oint\frac{g(z_1)g(z_2)}{z_1^2z_2^2}\frac{m_{\underline{F}}'(1/z_1)m_{\underline{F}}'(1/z_2)}{\left(m_{\underline{F}}(1/z_1) - m_{\underline{F}}(1/z_2)\right)^2}dz_1dz_2$$

$$-\frac{E(X_{11}^4) - 3}{4\pi^2}\oint\oint\frac{g(z_1)g(z_2)}{z_1^2z_2^2}\left(m_{\underline{F}}(1/z_1)m_{\underline{F}}(1/z_2)h_1(z_1, z_2)\right)''dz_1dz_2. \tag{3.8}$$

The contours in (3.7) and (3.8) are both contained in the analytic region for the functions $g_1, \ldots, g_k$ and both enclose the support of P_n^* for sufficiently large n. Moreover, the contours in (3.8) are disjoint.

Before we provide the proof of this result we emphasize the existence of the extra summand in the asymptotic mean. It has a very simple structure and can be calculated without much effort in practice. Indeed, the last integral in (3.7) can be rewritten using integration by parts in the following way (see, Appendix A.1 for detailed derivation)

$$-\frac{1}{2\pi i}\oint \frac{g(z)}{z^2}\frac{m'_F(1/z)}{m_F(1/z)}dz = -\frac{1}{\pi}\int_a^b g'(x)\arg\{m_F(1/x)\}dx, \tag{3.9}$$

where $m_F(1/x) \equiv \lim_{z\to x} m_F(1/z)$ for $x \in \mathbb{R}$ and the interval (a, b) contains the support of P.

On the other hand, the asymptotic variances of the linear spectral statistics for centered and non-centered sample covariance matrices coincide. For a discussion of assumption (v) we refer to Pan [10, Remark 2], and other references therein.

Proof of Theorem 3.2. The proof of Theorem 3.2 is based on the Stieltjes transform method and consists of a combination of arguments similar to those given by Bai and Silverstein [2] and Pan [10]. First, by the analyticity of the functions $g_1, \ldots, g_k$ and (3.3) it is sufficient to consider the Stieltjes transforms of the spectral e.d.f. of sample covariance matrices. Furthermore, recall from (3.6) that the Stieltjes transform of the e.d.f. of $\tilde{\mathbf{S}}_n^+$ can be decomposed as the sum of the Stieltjes transform of the e.d.f. of $\mathbf{S}_n^+$ and the additional term

$$\xi_n(z) = \frac{\mathbf{v}^\top \mathbf{A}^{-2}(z)\mathbf{v}}{\mathbf{u}^\top \mathbf{v} - \mathbf{v}^\top \mathbf{A}^{-1}(z)\mathbf{v}} - \frac{\mathbf{w}^\top \left(\mathbf{A}^{-1}(z) + \frac{\mathbf{A}^{-1}(z)\mathbf{v}\mathbf{v}^\top \mathbf{A}^{-1}(z)}{\mathbf{u}^\top \mathbf{v} - \mathbf{v}^\top \mathbf{A}^{-1}(z)\mathbf{v}}\right)^2 \mathbf{w}}{\mathbf{u}^\top \mathbf{u} + \mathbf{w}^\top \mathbf{A}^{-1}(z)\mathbf{w} + \frac{(\mathbf{w}^\top \mathbf{A}^{-1}(z)\mathbf{v})^2}{\mathbf{u}^\top \mathbf{v} - \mathbf{v}^\top \mathbf{A}^{-1}(z)\mathbf{v}}} \tag{3.10}$$

involving sample mean $\bar{\mathbf{y}}$ and $\mathbf{S}_n^+$. Thus, it is sufficient to show that this random variable converges almost surely on $\mathbb{C}^+ = \{z \in \mathbb{C} : \Im z > 0\}$ to a nonrandom quantity as $p/n \to c > 1$ and to determine its limit. As a result, Theorem 3.2 follows from Slutsky's theorem, the continuous mapping theorem and the results in Bai and Silverstein [2] and Pan and Zhou [11].

It is shown in Appendix A.2 that the function ξ_n in (3.10) can be represented as

$$\xi_n(z) = -\frac{1}{z} - \frac{\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2\theta'_n(z)}{1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2\theta_n(z)}, \tag{3.11}$$

where the function θ_n is given by

$$\theta_n(z) = -\frac{1}{z}\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + \frac{1}{z}\frac{1}{n}\mathbf{1}_n^\top ((1/n\mathbf{Y}_n^\top \mathbf{Y}_n)^{-1} - z\mathbf{I})^{-1}\mathbf{1}_n. \tag{3.12}$$

As a consequence, the asymptotic properties of ξ_n can be obtained analyzing the quantity

$$\begin{aligned}
\eta_n(z) &= \frac{1}{n}\mathbf{1}_n^\top ((1/n\mathbf{Y}_n^\top \mathbf{Y}_n)^{-1} - z\mathbf{I})^{-1}\mathbf{1}_n \\
&= -\frac{1}{z}\operatorname{tr}\left\{(1/n\mathbf{Y}_n^\top \mathbf{Y}_n)(1/n\mathbf{Y}_n^\top \mathbf{Y}_n - 1/z\mathbf{I})^{-1}1/n\mathbf{1}_n\mathbf{1}_n^\top\right\} \\
&= -\frac{1}{z} - \frac{1}{z^2}\operatorname{tr}\left\{(1/n\mathbf{Y}_n^\top \mathbf{Y}_n - 1/z\mathbf{I})^{-1}\boldsymbol{\Theta}_n\right\},
\end{aligned}$$

where we use the notation $\boldsymbol{\Theta}_n = 1/n\mathbf{1}_n\mathbf{1}_n^\top$. It now follows from Theorem 1 in Rubio and Mestre [12] that

$$\left|\operatorname{tr}\left\{(1/n\mathbf{Y}_n^\top \mathbf{Y}_n - 1/z\mathbf{I})^{-1}\boldsymbol{\Theta}_n\right\} - x_n(1/z)\right| \longrightarrow 0 \quad \text{a.s.},$$

where $x_n(1/z)$ is a unique solution in $\mathbb{C}^+$ of the equation

$$\frac{1 + 1/zx_n(1/z)}{x_n(1/z)} = \frac{c}{p}\operatorname{tr}\left(x_n(1/z)\mathbf{I} + \boldsymbol{\Sigma}_n^{-1}\right)^{-1}.$$

Note that $\operatorname{tr}(\boldsymbol{\Theta}_n) = 1$ and that Theorem 1 in Rubio and Mestre [12] is originally proven assuming the existence of moments of order $8 + \delta$. However, it is shown in Bodnar et al. [4] that only the existence of moments of order $4 + \delta$ is required for this statement.

In order to see how $x_n(1/z)$ relates to $m_F(1/z)$ we note that due to assumption (iii) $H_n \xrightarrow{\mathcal{D}} H$ as $n \to \infty$ and, thus, $x_n(1/z) \to x(1/z)$. This implies

$$\frac{1}{x_n(1/z)} + 1/z = \frac{c}{p}\operatorname{tr}\left(x_n(1/z)\mathbf{I} + \boldsymbol{\Sigma}_n^{-1}\right)^{-1} = c\int_{-\infty}^{\infty}\frac{\tau\,dH_n(\tau)}{x_n(1/z)\tau + 1} \longrightarrow c\int_{-\infty}^{\infty}\frac{\tau\,dH(\tau)}{x(1/z)\tau + 1},$$

which leads to

$$x(1/z) = -\left(1/z - c\int_{-\infty}^{\infty}\frac{\tau}{x(1/z)\tau + 1}dH(\tau)\right)^{-1}.$$

The last equation is the well-known Marchenko–Pastur equation for the Stieltjes transformation $m_{\underline{F}}(1/z)$ of the limiting distribution $\underline{F}$. Because the solution of this equation is unique we obtain

$$x(1/z) = m_{\underline{F}}(1/z).$$

As a result we get the following asymptotics for $1 + z\bar{\mathbf{y}}^\top\bar{\mathbf{y}} + z^2\theta_n(z)$ as $n \to \infty$

$$1 + z\bar{\mathbf{y}}^\top\bar{\mathbf{y}} + z^2\theta_n(z) \longrightarrow -\frac{m_{\underline{F}}(1/z)}{z} \quad \text{a.s.},$$

which ensures that

$$\xi_n(z) \longrightarrow -\frac{1}{z} - \frac{\left(-\frac{m_{\underline{F}}(1/z)}{z}\right)'}{-\frac{m_{\underline{F}}(1/z)}{z}} = -\frac{1}{z} - z\frac{-\frac{m'_{\underline{F}}(1/z)}{z^3} - \frac{m_{\underline{F}}(1/z)}{z^2}}{m_{\underline{F}}(1/z)} = \frac{1}{z^2}\frac{m'_{\underline{F}}(1/z)}{m_{\underline{F}}(1/z)} \quad \text{a.s.} \tag{3.13}$$

for $p/n \to c \in (1, +\infty)$ as $n \to \infty$. The assertion of Theorem 3.2 now follows taking into account the argument made at the beginning of the proof and (3.13). □

Acknowledgments

Appendix

A.1. Derivation of (3.9)

We select the contour to be a rectangle with sides parallel to the axes. It intersects the real axis at the points $a \neq 0$ and b such that the interval (a, b) contains the support of P. The horizontal sides are taken as a distance $y_0 > 0$ from the real axis. More precisely, the contour $\mathcal{C}$ is given by

$$\mathcal{C} = \{a + iy : |y| \leq y_0\} \cup \{x + iy_0 : x \in [a, b]\} \cup \{b + iy : |y| \leq y_0\} \cup \{x - iy_0 : x \in [a, b]\} \tag{A.1}$$

so that (a, b) contains $\left[0, \lim\sup_{n\to\infty}\lambda_{\max}(\mathbf{\Sigma}_n^{-1})/(1-\sqrt{c})^2\right]$ and is enclosed in the analytic region of function g. We calculate the four parts of the contour integral and then let y_0 tend to zero. First, we note that

$$\frac{d}{dz}\ln(m_{\underline{F}}(1/z)) = -\frac{1}{z^2}\frac{m'_{\underline{F}}(1/z)}{m_{\underline{F}}(1/z)}.$$

Then using integration by parts the last integral in (3.7) becomes

$$-\frac{1}{2\pi i}\oint \frac{g(z)}{z^2}\frac{m'_{\underline{F}}(1/z)}{m_{\underline{F}}(1/z)}dz = \frac{1}{2\pi i}\oint g(z)d(\ln m_{\underline{F}}(1/z))$$

$$= -\frac{1}{2\pi i}\oint g'(z)\ln m_{\underline{F}}(1/z)dz$$

$$= -\frac{1}{2\pi i}\oint g'(z)\left(\ln|m_{\underline{F}}(1/z)| + i\arg(m_{\underline{F}}(1/z))\right)dz, \tag{A.2}$$

where any branch of the logarithm may be taken. Naturally extending the Stieltjes transform on the negative imaginary axis and using $z = x + iy$ we get

$$|m_{\underline{F}}(1/z)| = \left|\int_{-\infty}^{\infty}\frac{dF(\lambda)}{\lambda - 1/z}\right| \leq \int_{-\infty}^{\infty}\frac{dF(\lambda)}{|\lambda - 1/z|} = \int_{-\infty}^{\infty}\frac{dF(\lambda)}{\sqrt{\left(\lambda - \frac{x}{|z|^2}\right)^2 + \frac{y^2}{|z|^4}}} \leq \frac{x^2 + y^2}{|y|}. \tag{A.3}$$

Next we note that any portion of the integral (A.2) which involves the vertical side can be neglected. Indeed, using (A.3), the fact that $|g'(z)| \leq K$ and (5.1) in Bai and Silverstein [2] for the left vertical side we have

$$\left|\frac{1}{2\pi i}\int_{-y_0}^{y_0}g'(a + iy)\ln m_{\underline{F}}(1/(a + iy))dy\right| \leq \frac{K}{2\pi}\int_{-y_0}^{y_0}\left(\ln|m_{\underline{F}}(1/(a + iy))| + |\arg(m_{\underline{F}}(1/(a + iy)))|\right)dy$$

$$\leq \frac{K}{2\pi}\int_{-y_0}^{y_0}\left(\ln\frac{a^2 + y^2}{|y|} + \pi\right)dy$$

$$= \frac{K}{\pi} \int_0^{y_0} \ln \frac{a^2 + y^2}{y} dy + K y_0$$

$$= \frac{K}{\pi} \left(y_0 \ln \frac{y_0^2 + a^2}{y_0} - y_0 + 2a \arctan(y_0/a) \right) + K y_0, \tag{A.4}$$

which converges to zero as $y_0 \to 0$. A similar argument can be used for the right vertical side. Consequently, only the remaining terms

$$-\frac{1}{2\pi} \int_a^b \Im \left[g'(x + i y_0) \right] \ln |m_{\underline{F}}(1/(x + i y_0))| dx - \frac{1}{2\pi} \int_a^b \Re \left[g'(x + i y_0) \right] \arg \left[m_{\underline{F}}(1/(x + i y_0)) \right] dx$$

$$-\frac{1}{2\pi} \int_a^b \Im \left[g'(x - i y_0) \right] \ln |m_{\underline{F}}(1/(x - i y_0))| dx - \frac{1}{2\pi} \int_a^b \Re \left[g'(x - i y_0) \right] \arg \left[m_{\underline{F}}(1/(x - i y_0)) \right] dx$$

have to be considered in the limit of the integral (A.2). Similarly, using the fact that

$$\sup_{x \in [a,b]} |\Im h(x + iy)| \le K|y| \tag{A.5}$$

for any real-valued analytic function h on the bounded interval $[a, b]$ (see equation (5.6) in Bai and Silverstein [2]), we obtain that the first and the third integrals are bounded in absolute value by $O(y_0 \ln y_0^{-1})$ and, thus, can be neglected. As a result the dominated convergence theorem leads to

$$-\frac{1}{2\pi i} \oint_{\mathcal{J}} g'(z) \left(\ln |m_{\underline{F}}(1/z)| + i \arg(m_{\underline{F}}(1/z)) \right) dz \xrightarrow[y_0 \to 0]{} -\frac{1}{\pi} \int_a^b g'(x) \arg \left[m_{\underline{F}}(1/x) \right] dx, \tag{A.6}$$

which proves (3.9).

A.2. Proof of the representations (3.11) and (3.12)

For a proof of (3.11) we introduce the notations

$$\mathbf{a} = \frac{1}{(\mathbf{u}^\top \mathbf{v})^{1/2}} \mathbf{v}, \qquad \mathbf{b} = \frac{(\mathbf{u}^\top \mathbf{v})^{1/2}}{\mathbf{u}^\top \mathbf{u}} \mathbf{u}.$$

Then

$$\frac{1}{(\mathbf{u}^\top \mathbf{u})^{1/2}} \mathbf{w} = \mathbf{b} - \mathbf{a},$$

and we obtain for (3.10)

$$\xi_n(z) = \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z) \mathbf{a}}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z) \mathbf{a}}$$

$$- \frac{(\mathbf{b} - \mathbf{a})^\top \left(\mathbf{A}^{-2}(z) + \frac{\mathbf{A}^{-2}(z)\mathbf{a}\mathbf{a}^\top \mathbf{A}^{-1}(z) + \mathbf{A}^{-1}(z)\mathbf{a}\mathbf{a}^\top \mathbf{A}^{-2}(z)}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a}} + \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a}(\mathbf{A}^{-1}(z)\mathbf{a}\mathbf{a}^\top \mathbf{A}^{-1}(z))}{(1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a})^2} \right) (\mathbf{b} - \mathbf{a})}{1 + (\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)(\mathbf{b} - \mathbf{a}) + \frac{((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a}}}.$$

A tedious but straightforward calculation now gives

$$\xi_n(z) = \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a} + \mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a}(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)(\mathbf{b} - \mathbf{a}) + \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a}((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a}}}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} + (1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a})(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)(\mathbf{b} - \mathbf{a}) + ((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}$$

$$- \frac{(1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a})(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-2}(z)(\mathbf{b} - \mathbf{a})}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} + (1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a})(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)(\mathbf{b} - \mathbf{a}) + ((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}$$

$$- \frac{2(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-2}(z)\mathbf{a}(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a} + \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a}((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a}}}{1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} + (1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a})(\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)(\mathbf{b} - \mathbf{a}) + ((\mathbf{b} - \mathbf{a})^\top \mathbf{A}^{-1}(z)\mathbf{a})^2}$$

$$= \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a} \{ \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} \} - \mathbf{b}^\top \mathbf{A}^{-2}(z)\mathbf{b} + 2\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{b}}{1 + \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} - 2\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} \{ \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} \} + (\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b})^2}$$

$$+ \frac{\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} \{ \mathbf{b}^\top \mathbf{A}^{-2}(z)\mathbf{b} \} - 2\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{b} \{ \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} \}}{1 + \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} - 2\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} \{ \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} \} + (\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b})^2}$$

$$= \frac{\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a} \{ \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} \} - \mathbf{b}^\top \mathbf{A}^{-2}(z)\mathbf{b} \{ 1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} \} + 2\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{b} \{ 1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} \}}{\left(\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} - 1 \right)^2 + \mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} \{ 1 - \mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} \}}. \tag{A.7}$$

Now note that $\xi_n(z)$ is a non-linear function of the quantities $\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a}$, $\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a}$, $\mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b}$, $\mathbf{b}^\top \mathbf{A}^{-2}(z)\mathbf{b}$, $\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b}$ and $\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{b}$, which can easily be expressed in terms of $\bar{\mathbf{y}}$ and $\mathbf{S}_n^+$. For example, we have

$$
\begin{aligned}
\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{a} &= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 (\mathbf{S}_n^+ - z\mathbf{I})^{-1} (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} \\
&= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top \mathbf{S}_n^+ (\mathbf{S}_n^+ - z\mathbf{I} + z\mathbf{I})(\mathbf{S}_n^+ - z\mathbf{I})^{-1}(\mathbf{S}_n^+)^2 \bar{\mathbf{y}} \right) \\
&= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}} + z\bar{\mathbf{y}}^\top \mathbf{S}_n^+ (\mathbf{S}_n^+ - z\mathbf{I} + z\mathbf{I})(\mathbf{S}_n^+ - z\mathbf{I})^{-1}(\mathbf{S}_n^+)^2 \bar{\mathbf{y}} \right) \\
&= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}} + z\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} + z^2 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}(\mathbf{S}_n^+ - z\mathbf{I} + z\mathbf{I})\mathbf{S}_n^+ \bar{\mathbf{y}} \right) \\
&= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}} + z\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} + z^2 \bar{\mathbf{y}}^\top \mathbf{S}_n^+ \bar{\mathbf{y}} + z^3 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}(\mathbf{S}_n^+ - z\mathbf{I} + z\mathbf{I})\bar{\mathbf{y}} \right) \\
&= \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}} + z\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} + z^2 + z^3 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^4 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} \right),
\end{aligned}
$$

where the last equality follows from the fact that $\bar{\mathbf{y}}^\top \mathbf{S}_n^+ \bar{\mathbf{y}} = 1$. In a similar way, namely adding and subtracting $z\mathbf{I}$ from $\mathbf{S}_n^+$ in a sequel we obtain representations for the remaining quantities of interest

$$
\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{a} = \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} + 2z + 3z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 4z^3 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} + z^4 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-2}\bar{\mathbf{y}} \right)
$$

$$
\mathbf{b}^\top \mathbf{A}^{-1}(z)\mathbf{b} = \frac{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}}{(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}})^2} \left(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} \right)
$$

$$
\mathbf{b}^\top \mathbf{A}^{-2}(z)\mathbf{b} = \frac{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^3 \bar{\mathbf{y}}}{(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}})^2} \left(\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} + z^2 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-2}\bar{\mathbf{y}} \right)
$$

$$
\mathbf{a}^\top \mathbf{A}^{-1}(z)\mathbf{b} = \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}}} \left(\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}} + z + z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^3 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} \right)
$$

$$
\mathbf{a}^\top \mathbf{A}^{-2}(z)\mathbf{b} = \frac{1}{\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}}} \left(1 + 2z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 3z^2 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} + z^3 \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-2}\bar{\mathbf{y}} \right).
$$

In the next step we substitute these results in (A.7). More precisely introducing the notations

$$
\theta_n(z) = \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}}, \qquad \alpha_n = 1/\bar{\mathbf{y}}^\top (\mathbf{S}_n^+)^2 \bar{\mathbf{y}},
$$

we have $\theta_n'(z) = \frac{\partial}{\partial z}\theta_n(z) = \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-2}\bar{\mathbf{y}}$ and obtain for $\xi_n(z)$ the following representation

$$
\begin{aligned}
\xi_n(z) &= \frac{\alpha_n^2 (\alpha_n^{-1} + 2z + 3z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 4z^3 \theta_n(z) + z^4 \theta_n'(z))(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))}{\alpha_n^2 z^2 (1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))^2 - \alpha_n^2 z(\alpha_n^{-1} + z + z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^3 \theta_n(z))(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))} \\
&\quad + \frac{\alpha_n^2 z(\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2 \theta_n'(z))(\alpha_n^{-1} + z + z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^3 \theta_n(z))}{\alpha_n^2 z^2 (1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))^2 - \alpha_n^2 z(\alpha_n^{-1} + z + z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^3 \theta_n(z))(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))} \\
&\quad - \frac{2\alpha_n^2 z(1 + 2z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 3z^2 \theta_n(z) + z^3 \theta_n'(z))(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))}{\alpha_n^2 z^2 (1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))^2 - \alpha_n^2 z(\alpha_n^{-1} + z + z^2 \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^3 \theta_n(z))(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))} \\
&= \frac{\alpha_n^2 \left((1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))(\alpha_n^{-1} - z^2 (\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2 \theta_n'(z))) \right)}{-\alpha_n z(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))} \\
&\quad + \frac{\alpha_n^2 z(\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2 \theta_n'(z))(\alpha_n^{-1} + z(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z)))}{-\alpha_n z(1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z))}.
\end{aligned}
$$

In order to simplify the following calculations we introduce the quantities

$$
\psi_n(z) = 1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z); \qquad \psi_n'(z) = \bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2 \theta_n'(z),
$$

which lead to

$$
\begin{aligned}
\xi_n(z) &= \frac{\alpha_n^2 \psi_n(z)(\alpha_n^{-1} - z^2 \psi_n'(z)) + \alpha_n^2 z\psi_n'(z)(\alpha_n^{-1} + z\psi_n(z))}{-\alpha_n z\psi_n(z)} \\
&= \frac{\alpha_n^2 \alpha_n^{-1}(\psi_n(z) + z\psi_n'(z))}{-\alpha_n z\psi_n(z)} = -\frac{\psi_n(z) + z\psi_n'(z)}{z\psi_n(z)} \\
&= -\frac{1}{z} - \frac{\psi_n'(z)}{\psi_n(z)} = -\frac{1}{z} - \frac{\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + 2z\theta_n(z) + z^2 \theta_n'(z)}{1 + z\bar{\mathbf{y}}^\top \bar{\mathbf{y}} + z^2 \theta_n(z)}.
\end{aligned}
$$

Finally, we derive the representation (3.12) $\theta_n(z)$ using Woodbury matrix inversion lemma (see, e.g., Horn and Johnsohn [5]):

$$
\begin{aligned}
\theta_n(z) &= \bar{\mathbf{y}}^\top (\mathbf{S}_n^+ - z\mathbf{I})^{-1}\bar{\mathbf{y}} \\
&= \bar{\mathbf{y}}^\top \left(1/n\mathbf{Y}_n(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-2}\mathbf{Y}_n^\top - z\mathbf{I}\right)^{-1}\bar{\mathbf{y}} \\
&= \bar{\mathbf{y}}^\top \left(-\frac{1}{z}\mathbf{I} - \frac{1}{z^2}1/n\mathbf{Y}_n(\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\left(\mathbf{I} - \frac{1}{z}(\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\right)^{-1}(\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\mathbf{Y}_n^\top\right)\bar{\mathbf{y}} \\
&= -\frac{1}{z}\bar{\mathbf{y}}^\top\bar{\mathbf{y}} - \frac{1}{z^2}\bar{\mathbf{y}}^\top 1/n\mathbf{Y}_n(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\left(\mathbf{I} - \frac{1}{z}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\right)^{-1}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\mathbf{Y}_n^\top\bar{\mathbf{y}} \\
&= -\frac{1}{z}\bar{\mathbf{y}}^\top\bar{\mathbf{y}} - \frac{1}{z^2}\frac{1}{n}\mathbf{1}_n^\top(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}(\mathbf{I} - \frac{1}{z}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1})^{-1}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)\mathbf{1}_n \\
&= -\frac{1}{z}\bar{\mathbf{y}}^\top\bar{\mathbf{y}} - \frac{1}{z^2}\frac{1}{n}\mathbf{1}_n^\top\left(\mathbf{I} - \frac{1}{z}(1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1}\right)^{-1}\mathbf{1}_n \\
&= -\frac{1}{z}\bar{\mathbf{y}}^\top\bar{\mathbf{y}} + \frac{1}{z}\frac{1}{n}\mathbf{1}_n^\top((1/n\mathbf{Y}_n^\top\mathbf{Y}_n)^{-1} - z\mathbf{I})^{-1}\mathbf{1}_n.
\end{aligned}
$$

References

[1] Z.D. Bai, B.Q. Miao, G.M. Pan, On asymptotics of eigenvectors of large sample covariance matrix, Ann. Probab. 35 (2007) 1532–1572.
[2] Z.D. Bai, J.W. Silverstein, CLT for linear spectral statistics of large dimensional sample covariance matrices, Ann. Probab. 32 (2004) 553–605.
[3] Z.D. Bai, J.W. Silverstein, Spectral Analysis of Large Dimensional Random Matrices, Springer, New York, 2010.
[4] T. Bodnar, A.K. Gupta, N. Parolya, Direct shrinkage estimation of large dimensional precision matrix, J. Multivariate Anal. 146 (2016) 223–236.
[5] R.A. Horn, C.R. Johnsohn, Matrix Analysis, Cambridge University Press, Cambridge, 1985.
[6] D.C. Hoyle, Accuracy of pseudo-inverse covariance learning—a random matrix theory analysis, IEEE Trans. Pattern Anal. Mach. Intell. 33 (2011) 1470–1481.
[7] T. Kubokawa, M. Srivastava, Estimation of the precision matrix of a singular wishart distribution and its application in high-dimensional data, J. Multivariate Anal. 99 (2008) 1906–1928.
[8] V.A. Marčenko, L.A. Pastur, Distribution of eigenvalues for some sets of random matrices, Sb. Math. 1 (1967) 457–483.
[9] C.R. Meyer, Generalized inversion of modified matrices, SIAM J. Appl. Math. 24 (1973) 315–323.
[10] G.M. Pan, Comparison between two types of large sample covariance matrices, Ann. Inst. H. Poincaré Probab. Statist. 50 (2014) 655–677.
[11] G.M. Pan, W. Zhou, Central limit theorem for signal-to-interference ratio of reduced rank linear receiver, Ann. Appl. Probab. 18 (2008) 1232–1270.
[12] F. Rubio, X. Mestre, Spectral convergence for a general class of random matrices, Statist. Probab. Lett. 81 (2011) 592–602.
[13] J. Sherman, W.J. Morrison, Adjustment of an inverse matrix corresponding to a change in one element of a given matrix, Ann. Math. Statist. 21 (1950) 124–127.
[14] J.W. Silverstein, Strong convergence of the empirical distribution of eigenvalues of large-dimensional random matrices, J. Multivariate Anal. 55 (1995) 331–339.
[15] M. Srivastava, Multivariate theory for analyzing high dimensional data, J. Japan Statist. Soc. 37 (2007) 53–86.
[16] Z. Zheng, Z.D. Bai, J. Yao, CLT for linear spectral statistics of a rescaled sample precision matrix, Random Matrices: Theory Appl. 04 (2015) 1550014. (43 pages).
[17] Z. Zheng, Z.D. Bai, J. Yao, Substitution principle for clt of linear spectral statistics of high-dimensional sample covariance matrices with applications to hypothesis testing, Ann. Statist. 43 (2015) 546–591.