Supplementary material of "Estimation of the number of spiked eigenvalues in a covariance matrix by bulk eigenvalue matching analysis"

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In Section A, we introduce two `GetQT` algorithms; each of them can be plugged into the main algorithm, BEMA. In Section B, we prove Theorem 1 and Theorem 2.

A `GetQT` algorithms

We present details of the `GetQT` algorithms used in BEMA. Under the general spiked covariance model (7), the empirical spectral distribution (ESD) converges to a fixed distribution $F_{\gamma}(x; \sigma^2, \theta)$. Write $\gamma_n = p/n$. The purpose of the algorithm $\texttt{GetQT}(y, \gamma_n, \theta)$ is as follows: Fixing $\sigma = 1$, given any $\theta > 0$ and $y \in [0, 1]$, it outputs the y-upper-quantile of the distribution $F_{\gamma_n}(x; 1, \theta)$.

A.1 The Monte Carlo simulation algorithm `GetQT1`

As explained in Section 3.1, $F_{\gamma_n}(\cdot; 1, \theta)$ is also the theoretical limit of the ESD under the following null covariance model:

$$\mathbf{\Sigma} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_p^2), \qquad \text{where } \sigma_k^2 \overset{iid}{\sim} \mathrm{Gamma}(\theta, \theta). \tag{A.1}$$

We can simulate data from (A.1) and use its ESD as a numerical approximation to $F_{\gamma_n}(\cdot; 1, \theta)$.

Write $\tilde{p} = \min\{n, p\}$ and $y = k/\tilde{p}$. When the population covariance matrix satisfies (A.1), the kth eigenvalue of the sample covariance matrix, $\hat{\lambda}_k$, is asymptotically close to the y-upper-quantile of $F_{\gamma_n}(\cdot; 1, \theta)$. We thereby use the mean of $\hat{\lambda}_k$, obtained by sampling the data matrix multiple times, to estimate the desired quantile. We note that model (A.1) only specifies how to sample $\mathbf{\Sigma}$, but it does not specify how to sample $\boldsymbol{X}_i$'s. Due to universality theory of eigenvalues (Knowles and Yin, 2017, Section 3.3), the choice of distribution of $\boldsymbol{X}_i$'s does not matter. For convenience, we sample $\boldsymbol{X}_i$'s from multivariate normal distributions. See Algorithm 3.

In the practical implementation, we use the following strategies to further reduce computation time and memory use: (i) When n is smaller than p, we no longer construct the $p \times p$ covariance

Algorithm 3. GetQT1.

Input: n, p, θ, k, and an integer B.

Output: An estimate of the $(k/\tilde{p})$-upper-quantile of $F_{\gamma_n}(\cdot; 1, \theta)$.

1. For $b = 1, 2, \ldots, B$, repeat: First generate $\boldsymbol{\Sigma}^{(b)}$ from (A.1), and then generate $\boldsymbol{X}_i^{(b)} \overset{iid}{\sim} N(0, \boldsymbol{\Sigma}^{(b)})$, $1 \le i \le n$. Write $\boldsymbol{X}^{(b)} = [\boldsymbol{X}_1^{(b)}, \ldots, \boldsymbol{X}_n^{(b)}]^\top \in \mathbb{R}^{n\times p}$. Construct the sample covariance matrix $\boldsymbol{S}^{(b)} = (1/n)(\boldsymbol{X}^{(b)})^\top \boldsymbol{X}^{(b)}$ and obtain its kth eigenvalue $\hat{\lambda}_k^{(b)}$.
2. Output $\frac{1}{B}\sum_{b=1}^{B} \hat{\lambda}_k^{(b)}$ as the estimated $(k/\tilde{p})$-upper-quantile.

matrix $\boldsymbol{S}^{(b)}$. Instead, we construct an $n \times n$ matrix $(1/n)\boldsymbol{X}^{(b)}(\boldsymbol{X}^{(b)})^\top$. This matrix shares the same nonzero eigenvalues as $\boldsymbol{S}^{(b)}$ but requires much less memory in eigen-decomposition. This strategy is especially useful for genomic data, where n is typically much smaller than p. (ii) In the main algorithm, Algorithm 2, `GetQT1` is applied multiple times to compute the $(k/\tilde{p})$-upper-quantile for a collection of k. We let the sampling step, Step 1 above, be shared across different values of k: For each $b = 1, 2, \ldots, B$, we obtain and store $\hat{\lambda}_k^{(b)}$ for all values of k; next, in Step 2, we output the estimated $(k/\tilde{p})$-upper-quantile simultaneously for all values of k. This strategy can significantly reduce the actual running time.

A.2 The deterministic algorithm `GetQT2`

This algorithm directly uses the definition of $F_{\gamma_n}(\cdot; , 1, \theta)$. Let $H_\theta(t)$ be the CDF of Gamma(θ, θ). Given a positive sequence ξ_n such that $\xi_n \to 0$ as $n \to \infty$, let $m_n(y) = m_n(y, \xi_n, \gamma_n, \theta) \in \mathbb{C}^+$ be the unique solution to the equation

$$y + \mathrm{i}\,\xi_n = -\frac{1}{m_n} + \gamma_n \int \frac{t}{1 + t m_n} dH_\theta(t). \tag{A.2}$$

Then, the density of $F_{\gamma_n}(\cdot; 1, \theta)$, denoted by $f_{\gamma_n}(y; 1, \theta)$, is approximated by

$$\hat{f}^*_{\gamma_n}(y; 1, \theta) = \frac{1}{\pi(\gamma_n \wedge 1)} \Im(m_n(y, \xi_n, \gamma_n, \theta)), \tag{A.3}$$

where $\Im(\cdot)$ denotes the imaginary part of a complex number. The choice of ξ_n needs to satisfy $\xi_n \gg n^{-1}$, in order to guarantee that the approximation is not governed by stochastic fluctuations (Knowles and Yin, 2017). We choose $\xi_n = n^{-2/3}$ for convenience.

The above motivates a three-step algorithm.

1. Fix a grid $y_1 < y_2 < \ldots < y_N$. Solve equation (A.2) to obtain $m_n(y_j)$ for $1 \le j \le N$.
2. Use equation (A.3) to obtain $\hat{f}^*_{\gamma_n}(y_j; 1, \theta)$, for $1 \le j \le N$. Obtain the whole density curve $\hat{f}_{\gamma_n}(y; 1, \theta)$ by linear interpolation.

Algorithm 4. GetQT2.

Input: n, p, θ, and $y \in [0,1]$.

Output: An estimate of the y-upper-quantile of $F_{\gamma_n}(\cdot;1,\theta)$.

Step 1: Write $\tilde{p} = n \wedge p$ and $\gamma_n = p/n$. Fix a grid $y_1 < y_2 < \dots y_{N-1} < y_N$. For each $1 \le j \le N$, compute $\hat{m}_n(y)$ as follows:

- For a tuning parameter $\delta > 0$, construct the set of grid points in $\mathbb{R} \times \mathbb{R}^+$:

$$S_{y,\gamma_n,\delta} = \left\{(a,b) : a = k\delta, b = \ell\delta,\ k,\ell \in \mathbb{Z},\ (a - 1/y_j)^2 + b^2 \le \gamma_n/y_j^2,\ a < (\gamma_n - 1)/2y_j\right\}.$$

- For each $(a,b) \in S_{y,\gamma_n,\delta}$ and $\xi_n = n^{-2/3}$, compute

$$\Delta(a,b) = \left| y + \mathrm{i}\,\xi_n + \frac{1}{m} - \gamma_n \int \frac{t}{1+tm} dH_\theta(t) \right|,$$

  where $H_\theta(t)$ is the CDF of Gamma(θ,θ). The integral above can be computed via standard Monte Carlo approximation (by sampling data from Gamma(θ,θ)).

- Find $(\hat{a},\hat{b}) = \mathrm{argmin}_{(a,b)\in S_{y,\gamma_n,\delta}} \Delta(a,b)$. Let $\hat{m}(y) = \hat{a} + \hat{b}\mathrm{i}$.

Step 2: Let $\hat{f}_{\gamma_n}(y_j;1,\theta) = \frac{1}{\pi(\gamma_n \wedge 1)}\Im(\hat{m}(y))$, for $1 \le j \le N$. For any $y_{j-1} < z < y_j$, let

$$\hat{f}_{\gamma_n}(z;1,\theta) = \frac{y_j - z}{y_j - y_{j-1}} \hat{f}_{\gamma_n}(y_{j-1};1,\theta) + \frac{z - y_{j-1}}{y_j - y_{j-1}} \hat{f}_{\gamma_n}(y_j;1,\theta).$$

Step 3: Find q such that $\int_q^{(1+\sqrt{\gamma_n})^2} \hat{f}_{\gamma_n}(z;1,\theta) = y$. Output q as the estimated y-upper-quantile.

3. Find q such that $\int_q^{(1+\sqrt{\gamma_n})^2} \hat{f}_{\gamma_n}(z;1,\theta)dz = y$. Output q as the estimated y-upper-quantile.

Step 2 is straightforward. Step 3 is also easy to implement, since $\hat{f}_{\gamma_n}(y;1,\theta)$ is a piece-wise linear function. Below, we describe Step 1 with more details.

In Step 1, fix y and write $m = a + b\mathrm{i}$, where $\mathrm{i} = \sqrt{-1}$, and $a \in \mathbb{R}$ and $b \in \mathbb{R}^+$ are the real and imaginary parts of m, respectively. We aim to find (a,b) so that m solves the complex equation (A.2). Pretending that $\xi_n = 0$, the equation (A.2) can be re-written as a set of real equations: [1]

$$\begin{cases} y = \gamma_n \int \frac{t}{1+2at+(a^2+b^2)t^2} dH_\theta(t), \\ \frac{1}{a^2+b^2} = \gamma_n \int \frac{t^2}{1+2at+(a^2+b^2)t^2} dH_\theta(t), \end{cases} \quad \Longleftrightarrow \quad \begin{cases} 2ay = \gamma_n \int \frac{2at}{1+2at+(a^2+b^2)t^2} dH_\theta(t), \\ 1 = \gamma_n \int \frac{(a^2+b^2)t^2}{1+2at+(a^2+b^2)t^2} dH_\theta(t). \end{cases}$$

First, by combining the above equations with $\gamma_n = \gamma_n \int \frac{1+2at+(a^2+b^2)t^2}{1+2at+(a^2+b^2)t^2} dH_\theta(t)$, we have

$$\gamma_n - 1 - 2ay = \gamma_n \int \frac{1}{1+2at+(a^2+b^2)t^2} dH_\theta(t) > 0.$$

[1] The second equation is obtained by letting the imaginary part of both hand sides of (A.2) be equal. The first equation is obtained by letting the real part of both hand sides of (A.2) be equal and then substituting $\frac{a}{a^2+b^2}$ by a times the second equation.

It yields that $a < (\gamma_n - 1)/2y$. Second, by Cauchy-Schwarz inequality, $\left[\int \frac{t}{1+2at+(a^2+b^2)t^2} dH_\theta(t)\right]^2 \leq \int \frac{1}{1+2at+(a^2+b^2)t^2} dH_\theta(t) \cdot \int \frac{t^2}{1+2at+(a^2+b^2)t^2} dH_\theta(t)$. It follows that

$$y^2 \leq (\gamma_n - 1 - 2ay) \cdot \frac{1}{a^2+b^2}.$$

Re-arranging the terms gives $(a - 1/y)^2 + b^2 \leq \gamma_n/y^2$. So far, we have obtained a feasible set of (a, b) for the solution of (A.2) when $\xi_n = 0$:

$$S_{y,\gamma_n} = \left\{(a, b) : (a - 1/y)^2 + b^2 \leq \gamma_n/y^2,\ a < (\gamma_n - 1)/2y\right\}. \tag{A.4}$$

Since ξ_n is very close to 0, we use the same feasible set when solving (A.2). Observing that S_{y,γ_n} is bounded, we solve equation (A.2) by a grid search on this feasible set. See Algorithm 4.

A.3 Comparison

We compare the performance of two `GetQT` algorithms on a numerical example where $(n, p, \theta) = (10000, 1000, 1)$. The results are in Figure 1. To generate this figure, first, we simulate eigenvalues $\{\hat{\lambda}_k^{(b)}\}_{1\leq k\leq p, 1\leq b\leq B}$ as in Step 1 of `GetQT1`, where $B = 20$, and plot the histogram of eigenvalues. Next, we plot the estimated density $\hat{f}_{\gamma_n}(y; 1, \theta)$ from `GetQT2` (tuning parameter is $\delta = 0.05$). The estimated density fits the histogram well, suggesting that the steps in `GetQT2` for estimating $f_{\gamma_n}(y; 1, \theta)$ are successful. Furthermore, the estimated quantiles from two algorithms are very close to each other.

In terms of numerical performance, the two `GetQT` algorithms are similar. We now discuss the computing time. The main computational cost of `GetQT1` comes from computing the eigenvalues of $\boldsymbol{S}^{(b)}$ at each iteration. As we have mentioned in the end of Section A.1, if $p < n$, we conduct eigen-decomposition on an $p \times p$ matrix; if $n < p$, we conduct eigen-decomposition on an $n \times n$ matrix. Therefore, as long as $\min\{n, p\}$ is not too large, `GetQT1` is fast.

Compared with `GetQT1`, the advantage of `GetQT2` is that it does not need to compute any eigen-decomposition. As a result, when $\min\{n, p\}$ is large, `GetQT2` is much faster than `GetQT1` (and `GetQT2` also requires less memory use). The computational cost of `GetQT2` is proportional to the number of grid points in the algorithm, governed by the tuning parameter δ. Sometimes, we need to choose δ sufficiently small to guarantee the accuracy of computing $\hat{m}(y, \gamma_n, \theta)$, which significantly increases the cost of grid search. Our experience suggests that `GetQT2` is faster than `GetQT1` only in the case that $\min\{n, p\}$ is larger than 10^4.

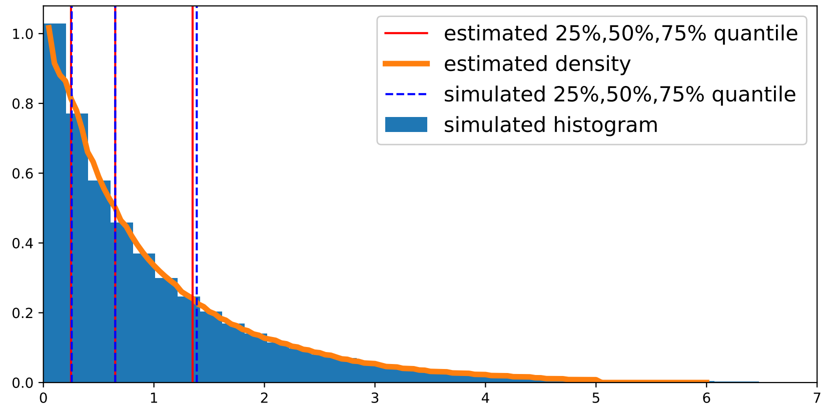

Figure 1: Comparison of two `GetQT` algorithms. The simulated histogram is from `GetQT1`, and the density curve is estimated by `GetQT2`.

A.4 Modifications under Model (13)

Section 4.2 introduces Model (13), as a proxy of Model (2), to facilitate the theoretical analysis. In Model (13), the diagonal entries of $\boldsymbol{D}$ are *iid* generated from a truncated Gamma distribution. In Section 4.2, we described how to adapt Algorithm 2 to this setting, where the key is to modify `GetQT` so that it can compute the y-upper-quantile of the distribution $F_\gamma(\cdot; 1, \theta, T_1, T_2)$, for any given y and (θ, T_1, T_2).

To modify `GetQT1`, we note that $F_{\gamma_n}(\cdot; 1, \theta, T_1, T_2)$ is the theoretical limit of the ESD under the null covariance model:

$$\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_p^2), \qquad \text{where } \sigma_k^2 \overset{iid}{\sim} \mathrm{TruncGamma}(\theta, \theta, T_1, T_2). \tag{A.5}$$

We can simulate data from (A.5) and use its ESD as a numerical approximation to $F_{\gamma_n}(\cdot; 1, \theta, T_1, T_2)$. In Algorithm 3, we only need to modify Step 1 so that $\boldsymbol{\Sigma}^{(b)}$ is generated from (A.5).

To modify `GetQT2`, we solve (A.2) with $H_\theta(t)$ replaced by $H_{\theta,T_1,T_2}(t)$, where $H_{\theta,T_1,T_2}(\cdot)$ is the CDF of TruncGamma$(\theta, \theta, T_1, T_2)$. We note that the feasible set in (A.4) is derived without using the explicit form of $H_\theta(t)$, so it continues to apply. In Algorithm 4, we only need to modify the definition of $\Delta(a, b)$ to

$$\Delta(a, b) = \left| y + \mathrm{i}\,\xi_n + \frac{1}{m} - \gamma_n \int \frac{t}{1 + tm} dH_{\theta,T_1,T_2}(t) \right|,$$

and the other steps remain the same.

B Proofs

B.1 Proof of Theorem 1

Let $z_k = \hat{\lambda}_k - \sigma^2 q_k$, for all $1 \le k \le \tilde{p}$. It follows that

$$\hat{\sigma}^2 = \frac{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} q_k(\sigma^2 q_k + z_k)}{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} q_k^2} = \sigma^2 + \frac{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} q_k z_k}{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} q_k^2}.$$

It follows that

$$|\hat{\sigma}^2 - \sigma^2| \le \underbrace{\frac{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} |q_k|}{\sum_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} q_k^2}}_{\equiv B_{n,p}(\alpha)} \times \max_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} |z_k|.$$

We recall that q_k is the $(k/\tilde{p})$-upper-quantile of a standard Machenko-Pastur distribution associated with $\gamma_n = p/n$. Note that $p/n \to \gamma$ and $\alpha \le k/\tilde{p} \le 1 - \alpha$, where $\gamma > 0$ and $\alpha \in (0, 1/2)$ are constants. It follows immediately that there is a constant $C_1 = C_1(\alpha, \gamma)$ such that $B_{n,p}(\alpha) \le C_1$. As a result,

$$|\hat{\sigma}^2 - \sigma^2| \le C_1 \max_{\alpha\tilde{p} \le k \le (1-\alpha)\tilde{p}} |\hat{\lambda}_k - \sigma^2 q_k|. \tag{B.6}$$

We bound the right hand side of (B.6). By Assumption 1, the data vectors $\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_n$ are obtained from a random matrix $\boldsymbol{Y} = [\boldsymbol{Y}_1, \boldsymbol{Y}_2, \ldots, \boldsymbol{Y}_n]^\top \in \mathbb{R}^{n \times p}$, where the entries of $\boldsymbol{Y}$ are independent variables with zero mean and unit variance. Given $\boldsymbol{Y}$, define $\boldsymbol{X}_1^*, \boldsymbol{X}_2^*, \ldots, \boldsymbol{X}_n^*$ by

$$\boldsymbol{X}_i^*(j) = \sigma \cdot \boldsymbol{Y}_i(j), \qquad 1 \le i \le n, 1 \le j \le p.$$

Then, $\boldsymbol{X}_1^*, \ldots, \boldsymbol{X}_n^*$ follow a "null" model that is similar to the factor model in Assumption 1 but corresponds to $K = 0$. Let $\boldsymbol{S}^*$ be the sample covariance matrix of $\boldsymbol{X}_1^*, \ldots, \boldsymbol{X}_n^*$. Then, $\boldsymbol{S}^*$ serves as a reference matrix for $\boldsymbol{S}$. The *eigenvalue sticking* result says that eigenvalues of $\boldsymbol{S}$ "stick" to eigenvalues of the reference matrix. The precise statement is as follows: Let $\hat{\lambda}_1^* > \hat{\lambda}_2^* > \ldots > \hat{\lambda}_{\tilde{p}}^*$ be the nonzero eigenvalues of $\boldsymbol{S}^*$. When the entries of $\boldsymbol{Y}$ satisfy the regularity conditions stated in Theorem 1, by Theorem 2.7 of Bloemendal et al. (2016), there is a constant $C_2 = C_2(\alpha, \gamma, \sigma^2)$ such that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P}\Big\{\max_{(\alpha/2)\tilde{p} \le j \le (1-\alpha/2)\tilde{p}} |\hat{\lambda}_{j+K_1} - \hat{\lambda}_j^*| > C_2 n^{-(1-\epsilon)}\Big\} \le n^{-s}, \tag{B.7}$$

where K_1 is the total number of spiked eigenvalues in Model (3) such that $\lambda_k = \sigma^2(\sqrt{\gamma} + \tau_k)$ for some $\tau_k \ge n^{-1/3}$. It remains to study $\hat{\lambda}_j^*$. Its large deviation bound can be found in Pillai and Yin (2014) (also, see Theorem 3.3 of Ke (2016)). There is a constant $C_3 = C_3(\alpha, \gamma, \sigma^2) > 0$ such that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P}\Big\{\max_{(\alpha/2)\tilde{p} \le j \le (1-\alpha/2)\tilde{p}} |\hat{\lambda}_j^* - \sigma^2 q_j| > C_3 n^{-(1-\epsilon)}\Big\} \le n^{-s}. \tag{B.8}$$

Furthermore, since $K_1 \leq K$ and K is fixed, there is a constant $C_4 = C_4(\gamma, K)$ such that

$$\max_{(\alpha/2)\tilde{p} \leq j \leq (1-\alpha/2)\tilde{p}} |q_j - q_{j+K_1}| \leq C_4 n^{-1}. \tag{B.9}$$

Combining (B.7)-(B.9) gives that, for any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P}\Big\{ \max_{(\alpha/2)\tilde{p} \leq j \leq (1-\alpha)\tilde{p}} |\hat{\lambda}_{j+K_1} - \sigma^2 q_{j+K_1}| > Cn^{-(1-\epsilon)} \Big\} \leq n^{-s}.$$

We plug it into (B.6). The claim follows immediately. □

B.2 Proof of Theorem 2

Denote by $T_{n,p}(\hat{\sigma}^2, \beta_n)$ the threshold used in Algorithm 1. It satisfies that

$$T_{n,p}(\hat{\sigma}^2, \beta_n) = \hat{\sigma}^2[(1+\sqrt{\gamma}_n)^2 + \omega_n], \qquad \text{where } \omega_n = O(n^{-2/3} t_{1-\beta_n}). \tag{B.10}$$

Here, $t_{1-\beta_n}$ is the $(1-\beta_n)$-quantile of Tracy-Widom distribution. Note that $\tau_n \gg n^{-1/3}$. We can choose $\beta_n \to \infty$ appropriately slow such that $1 \ll t_{1-\beta_n} \ll n^{2/3}\min\{\tau_n^2, 1\}$. It follows that

$$n^{-2/3} \;\ll\; \omega_n \;\ll\; \min\{\tau_n^2,\; 1\}. \tag{B.11}$$

First, we derive a lower bound for $\hat{\lambda}_K$ and show that $\hat{K} \geq K$ with probability $1-o(1)$. Recall that λ_k denotes the kth largest eigenvalue of $\mathbf{\Sigma}$. In view of Model (3), it is true that $\lambda_k = \mu_k + \sigma^2$ for $1 \leq k \leq K$ and $\lambda_k = \sigma^2$, for $K < k \leq p$. Introduce

$$\lambda_k^* = \lambda_k\Big(1 + \frac{\gamma_n}{\lambda_k/\sigma^2 - 1}\Big), \qquad 1 \leq k \leq K.$$

Write $\delta_k = \lambda_k/\sigma^2 - 1$, for $k = 1, 2, \ldots, K$. Let $g(t) = (1+t)(1+\gamma_n/t)$. Then,

$$\lambda_k^* = \sigma^2 \cdot g(\delta_k), \qquad 1 \leq k \leq K.$$

The function g satisfies that $g(\sqrt{\gamma_n}) = (1+\sqrt{\gamma_n})^2$ and $g'(t) \geq 1 - \sqrt{\gamma_n}/t$. Hence, it is monotone increasing in $(\sqrt{\gamma_n}, \infty)$. For any $\tau > 0$ and $t > \sqrt{\gamma_n} + \tau$, we have $g(t) \geq g(\sqrt{\gamma_n}) + g'(\sqrt{\gamma_n}+\tau)\cdot\tau \geq (1+\sqrt{\gamma_n})^2 + \tau^2/(\sqrt{\gamma}_n + \tau)$. It follows that

$$\lambda_K^* \geq \sigma^2\Big[(1+\sqrt{\gamma_n})^2 + \frac{\delta_K^2}{\sqrt{\gamma_n} + \delta_K}\Big]. \tag{B.12}$$

At the same time, by Theorem 2.3 of Bloemendal et al. (2016), with probability $1-o(1)$,

$$|\hat{\lambda}_K - \lambda_K^*| \leq C_2\sigma^2 n^{-1/2} \begin{cases} \delta_K^{1/2}, & \text{if } \delta_K < 1, \\ 1 + \delta_K/(1+\sqrt{\gamma_n}), & \text{if } \delta_K \geq 1, \end{cases} \tag{B.13}$$

for a constant $C_2 > 0$. If $\delta_K \geq 1$, then (B.12) implies $\lambda_K^* - \sigma^2(1+\sqrt{\gamma_n})^2 \geq C_3\sigma^2\delta_K$, for a constant $C_3 > 0$, and (B.13) yields that $|\hat{\lambda}_K - \lambda_K^*| \leq C_2\sigma^2(1+\delta_K)n^{-1/2}$. It follows that

$$\hat{\lambda}_K - \sigma^2(1+\sqrt{\gamma_n})^2 \;\geq\; (C_3/2)\cdot\sigma^2\delta_K \;\geq\; (C_3/2)\cdot\sigma^2.$$

If $\delta_K < 1$, then (B.12) yields that $\lambda_K^* - \sigma^2(1+\sqrt{\gamma_n})^2 \geq C_4\sigma^2\delta_K^2$, for a constant $C_4 > 0$, and (B.13) yields that $|\hat{\lambda}_K - \lambda_K^*| \leq C_2\sigma^2\delta_K^{1/2}n^{-1/2}$. It follows that

$$\hat{\lambda}_K - \sigma^2(1+\sqrt{\gamma_n})^2 \;\geq\; C_4\sigma^2\delta_K^2 - \frac{C_2\sigma^2\delta_K^2}{\sqrt{n\delta_K^3}} \;\geq\; (C_4/2)\cdot\sigma^2\delta_K^2,$$

where the last inequality is because $\delta_K \geq \tau_n \gg n^{-1/3}$. We combine the two cases and note that $\delta_K \geq \tau_n$. It gives that

$$\mathbb{P}\Big\{\hat{\lambda}_K \geq \sigma^2\big[(1+\sqrt{\gamma_n})^2 + C\min\{\tau_n^2,\,1\}\big]\Big\} = 1 - o(1).$$

Furthermore, by Theorem 1, $|\hat{\sigma}^2 - \sigma^2| \prec n^{-1} \ll \min\{\tau_n^2,\,1\}$. Hence, we can replace σ^2 by $\hat{\sigma}^2$ in the above equation, i.e.,

$$\mathbb{P}\Big\{\hat{\lambda}_K \geq \hat{\sigma}^2\big[(1+\sqrt{\gamma_n})^2 + C\min\{\tau_n^2,\,1\}\big]\Big\} = 1 - o(1). \tag{B.14}$$

We compare $\hat{\lambda}_K$ with the threshold in (B.10). Since $\omega_n \ll \min\{\tau_n^2, 1\}$, it is implied from (B.14) that $\hat{\lambda}_K$ exceeds this threshold with probability $1 - o(1)$. Therefore,

$$\mathbb{P}\Big\{\hat{K} \geq K\Big\} = 1 - o(1).$$

Next, we derive an upper bound for $\hat{\lambda}_{K+1}$ and show that $\hat{K} \leq K$ with probability $1 - o(1)$. We apply Theorem 2.3 of Bloemendal et al. (2016) again: For any $\epsilon > 0$ and $s > 0$,

$$\mathbb{P}\Big\{\hat{\lambda}_{K+1} - \sigma^2(1+\sqrt{\gamma_n})^2 \leq \sigma^2 n^{-(2/3-\epsilon)}\Big\} = 1 - o(1). \tag{B.15}$$

Since $\omega_n \gg n^{-2/3}$, we can take ϵ arbitrarily small to make $n^{-(2/3-\epsilon)} \leq \omega_n/2$. We also apply the large deviation bound for $\hat{\sigma}^2$ in Theorem 1 to replace σ^2 by $\hat{\sigma}^2$. It follows immediately that

$$\mathbb{P}\Big\{\hat{\lambda}_{K+1} \leq \hat{\sigma}^2\big[(1+\sqrt{\gamma}_n)^2 + \omega_n/2\big]\Big\} = 1 - o(1). \tag{B.16}$$

We compare $\hat{\lambda}_{K+1}$ with the threshold in (B.10). It is seen that $\hat{\lambda}_{K+1}$ is below this threshold with probability $1 - o(1)$. Therefore,

$$\mathbb{P}\Big\{\hat{K} \leq K\Big\} = 1 - o(1).$$

The claim follows immediately. $\square$

B.3 Proof of Theorem 3

Throughout this proof, we let C be a generic constant, whose meaning may vary from occurrence to occurrence. Let $F_\gamma(\cdot;\sigma^2,\theta,T_1,T_2)$ be the theoretical limit of ESD, whose definition is given in Lemma 1. We replace γ by $\gamma_n = p/n$ in this definition, write $\bar{F}_{\gamma_n} = 1 - F_{\gamma_n}$ and let $q_i(\sigma^2,\theta) = \bar{F}_{\gamma_n}^{-1}(y;\sigma^2,\theta,T_1,T_2)$ denote the $(i/\tilde{p})$-upper-quantile of this distribution, where $\tilde{p} = n \wedge p$. We use (σ_0^2, θ_0) to denote the true parameters. Write $s_n = \lceil \alpha\tilde{p} \rceil$ and

$$\hat{R}(\sigma^2,\theta) = \sum_{s_n \le i \le \tilde{p}-s_n} [\hat{\lambda}_i - q_i(\sigma^2,\theta)]^2, \qquad R(\sigma^2,\theta) = \sum_{s_n \le i \le \tilde{p}-s_n} [q_i(\sigma_0^2,\theta_0^2) - q_i(\sigma^2,\theta)]^2.$$

Let $\Delta = \sum_{s_n \le i \le \tilde{p}-s_n} |\hat{\lambda}_i - q_i(\sigma_0^2,\theta_0)|^2$. By direct calculations and Cauchy-Schwarz inequality,

$$\begin{aligned}
|\hat{R}(\sigma^2,\theta) - R(\sigma^2,\theta)| &\le 2 \sum_{s_n \le i \le \tilde{p}-s_n} |q_i(\sigma_0^2,\theta_0) - q_i(\sigma,\theta)| \cdot |\hat{\lambda}_i - q_i(\sigma_0^2,\theta_0)| \\
&\quad + \sum_{s_n \le i \le \tilde{p}-s_n} |\hat{\lambda}_i - q_i(\sigma_0^2,\theta_0)|^2 \\
&\le 2\sqrt{R(\sigma^2,\theta)}\sqrt{\Delta} + \Delta.
\end{aligned}$$

It follows that $\hat{R}(\sigma^2,\theta) \le R(\sigma^2,\theta) + 2\sqrt{R(\sigma^2,\theta)}\sqrt{\Delta} + \Delta = \big(\sqrt{R(\sigma^2,\theta)} + \sqrt{\Delta}\big)^2$. In the above inequality, we can switch $\hat{R}(\sigma^2,\theta)$ and $R(\sigma^2,\theta)$ and similarly derive that $R(\sigma^2,\theta) \le \big(\sqrt{\hat{R}(\sigma^2,\theta)} + \sqrt{\Delta}\big)^2$. As a result,

$$\Big|\sqrt{\hat{R}(\sigma^2,\theta)} - \sqrt{R(\sigma^2,\theta)}\Big| \le \sqrt{\Delta}. \tag{B.17}$$

We now bound Δ. By Lemma 1, for all $K < i \le \tilde{p}$,

$$|\hat{\lambda}_i - q_i(\sigma_0^2,\theta_0)| \prec [i \wedge (\tilde{p}+1-i)]^{-1/3} n^{-2/3}.$$

We note that the stochastic dominance in Lemma 1 can be made 'uniform' over i; i.e., the integer $N(\epsilon, s)$ in Definition 3 is shared by all $K < i \le \tilde{p}$ (Knowles and Yin, 2017). Hence, summing over i preserves 'stochastic dominance.' Additionally, $\sum_{i=s_n}^{\tilde{p}/2} i^{-2/3} n^{-4/3} \le Cn^{-1}\big[\frac{1}{\tilde{p}}\sum_{i=s_n}^{\tilde{p}/2} (i/\tilde{p})^{-2/3}\big] \le Cn^{-1}\int_{s_n/n}^{1/2} x^{-2/3}dx \le Cn^{-1}$. Combining the above arguments gives

$$\begin{aligned}
\sum_{s_n \le i \le \tilde{p}-s_n} |\hat{\lambda}_i - q_i(\sigma_0^2,\theta_0)|^2 &\prec \sum_{s_n \le i \le \tilde{p}-s_n} [i \wedge (\tilde{p}+1-i)]^{-2/3} n^{-4/3} \\
&\prec \sum_{s_n \le i \le \tilde{p}/2} i^{-2/3} n^{-4/3} \quad \prec \quad n^{-1}.
\end{aligned}$$

This gives $\Delta \prec n^{-1}$. We plug it into (B.17) to get

$$\Big|\sqrt{\hat{R}(\sigma^2,\theta)} - \sqrt{R(\sigma^2,\theta)}\Big| \prec n^{-1/2}. \tag{B.18}$$

Since Δ does not depend on (σ^2, θ), the 'stochastic dominance' here is uniform for all $(\sigma^2, \theta) \in \mathcal{J}_{\sigma^2} \times \mathcal{J}_\theta$. We claim that there exists a constant $c_0 > 0$ such that for any (σ^2, θ) in $\mathcal{J}_{\sigma^2} \times \mathcal{J}_\theta$,

$$R(\sigma^2, \theta) \geq c_0 n \cdot \big[(\sigma^2 - \sigma_0^2)^2 + (\theta - \theta_0)^2\big]. \tag{B.19}$$

Note that $R(\sigma_0^2, \theta_0) = 0$. Combining it with (B.18)-(B.19) gives

$$\sqrt{\hat{R}(\sigma_0^2, \theta_0)} \prec n^{-1/2}, \qquad \sqrt{c_0 n}\sqrt{(\hat{\sigma}^2 - \sigma_0^2)^2 + (\hat{\theta} - \theta_0)^2} \leq \sqrt{\hat{R}(\hat{\sigma}^2, \hat{\theta})} + O_\prec(n^{-1/2}),$$

where a random variable is $O_\prec(b_n)$ if its absolute value is $\prec b_n$. Since $(\hat{\sigma}^2, \hat{\theta})$ minimizes $\hat{R}(\sigma^2, \theta)$, we have $\hat{R}(\hat{\sigma}^2, \hat{\theta}) \leq \hat{R}(\sigma_0^2, \theta_0) \prec n^{-1}$. It follows that

$$\sqrt{(\hat{\sigma}^2 - \sigma_0^2)^2 + (\hat{\theta} - \theta_0)^2} \prec n^{-1}.$$

This proves the claim.

What remains is to show (B.19). Define the quantile function $h_{\sigma^2,\theta}(\alpha) = \bar{F}_{\gamma_n}^{-1}(\alpha; \sigma^2, \theta, T_1, T_2)$. Then, $q_i(\sigma^2, \theta) = h_{\sigma^2,\theta}(i/\tilde{p})$. We can re-write

$$R(\sigma^2, \theta) = \sum_{i=s_n}^{\tilde{p}-s_n} \big[h_{\sigma^2,\theta}(i/\tilde{p}) - h_{\sigma_0^2,\theta_0}(i/\tilde{p})\big]^2.$$

Introduce $R^*(\sigma^2, \theta) = \tilde{p}\int_0^1 [h_{\sigma^2,\theta}(\alpha) - h_{\sigma_0^2,\theta_0}(\alpha)]^2 d\alpha$. Then, $\tilde{p}^{-1}R(\sigma^2, \theta)$ is the Riemann approximation of the integral $\tilde{p}^{-1}R^*(\sigma^2, \theta)$. Note that $s_n/\tilde{p} = o(1)$. Furthermore, $h_{\sigma^2,\theta}(\alpha)$ is uniformly square integrable for $(\sigma^2, \theta) \in \mathcal{J}_{\sigma^2} \times \mathcal{J}_\theta$ (the proof is very similar to the analysis of C_2 below; we thus omit it). Hence, the Riemann approximation error is negligible. Particularly, there exists a constant $c_1 \in (0, 1)$ such that

$$R(\sigma^2, \theta) \geq c_1 \cdot R^*(\sigma^2, \theta). \tag{B.20}$$

It suffices to study $R^*(\sigma^2, \theta)$. The next lemma is proved in Section B.6.

Lemma B.1. *Let $F(x)$ be a distribution on $(0, \infty)$ with a continuous density $f(x)$. Let $\bar{F}(x) = 1 - F(x)$, $h_F(\alpha) = \bar{F}^{-1}(\alpha)$, and $\mu_m(f) = \int x^m f(x)dx$, $m \geq 1$. For another distribution $G(x)$ on $(0, \infty)$ with a continuous density $g(x)$, we define $\bar{G}(x)$, $h_G(\alpha)$, and $\mu_m(g)$ similarly. Suppose $\int x^2|\bar{F}(x) - \bar{G}(x)|dx < \infty$. Let $\check{g}(x, y) = \max_{z\in[x,y]\cup[y,x]} g(z)$ for $x, y \in (0, \infty)$. We assume that $C_1 \equiv \int_0^1 \big[\frac{\check{g}(h_F(\alpha), h_G(\alpha))}{f(h_F(\alpha))}\big]^2 d\alpha < \infty$ and $C_2 \equiv \int_0^1 \big[\frac{h_F(\alpha)\check{g}(h_F(\alpha), h_G(\alpha))}{f(h_F(\alpha))}\big]^2 d\alpha < \infty$. Then,*

$$\int_0^1 [h_G(\alpha) - h_F(\alpha)]^2 d\alpha \geq \frac{|\mu_1(f) - \mu_1(g)|^2}{4C_1}, \qquad \int_0^1 [h_G(\alpha) - h_F(\alpha)]^2 d\alpha \geq \frac{|\mu_2(f) - \mu_2(g)|^2}{4C_2}.$$

We apply Lemma B.1 to $F(\cdot) = F_{\gamma_n}(\cdot; \sigma_0^2, \theta_0, T_1, T_2)$ and $G(\cdot) = F_{\gamma_n}(\cdot; \sigma^2, \theta, T_1, T_2)$. Define

$$\mu_1(\sigma^2, \theta) = \int x\, dF_{\gamma_n}(x; \sigma^2, \theta, T_1, T_2), \qquad \mu_2(\sigma^2, \theta) = \int x^2\, dF_{\gamma_n}(x; \sigma^2, \theta, T_1, T_2).$$

We now show that the quantities C_1, C_2 in Lemma B.1 are uniformly upper bounded by constants for all $(\sigma^2, \theta) \in \mathcal{J}_\sigma^2 \times J_\theta$. We only study C_2, and the analysis of C_1 is similar. By Knowles and Yin (2017); Ding (2020), the support of $F_{\gamma_n}(\cdot; \sigma^2, \theta, T_1, T_2)$ is in a compact subset of $(0, \infty)$, and the density is upper bounded by a constant; these constants are uniform for $(\sigma^2, \theta) \in \mathcal{J}_{\sigma^2} \times \mathcal{J}_\theta$. It follows that

$$C_2 \leq C \int_0^1 \Big[\frac{1}{f(h_F(\alpha))}\Big]^2 d\alpha = \int \frac{1}{f^2(x)} f(x) dx = \int \frac{1}{f(x)} dx.$$

Here we have used a change of variable $x = h_F(\alpha)$, where $\alpha = 1 - F(x)$ and $d\alpha = f(x)dx$. We then apply Theorem 3.3 of Ji (2020). Note that $F(\cdot) = F_{\gamma_n}(\cdot; \sigma_0^2, \theta_0, T_1, T_2)$ is the free multiplicative convolution between a truncated Gamma distribution and the standard MP distribution. These two distributions are compacted supported and have power law behavior on left/right ends. The conditions in Theorem 3.3 of Ji (2020) are satisfied for $t_\pm^\mu = 0$ (truncated Gamma) and $t_\pm^\nu = 1/2$ (MP law). By that theorem, the density of $F(\cdot)$ has a square-root decay at the left/right edge: Let $[b^-, b^+]$ be the support of $F(\cdot)$; then, $C^{-1} \leq f(x)/\sqrt{(x - b^-)(b^+ - x)} \leq C$ for $x \in [b^-, b^+]$. It yields hat

$$C_2 \leq \int_{b^-}^{b^+} \frac{C}{\sqrt{(x - b^-)(b^+ - x)}} dx = O(1).$$

We have verified that C_1 and C_2 in Lemma B.1 are uniformly upper bounded. As a result,

$$R^*(\sigma^2, \theta) \geq Cn\Big(\big|\mu_1(\sigma^2, \theta) - \mu_1(\sigma_0^2, \theta_0)\big|^2 + \big|\mu_2(\sigma^2, \theta) - \mu_2(\sigma_0^2, \theta_0)\big|^2\Big). \tag{B.21}$$

Below, we study $\mu_1(\sigma^2, \theta)$ and $\mu_2(\sigma^2, \theta)$. Note that $\mathrm{Gamma}(\theta, \theta/\sigma^2, \sigma^2 T_1, \sigma^2 T_2)$ is equivalent to $\sigma^2 \cdot \mathrm{Gamma}(\theta, \theta, T_1, T_2)$. Then, the distributions $F_{\gamma_n}(\cdot; \sigma^2, \theta, T_1, T_2)$ and $F_{\gamma_n}(\cdot; 1, \theta, T_1, T_2)$ also have such a connection. This implies $\mu_1(\sigma^2, \theta) = \sigma^2 \cdot \mu_1(1, \theta)$ and $\mu_2(\sigma^2, \theta) = \sigma^4 \cdot \mu_2(1, \theta)$. Define

$$\kappa(\theta) = \mu_2(\sigma^2, \theta)/[\mu_1(\sigma^2, \theta)]^2.$$

Consider a mapping M from $\mathbb{R}^2$ to $\mathbb{R}^2$, where $M(x, y) = (x, y/x^2)$. It maps $(\mu_1(\sigma^2, \theta), \mu_2(\sigma^2, \theta))$ to $(\mu_1(\sigma^2, \sigma^2), \kappa(\theta))$. The Jacobian matrix is

$$\begin{bmatrix} 1 & 0 \\ -2y/x^3 & 1/x^2 \end{bmatrix}.$$

When $(\sigma^2, \theta) \in \mathcal{J}_{\sigma^2} \times \mathcal{J}_\theta$, the vector $(\mu_1(\sigma^2, \theta), \mu_2(\sigma^2, \theta))$ is in a compact set. The spectral norm of Jacobian is uniformly upper bounded. It follows that

$$\begin{aligned} &\big|\mu_1(\sigma^2, \theta) - \mu_1(\sigma_0^2, \theta_0)\big|^2 + \big|\mu_2(\sigma^2, \theta) - \mu_2(\sigma_0^2, \theta_0)\big|^2 \\ \geq\ & C\Big(\big|\mu_1(\sigma^2, \theta) - \mu_1(\sigma_0^2, \theta_0)\big|^2 + \big|\kappa(\theta) - \kappa(\theta_0)\big|^2\Big). \end{aligned} \tag{B.22}$$

We then study $\mu_1(\sigma^2,\theta)$ and $\kappa(\theta)$. Denote by $\hat{F}(\cdot;\sigma^2,\theta,T_1,T_2)$ the ESD when (σ^2,θ) are true parameters. Write $\hat{\mu}_1(\sigma^2,\theta)=\int x d\hat{F}(x;\sigma^2,\theta,T_1,T_2)$ and $\hat{\mu}_2(\sigma^2,\theta)=\int x^2 d\hat{F}(x;\sigma^2,\theta,T_1,T_2)$. The converges of ESD to its theoretical limit yields that $|\hat{\mu}_1(\sigma^2,\theta)-\mu_1(\sigma^2,\theta)|\to 0$ and $|\hat{\mu}_2(\sigma^2,\theta)-\mu_2(\sigma^2,\theta)|\to 0$ in probabiliy. In fact, we have a stronger result (Knowles and Yin, 2017):

$$\big|\mathbb{E}[\hat{\mu}_1(\sigma^2,\theta)]-\mu_1(\sigma^2,\theta)\big|\prec n^{-1},\qquad \big|\mathbb{E}[\hat{\mu}_2(\sigma^2,\theta)]-\mu_2(\sigma^2,\theta)\big|\prec n^{-1}. \tag{B.23}$$

Here the expectation is with respect to the null model (i.e., $K=0$) with true parameters (σ^2,θ). The left hand sides above are non-stochastic quantities, and "$\prec n^{-1}$" is interpreted as "$\leq n^{-1+\epsilon}$ for any $\epsilon>0$." Since $\mu_1(\sigma^2,\theta)$ and $\mu_2(\sigma^2,\theta)$ are uniformly upper/lower bounded, it follows that

$$\Big|\hat{\kappa}(\theta)-\frac{\mathbb{E}[\hat{\mu}_2(\sigma^2,\theta)]}{\big(\mathbb{E}[\hat{\mu}_1(\sigma^2,\theta)]\big)^2}\Big|\prec n^{-1}. \tag{B.24}$$

By definition, we can also write $\hat{\mu}_1=\frac{1}{\tilde{p}}\sum_{i=1}^{\tilde{p}}\hat{\lambda}_i=\frac{1}{\tilde{p}}\mathrm{tr}(\boldsymbol{S})$ and $\hat{\mu}_2=\frac{1}{\tilde{p}}\sum_{i=1}^{\tilde{p}}\hat{\lambda}_i^2=\frac{1}{\tilde{p}}\|\boldsymbol{S}\|_F^2$, where $\boldsymbol{S}=\frac{1}{n}\boldsymbol{X}^\top\boldsymbol{X}$ is the sample covariance matrix under the null model of $K=0$. By Assumption 1, $\boldsymbol{X}=\boldsymbol{Y}\boldsymbol{\Sigma}^{1/2}$, where $\boldsymbol{Y}$ contains *iid* zero-mean, unit variance entries. Note that our purpose here is to approximate the moments of the theoretical limit of ESD, and we are flexible to choose the eigenvectors in $\boldsymbol{\Sigma}$. We choose $\boldsymbol{\xi}_k$ as the kth standard basis, and so $\boldsymbol{\Sigma}=\mathrm{diag}(\sigma_1^2,\sigma_2^2,\ldots,\sigma_p^2)$. By direct calculations,

$$\begin{aligned}
\mathbb{E}[\hat{\mu}_1(\sigma^2,\theta)] &= \frac{1}{n\tilde{p}}\mathbb{E}\Bigg[\sum_{j=1}^{p}\Big(\sum_{i=1}^{n}\sigma_j^2Y_{ij}^2\Big)\Bigg]=(\gamma_n\vee 1)\cdot\mathbb{E}[\sigma_1^2],\\
\mathbb{E}[\hat{\mu}_2(\sigma^2,\theta)] &= \frac{1}{n^2\tilde{p}}\mathbb{E}\Bigg[\sum_{j=1}^{p}\Big(\sum_{i=1}^{n}\sigma_j^2Y_{ij}^2\Big)^2+\sum_{1\leq j\neq\ell\leq p}\Big(\sum_{i=1}^{n}\sigma_j\sigma_\ell Y_{ij}Y_{i\ell}\Big)^2\Bigg]\\
&= \frac{1}{n^2\tilde{p}}\Big[np\,\mathbb{E}[\sigma_1^4]\,\mathbb{E}[Y_{11}^4]+pn(n-1)\,\mathbb{E}[\sigma_1^4]+p(p-1)n\big(\mathbb{E}[\sigma_1^2]\big)^2\Big]\\
&= O(n^{-1})+(\gamma_n\vee 1)\cdot\mathbb{E}[\sigma_1^4]+\gamma_n(\gamma_n\vee 1)\cdot\big(\mathbb{E}[\sigma_1^2]\big)^2.
\end{aligned}$$

Note that $\sigma_1^2/\sigma^2\sim\mathrm{Gamma}(\theta,\theta,T_1,T_2)$. The density of $\mathrm{Gamma}(\theta,\theta,T_1,T_2)$ is equal to $x^{\theta-1}e^{-\theta x}\cdot(\int_{T_1}^{T_2}z^{\theta-1}e^{-\theta z}dz)^{-1}$. We immediately have

$$\begin{aligned}
\mathbb{E}[\hat{\mu}_1(\sigma^2,\theta)] &= (\gamma_n\vee 1)\sigma^2\cdot\frac{\int_{T_1}^{T_2}x^{\theta}\exp(-\theta x)dx}{\int_{T_1}^{T_2}x^{\theta-1}\exp(-\theta x)dx}\\
\mathbb{E}[\hat{\mu}_2(\sigma^2,\theta)] &= O(\frac{1}{n})+(\gamma_n\vee 1)\frac{\sigma^4\int_{T_1}^{T_2}x^{\theta+1}\exp(-\theta x)dx}{\int_{T_1}^{T_2}x^{\theta-1}\exp(-\theta x)dx}+\gamma_n(\gamma_n\vee 1)\frac{\sigma^4\big[\int_{T_1}^{T_2}x^{\theta}\exp(-\theta x)dx\big]^2}{\big[\int_{T_1}^{T_2}x^{\theta-1}\exp(-\theta x)dx\big]^2}.
\end{aligned}$$

Define $\Psi(\theta)=\Psi(\theta;T_1,T_2)\equiv(\int_{T_1}^{T_2}x^{\theta}e^{-\theta x}dx)/(\int_{T_1}^{T_2}x^{\theta-1}e^{-\theta x}dx)$. Let $\Phi(\theta)$ be the same as in the statement of this theorem. We plug the above equations into (B.23)-(B.24) to get

$$\begin{aligned}
\mu_1(\sigma^2,\theta) &= (\gamma_n\vee 1)\sigma^2\cdot\Psi(\theta)+O_{\prec}(n^{-1}),\\
\kappa(\theta) &= \frac{1}{(\gamma_n\vee 1)}\cdot\Phi(\theta)+\frac{\gamma_n}{(\gamma_n\vee 1)}+O_{\prec}(n^{-1}).
\end{aligned} \tag{B.25}$$

Consider the mapping from (σ^2, θ) to $(\mu_1(\sigma^2, \theta),\ \kappa(\theta))$. The Jacobian matrix is

$$J = (\gamma_n \vee 1) \begin{bmatrix} \Psi(\theta) & \sigma^2 \cdot \Psi'(\theta) \\ 0 & \frac{1}{(\gamma_n \vee 1)^2} \cdot \Phi'(\theta) \end{bmatrix} + O_{\prec}(n^{-1}).$$

First, since $\mathcal{J}_\theta$ is a bounded set, $\Psi(\theta)$, $\Psi'(\theta)$ and $\Phi'(\theta)$ are uniformly upper bounded by constants. Second, we have $\Psi(\theta) > 0$ in a fixed compact set $\mathcal{J}_\theta$. As a result, $\Psi(\theta)$ must be uniformly lower bounded by a constant. Last, the assumption says that $\inf_{\theta \in \mathcal{J}_\theta} |\Phi'(\theta)| \geq \omega$, for a constant $\omega > 0$. Combining these arguments with the formula of the inverse of a 2×2 matrix, we have $\|J^{-1}\| \leq C$. It follows that

$$\begin{aligned} & \left|\mu_1(\sigma^2, \theta) - \mu_1(\sigma_0^2, \theta_0)\right|^2 + \left|\kappa(\theta) - \kappa(\theta_0)\right|^2 \\ \geq\ & C\Big(|\sigma^2 - \sigma_0^2|^2 + |\theta - \theta_0|^2\Big). \end{aligned} \tag{B.26}$$

We plug (B.26) into (B.22), and then into (B.21), and then combine it with (B.20). It gives (B.19). □

B.4 Proof of Lemma 2

Write

$$J_1(\theta) = (\int_{t_1}^{t_2} x^{\theta+1} exp(-\theta x)dx)(\int_{t_1}^{t_2} x^{\theta-1} exp(-\theta x)dx), \qquad J_2(\theta) = (\int_{t_1}^{t_2} x^{\theta} exp(-\theta x)dx)^2.$$

Then $\Psi(\theta) = J_1(\theta)/J_2(\theta)$ and

$$\Psi'(\theta) = \frac{J_1'(\theta)J_2(\theta) - J_1(\theta)J_2'(\theta)}{J_2(\theta)^2}. \tag{B.27}$$

By direct calculations,

$$\begin{aligned} J_1'(\theta) =& (\int_{t_1}^{t_2} \log(x)x^{\theta+1}exp(-\theta x)dx - \int_{t_1}^{t_2} x^{\theta+2}exp(-\theta x)dx)(\int_{t_1}^{t_2} x^{\theta-1}exp(-\theta x)dx) \\ &+ (\int_{t_1}^{t_2} \log(x)x^{\theta-1}exp(-\theta x)dx - \int_{t_1}^{t_2} x^{\theta}exp(-\theta x)dx)(\int_{t_1}^{t_2} x^{\theta+1}exp(-\theta x)dx), \\ J_2'(\theta) =& 2(\int_{t_1}^{t_2} x^{\theta}exp(-\theta x)dx)(\int_{t_1}^{t_2} \log(x)x^{\theta}exp(-\theta x)dx - \int_{t_1}^{t_2} x^{\theta+1}exp(-\theta x)dx). \end{aligned}$$

Let $L(\alpha, \theta; t_1, t_2)$ denote $\int_{t_1}^{t_2} \log(x)x^{\alpha}exp(-\theta x)dx$ and $I(\alpha, \theta; t_1, t_2)$ denote $\int_{t_1}^{t_2} x^{\alpha}exp(-\theta x)dx$. When not causing any confusion, we write them as $L(\alpha)$ and $I(\alpha)$. Then

$$J_1(\theta) = I(\theta+1) \times I(\theta-1), \quad J_2(\theta) = I(\theta)^2$$

$$J_1'(\theta) = (L(\theta+1) - I(\theta+2)) \times I(\theta-1) + (L(\theta-1) - I(\theta)) \times I(\theta+1)$$

$$J_2'(\theta) = 2(L(\theta) - I(\theta+1)) \times I(\theta)$$

Plugging them into (B.27), we have

$$\Psi'(\theta) = \frac{I(\theta+1)I(\theta-1)}{I(\theta)^2}\Big(\Big(\frac{L(\theta+1)}{I(\theta+1)}+\frac{L(\theta-1)}{I(\theta-1)}-2\frac{L(\theta)}{I(\theta)}\Big)-\Big(\frac{I(\theta+2)}{I(\theta+1)}+\frac{I(\theta)}{I(\theta-1)}-2\frac{I(\theta+1)}{I(\theta)}\Big)\Big).$$

Recall that we are interested in $\theta \in \mathcal{J}_\theta = [c, d]$. For $\alpha \in [c-1, d+2]$ and $\theta \in [c, d]$,

$$\int_0^\infty \log(x)x^\alpha exp(-\theta x)dx - L(\alpha, \theta; t_1, t_2) = \int_0^{t_1} \log(x)x^\alpha exp(-\theta x)dx + \int_{t_2}^\infty \log(x)x^\alpha exp(-\theta x)dx,$$

$$\Big|\int_0^{t_1} \log(x)x^\alpha exp(-\theta x)dx\Big| \leq \int_0^{t_1} (-\log(x))x^{c-1}exp(-cx)dx \to 0, \quad \text{as } t_1 \to 0,$$

$$\Big|\int_{t_2}^\infty \log(x)x^\alpha exp(-\theta x)dx\Big| \leq \int_{t_2}^\infty \log(x)x^{d+2}exp(-cx)dx \to 0, \quad \text{as } t_2 \to \infty.$$

This implies for $\alpha \in [c-1, d+2], \theta \in [c, d]$, as $(t_1, t_2) \to (0, \infty)$, $L(\alpha, \theta; t_1, t_2)$ uniformly converges to $L_0(\alpha, \theta) = \int_0^\infty \log(x)x^\alpha exp(-\theta x)dx$. By a similar argument, we can show that $I(\alpha, \theta; t_1, t_2)$ uniformly converges to $I_0(\alpha, \theta) = \int_0^\infty x^\alpha exp(-\theta x)dx$. From the uniform convergence and the fact that $I_0(\alpha, \theta)$ is lower bounded by a common positive constant when $\alpha \in [c-1, d+2], \theta \in [c, d]$, we know that as $(t_1, t_2) \to (0, \infty)$ we have $\Psi'(\theta)$ uniformly converges to

$$\frac{I_0(\theta+1)I_0(\theta-1)}{I_0(\theta)^2}\Big(\Big(\frac{L_0(\theta+1)}{I_0(\theta+1)}+\frac{L_0(\theta-1)}{I_0(\theta-1)}-2\frac{L_0(\theta)}{I_0(\theta)}\Big)-\Big(\frac{I_0(\theta+2)}{I_0(\theta+1)}+\frac{I_0(\theta)}{I_0(\theta-1)}-2\frac{I_0(\theta+1)}{I_0(\theta)}\Big)\Big),$$

for all $\theta \in [c, d]$. Here, $L_0(\alpha)$ and $I_0(\alpha)$ are short for $L_0(\alpha, \theta)$ and $I_0(\alpha, \theta)$. Let $Z \sim \text{Gamma}(\alpha, \theta)$ and let ψ denote the digamma function. By properties of the Gamma distribution,

$$\frac{I_0(\alpha, \theta)}{I_0(\alpha-1, \theta)} = \mathbb{E}(Z) = \frac{\alpha}{\theta}, \quad \frac{L_0(\alpha-1, \theta)}{I_0(\alpha-1, \theta)} = \mathbb{E}(\log(Z)) = \psi(\alpha) - \log(\theta).$$

Therefore, $\Psi'(\theta)$ uniformly converges to

$$\frac{\theta+1}{\theta}\Big(\Big(\psi(\theta+2)+\psi(\theta)-2\psi(\theta+1)\Big)-\Big(\frac{\theta+2}{\theta}+\frac{\theta}{\theta}-2\times\frac{\theta+1}{\theta}\Big)\Big) = \frac{\theta+1}{\theta}\Big(\frac{1}{\theta+1}-\frac{1}{\theta}\Big) = -\frac{1}{\theta^2}.$$

The first equation uses the recurrence relation of digamma function. By the uniform convergence, for any $\delta > 0$ there exists $0 < T_1^* < T_2^* < \infty$ such that $\sup_{\theta\in[c,d]} |\Psi'(\theta) - (-\frac{1}{\theta^2})| \leq \delta$. The claim follows by choosing $\delta = 1/d^2 - \omega$. □

B.5 Proof of Theorem 4

Let $d_j = \sigma_j^2 + \mu_j$ for $1 \leq k \leq K$ and $d_j = \sigma_j^2$ for $K+1 \leq j \leq p$. Then, $d_1, d_2, \ldots, d_p$ are all the eigenvalues of $\mathbf{\Sigma}$. Define

$$\hat{G}(x) = -\frac{1}{x} + \frac{\gamma}{p}\sum_{j=1}^p \frac{1}{x+\sigma_j^{-2}}. \tag{B.28}$$

By Lemma 2.2 and Condition 3.6 of Ding (2020), this function $\hat{G}(x)$ has 2 critical points $0 > \hat{x}_1 > \hat{x}_2$; furthermore, conditioning on $\mathbf{\Sigma}$, the ESD converges to a limit whose support is $[\hat{G}(\hat{x}_2), \hat{G}(\hat{x}_1)]$.

We apply Theorem 3.2 of Ding (2020). Using the first claim there, if $-1/d_k \geq \hat{x}_1 + n^{1/3}$ for each $1 \leq k \leq K$, then

$$|\hat{\lambda}_k - \hat{G}(-1/d_k)| \prec n^{-1/2}(-1/d_k - \hat{x}_1)^{1/2}, \qquad 1 \leq k \leq K.$$

Using the second claim there,

$$|\hat{\lambda}_{K+1} - \hat{G}(\hat{x}_1)| \prec n^{-2/3}.$$

The above "stochastic dominance" arguments are conditioning on $\mathbf{\Sigma}$. Under Model (13) for $\mathbf{\Sigma}$, $\hat{G}(x)$ converges weakly to $G(x)$ defined in (16), and the critical points $(\hat{x}_1, \hat{x}_2)$ also converge to (x_1^*, x_2^*), the critical points of $G(x)$, almost surely. Replacing $\hat{G}(\cdot)$ and $\hat{x}_1$ by $G(\cdot)$ and x_1^* in the above inequalities has a negligible effect (e.g., see Example 3.9 of Ding (2020)). It follows that

$$\max_{1 \leq k \leq K} |\hat{\lambda}_k - G(-1/d_k)| \prec n^{-1/2}, \qquad |\hat{\lambda}_{K+1} - G(x_1^*)| \prec n^{-2/3}.$$

Note that $d_k = \sigma_k^2 + \mu_k \geq \mu_K + T_1$. The assumption of $-1/(T_1 + \mu_K) \geq x_1^* + \tau$ guarantees that $G(-1/d_k) \geq G(-1/(T_1 + \mu_K)) \geq G(x_1^* + \tau) \geq G(x_1^*) + c$, where $c > 0$ is a constant. Therefore,

$$\min_{1 \leq k \leq K} \{\hat{\lambda}_k\} - G(x_1^*) \ \geq \ c + O_{\prec}(n^{-1/2}), \qquad \hat{\lambda}_{K+1} - G(x_1^*) \ \prec \ n^{-2/3}, \tag{B.29}$$

where $O_{\prec}(b_n)$ means the absolute value is $\prec b_n$.

The estimator $\hat{K}$ is obtained by thresholding the empirical eigenvalues at $\hat{T}_\beta$ as in (15). Let $\hat{\lambda}_1^* = \hat{\lambda}_1^*(\sigma^2, \theta)$ be the largest empirical eigenvalue under the null model ($K = 0$) with parameters (σ^2, θ). Applying Theorem 3.2 of Ding (2020) again, for the same x_1^* as above,

$$|\hat{\lambda}_1^*(\sigma^2, \theta) - G(x_1^*)| \prec n^{-2/3}.$$

In Theorem 3, we have shown $|\hat{\sigma}^2 - \sigma^2| \prec n^{-1}$ and $|\hat{\theta} - \theta| \prec n^{-1}$. Now, let $\hat{x}_1^*$ be the largest critical point of $G(x)$ in (16), except that (σ^2, θ) is replaced by $(\hat{\sigma}^2, \hat{\theta})$. Then, we have $|G(\hat{x}_1^*) - G(x_1^*)| = O\big(\sqrt{|\hat{\sigma}^2 - \sigma^2|^2 + |\hat{\theta} - \theta|^2}\big) \prec n^{-1}$ and $|\hat{\lambda}_1^*(\hat{\sigma}^2, \hat{\theta}) - G(\hat{x}_1^*)| \prec n^{-2/3}$. Combining these claims gives

$$|\hat{\lambda}_1^*(\hat{\sigma}^2, \hat{\theta}) - G(x_1^*)| \prec n^{-2/3}.$$

Note that $\hat{T}_\beta$ is the $(1 - \beta)$-quantile of $\hat{\lambda}_1^*(\hat{\sigma}^2, \hat{\theta})$ (it means the quantile of $\hat{\lambda}_1^*(\sigma^2, \theta)$ evaluated at $(\sigma^2, \theta) = (\hat{\sigma}^2, \hat{\theta})$). The above inequality implies that there exists $\beta \to 0$ properly slow such that

$$n^{-2/3} \ \ll \ \hat{T}_\beta - G(x_1^*) \ \ll \ 1. \tag{B.30}$$

It follows from (B.29) and (B.30) that $\hat{K} = K$. $\square$

B.6 Proof of Lemma B.1

We only show the second inequality. The proof of the first inequality is similar and thus omitted. Note that $f(x) - g(x)$ is the derivative of $\bar{G}(x) - \bar{F}(x)$. Using integration by part, we have

$$\mu_2(f) - \mu_2(g) = \int x^2[f(x) - g(x)]dx = 2\int x[\bar{F}(x) - \bar{G}(x)]dx. \tag{B.31}$$

We consider a change of variable from x to $\alpha = \bar{F}(x)$. Note that $x = h_F(\alpha)$. It follows that

$$\begin{aligned}\int x[\bar{F}(x) - \bar{G}(x)]dx &= \int_0^1 h_F(\alpha)\big[\alpha - \bar{G}(h_F(\alpha))\big]h_F'(\alpha)d\alpha \\ &= \int_0^1 h_F(\alpha)\big[\bar{G}(h_G(\alpha)) - \bar{G}(h_F(\alpha))\big]h_F'(\alpha)d\alpha.\end{aligned}$$

By mean value theorem, there is x^* between $h_F(\alpha)$ and $h_G(\alpha)$ such that $\bar{G}(h_G(\alpha)) - \bar{G}(h_F(\alpha)) = -g(x^*)[h_G(\alpha) - h_F(\alpha)]$. Recall that $\breve{g}(x,y) = \max_{z\in[x,y]\cup[y,x]} g(z)$. It follows that $|\bar{G}(h_G(\alpha)) - \bar{G}(h_F(\alpha)| \leq \breve{g}(h_F(\alpha), h_G(\alpha)) \cdot |h_G(\alpha) - h_F(\alpha)|$. We plug it into the above equation to get

$$\Big|\int x[\bar{F}(x) - \bar{G}(x)]dx\Big| \leq \int_0^1 |h_G(\alpha)) - h_F(\alpha)| \cdot \big|h_F(\alpha)\,\breve{g}\big(h_F(\alpha), h_G(\alpha)\big)h_F'(\alpha)\big|d\alpha.$$

Since $h_F(\cdot) = \bar{F}^{-1}$, we have $h_F'(\alpha) = -1/f(h_F(\alpha))$. It follows that

$$\begin{aligned}\Big|\int x[\bar{F}(x) - \bar{G}(x)]dx\Big| &\leq \int_0^1 |h_G(\alpha) - h_F(\alpha)| \cdot \frac{h_F(\alpha)\cdot\breve{g}(h_F(\alpha), h_G(\alpha))}{f(h_F(\alpha))}d\alpha \\ &\leq \sqrt{\int_0^1 |h_G(\alpha) - h_F(\alpha)|^2 d\alpha}\,\sqrt{\int_0^1 \Big[\frac{h_F(\alpha)\cdot\breve{g}(h_F(\alpha), h_G(\alpha))}{f(h_F(\alpha))}\Big]^2 d\alpha} \\ &\leq \sqrt{\int_0^1 |h_G(\alpha) - h_F(\alpha)|^2 d\alpha}\cdot\sqrt{C_2}.\end{aligned} \tag{B.32}$$

Combining (B.31)-(B.32) gives the claim. □

C Robustness of BEMA on real data

For the two real data sets in Section 6, we apply BEMA with different values of α. The results are presented in the tables below. Both the point estimator and the confidence interval are very stable as long as α is in a reasonable range.

References

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	BEMA (0.1)	BEMA (0.2)	BEMA (0.3)	BEMA (0.4)
$\hat{\theta}$	0.343	0.288	0.281	0.270
$\hat{\sigma}^2$	0.869	0.926	0.949	1
$\hat{K}$ ($\beta = 0.1$)	1	1	1	1
90% quantile	16.074	19.231	20.261	21.944
10% quantile	9.379	10.872	11.186	12.098
confidence interval	[1,4]	[1,4]	[1,4]	[1,2]

Table 1: Lung Cancer data. BEMA is applied with $\alpha \in \{0.1, 0.2, 0.3, 0.4\}$ (denoted as BEMA (α) in the table). The quantiles are from Gamma$(\hat{\theta}, \hat{\theta}/\hat{\sigma}^2)$, and they are used to construct the 80% confidence interval.

	BEMA (0.1)	BEMA (0.2)	BEMA (0.3)	BEMA (0.4)
$\hat{\theta}$	4.256	4.239	4.198	4.261
$\hat{\sigma}^2$	0.3779	0.3780	0.3782	0.3783
$\hat{K}$ ($\beta = 0.1$)	28	28	28	28
90% quantile	6.895	6.899	6.909	6.903
10% quantile	6.822	6.829	6.838	6.831
confidence interval	[28,30]	[28,30]	[28,29]	[28,30]

Table 2: 1000 Genomes data. BEMA is applied with $\alpha \in \{0.1, 0.2, 0.3, 0.4\}$ (denoted as BEMA (α) in the table). The quantiles are from Gamma$(\hat{\theta}, \hat{\theta}/\hat{\sigma}^2)$, and they are used to construct the 80% confidence interval.

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