Principal components of spiked covariance matrices in the supercritical regime

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In this paper, we study the asymptotic behavior of the extreme eigenvalues and eigenvectors of the spiked covariance matrices, in the supercritical regime. Specifically, we derive the joint distribution of the extreme eigenvalues and the generalized components of their associated eigenvectors in this regime.

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1. Introduction

In this paper, we consider the sample covariance matrices of the form

\[ Q = TXX^*T^*, \]

(1.1)

where \( T \) is a \( M \times M \) deterministic matrix and \( X \) is a \( M \times N \) random matrix with independent entries. Further, we assume that the population covariance matrix \( \Sigma := TT^* \) admits the following form

\[ \Sigma = I_M + S, \]

(1.2)

where \( S \) is a fixed-rank deterministic Hermitian matrix.

Throughout the paper, we make the following assumptions.

Assumption 1.1.

(i)(On dimensions): We assume that \( M \equiv M(N) \) and \( N \) are comparable and there exist constants \( \tau_2 > \tau_1 > 0 \) such that

\[ y \equiv y_N = M/N \in (\tau_1, \tau_2). \]

(ii)(On \( S \)): We assume that \( S \) admits the following spectral decomposition

\[ S = \sum_{i=1}^r d_i v_i v_i^*, \]

(1.3)

where \( r \geq 1 \) is a fixed integer. Here \( d_1 > \cdots > d_r > 0 \) are the ordered eigenvalues of \( S \), and \( v_i = (v_{i1}, \ldots, v_{iM})^T \)'s are the associated unit eigenvectors.

(iii)(On \( X \)): For the matrix \( X = (x_{ij}) \), we assume that the entries \( x_{ij} \equiv x_{ij}(N) \) are real random variables satisfying

\[ \mathbb{E} x_{ij} = 0, \quad \mathbb{E} x_{ij}^2 = 1/N. \]

Moreover, we assume the existence of large moments, i.e., for any integer \( p \geq 3 \), there exists a constant \( C_p > 0 \), such that

\[ \mathbb{E} |\sqrt{N} x_{ij}|^p \leq C_p < \infty. \]

We further assume that all \( \sqrt{N} x_{ij} \)'s possess the same 3rd and 4th cumulants, which are denoted by \( \kappa_3 \) and \( \kappa_4 \) respectively.

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We denote by $\mu_1 \geq \cdots \geq \mu_M$ the ordered eigenvalues of $Q$ and $\xi_i$ the unit eigenvector associated with $\mu_i$. The matrix model $Q$ is usually referred to as the spiked covariance matrix in literature. In the context of Random Matrix Theory (RMT), this model was first studied by Johnstone in [26]. The primary interest of the spiked model $Q$ lies in the asymptotic behavior of a few largest $\mu_i$'s and the associated $\xi_i$'s when $N$ is large, under various assumptions of $d_i$'s and $v_i$'s. Significant progress has been made on this topic, in the last few years. It has been well known since the seminal work of Baik, Ben Arous and Péché [3] that the largest eigenvalues $\mu_i$'s undergo a phase transition (BBP transition) w.r.t. the size of $d_i$'s. On the level of the first order limit, when $d_i > \sqrt{y}$, the eigenvalue $\mu_i$ jumps out of the support of the Marchenko-Pastur law (MP law) and converges to a limit determined by $d_i$, while in the case of $d_i \leq \sqrt{y}$ it sticks to the right end of the MP law $(1 + \sqrt{y})^2$. On the level of the second order fluctuation, it was revealed in [3] that a phase transition for $\mu_i$ takes place in the regime $d_i - \sqrt{y} \sim N^{-\frac{1}{2}}$. Specifically, if $d_i - \sqrt{y} \ll N^{-\frac{1}{2}}$ (subcritical regime), the eigenvalue $\mu_i$ still admits the Tracy-Widom type distribution; if $d_i - \sqrt{y} \gg N^{-\frac{1}{2}}$ (supercritical regime), the eigenvalue $\mu_i$ is asymptotically Gaussian; while if $d_i - \sqrt{y} \sim N^{-\frac{1}{2}}$ (critical regime), the limiting distribution of the eigenvalue $\mu_i$ is a mixture of Tracy-Widom and Gaussian. The works [26] and [3] are on real and complex spiked Gaussian covariance matrices respectively. On extreme eigenvalues, further study for more generally distributed covariance matrices can be found in [4, 16, 8, 37, 1, 2, 11, 21]. The limiting behavior of the extreme eigenvalues have also been studied for various related models, such as the finite-rank deformation of Wigner matrices [16, 8, 18, 19, 24, 29, 30, 38, 40], the signal-plus-noise model [9, 33, 20], the general spiked $\beta$ ensemble [12, 13], and also the finite-rank deformation of general unitary/orthogonal invariant matrices [16, 6, 7].

In contrast, the study on the limiting behavior of the eigenvectors associated with the extreme eigenvalues is much less. On the level of the first order limit, it is known that the $\xi_i$'s are delocalized and purely noisy in the subcritical regime, but has a bias on the direction of $v_i$ in the supercritical regime. We refer to [10, 9, 15, 20, 37, 11, 21] for more details of such a phenomenon. It was recently noticed in [11] that a $d_i$ close to the critical point can cause a bias even for the non-outlier eigenvectors. On the level of the second order fluctuation, it was proved in [11] that the eigenvectors are asymptotically Gaussian in the subcritical regime, for the spiked covariance matrices. In the supercritical regime, a non-universality phenomenon was shown in [17] and [5] for the eigenvector distribution for the finite-rank deformation of Wigner matrices and the signal-plus-noise model, respectively. The non-universality phenomenon in the supercritical regime has been previously observed in [18, 29, 30] for the extreme eigenvalues of the finite-rank deformation of Wigner matrices. Here we also refer to [36, 27, 23] for related study on the extreme eigenstructures of various finite-rank deformed models from more statistical perspective.

In this paper, we will establish the joint distribution of the extreme eigenvalues and the associated eigenvectors for the spiked covariance matrices, in the supercritical regime. This is the primary goal of the Principal Component Analysis from statistics point of view. More specifically, in this paper, we are interested in the joint distribution of the largest $\mu_i$'s and the generalized component of the top eigenvectors, i.e., the projections of those eigenvectors onto a general direction. More specifically, let $w \in S^{M-1}$ be any deterministic unit vector. We will study the limiting distribution of $(\mu_i, |\langle w, \xi_i \rangle|^2)$ in the supercritical regime.

Since we will focus on the supercritical regime, we further make the following assumption. For brevity, in the sequel, we use the notation $[1, m] := \{1, \cdots, m\}$.

**Assumption 1.2.** There exists a fixed $\delta > 0$ and an integer $r_0 \in [1, r]$ such that for $i \in [1, r_0]$,

\[ d_i \geq y^{1/2} + \delta \quad \text{and} \quad \min_{j \neq i \in [1, r_0]} |d_j - d_i| \geq \delta. \tag{1.4} \]

**Remark 1.3.** The first inequality ensures the existence of the supercritical regime, and the second inequality ensures that those outlying eigenvalues are well-separated from each other. In both inequalities, the fixed constant $\delta$ may be replaced by smaller $N$-dependent ones. One can also consider the case that $d_i$'s are not simple, i.e., the multiplicity of certain $d_i$ is larger than 1. We refer to [11] for related discussion. Further extension along this direction will be considered in the future work.

Our main results will be stated in Theorem 1.6, after necessary notations are introduced. For simplicity, we will work with the setting

\[ T = \Sigma^1. \tag{1.5} \]

But our results hold for more general $T$ satisfying $\Sigma = TT^*$. Extension along this direction has been discussed in Section 8 of [11]. We refer to Remark 1.9 for more details.
For any \( w \in S_{R}^{M-1} \), we do the decomposition
\[
  w = \sum_{j=1}^{r} \langle w, v_j \rangle v_j + u, \quad \text{where } u \in \text{Span}\{v_1, \ldots, v_r\}.
\] (1.6)

Hereafter, we take (1.6) as the definition of \( u \). Further, we introduce the following two shorthand notations
\[
  s_i := \frac{2\sqrt{1 + d_i(d_i - y)}}{d_i^2(d_i + y)} \left( \sum_{j \neq i} \langle w, v_j \rangle \frac{d_j \sqrt{d_j + 1}}{d_j - d_i} v_j + u \right),
\]
\[
  \hat{v}_i := \langle w, v_i \rangle \frac{y(1 + d_i)}{d_i^2(d_i + y)} \left( 1 + \frac{d_i(1 + 1)}{d_i + y} \right) v_i.
\] (1.7)

For any vectors \( a_\gamma = (a_\gamma(i)) \in \mathbb{R}^M \), \( \gamma = 1, 2, 3 \), we set the notations
\[
  s_k(a_1) := \sum_{j=1}^{M} a_1(j)^k, \quad s_{k,l}(a_1, a_2) := \sum_{j=1}^{M} a_1(j)^k a_2(j)^l,
\]
\[
  s_{k,l,t}(a_1, a_2, a_3) := \sum_{j=1}^{M} a_1(j)^k a_2(j)^l a_3(j)^t.
\] (1.8)

We adopt the notion of stochastic domination introduced in [22], which provides a precise statement of the form “\( X_N \) is bounded by \( Y_N \) up to a small power of \( N \) with high probability”.

**Definition 1.4. (Stochastic domination)** Let
\[
  X = (X_N(u) : N \in \mathbb{N}, u \in U_N), \quad Y = (Y_N(u) : N \in \mathbb{N}, u \in U_N)
\]
be two families of nonnegative random variables, where \( U_N \) is a possibly \( N \)-dependent parameter set. We say that \( X \) is bounded by \( Y \), uniformly in \( u \), if for all small \( \epsilon > 0 \) and large \( \phi > 0 \), we have
\[
  \sup_{u \in U_N} \mathbb{P}(X_N(u) > N^\epsilon Y_N(u)) \leq N^{-\phi}
\]
for large \( N \geq N_0(\epsilon, \phi) \). Throughout the paper, we use the notation \( X = O_\prec(Y) \) or \( X \prec Y \) when \( X \) is stochastically bounded by \( Y \) uniformly in \( u \).

In addition, we also say that an \( n \)-dependent event \( E \equiv E(n) \) holds with high probability if, for any large \( \varphi > 0 \),
\[
  \mathbb{P}(E) \geq 1 - n^{-\varphi},
\]
for sufficiently large \( n \geq n_0(\varphi) \).

It is convenient to introduce the following notion of convergence in distribution.

**Definition 1.5.** Two sequences of random vectors, \( X_n \in \mathbb{R}^k \) and \( Y_n \in \mathbb{R}^k \), \( n \geq 1 \), are asymptotically equal in distribution, denoted as \( X_n \simeq Y_n \), if they are tight and satisfy
\[
  \lim_{n \to \infty} \mathbb{E}[f(X_n)] = \mathbb{E}[f(Y_n)] = 0
\]
for any bounded continuous function \( f : \mathbb{R}^k \to \mathbb{R} \).

Furthermore, for a vector \( a \), we use \( \|a\| \) to denote its \( \ell^2 \)-norm. Let \( \{e_i\}_{i=1}^{M} \) be the standard basis of \( \mathbb{R}^M \). For a random variable \( \xi \), we denote its \( l \)th cumulant by \( \kappa_l(\xi) \).

With the above notations, we can now state our main Theorem.

**Theorem 1.6.** Suppose that Assumptions 1.1, 1.2 and the setting (1.5) hold. Then for any deterministic unit vector \( w \in S_{R}^{M-1} \) and \( i \in [1, r_0] \), there exist random variables \( \Upsilon_i, \Theta_i^w \) and \( \Lambda_i^w \) such that
\[
  \mu_i = 1 + d_i + y \frac{y}{d_i} + \frac{1}{\sqrt{N}} \Upsilon_i + O_\prec \left( \frac{1}{\sqrt{N}} \right),
\] (1.9)
and
\[
  |\langle w, \xi_i \rangle|^2 = \frac{d_i^2 - y}{d_i(d_i + y)} |\langle w, v_i \rangle|^2 + \frac{\langle w, v_i \rangle}{\sqrt{N}} \Theta_i^w + \frac{1}{N} \Lambda_i^w + O_\prec \left( \frac{|\langle w, v_i \rangle|}{N} \right) + O_\prec \left( \frac{N^{-\frac{3}{2}}}{} \right),
\] (1.10)
and
\[
  (\Upsilon_i, \Theta_i^w, \Lambda_i^w) \simeq \mathcal{N}(0, V_i^w).
\] (1.11)
Here, $\mathcal{N}(0, \mathcal{V}^w)$ represents a Gaussian vector with mean 0 and covariance matrix $\mathcal{V}^w_i$ defined entrywise by

$$
\mathcal{V}^w_i(1, 1) = \frac{(1 + d_i)^2(d_i^2 - y)^2}{d_i^4} \frac{2d_i^2}{d_i^2 - y} + \kappa_4s_4(v_{ij}),
$$

$$
\mathcal{V}^w_i(1, 2) = (w, v_{ij}) \frac{2y(1 + d_i)^3}{d_i(d_i + y)^2} + \frac{(1 + d_i)(d_i^2 - y)}{d_i^2} \kappa_4s_{1,3}(\hat{v}_i + s_i, v_{ij}),
$$

$$
\mathcal{V}^w_i(1, 3) = -\frac{d_i + 1}{2d_i} \sqrt{\frac{(d_i + y)(d_i^2 - y)}{d_i}} s_{1,3}(s_i, v_{ij}),
$$

$$
\mathcal{V}^w_i(2, 2) = \frac{d_i^2}{d_i^2 - y} \|\hat{v}_i + s_i\|^2 + \kappa_4s_{2,2}(\hat{v}_i + s_i, v_{ij})
$$

$$
+ (w, v_{ij}) \frac{d_i y + d_i + 2y}{d_i + y} s_{1,1}(\hat{v}_i, v_{ij}) + (w, v_{ij}) \frac{2y(1 + d_i)(d_i^2 - y)}{d_i^2(d_i + y)^3},
$$

$$
\mathcal{V}^w_i(2, 3) = \frac{1}{2} \sqrt{\frac{d_i d_i + y}{d_i^2 - y}} \left( \frac{d_i^2}{d_i^2 - y} \|s_i\|^2 + \kappa_4s_{2,2}(s_i, v_{ij}) - \kappa_4s_{1,1,2}(s_i, v_{ij}) \right),
$$

$$
\mathcal{V}^w_i(3, 3) = \frac{d_i(d_i + y)}{4(d_i^2 - y)} \left( \frac{d_i^2}{d_i^2 - y} \|s_i\|^2 + \kappa_4s_{2,2}(s_i, v_{ij}) \right). \quad (1.12)
$$

Remark 1.7. Here we remark that in the supercritical regime, a generalized CLT for the eigenvalues has been established in [1] previously. On eigenvectors, in the supercritical regime, a large deviation estimate for the generalized components of the eigenvectors has also been given in [11]. In addition, the Gaussianity of the generalized components of eigenvectors in the subcritical regime has been proved in [11].

Remark 1.8. In Assumption 1.1, we assume that the third and fourth cumulants of all $\sqrt{N}x_{ij}$’s are the same. But our proof can be directly adapted to the more general setting that the third and fourth cumulants of $\sqrt{N}x_{ij}$’s are (ij)-dependent.

Remark 1.9. In (1.5), we assumed $T = \Sigma^{\pm}$. But our result holds under much more general assumption on T. We can indeed extend our result to the matrix $Q = TXX^*T^*$ with $(M + k) \times N$ random matrix X and $M \times (M + k)$ matrix T. As long as $k \in \mathbb{N}$ is fixed and $TT^* = \Sigma$ satisfying (1.2), our result remains true. Such an extension has been discussed in Section 8 of [11]. The discussion in [11] relies on the rewriting $Q = TXX^*T^* = \Sigma^{\pm}YY^*\Sigma^{\pm}$, where $Y = (I_M 0)O$. Here 0 is the $M \times k$ zero matrix and $O$ is some $(M + k) \times (M + k)$ orthogonal matrix. It will be clear that our arguments in the proof of Theorem 1.6 are valid, as long as the isotropic local law of the matrix $XX^*$ (c.f., Theorem 2.1) holds. So here it would be sufficient to have the isotropic local law for the matrix $YY^*$, which has been demonstrated in Theorem 8.1 of [11].

In the sequel, we provide some simple examples with special choices of $w$.

Example 1.10. Let $w = v_i$. The expansion (1.10) can be simplified to

$$
|\langle v_i, \xi_i \rangle|^2 = \frac{d_i^2}{d_i^2 - y} \|\hat{v}_i\|^2 + \frac{1}{\sqrt{N}} \Theta_i + O_\infty \left( \frac{1}{N} \right), \quad (1.13)
$$

and $\Theta_i \simeq \mathcal{N}(0, \mathcal{V}_i(2, 2))$ with explicit expression

$$
\mathcal{V}_i(2, 2) = \frac{d_i^2}{d_i^2 - y} \|\hat{v}_i\|^2 + \frac{d_i y + d_i + 2y}{d_i + y} s_{1,1}(\hat{v}_i, v_{ij}) + \frac{y(1 + d_i)(d_i^2 - y)}{d_i^2(d_i + y)^3} + \kappa_4s_{2,2}(\hat{v}_i, v_{ij}). \quad (1.14)
$$

Here

$$
\hat{v}_i = \frac{y(1 + d_i)}{d_i^2(d_i + y)^3} \left( 1 + \frac{d_i(d_i + 1)}{d_i + y} \right) v_i.
$$

Example 1.11. Let $w \in \{v_i\}^\perp$. In this case, we have $\hat{v}_i = 0$. We then get from (1.10) that

$$
|\langle w, \xi_i \rangle|^2 = \frac{1}{N} \langle \Lambda^w_i \rangle^2 + O_\infty(N^{-\frac{1}{2}}), \quad (1.15)
$$

and $\Lambda^w_i \simeq \mathcal{N}(0, \mathcal{V}_i^w(3, 3))$ where

$$
\mathcal{V}_i^w(3, 3) = \frac{d_i(d_i + y)}{4(d_i^2 - y)} \left( \frac{d_i^2}{d_i^2 - y} \|s_i\|^2 + \kappa_4s_{2,2}(s_i, v_{ij}) \right). \quad (1.15)
$$
with \( \zeta \), defined in the first equation of (1.7).

**Organization**: The paper is organized as the following: In Section 2, we introduce some basic notions and preliminary results for later discussion. Section 3 is devoted to the Green function representations of our eigenvalue and eigenvector statistics. Then in Section 4, we prove our main result, Theorem 1.6, based on a key technical recursive moment estimate for some Green function statistics, see Proposition 4.2. The proof of Proposition 4.2 is then postponed to Section 5. In addition, in Appendix A, we collect some basic formulas concerning the derivatives of Green function, for the convenience of the reader.

2. **Preliminaries**

In this section, we collect some basic notions and preliminary results which will be used in the proof of our main theorem. A key technical input is the isotropic local law from [14, 31].

2.1. **Basic notions.** In the sequel, we denote the Green function of \( Q \) by

\[
G(z) := (Q - z)^{-1}, \quad z \in \mathbb{C}^+.
\]

The matrix \( Q \) can be regarded as a finite-rank perturbation of the matrix \( H := XX^* \). In the sequel, we also need to consider \( H := X^*X \) which shares the same non-zero eigenvalues with \( H \). We further denote the Green functions of \( H \) and \( \mathcal{H} \) respectively by

\[
G_1(z) := (XX^* - z)^{-1}, \quad G_2(z) := (X^*X - z)^{-1}, \quad z \in \mathbb{C}^+.
\]

(2.1)

We also denote the normalized traces of \( G_1(z) \) and \( G_2(z) \) by

\[
m_{1N}(z) := \frac{1}{M} \text{Tr} G_1(z) = \int (x - z)^{-1} dF_{1N}(x), \quad m_{2N}(z) := \frac{1}{N} \text{Tr} G_2(z) = \int (x - z)^{-1} dF_{2N}(x),
\]

where \( F_{1N}(x) \), \( F_{2N}(x) \) are the empirical distributions of \( H \) and \( \mathcal{H} \) respectively, i.e.,

\[
F_{1N}(x) := \frac{1}{M} \sum_{i=1}^{M} \mathbb{I}(\lambda_i(H) \leq x), \quad F_{2N}(x) := \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(\lambda_i(\mathcal{H}) \leq x).
\]

Here we used \( \lambda_i(H) \) and \( \lambda_i(\mathcal{H}) \) to denote the \( i \)-th largest eigenvalue of \( H \) and \( \mathcal{H} \), respectively.

It is well-known since [35] that \( F_{1N}(x) \) and \( F_{2N}(x) \) converge weakly (a.s.) to the Marchenko-Pastur laws \( \nu_{MP,1} \) and \( \nu_{MP,2} \) (respectively) given below

\[
\nu_{MP,1}(dx) := \frac{1}{2 \pi x y} \sqrt{((\lambda_+ - x)(x - \lambda_-))} \, dx + \left(1 - \frac{1}{y}\right) \delta(dx),
\]

\[
\nu_{MP,2}(dx) := \frac{1}{2 \pi x} \sqrt{((\lambda_+ - x)(x - \lambda_-))} \, dx + (1 - y) \delta(dx),
\]

(2.2)

where \( \lambda_\pm := (1 \pm \sqrt{y})^2 \). Note that \( m_{1N} \) and \( m_{2N} \) can be regarded as the Stieltjes transforms of \( F_{1N} \) and \( F_{2N} \), respectively. We further define their deterministic counterparts, i.e., Stieltjes transforms of \( \nu_{MP,1}, \nu_{MP,2} \), by \( m_1(z), m_2(z) \), respectively, i.e.,

\[
m_1(z) := \int (x - z)^{-1} \nu_{MP,1}(dx), \quad m_2(z) := \int (x - z)^{-1} \nu_{MP,2}(dx).
\]

From the definition (2.2), it is elementary to compute

\[
m_1(z) = \frac{1 - y - z + i \sqrt{(\lambda_+ - z)(z - \lambda_-)}}{2zy}, \quad m_2(z) = \frac{y - 1 - z + i \sqrt{(\lambda_+ - z)(z - \lambda_-)}}{2z},
\]

(2.3)

where the square root is taken with a branch cut on the negative real axis. Equivalently, we can also characterize \( m_1(z), m_2(z) \) as the unique solutions from \( \mathbb{C}^+ \) to \( \mathbb{C}^+ \) to the equations

\[
zm_1^2 + [z - (1 - y)]m_1 + 1 = 0, \quad zm_2^2 + [z + (1 - y)]m_2 + 1 = 0.
\]

(2.4)

Using (2.3) and (2.4), one can easily derive the following identities

\[
m_1 = -\frac{1}{z(1 + m_2)}, \quad 1 + zm_1 = \frac{1 + zm_2}{y}, \quad m_1 ((zm_2)' + 1) = \frac{m_1'}{m_1},
\]

(2.5)

which will be used in the later discussions.
2.2. Isotropic local law. In this section, we state the isotropic local law from [14, 31] together with some consequences which will serve as the main technical inputs in the proofs. We first introduce the following domain. For a small (but fixed) $\tau > 0$, we set
\[ \mathcal{D} \equiv \mathcal{D}(\tau) := \{ z = E + \mathbf{i} \eta \in \mathbb{C} : \lambda_{+} + \tau \leq E \leq \tau^{-1}, 0 < \eta \leq \tau^{-1} \}. \tag{2.6} \]
Conventionally, for $a = 1, 2$, we denote by $\mathcal{G}_a^0$ and $\mathcal{G}_a^{(l)}$ the $l$-th power of $\mathcal{G}_a$ and the $l$-th derivative of $\mathcal{G}_a$ w.r.t. $z$, respectively. With the above notation, we have

**Theorem 2.1.** Let $\tau > 0$ in (2.6) be a small but fixed constant. Let $\mathbf{u}, \mathbf{v} \in \mathbb{C}^M$ be two deterministic unit vectors. Suppose $X$ satisfies Assumption 1.1. Then, for any given $l \in \mathbb{N}$ and $a = 1, 2$, we have
\[
\begin{align*}
|\langle \mathbf{u}, \mathcal{G}_a^{(l)}(z)\mathbf{v} \rangle - m_a^{(l)}(z)\langle \mathbf{u}, \mathbf{v} \rangle| &= O_\prec\left( \frac{3m_a(z)}{\eta N} \right), \\
|\langle \mathbf{u}, \mathbf{X}^* \mathcal{G}_a^l(z)\mathbf{v} \rangle| &= O_\prec\left( \frac{3m_a(z)}{\eta N} \right), \\
|m_{a\mathcal{N}}(z) - m_a(z)| &= O_\prec\left( \frac{1}{N} \right),
\end{align*}
\]
uniformly in $z \in \mathcal{D}$.

**Remark 2.2.** The case of $l = 0$ is directly from the isotropic law in Theorem 3.12 of [14] and the anisotropic law in Theorem 3.7 of [31]. For other $l \geq 1$, we can derive the estimate easily from the case $l = 0$ by using Cauchy integral. We also remark here that the original isotropic local laws in [14, 31] were stated in much larger domains which also include the bulk and edge regimes of the MP law. But here we only need the result for the domain far away from the support of the MP law.

Further, in the following lemma, we collect some basic estimates of $m_1$ and $m_2$ which can be verified by elementary computations.

**Lemma 2.3.** Recall the definition of $m_1$ and $m_2$ in (2.3). For $a = 1, 2$, we have
\[ |m_a(z)| \sim |m_a(z)| \sim 1 \quad 3m_a \sim \frac{\eta}{\sqrt{\kappa + \eta}}, \tag{2.10} \]
uniformly in $z \in \mathcal{D}$, where $\kappa = |E - \lambda_{+}|$.

**Remark 2.4.** Following from Theorem 2.1 and Lemma 2.3, we can easily have the boundedness of $\mathbf{u}^* \mathcal{G}_a^0 \mathbf{v}$, $\mathbf{u}^* \mathbf{X} \mathcal{G}_a^0 \mathbf{v}$ and $\mathbf{u}^* \mathbf{X}^* \mathcal{G}_a^0 \mathbf{X}^* \mathbf{v}$ for any positive integer $a$ and deterministic unit vectors $\mathbf{u}$ and $\mathbf{v}$ of appropriate dimensions. Actually, in our regime, $z \in \mathcal{D}$, the boundedness of all these quantities follows more directly from the rigidity of the largest eigenvalue of $H$ (c.f., (2.12)), which guarantees that $\|\mathcal{G}\|_{\text{op}} \leq C$ with high probability.

Using the isotropic local law, one can also get the following result, which gives the location of the outlier and the extremal non-outlier.

**Lemma 2.5.** (Theorem 2.3 of [11]) Under Assumption 1.1 and (1.4), we have for $i \in [1, r_0]$
\[ |\mu_i - \Theta(d_i)| \prec N^{-\frac{1}{3}}, \quad |\mu_{r_0 + 1} - \lambda_{+}| \prec N^{-2/3}, \]
where
\[
\Theta(z) := 1 + z + \eta z^{-1}, \quad \text{for } z \in \mathbb{C}, \quad \Re z > \sqrt{\eta}. \tag{2.11}
\]
Further, for the largest eigenvalue of $H$, denoted by $\lambda_1(H)$, we have the rigidity estimate
\[ |\lambda_1(H) - \lambda_{+}| \prec N^{-\frac{1}{2}}. \tag{2.12} \]
We refer to Theorem 3.1 of [39], for instance.

2.3. Auxiliary lemmas. The following **cumulant expansion formula** plays a central role in our computation, whose proof can be found in [34, Proposition 3.1] or [28, Section II], for instance.

**Lemma 2.6.** (Cumulant expansion formula) For a fixed $\ell \in \mathbb{N}$, let $f \in C^{\ell+1}(\mathbb{R})$. Supposed $\xi$ is a centered random variable with finite moments to order $\ell + 2$. Recall the notation $\kappa_k(\xi)$ for the $k$-th cumulant of $\xi$. Then we have
\[ \mathbb{E}(\xi f(\xi)) = \sum_{k=1}^{\ell} \frac{\kappa_{k+1}(\xi)}{k!} \mathbb{E}(f^{(k)}(\xi)) + \mathbb{E}(r_{\ell}(\xi f(\xi))), \tag{2.13} \]
where the error term \( r_\ell(\xi f(\xi)) \) satisfies
\[
|\mathbb{E}(r_\ell(\xi f(\xi)))| \leq C_\ell \mathbb{E}(|\xi|^{\ell+2}) \sup_{t \leq s} |f^{\ell+1}(t)| + C_\ell \mathbb{E}(|\xi|^s \mathbb{1}(|\xi| > s)) \sup_{t \in \mathbb{R}} |f^{\ell+1}(t)|
\] (2.14)
for any \( s > 0 \) and \( C_\ell \) satisfied \( C_\ell \leq (C \ell)! / \ell! \) for some constant \( C > 0 \).

Next we collect some basic identities for the Green functions in (2.1) without proof.

**Lemma 2.7.** For any integer \( l \geq 1 \), we have
\[
\mathcal{G}_l^i = \frac{1}{(l-1)!} \frac{\partial^{l-1} \mathcal{G}_1}{\partial x^{l-1}} = \frac{1}{(l-1)!} \mathcal{G}_1^{l-1},
\] (2.15)
\[
\mathcal{G}_l^i X X^* = \mathcal{G}_1^{l-1} + z \mathcal{G}_1^i, \quad X^* \mathcal{G}_1^i X = \mathcal{G}_2^i X^* X = \mathcal{G}_1^{l-1} + z \mathcal{G}_2^i.
\] (2.16)

Further, for \( a \in [1, M] \) and \( b \in [1, N] \), we denote by \( E_{ab} \) the \( M \times N \) matrix with entries \( (E_{ab})_{cd} = \delta_{ac} \delta_{bd} \). Let
\[
\mathcal{P}_{ab}^l = E_{ab} (E_{ab})^*, \quad \mathcal{P}_i^l = E_{ab} X^*, \quad \mathcal{P}_{ab} = X (E_{ab}).
\] (2.17)

For any integer \( l \geq 1 \), it is also elementary to compute that
\[
\frac{\partial \mathcal{G}_1^i}{\partial x_{ab}} = - \sum_{\alpha=1}^2 \sum_{l_1, l_2 \geq 1} \mathcal{G}_1^{l_1} \mathcal{P}_{ab}^l \mathcal{P}_{ab}^{l_2}.
\] (2.18)

Repeatedly applying the identity (2.18), we can get the formulas for higher order derivatives of \( \mathcal{G}_1^i \) w.r.t. \( x_{ab} \). Moreover, by (2.18) and the product rule, we can easily deduce the derivatives of \( X^* \mathcal{G}_1^i \) w.r.t. \( x_{ab} \).

For the convenience of the reader, we collect more basic formulas of the derivatives of Green functions in Appendix A.

### 3. Green function representation

In this section, we express \( \mu_i \) and \( |(w, \xi_i)^2| \) in terms of the Green function \( \mathcal{G}_1(z) \) in (2.1). This representation will allow us to work with the Green function instead of the eigenvalue and eigenvector statistics. We also remark here that similar derivation of the Green function representation has appeared in previous work such as [29, 11]. But here for eigenvectors, we need to do it up to a higher order precision, in order to capture all contributing terms for the fluctuation.

We start with a few more notations. We define the centered Green function by
\[
\Xi(z) := \mathcal{G}_1(z) - m_1(z) \mathbb{I},
\] (3.1)
and introduce its quadratic forms
\[
\chi_{ij}(z) = v_i^* \Xi(z) v_j, \quad \chi_{w}(z) = u^* \Xi(z) v, \quad i, j \in [1, r],
\] (3.2)
where \( u \) is defined in (1.6). For brevity, we further set
\[
\tilde{w} := \Sigma^{-\frac{1}{2}} w = \sum_{j=1}^r \tilde{w}_j v_j + u \quad \text{with} \quad \tilde{w}_j := \frac{(w, v_j)}{\sqrt{1 + d_j}}.
\] (3.3)

Also, for \( d > 0 \), we define the following functions
\[
f(d) := \frac{1}{d} (d + 1)(d^2 - y), \quad g(d) := \frac{1}{d} (d + 1)(d + y)(d^2 - y),
\] (3.4)
and for \( i \in [1, r] \), we set for \( d \neq d_i \),
\[
\nu_i(d) := \frac{d_i (d + 1)}{d_i - d}.
\] (3.5)

With the above notations, we have the following lemma.

**Lemma 3.1.** Under Assumptions 1.1, 1.2, and the setting (1.5), for \( i \in [1, r_0] \), we have
\[
\mu_i = \theta(d_i) - (d_i^2 - y) \theta(d_i) \chi_{ii}(\theta(d_i)) + O_h \left( \frac{1}{N} \right),
\] (3.6)
and
\[ |(w, \xi)_i|^2 = \frac{d_i^2 - y}{d_i(d_i + y)} |(w, v_i)|^2 - 2d_i(d_i + 1)^2 \tilde{w}_i^2 \chi_{ii}(\theta(d_i)) - f(d_i)^2 \tilde{w}_i^2 \chi'_{ii}(\theta(d_i)) \\
- 2f(d_i) \tilde{w}_i \left( \sum_{j \neq i} \nu_j(d_j) \tilde{w}_j \chi_{ij}(\theta(d_i)) + \chi_{ii}(\theta(d_i)) \right) \\
+ g(d_i) \left( \sum_{j \neq i} \nu_j(d_j) \tilde{w}_j \chi_{ij}(\theta(d_i)) + \chi_{ii}(\theta(d_i)) \right)^2 + O_{\infty} \left( \frac{\tilde{w}_i}{N} \right) + O_{\infty}(N^{-\frac{2}{5}}). \quad (3.7) \]

**Remark 3.2.** Lemma 3.1 suggests that the joint distribution of \( \mu_i \) and \(|(w, \xi)_i|^2\) is ultimately governed by the joint distribution of \( \chi_{ij}(z) \) (1 \( \leq j \leq r \)), \( \chi_{ii}(z) \) and \( \chi_{ii}(z) \). We can also rewrite (3.7) as
\[ |(w, \xi)_i|^2 = \frac{d_i^2 - y}{d_i(d_i + y)} |(w, v_i)|^2 - \frac{\tilde{w}_i}{\sqrt{N}} l_i^* \chi_i + \frac{1}{N} \chi_{ii}^* A_i \chi_i + O_{\infty} \left( \frac{\tilde{w}_i}{N} \right) + O_{\infty}(N^{-\frac{2}{5}}), \]
by defining the random vector
\[ \chi_i = \chi(\theta(d_i)) := \sqrt{N} \left( \chi_{ii}(\theta(d_i)), \ldots, \chi_{ir}(\theta(d_i)), \chi_{ri}(\theta(d_i)), \chi_{rr}(\theta(d_i)) \right)^*, \]
the deterministic vector \( l_i = (l_i(j)) \in \mathbb{R}^{r+2} \) with components
\[ l_i(j) = \begin{cases} 2d_i(d_i + 1)^2 \tilde{w}_i, & \text{if } j = i; \\
2f(d_i) \nu_j(d_j) \tilde{w}_i, & \text{if } 1 \leq j \neq i \leq r; \\
2f(d_i), & \text{if } j = r + 1; \\
f(d_i)^2 \tilde{w}_i, & \text{if } j = r + 2, \end{cases} \]
and the \((r + 2) \times (r + 2)\) symmetric matrix \( A_i \) whose non-zero entries are given by
\[ A_i(j, k) = \begin{cases} g(d_i) \nu_j(d_i) \nu_k(d_k) \tilde{w}_j \tilde{w}_k, & \text{if } 1 \leq j, k \leq r \text{ and } j, k \neq i; \\
g(d_i) \nu_i(d_i) \tilde{w}_j, & \text{if } 1 \leq j \neq i \leq r \text{ and } k = r + 1; \\
g(d_i) \nu_j(d_j), & \text{if } j = k = r + 1. \end{cases} \]

**Proof of Lemma 3.1.** First, the proof of (3.6) can be done similarly to the proof of Proposition 7.1 in [29]. For the convenience of the reader, we state the details below. Recall (1.2) together with (1.3). We rewrite \( S \) as
\[ S = V \text{diag}(d_1, \ldots, d_r)V^*, \]
by setting \( V = (v_1, \ldots, v_r) \). Therefore, we have
\[ \Sigma^{-1} = I - VDV^*. \]
with
\[ D = \text{diag} \left( \frac{d_1}{1 + d_1}, \ldots, \frac{d_r}{1 + d_r} \right). \]
Then, by elementary calculation, we have
\[ Q - z = \Sigma^{1/2} G^{-1}(z) (I + zG(z)V^*) \Sigma^{1/2}. \]
Notice that \( \mu_i \) is the \( i \)th largest real value such that \( \det(Q - \mu_i) = 0 \). Further by the fact that \( \mu_i \) stays away from the spectrum of \( H \) with high probability (c.f., Lemma 2.5, Assumption 1.2), together with the identity \( \det(I_M + zG(z)V^*) = \det(D) \det(D^{-1} + zV^* G(z)V) \), we have that \( \mu_i \) is the \( i \)th largest real solution to the equation \( \det(D^{-1} + zV^* G(z)V) = 0 \) with high probability.

For \( z \in [\lambda_+ + \delta, K] \) with sufficiently small constant \( \delta > 0 \) and sufficiently large constant \( K > 0 \), we define the matrices \( A(x) = (A_{ij}(x)) \) and \( \tilde{A}(x) = (\tilde{A}_{ij}(x)) \) by setting
\[ A_{ij}(x) = (1 + d_{i}^{-1}) \delta_{ij} + xv_i^* G_i(x)v_j - x(m_1(x)) \delta_{ij}, \quad \tilde{A}_{ij}(x) = \delta_{ij}((1 + d_{i}^{-1}) + xv_i^* G_i(x)v_i - x(m_1(x))), \]
Further, we denote the eigenvalues of \( A(x) \) and \( \tilde{A}(x) \) by \( a_1(x) \leq \ldots \leq a_r(x) \) and \( \tilde{a}_1(x) \leq \ldots \leq \tilde{a}_r(x) \) respectively. Apparently, one has
\[ \tilde{a}_i(x) = (1 + d_{i}^{-1}) + xv_i^* G_i(x)v_i - x(m_1(x)), \quad (3.9) \]
with high probability by the isotropic local law (2.7) and the Assumption 1.2. We then claim that, in order to prove (3.6), it suffices to show the following two estimates

\[ \mu_i m_1(\mu_i) = -a_i(\theta(d_i)) + O_{\prec}(\frac{1}{N}), \]  

(3.10)

\[ a_i(\theta(d_i)) = \tilde{a}_i(\theta(d_i)) + O_{\prec}(\frac{1}{N}). \]  

(3.11)

Combining (3.9), (3.10) and (3.11), we have

\[ \mu_i m_1(\mu_i) - \theta(d_i)m_1(\theta(d_i)) = -(1 + d_i^{-1}) - \theta(d_i)v_1^*G_1(\theta(d_i))v_i. \]

Expanding \( \mu_i m_1(\mu_i) \) around \( \theta(d_i)m_1(\theta(d_i)) \) with the aid of Lemma 2.5 will then lead to (3.6). Therefore, what remains is to prove (3.10) and (3.11).

We start with (3.10). First, by the fact that \( \mu_i \) is a solution to \( \text{det}(D^{-1} + zV^*G_1(z)V) = 0 \), it is easy to see that \( \mu_i m_1(\mu_i) = -a_k(\mu_i) \) for some \( k \). But by isotropic local law (2.7) and Lemma 2.5, we see that \( A = \tilde{A} + O_{\prec}(N^{-\frac{1}{2}}) \), where \( O_{\prec}(N^{-\frac{1}{2}}) \) represents a matrix bounded in operator norm by \( O_{\prec}(N^{-\frac{1}{2}}) \). This leads to the estimate \( a_k(\mu_i) = \tilde{a}_k(\mu_i) + O_{\prec}(N^{-\frac{1}{2}}) \). Further, by (2.7) and Lemma 2.5 one can easily show that \( \mu_i m_1(\mu_i) = -(1 + d_i^{-1}) + O_{\prec}(N^{-\frac{1}{2}}) \) and \( \tilde{a}_k(\mu_i) = (1 + d_i^{-1}) + O_{\prec}(N^{-\frac{1}{2}}) \). Therefore, due to the fact that \( d_i \)'s are well separated, we have \( \mu_i m_1(\mu_i) = -a_i(\mu_i) \) with high probability. Next, by the isotropic law (2.7), one can also check that

\[ \|\partial_{zz}A(z)\|_{\text{op}} < \frac{1}{\sqrt{N}}. \]

This together with Lemma 2.5 leads to

\[ |a_i(\mu_i) - a_i(\theta(d_i))| < \frac{1}{N}. \]

Combining the above with the fact \( \mu_i m_1(\mu_i) = -a_i(\mu_i) \) with high probability, we arrive at (3.10).

Next, we prove (3.11). Observe that the diagonal entries of \( A - \tilde{A} \) are 0, and \( \tilde{A} \) is a diagonal matrix. So expanding the eigenvalues of \( A \) around the eigenvalues of \( \tilde{A} \) using the perturbation theory, we see that the first order term vanishes. Hence, it suffices to estimate the second order term. More specifically, we have

\[ |a_i(\theta(d_i)) - \tilde{a}_i(\theta(d_i))| < \frac{\|A - \tilde{A}\|_{\text{op}}^2}{\min_{j \neq i}|\tilde{a}_j(\theta(d_i)) - \tilde{a}_i(\theta(d_i))|} < \frac{1}{N}, \]

where the last step follows from the fact that \( \tilde{a}_k(\theta(d_i)) = 1 + d_k^{-1} + O_{\prec}(N^{-\frac{1}{2}}) \) and the fact that the \( d_i \)'s are well separated. This concludes the proof of (3.11).

Then, we turn to prove (3.7). Let \( \Gamma_i \) be the boundary of a disc centered at \( d_i \) with sufficiently small (but fixed) radius, such that this disc is away from \( \lambda_+ \) by a constant order distance and also \( \Gamma_i \)'s are well-separated from each other by a constant order distance for all \( i \in [1, r_0] \). Notice that this can be guaranteed by Assumption 1.2. According to Lemma 2.5, together with the Cauchy integral, we have the following equality with high probability

\[ |\langle w, \xi_i \rangle|^2 = -\frac{1}{2\pi i} \oint_{\Gamma_i} w^*G(z)w \, dz, \]  

(3.12)

where \( \theta(\Gamma_i) \) is the image of \( \Gamma_i \) under the map \( \theta(\cdot) \) defined in (2.11). With the notations for \( V, S, D \) and \( \Sigma^{-1} \), using the setting (1.5), we can write

\[ G(z) = \left( \Sigma^\frac{1}{2} XX^* \Sigma + zI \right)^{-1} = \Sigma^{-\frac{1}{2}} \left( G_1^{-1}(z) + z\Sigma^{-\frac{1}{2}} S \Sigma^{-\frac{1}{2}} \right)^{-1} \Sigma^{-\frac{1}{2}} \]

\[ = \Sigma^{-\frac{1}{2}} \left( G_1^{-1}(z) + zV^* DV\right)^{-1} \Sigma^{-\frac{1}{2}}. \]

Then, it follows from the matrix inversion lemma that

\[ G(z) = \Sigma^{-\frac{1}{2}} G_1(z) \Sigma^{-\frac{1}{2}} - z \Sigma^{-\frac{1}{2}} G_1(z)V \left( D^{-1} + zV^* G_1(z)V \right)^{-1} V^* G_1(z) \Sigma^{-\frac{1}{2}}. \]

With the notation introduced in (3.3), we can further write

\[ w^* G(z) w = \hat{w}^* G_1(z) \hat{w} - z \hat{w}^* G_1(z)V \left( D^{-1} + zV^* G_1(z)V \right)^{-1} V^* G_1(z) \hat{w}. \]  

(3.13)
Plugging (3.13) into (3.12), and noticing that the contour integral of $\tilde{w}^* G_1(z)\tilde{w}$ on $\theta(\Gamma_1)$ is zero with high probability by Assumption 2 and the rigidity of eigenvalues of $H$ (c.f., (2.12)), one has

$$|(\omega, \xi_i)|^2 = \frac{1}{2\pi i} \oint_{\theta(\Gamma_1)} z\tilde{w}^* G_1(z)V(D^{-1} + zV^* G_1(z)V)^{-1}V^* G_1(z)\tilde{w} \, dz,$$

with high probability.

For the integrand in (3.14), we first recall the notation in (3.1) and then we apply resolvent expansion

$$\left(D^{-1} + zV^* G_1(z)V\right)^{-1} = L(z) - zL(z)V^* \Xi(z)VL(z) + (zL(z)V^* \Xi(z)V)^2\left(D^{-1} + zV^* G_1(z)V\right)^{-1},$$

where

$$L(z) := (D^{-1} + zm_1(z))^{-1}.$$

With (3.15), we can further rewrite (3.14) as

$$|(\omega, \xi_i)|^2 = \frac{1}{2\pi i} \oint_{\theta(\Gamma_1)} z(m_1(z)\tilde{w}^* V + \tilde{w}^* \Xi(z)V)(L(z) - zL(z)V^* \Xi(z)VL(z) + (zL(z)V^* \Xi(z)V)^2\left(D^{-1} + zV^* G_1(z)V\right)^{-1})(m_1(z)V^* \tilde{w} + V^* \Xi(z)\tilde{w}) \, dz.$$

Applying (2.7), we can further write

$$|(\omega, \xi_i)|^2 = S_1 + S_2 + S_3 + O_\ll(N^{-\frac{2}{3}}),$$

by defining

$$S_1 := \frac{1}{2\pi i} \oint_{\theta(\Gamma_1)} zm_1^2(z)\tilde{w}^* VL(z)V^* \tilde{w} \, dz,$$

$$S_2 := \frac{1}{2\pi i} \oint_{\theta(\Gamma_1)} \left(2zm_1(z)\tilde{w}^* VL(z)V^* \Xi(z)\tilde{w} - z^2m_1^2(z)\tilde{w}^* VL(z)V^* \Xi(z)VL(z)V^* \tilde{w}\right) \, dz,$$

$$S_3 := \frac{1}{2\pi i} \oint_{\theta(\Gamma_1)} \left(z\tilde{w}^* \Xi(z)VL(z)V^* \Xi(z)\tilde{w} - 2z^2m_1(z)\tilde{w}^* (VL(z)V^* \Xi(z))^2\tilde{w} + z^3m_1^2(z)\tilde{w}^* (VL(z)V^* \Xi(z))^2VL(z)V^* \tilde{w}\right) \, dz.$$

It remains to estimate $S_1$, $S_2$ and $S_3$. From the definitions in (2.3) and (2.11), it is easy to check the identity

$$1 + z^{-1} + \theta(z)m_1(\theta(z)) = 0.$$

(3.16)

With the above identity, we see that

$$VL(\theta(z))V^* = \sum_{j=1}^r \frac{\nu_j v_j^*}{1 + d_j^{-1} + \theta(z)m_1(\theta(z))} = \sum_{j=1}^r \frac{zd_j v_j v_j^*}{z - d_j}.$$

Therefore, by the residue theorem,

$$S_1 = \frac{1}{2\pi i} \oint_{\Gamma_1} \theta(z)\theta'(z)m_1^2(\theta(z))\tilde{w}^* VL(\theta(z))V^* \tilde{w} \, dz$$

$$= \theta(d_i)\theta'(d_i)m_1^2(\theta(d_i))d_i^2(\tilde{w}^* v_i)^2 = \frac{d_i^2 - y}{d_i(d_i + y)}|(\omega, v_i)|^2.$$

(3.17)

Similarly, using (3.16), we can get

$$S_2 = \frac{1}{2\pi i} \oint_{\Gamma_1} \left(2\theta(z)\theta'(z)m_1(\theta(z))\sum_{j=1}^r \frac{zd_j}{z - d_j} (\tilde{w}^* v_j)\tilde{w}^* \Xi(\theta(z))v_j \right.$$

$$- \theta^2(z)\theta'(z)m_1^2(\theta(z))\sum_{j,k=1}^r \frac{z^2d_j d_k}{(z - d_j)(z - d_k)} (\tilde{w}^* v_j)(\tilde{w}^* v_k)\Xi(\theta(z))v_j v_k \bigg) \, dz.$$
Further by the residue theorem together with the definition of $\theta$ and $m$ in (2.3) and (2.11), we can get
\[
S_2 = -2\frac{(d_i + 1)(d_i^2 - y)}{d_i} \tilde{w}_i \tilde{w}_j \Xi(\theta(d_i))v_i - 2\frac{(d_i + 1)^2(d_i^2 - y)}{d_i} \sum_{j \neq i} \frac{d_j}{d_i - d_j} \tilde{w}_i \tilde{w}_j \chi_{ij}(\theta(d_i))
\]
\[
- \frac{(d_i + 1)^2(d_i^2 - y)^2}{d_i^2} \tilde{w}_i^2 \chi_{ii}(\theta(d_i)) - 2\frac{(d_i + 1)(d_i^2 + y)}{d_i} \tilde{w}_i^2 \chi_{ii}(\theta(d_i)),
\]
where we also recalled the notations in (3.2). With the functions defined in (3.4) and (3.5), we can further write
\[
S_2 = -2d_i(d_i + 1)^2 \tilde{w}_i^2 \chi_{ii}(\theta(d_i)) - 2f(d_i) \sum_{j \neq i} \nu_i(d_j) \tilde{w}_j \tilde{w}_i \chi_{ji}(\theta(d_i))
\]
\[
- 2f(d_i) \tilde{w}_i \chi_{ii}(\theta(d_i)) - f(d_i)^2 \tilde{w}_i^2 \chi_{ii}(\theta(d_i)).
\]  
(3.18)

Observe from the isotropic local law (2.7) and Assumption 1.2 that $S_2 = O_\prec(\tilde{w}_i/\sqrt{N})$. Hence, it can degenerate when $\tilde{w}_i$ is small or even 0. Hence, it is necessary to consider the fluctuation of the term $S_3$ as well. In the sequel, we turn to estimate $S_3$. We estimate the integrals of three terms in the integrand separately. First, using the residue theorem together with the notations in (3.2) and (3.4), we have
\[
\frac{1}{2\pi i} \oint_{\gamma(i)} z \tilde{w}^* \Xi(z)V_L(z)V^* \Xi(z) \tilde{w} dz = \theta(d_i) \theta'(d_i) d_i^2 \left( \tilde{w}^* \Xi(\theta(d_i))v_i \right)^2
\]
\[
= g(d_i) \left( \sum_{j,k=1}^r \tilde{w}_j \tilde{w}_k \chi_{ij}(\theta(d_i)) \chi_{ik}(\theta(d_i)) + \chi_{ii}(\theta(d_i)) + 2 \sum_{j=1}^r \tilde{w}_j \chi_{ij}(\theta(d_i)) \chi_{ii}(\theta(d_i)) \right).
\]  
(3.19)

For the second part of the integral, we have
\[
- \frac{1}{2\pi i} \oint_{\gamma(i)} 2z^2 m_1(z) \tilde{w}^* (V_L(z)V^* \Xi(z))^2 \tilde{w} dz
\]
\[
= \left. -2\theta^2(d_i) \theta'(d_i) m_1(\theta(d_i)) \sum_{j \neq i} \frac{d_j^3 d_j}{d_i - d_j} (\tilde{w}^* v_j) \tilde{w}^* \Xi(\theta(d_i))v_i \chi_{ij}(\theta(d_i)) \right|_{z=d_i}
\]
\[
- 2\theta^2(d_i) \theta'(d_i) m_1(\theta(d_i)) \sum_{j \neq i} \frac{d_j^3 d_j}{d_i - d_j} (\tilde{w}^* v_j) \tilde{w}^* \Xi(\theta(d_i))v_j \chi_{ij}(\theta(d_i))
\]
\[
- 2d_i^2 (\tilde{w}^* v_i) \left( \left( \theta^2(z) m_1(\theta(z)) \tilde{w}^* \Xi(\theta(z))v_i \chi_{ii}(\theta(z)) \right) \right)^{1/2}
\]  
Then, by using the isotropic law (2.7), Assumption 1.2, and the notations in (3.2) and (3.4), we have
\[
- \frac{1}{2\pi i} \oint_{\gamma(i)} 2z^2 m_1(z) \tilde{w}^* (V_L(z)V^* \Xi(z))^2 \tilde{w} dz
\]
\[
= -2d_i^3 \theta^2(d_i) \theta'(d_i) m_1(\theta(d_i)) \sum_{j \neq i} \frac{d_j^3}{d_i - d_j} (\tilde{w}^* v_j) \tilde{w}^* \Xi(\theta(d_i))v_i \chi_{ij}(\theta(d_i)) + O_\prec \left( \tilde{w}_i / \sqrt{N} \right)
\]
\[
= 2g(d_i) \sum_{j \neq i} \left( 1 + d_j \right) \frac{d_j}{d_i - d_j} \tilde{w}_j \tilde{w}_i \chi_{ij}(\theta(d_i)) \left( \sum_{k \neq i} \tilde{w}_k \chi_{ik}(\theta(d_i)) + \chi_{ii}(\theta(d_i)) \right) + O_\prec \left( \tilde{w}_i / \sqrt{N} \right).
\]  
(3.20)

Analogously, the last part of the integral can be estimated by
\[
\frac{1}{2\pi i} \oint_{\gamma(i)} z^3 m_1^2(z) \tilde{w}^* (V_L(z)V^* \Xi(z))^2 V_L(z)V^* \tilde{w} dz
\]
\[
= g(d_i) \sum_{k,l \neq i} \left( 1 + d_k \right) \frac{d_k}{d_i - d_k} \tilde{w}_k \tilde{w}_i \chi_{ik}(\theta(d_i)) \chi_{il}(\theta(d_i)) + O_\prec \left( \tilde{w}_i / \sqrt{N} \right).
\]  
(3.21)

Combining (3.19)-(3.21), after necessary simplification, we arrive at
\[
S_3 = g(d_i) \left( \chi_{ii}(\theta(d_i)) + 2 \sum_{j \neq i} \nu_i(d_j) \tilde{w}_j \tilde{w}_i \chi_{ij}(\theta(d_i)) \chi_{ii}(\theta(d_i)) \right)
\]
\[
+ \sum_{j,k \neq i} \nu_i(d_j) \nu_k(d_k) \tilde{w}_j \tilde{w}_i \chi_{ij}(\theta(d_i)) \chi_{ik}(\theta(d_i)) + O_\prec \left( \tilde{w}_i / \sqrt{N} \right).
\]  
(3.22)

By (3.17), (3.18) and (3.22), we can conclude the proof of Lemma 3.1. □
4. Proof of Theorem 1.6

In this section, we state the proof of the main result Theorem 1.6, based on Proposition 4.2, whose proof will be stated in Section 5. The starting point is Lemma 3.1 and Remark 3.2, which state that the study of $|\langle w, \xi_n \rangle|^2$ can be reduced to the study of the random vector

$$\chi_i(z) := \sqrt{N} \left( \chi_{i1}(z), \ldots, \chi_{ir}(z), \chi_{ui}(z), \chi_{ui}(z)^T \right)$$

at $z = \theta(d_i)$. It suffices to show that $\chi_i(z)$ is asymptotically real Gaussian. Before we give the precise statement, let us introduce some necessary notations. For brevity, in the sequel, we will very often omit the $z$-dependence from the notations. For instance, we will write $m_{1,2}(z)$ as $m_{1,2}$.

In the sequel, we fix an $i \in [1, r_0]$. Define a symmetric matrix $M_i \equiv M_i(z) \in \mathbb{C}^{(r+2) \times (r+2)}$ with diagonal entries

$$M_i(j, j) = \begin{cases} 2m_2'(zmn_1), & \text{if } j = i; \\ m_2'(zmn_1)^2, & \text{if } 1 \leq j \neq i \leq r; \\ 2(m_1m_1'(zmn_1)^2 + (m_1')^2(zmn_1)^2 + \frac{1}{2}m_2'(zmn_1)^2), & \text{if } j = r + 2 \\ m_1m_1'(zmn_1)^2, & \text{if } j = r + 1; \\ 2m_1m_1'(zmn_1)^2 + (m_1')^2(zmn_1)^2, & \text{if } j = r + 2. \end{cases}$$

and the only non-zero off-diagonal entry

$$M_i(i, r + 2) = (m_2'(zmn_1))'.$$

Recall the notations defined in (1.8). We then further define the symmetric matrix $K_i \equiv K_i(z) \in \mathbb{C}^{(r+2) \times (r+2)}$ whose $r \times r$ upper left corner is given by

$$K_i(j, k) = s_{1,1,2}(v_j, v_k, v_i)(zm_{2m_1}^2), \quad \text{for } 1 \leq j, k \leq r,$$

and the remaining entries are

$$K_i(j, k) = \begin{cases} s_{1,1,2}(v_j, u, v_i)(zm_{2m_1}^2), & \text{if } 1 \leq j \leq r \text{ and } k = r + 1; \\ s_1(v_i)((zm_{2m_1}^2)^2)', & \text{if } j = k = r + 2; \\ s_1(v_i)((zm_{2m_1}^2)^2)', & \text{if } j = k = r + 2; \\ s_1(v_i)((zm_{2m_1}^2)^2)', & \text{if } j = k = r + 2; \end{cases}$$

We further denote

$$V_i(z) := M_i(z) + \kappa_i K_i(z).$$

Lemma 4.1. Under the assumptions of Theorem 1.6, we have

$$\chi_i(\theta(d_i)) \sim N(0, V_i(\theta(d_i))).$$

With the above lemma, we now can finish the proof of Theorem 1.6.

Proof of Theorem 1.6. Recall Lemma 3.1. Then, by setting

$$\Upsilon_i = -\sqrt{N} (d_i^2 - y) \theta(d_i) \chi_i(\theta(d_i)),
\Theta_i' = -2\sqrt{N} d_i(1 + d_i)^{3/2} \bar{w} \chi_i(\theta(d_i)) - \sqrt{N} f(d_i)^2 (1 + d_i)^{-1/2} \bar{w} \chi_i(\theta(d_i))
- 2\sqrt{N} f(d_i)(1 + d_i)^{-1/2} \left( \sum_{j \neq i} \nu_i(d_j) \bar{w} \chi_i(\theta(d_i)) + \chi_{ui}(\theta(d_i)) \right),$$

$$\Lambda_i = \sqrt{N} \bar{g}(d_i) \left( \sum_{j \neq i} \nu_i(d_j) \bar{w} \chi_i(\theta(d_i)) + \chi_{ui}(\theta(d_i)) \right),$$

we get (1.9) and (1.10) in Theorem 1.6. Next, notice that $\Upsilon_i$, $\Theta_i'$ and $\Lambda_i'$ are all linear combinations of the components of $\chi_i(\theta(d_i))$. Then by Lemma 4.1, they are also asymptotically jointly Gaussian with mean 0. Further, elementary calculation of the quadratic forms of the entries of $V_i(\theta(d_i))$ using the
following basic facts at \( z = \theta(d_i) \)
\[
m_i^2(zm_1)' = \frac{d_i + y}{(d_i + y)^2(d_i^2 - y)}.
\]
\[
m_{1m}'(zm_1)' + m_i^2(zm_1)' = \frac{d_i d_i^3 + 4d_i^3 y - 3d_i^2 y + d_i^2 y^2 + y^3 + y^3}{(d_i + y)^2(d_i^2 - y)^3}.
\]
\[
zm_2 m_1^2 = -\frac{1}{d_i(d_i + y)}, \quad (zm_2 m_1^2)' = \frac{2d_i + y}{(d_i + y)^2(d_i^2 - y)}.
\]
eventually leads to the covariance matrix of \((\Upsilon, \Theta^w, \Lambda_w)\), which is stated in Theorem 1.6.

This completes the proof of Theorem 1.6.

In the rest of this section, we prove Lemma 4.1, based on our key technical result, Proposition 4.2. In order to show the asymptotic Gaussianity of \(\chi_i(\theta(d_i))\), it suffices to show that all linear combinations of the components of \(\chi_i(\theta(d_i))\) are asymptotic Gaussian. Our proof will be based on a moment estimate. This requires a deterministic bound for the Green function, in order to control the contribution of the bad event in the isotropic local laws. To this end, we introduce a tiny imaginary part to the parameter \(z\), such that the Green functions can be bounded by \(1/3z\) deterministically. Specifically, in the sequel, we set
\[
z = \theta(d_i) + iN^{-K},
\]
for some sufficiently large constant \(K\). For a fixed deterministic \((r+2)\)-dim column vector \(c = (c_1, \cdots, c_{r+2})^\ast\), we define
\[
P := c^\ast \chi_i(z),
\]
where \(z\) is given in (4.6). Notice that \(|P| \prec 1\) by the isotropic local law. Here we omit the dependence of \(P\) on \(c\) and the index \(i\) for simplicity. Hereafter we always assume that \(c\) and \(i\) are fixed. The following proposition is our main technical task.

**Proposition 4.2** (Recursive moment estimate). Let \(\mathcal{P}\) be defined in (4.7) with \(z\) given in (4.6). Under the assumption of Theorem 1.6, we have
\[
(i) \quad \mathbb{E}P = O_{\prec}(N^{-\frac{1}{2}}),
\]
\[
(ii) \quad \mathbb{E}P^l = (l - 1)\mathcal{V}_i c \mathbb{E}P^{l-2} + O_{\prec}(N^{-\frac{1}{2}}),
\]
where \(\mathcal{V}_i c = c^\ast \chi_i(\theta(d_i))c\) with \(\mathcal{V}_i(\theta(d_i))\) defined in (4.4).

With the above proposition, we can now show the proof of Lemma 4.1.

**Proof of Lemma 4.1.** By Proposition 4.2, one observes that \(\mathcal{P}(z)\) is asymptotically Gaussian with mean 0 and variance \(\mathcal{V}_i c\). By the definition of \(z\) in (4.6), and a simple continuity argument for the Green function, one can easily see that \(\mathcal{P}(\theta(d_i))\) admits the same asymptotic distribution as \(\mathcal{P}(z)\), when \(K\) is chosen to be sufficiently large. Further implied by the fact that \(\mathcal{V}_i c = c^\ast \chi_i(\theta(d_i))c\) and the arbitrariness of \(c\), we have
\[
\chi_i(\theta(d_i)) \simeq N(0, \mathcal{V}_i(\theta(d_i)))
\]
This concludes the proof of Lemma 4.1. \(\Box\)

5. Proof of Proposition 4.2

This section is devoted to the proof of Proposition 4.2, the recursive moment estimates of \(\mathcal{P}\) defined in (4.7). The basic strategy is to use the cumulant expansion formula in Lemma 2.6 to the functionals of Green functions. In the context of Random Matrix Theory, such an idea dates back to [28]. We also refer to [32, 25] for some recent applications of this strategy for other problems in Random Matrix Theory.

First, we will see that all the random terms we will encounter in the proof are one of the following forms: \(\eta_1^s \bar{G}^\ast_1 \eta_2, \eta_1^s X^\ast \bar{G}^\ast_1 X \eta_2, \eta_1^s \bar{G}^\ast_1 \eta_2\), for some fixed \(s \in \mathbb{N}\) and some deterministic vectors \(\eta_1, \eta_2\) which are bounded by some constant \(C > 0\) in \(l^2\)-norm. Notice that under the choice of \(z\) in (4.6), we have the deterministic bound
\[
|\eta_1^s \bar{G}^\ast_1 \eta_2| \leq C(3z)^{-s}.
\]
Similarly, by Cauchy-Schwarz inequality, we have
\[ |\eta_1^* X G_1^* \eta_2| \leq \|\eta_1\| \|X G_1^* \eta_2\| \leq C \left( \eta_2^* G_1^* (z) X^* G_1^* (z) \eta_2 \right)^{\frac{1}{2}} \]
\[ = \left( \eta_2^* G_1^* (z) (I + z G_1^*)^{-1} (z) \eta_2 \right)^{\frac{1}{2}} \leq C (3z)^{-s}, \]  
(5.2)
and
\[ |\eta_1^* X G_1^* X \eta_2| = |\eta_1^* X^* G_2^* \eta_2| = |\eta_1^* G_2^* \eta_2 + z \eta_1^* G_2^* \eta_2| \leq C (3z)^{-s}. \]  
(5.3)

The above deterministic bounds allow us to use the high probability bounds for the aforementioned quantities (following from the isotropic local law) directly in the calculation of the expectations in (4.8) and (4.9).

The main tool for the proof is the cumulant expansion formula in Lemma 2.6. By introducing the following two column vectors
\[ y_1 = (y_1)_a = \sum_{j=1}^r c_j v_j + c_{r+1} u, \quad y_2 = (y_2)_a = c_{r+2} v_i, \]  
(5.4)
we can rewrite
\[ \mathcal{P} = \sqrt{N} y_1^* (G_1 - m_1) v_i + \sqrt{N} y_2^* (G_1^2 - m_1^2) v_i, \]  
(5.5)
Hence, we can write
\[ \mathbb{E}(\mathcal{P}^t) = \sqrt{N} \mathbb{E} \sum_{t=1}^2 y_t^* \left( G_1^t - \frac{m_1}{(t-1)!} \right) v_i \mathcal{P}^{t-1}. \]  
(5.6)
Using the identity
\[ G_1^t = z^{-1} (H G_1^t - G_1^{t-1}), \quad t = 1, 2, \]
we rewrite (5.6) as
\[ \mathbb{E}(\mathcal{P}^t) = \sqrt{N} \mathbb{E} \sum_{t=1}^2 y_t^* \left( \frac{1}{1 + m_2 z} H G_1^t + \frac{m_2}{1 + m_2 z} G_1^t - \frac{1}{(1 + m_2 z)^2} G_1^{t-1} - \frac{m_1}{(t-1)!} \right) v_i \mathcal{P}^{t-1}, \]
Using the first identity in (2.5), we further have
\[ \mathbb{E}(\mathcal{P}^t) = -m_1 \mathbb{E} \sum_{t=1}^2 \sqrt{N} y_t^* \left( H G_1^t + z m_2 G_1^t - G_1^{t-1} + \frac{m_1}{(t-1)!} m_1 \right) v_i \mathcal{P}^{t-1}. \]  
(5.7)

Now, we apply the cumulant expansion formula to the terms \( \sqrt{N} \mathbb{E} y_t^* H G_1^t v_i \mathcal{P}^{t-1} \) for \( t = 1, 2 \). For simplicity, we use the following shorthand notation for the summation
\[ \sum_{q,k} = \sum_{q=1}^M \sum_{k=1}^N, \]
and similar shorthand notations are used for single index sums.

By Lemma 2.6, we have
\[ \sqrt{N} \mathbb{E} y_t^* H G_1^t v_i \mathcal{P}^{t-1} = \sqrt{N} \mathbb{E} \sum_{q,k} y_{tq} x_{qk} (X^* G_1^t v_i)_{k} \mathcal{P}^{t-1} \]
\[ = \sqrt{N} \mathbb{E} \sum_{q,k} y_{tq} \sum_{a=1}^3 \frac{k_{a+1} (x_{qk})}{a!} \frac{\partial^{a}}{\partial x_{qk}^{a}} ((X^* G_1^t v_i)_{k} \mathcal{P}^{t-1}) + R_{t,s}, \]  
(5.8)
where \( R_{t,s} \) satisfies
\[ |R_{t,s}| \leq \sqrt{N} \sum_{q,k} \left( C \mathbb{E} (|x_{qk}|^3) \mathbb{E} \left( \sup_{|x_{qk}| \leq c} |y_{tq} \frac{\partial^{3}}{\partial x_{qk}^{3}} ((X^* G_1^t v_i)_{k} \mathcal{P}^{t-1})| \right) + C \mathbb{E} (|x_{qk}|^3 \mathbb{1} (|x_{qk}| > c)) \mathbb{E} \left( \sup_{x_{qk} \in \mathbb{R}} |y_{tq} \frac{\partial^{3}}{\partial x_{qk}^{3}} ((X^* G_1^t v_i)_{k} \mathcal{P}^{t-1})| \right) \right) \]
for any \( c > 0 \) and any \( C \) satisfying \( C \leq (Ct)^{y!/l!} \) with some positive constant \( C \).
By the product rule, we have
\[
\frac{\partial^{\alpha}}{\partial x_{q_k}^{\alpha}} \left( (X^* G_1^t v_i)_k \mathcal{P}_t^{l-1} \right) = \sum_{\alpha_1, \alpha_2 \geq 0} \left( \begin{array}{l}
\alpha_1 \alpha_2 \\
\alpha_1 \alpha_2 = \alpha
\end{array} \right) \frac{\partial^{\alpha_1} (X^* G_1^t v_i)_k}{\partial x_{q_k}^{\alpha_1}} \frac{\partial^{\alpha_2} \mathcal{P}_t^{l-1}}{\partial x_{q_k}^{\alpha_2}}.
\] (5.9)

In the sequel, for brevity, we set the notation
\[
h_{t,s}(\alpha_1, \alpha_2) := \sqrt{N} \sum_{q,k} y_q \frac{K_{\alpha_1+\alpha_2}(x_{q_k})}{(\alpha_1+\alpha_2)!} \left( \begin{array}{l}
\alpha_1 + \alpha_2 \\
\alpha_1
\end{array} \right) \frac{\partial^{\alpha_1} (X^* G_1^t v_i)_k}{\partial x_{q_k}^{\alpha_1}} \frac{\partial^{\alpha_2} \mathcal{P}_t^{l-1}}{\partial x_{q_k}^{\alpha_2}}, \quad t, s = 1, 2.
\] (5.10)

Note that \( h_{t,s}(\alpha_1, \alpha_2) \) depends on \( l \) and \( i \). However, we drop this dependence for brevity.

Using (5.9) and the notation (5.10) to (5.8), we can now write
\[
\sqrt{N} \mathbb{E} y_t^* H G_1^t v_i \mathcal{P}_t^{l-1} = \sum_{\alpha_1, \alpha_2 \geq 0} \mathbb{E} h_{t,s}(\alpha_1, \alpha_2) + R_{t,s}.
\] (5.11)

In the sequel, we estimate \( h_{t,s}(\alpha_1, \alpha_2) \) and the remainder terms \( R_{t,s} \) for \( s, t = 1, 2 \). We collect the estimates in the following lemma, whose proof will be postponed to the end of this section.

**Lemma 5.1.** Let \( l \) be any fixed positive integer. With the convention \( m_a^{-1}/(-1)! = 1 \) for \( a = 1, 2 \), we have the following estimates on \( h_{t,s}(\alpha_1, \alpha_2) \) and \( R_{t,s} \) where \( t, s = 1, 2 \).

1. For \( h_{t,s}(\alpha_1, \alpha_2) \), the nonnegligible terms are
\[
h_{t,s}(1, 0) = -\sqrt{N} \left( zm_2 y_t^* G_1^t v_i + \sum_{1 \leq s_1, s_2 \leq 1} \frac{(zm_2)^{(s_1)} y_t^* G_1^{s_2} v_i}{s_1!} \right) \mathcal{P}_t^{l-1} + O_\prec (N^{-\frac{1}{2}}),
\] (5.12)
\[
h_{t,s}(0, 1) = -(l - 1) \sum_{b=1}^{2} \left( y_t^* y_i^* y_{b+1} y_{b+2} v_i \right) \sum_{0 \leq b_1, b_2 \leq b-1} \frac{m_1^{(b_1)} (zm_1)^{(b_2)} v_i}{b_1! (s+b)!} \mathcal{P}_t^{l-2} + O_\prec (N^{-\frac{1}{2}}),
\] (5.13)
\[
h_{t,s}(1, 2) = -(l - 1) \kappa_4 \sum_{b=0}^{s-1} s_{1, 2, 3} \left( y_t^* y_{b+1} y_i^* (zm_2)^{(b)} v_i \right) \mathcal{P}_t^{l-2} + O_\prec (N^{-\frac{1}{2}}).
\] (5.14)

2. Except for the terms in (5.12)-(5.14), all the other \( h_{t,s}(\alpha_1, \alpha_2) \) terms with \( \alpha_1 + \alpha_2 \leq 3 \) can be bounded by \( O_\prec (N^{-\frac{1}{2}}) \).

3. For the remainder terms, we have
\[
R_{t,s} = O_\prec (N^{-\frac{1}{2}}).
\] (5.15)

Now we show the proof of Proposition 4.2, based on Lemma 5.1.

**Proof of Proposition 4.2.** First we show the proof of (4.8). Using Lemma 5.1 with \( l = 1 \), we can rewrite (5.11) as
\[
\sqrt{N} \mathbb{E} y_t^* H G_1^t v_i = \mathbb{E} h_{1,1}(1, 0) + O_\prec (N^{-\frac{1}{2}}).
\]

Plugging the above estimate into (5.7) with \( l = 1 \), we obtain
\[
\mathbb{E} \mathcal{P} = -m_1 \left( \mathbb{E} h_{1,1}(1, 0) + \sqrt{N} zm_2 \mathbb{E} y_t^* G_1^t v_i + \mathbb{E} h_{2,2}(1, 0) + \sqrt{N} zm_2 \mathbb{E} y_t^* G_1^t v_i \right).
\] (5.16)

Applying (5.12) with \( l = 1 \), we have,
\[
h_{1,1}(1, 0) = -\sqrt{N} zm_2 y_t^* G_1^t v_i + O_\prec (N^{-\frac{1}{2}}),
\]
\[
h_{2,2}(1, 0) = -\sqrt{N} zm_2 y_t^* G_1^t v_i - \sqrt{N} (zm_2)^{y_t^* G_1^t v_i} + O_\prec (N^{-\frac{1}{2}}).
\]

We substitute the above two estimates into (5.16) and get
\[
\mathbb{E} \mathcal{P} = \frac{m_1}{m_1} \sqrt{N} \mathbb{E} y_t^* (G_1 - m_1) v_i + O_\prec (N^{-\frac{1}{2}}),
\] (5.17)
where we used the last equation in (2.5). Applying the similar arguments as (5.7) and (5.11) to the RHS of (5.17), for \( l = 1 \), we will get
\[
\mathbb{E} \mathcal{P} = -m'_1 \sqrt{N} \mathbb{E} y^*_2 (H \mathcal{G}_1 + zm_2 \mathcal{G}_1) v_i + O_\prec (N^{-\frac{1}{2}})
\]
\[
= -m'_1 \left( \mathbb{E} h_{2,1}(1,0) + \sqrt{N} zm_2 \mathbb{E} y^*_2 \mathcal{G}_1 v_i \right) + O_\prec (N^{-\frac{1}{2}}) = O_\prec (N^{-\frac{1}{2}}),
\]
where the last step follows from (5.12) with \( (t, s) = (2, 1) \). This proves (4.8).

Next we turn to prove (4.9). By (5.11) and Lemma 5.1, we observe that
\[
\sqrt{N} \mathbb{E} y^*_1 \mathcal{G}_1 v_i \mathcal{P}^{l-1} = \mathbb{E} h_{t,t}(1,0) + \mathbb{E} h_{t,t}(0,1) + \mathbb{E} h_{t,t}(1,2) + O_\prec (N^{-\frac{1}{2}}), \quad t = 1, 2. \tag{5.18}
\]
Further, using (5.12) to the first term in the RHS of (5.18), we see
\[
\sqrt{N} \mathbb{E} y^*_1 \mathcal{G}_1 v_i \mathcal{P}^{l-1} = - zm_2 \sqrt{N} \mathbb{E} y^*_2 \mathcal{G}_1 v_i \mathcal{P}^{l-1} + \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{1,1}(1,2) + O_\prec (N^{-\frac{1}{2}}) \tag{5.19}
\]
and
\[
\sqrt{N} \mathbb{E} y^*_1 \mathcal{P}^{l-1} = zm_2 \sqrt{N} \mathbb{E} y^*_2 \mathcal{P}^{l-1} - \sqrt{N} (zm_2) \mathbb{E} y^*_2 \mathcal{P}^{l-1}
\]
\[
+ \mathbb{E} h_{2,2}(0,1) + \mathbb{E} h_{2,2}(1,2) + O_\prec (N^{-\frac{1}{2}}). \tag{5.20}
\]
Plugging (5.15), (5.19) and (5.20) into (5.7), one gets
\[
\mathbb{E} \mathcal{P} = -m_1 \left( \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{1,1}(1,2) + \mathbb{E} h_{2,2}(0,1) + \mathbb{E} h_{2,2}(1,2) \right)
\]
\[
- \sqrt{N} ((zm_2)' + 1) \mathbb{E} y^*_2 \mathcal{G}_1 v_i \mathcal{P}^{l-1} + \frac{m'}{m_1} \sqrt{N} y^*_2 v_i \mathcal{P}^{l-1} + O_\prec (N^{-\frac{1}{2}}). \tag{5.21}
\]
Using the last equation of (2.5), we further obtain from (5.21) that
\[
\mathbb{E} \mathcal{P} = -m_1 \left( \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{1,1}(1,2) + \mathbb{E} h_{2,2}(0,1) + \mathbb{E} h_{2,2}(1,2) \right)
\]
\[
+ \frac{m'}{m_1} \mathbb{E} y^*_2 (\mathcal{G}_1 - m_1) v_i \mathcal{P}^{l-1} + O_\prec (N^{-\frac{1}{2}}). \tag{5.22}
\]
Similarly to (5.7), by using the first identity in (2.5), one can write
\[
\mathcal{G}_1 - m_1 = -m_1 H \mathcal{G}_1 = zm_1 m_2 \mathcal{G}_1.
\]
Then, using Lemma 5.1, we get
\[
\frac{m'}{m_1} \mathbb{E} y^*_2 (\mathcal{G}_1 - m_1) v_i \mathcal{P}^{l-1} = -m'_1 \mathbb{E} \sqrt{N} y^*_2 (H \mathcal{G}_1 + zm_2 \mathcal{G}_1) v_i \mathcal{P}^{l-1}
\]
\[
= -m'_1 \left( \mathbb{E} h_{2,1}(0,1) + \mathbb{E} h_{2,1}(1,2) \right) + O_\prec (N^{-\frac{1}{2}}). \tag{5.23}
\]
Plugging (5.23) into (5.22) yields
\[
\mathbb{E} \mathcal{P} = -m_1 \left( \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{1,1}(1,2) + \mathbb{E} h_{2,2}(0,1) + \mathbb{E} h_{2,2}(1,2) \right)
\]
\[
- m'_1 \left( \mathbb{E} h_{2,1}(0,1) + \mathbb{E} h_{2,1}(1,2) \right) + O_\prec (N^{-\frac{1}{2}}).
\]
It remains to compute the explicit formula for the RHS of the above equation. First, using (5.13), we get
\[
- m_1 \left( \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{2,2}(0,1) \right) - m'_1 \mathbb{E} h_{2,1}(0,1)
\]
\[
= (l - 1) \left( \left( y^*_2 y_1 + (y^*_1 v)^2 \right) m_1^2 (zm_1)' + \left( y^*_2 y_1 + y^*_1 v \right) v_2 (y^*_2 v_1) \right)
\]
\[
+ \left( y^*_2 y_2 + (y^*_2 v)^2 \right) (m_1 m_1' (zm_1)'' + m_1' (zm_1)' + \frac{1}{6} m_1^2 (zm_1)''') \mathcal{P}^{l-2}.
\]
Recall the definitions for \( y_1 \) and \( y_2 \) in (5.4) and the matrix \( M_i \) in (4.1) and (4.2). By elementary calculation, we arrive at
\[
- m_1 \left( \mathbb{E} h_{1,1}(0,1) + \mathbb{E} h_{2,2}(0,1) \right) - m'_1 \mathbb{E} h_{2,1}(0,1)
\]
\[
= (l - 1) \left( \sum_{j=1}^{r+2} M_i(j, j)c_j^2 + 2M_i(i, r + 2)c_r c_{r+2} \right) \mathcal{P}^{l-2}
\]
\[
= (l - 1) c^* \mathcal{M}_i c \mathcal{P}^{l-2}. \tag{5.24}
\]
Next, by (5.14), we have

\[- m_1(\mathbb{E} h_{1,1}(1,2) + \mathbb{E} h_{2,2}(1,2)) = m_1^\prime \mathbb{E} h_{2,1}(1,2)\]

\[
= (l - 1)\kappa_4 \left( s_{2,2}(y_1, v_i)(zm_2 m_1^2)^2 + 2s_{1,2}(y_1, v_i)(zm_2 m_1^2)^2 \right) + 2s_{1,2}(y_1, v_i)(zm_2 m_1^2)(zm_2 m_1^2) \mathbb{E} \mathbb{P}^{l-2},
\]

which, by the definitions of \( y_1 \) and \( y_2 \) in (5.4) and the matrix \( K \) in (4.3), can be simplified to

\[- m_1(\mathbb{E} h_{1,1}(1,2) + \mathbb{E} h_{2,2}(1,2)) = m_1^\prime \mathbb{E} h_{2,1}(1,2)\]

\[
= (l - 1)\kappa_4 \left( \sum_{j=1}^{r+2} \kappa_i(j, j)c_j^2 + \sum_{1 \leq i \neq k \leq r+2} 2\kappa_i(j, k)c_j c_k \right) \mathbb{E} \mathbb{P}^{l-2}
\]

\[
= (l - 1)\kappa_4 c^* \kappa_i c \mathbb{E} \mathbb{P}^{l-2}.
\]

Combining (5.24) and (5.25), we complete the proof of (4.9) in Proposition 4.2. Hence, we conclude the proof of Proposition 4.2.

The rest of this section is devoted to the proof of Lemma 5.1. It is convenient to first introduce the next lemma, which will be used to control the negligible terms in the proof of Lemma 5.1.

**Lemma 5.2.** For a fixed integer \( n \geq 1 \), let \( \eta_i = (\eta_{i1}, \ldots, \eta_{iM})^T \in \mathbb{C}^M, i \in [0, n] \) be any given deterministic vectors with \( \max_i ||\eta_i|| \leq C \) for some positive constant \( C \). For any positive integers \( s_0, s_1, \cdots, s_n \) and \( a = 0, 1 \), we have the following estimates:

\[
\sum_q \left| \eta_0 (G_i^{s_0})^a \left( \prod_{t=1}^n \eta_t \right) \right| = O_\prec(1),
\]

(5.26)

\[
\sum_k \left| (X^* G_i^{s_1}) (X^* G_i^{s_1} \eta_1) \right| = O_\prec(1).
\]

(5.27)

**Proof of Lemma 5.2.** The first estimate (5.26) can be proved by (2.15) and the isotropic local law (2.7) as follows:

\[
\sum_q \left| \eta_0 (G_i^{s_0})^a \left( \prod_{t=1}^n \eta_t \right) \right| = \sum_q \left| \eta_0 (G_i^{s_0})^a \left( \prod_{t=1}^n \eta_t \right) \right| = \sum_q \left| \eta_0 \left( \prod_{t=1}^n \eta_t \right) \right| = \sum_q \left| \eta_0 \left( \prod_{t=1}^n \eta_t \right) \right| = O_\prec(1).
\]

To prove (5.27), we notice that by (2.8),

\[
\sum_k (X^* G_i^{s_1} \eta_1) \right| = \sqrt{N} 1_N^* X^* G_i^{s_1} \eta_1 = O_\prec(1),
\]

where \( \sqrt{N} 1_N \in \mathbb{R}^M \) is the all-ones vector. Further, by (2.16) and the isotropic local law Theorem 2.1, we get

\[
\sum_k \left| (X^* G_i^{s_1} X) (X^* G_i^{s_1} \eta_1) \right| = \sum_k \left| (G_i^{s_0-1} + z G_i^{s_0}) (X^* G_i^{s_1} \eta_1) \right|
\]

\[
= \sum_k \left| \frac{m_2(s_0-2)}{(s_0-2)!} + \frac{m_2(s_0-1)}{(s_0-1)!} + O\left( (N^{-\frac{3}{2}}) \right) \right| (X^* G_i^{s_1} \eta_1) = O_\prec(1), \quad a = 0, 1
\]

with the convention \( m_2^{(-1)}/(1!) = 1 \).

With Lemma 5.2, we can now prove Lemma 5.1.
Proof of Lemma 5.1. In this proof, we fix $l$ and $i$. First, we compute $h_{t,s}(1,0)$ for $t, s = 1, 2$. Recall the definition in (5.10). By (A.2), we have

$$h_{t,s}(1,0) = N^{-\frac{1}{2}} \sum_{q,k} y_{q} \frac{\partial (X^* G_t^s v_i)_k}{\partial x_{qk}} P^{l-1}$$

$$= N^{-\frac{1}{2}} \sum_{q,k} y_{q} \left( (G_t^s v_i)_q - \sum_{a=1}^{2} \sum_{s_1, s_2 \geq 1, s_1 + s_2 = s + 1} (X^* G_t^{s_1} G_a^{s_2} v_i)_k \right) P^{l-1},$$

where $G_a^{s_k}, a = 1, 2$ are defined in (2.17). Taking the sum over $q, k$, we get

$$h_{t,s}(1,0) = \sqrt{N} y_i G_t^s v_i - N^{-\frac{1}{2}} \sum_{s_1, s_2 \geq 1} y_i G_t^{s_1} X^* G_t^{s_2} v_i + y_i G_t^{s_1} v_i \text{Tr}(X^* G_t^{s_1} X) P^{l-1}. \quad (5.28)$$

By the identity in (2.16), Theorem 2.1, and the fact $|P| \ll 1$, we further get

$$N^{-\frac{1}{2}} \sum_{s_1, s_2 \geq 1, s_1 + s_2 = s + 1} y_i G_t^{s_1} X^* G_t^{s_2} v_i = O(N^{-\frac{1}{2}}). \quad (5.29)$$

Substituting (5.29) into (5.28), we get

$$h_{t,s}(1,0) = \sqrt{N} y_i G_t^s v_i - \sqrt{N} \sum_{s_1, s_2 \geq 1} y_i G_t^{s_1} v_i \text{Tr}(X^* G_t^{s_1} X) P^{l-1} + O(N^{-\frac{1}{2}}). \quad (5.30)$$

Using the second identity in (2.16), and Theorem 2.1, we have

$$\frac{1}{N} \text{Tr}(X^* G_t^{s_1} X) = \frac{1}{N} \text{Tr}(G_t^{s_1 - 1}) + z G_t^{s_1} = \frac{m_2 (s_1 - 2)}{(s_1 - 2)!} + \frac{z m_2 (s_1 - 1)}{(s_1 - 1)!} + O(N^{-1}). \quad (5.31)$$

Then we obtain from (5.30) that

$$h_{t,s}(1,0) = -\sqrt{N} z m_2 y_i G_t^{s_1} v_i P^{l-1}$$

$$- \sqrt{N} \sum_{2 \leq s_1 \leq s_1, 1 \leq s_2 \leq s_1} \left( \frac{m_2 (s_1 - 2)}{(s_1 - 2)!} + \frac{z m_2 (s_1 - 1)}{(s_1 - 1)!} \right) y_i G_t^{s_2} v_i P^{l-1} + O(N^{-\frac{1}{2}}). \quad (5.32)$$

Further by the simple fact

$$\frac{z m_a}{l!} + \frac{m_a (l-1)}{(l-1)!} = \frac{1}{l!}(z m_a)^{(l)}, \quad a = 1, 2, \quad (5.33)$$

we can conclude the proof of (5.12) from (5.32).

Next, we turn to estimate $h_{t,s}(0,1)$, which by the definition in (5.10) reads

$$h_{t,s}(0,1) = (l - 1) N^{-\frac{1}{2}} \sum_{q,k} y_{q} (X^* G_t^s v_i)_k \frac{\partial P}{\partial x_{qk}} P^{l-2}. \quad (5.34)$$

Using the formula (A.6) to (5.34), we get

$$h_{t,s}(0,1) = -(l - 1) \sum_{b=1}^{2} \sum_{b_1 + b_2 = b} \left( (y_i G_t^{b_1} y_i)(v_i G_t^{b_2} X X^* G_t^s v_i) + (y_i G_t^{b_2} v_i)(y_i G_t^{b_1} X X^* G_t^s v_i) \right) P^{l-2}. \quad (5.35)$$

By (2.16), we have

$$G_t^{b_1} X X^* G_t^s = G_t^{b_1 + s - 1} + z G_t^{b_1 + s}, \quad a = 1, 2.$$
Hence, by (2.7) and the bound $|P| \prec 1$, one gets from (5.35) that

$$
\begin{align*}
hts(0,1) &= -(l-1) \sum_{b=1}^{2} \sum_{b_1, b_2 \geq 1 \atop b_1 + b_2 = b+1} \left( m_{b_1-1} m_{b_2-1} \right) \left( m_{s+b_1-2} m_{s+b_2-2} \right) + z m_{l-1} \left| y_k y_j \right| \\
& \quad + m_{l-1} \left( m_{l-1} \right) \left( m_{s+b_1-1} m_{s+b_2-1} \right) \left( m_{s+b_1-1} m_{s+b_2-1} \right) \left| y_k y_j v_k v_j \right| p_l^{l-2} + O_{\prec}(N^{-\frac{l}{2}}).
\end{align*}
$$

Using (5.33) to (5.36), we can conclude the proof of (5.13).

Next, we show (5.14). First, by the definition in (5.10), we have

$$
\begin{align*}
hts(1,2) &= \frac{\kappa_4}{2N^2} \sum_{q,k} y_{q,k} \left[ \frac{d(X^*G_1^q v_i)_k}{dq} \right] \left( l-1 \right) \left( \frac{d^2 P}{dx_{qk}} \right) p_l^{l-2} + (l-1)(l-2) \left( \frac{dP}{dx_{qk}} \right)^2 p_l^{l-3} \\
&= \kappa_4 (l-1)J_1 + \kappa_4 (l-1)(l-2)J_2,
\end{align*}
$$

where $\kappa_4 (l-1)J_1$ and $\kappa_4 (l-1)(l-2)J_2$ correspond to the sum involving the first and the second terms in the parenthesis in the first step, respectively. In the following, we shall give the estimates of $J_1$ and $J_2$.

To estimate $J_1$, using (A.8) and (A.2), we see

$$
\begin{align*}
J_1 &= \frac{1}{2N^2} \sum_{q,k} y_{q,k} \left[ \frac{d(X^*G_1^q v_i)_k}{dq} \right] \left( l-1 \right) \left( \frac{d^2 P}{dx_{qk}} \right) p_l^{l-2} \\
&= \frac{1}{N} \sum_{q,k} y_{q,k} \left( (G_1^q v_i)_q \right) - \sum_{a=1}^{2} \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s+1} \left( X^*G_1^a \circ G_2^{a_2} v_i \right)_k \\
& \quad \times \sum_{b=1}^{2} \sum_{a_1, a_2 = 1 \atop a_1 + a_2 = a+1} \left( G_1^{a_1} \circ G_2^{a_2} \right) v_i p_l^{l-2}. \tag{5.38}
\end{align*}
$$

Further, we claim that

$$
\begin{align*}
J_1 &= \frac{1}{N} \sum_{q,k} y_{q,k} \left( (G_1^q v_i)_q \right) - \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s+1} \left( X^*G_1^{s_1} \circ G_2^{s_2} v_i \right)_k \\
& \quad \times \sum_{b=1}^{2} \sum_{a_1, a_2 = 1 \atop a_1 + a_2 = a+1} \left( G_1^{a_1} \circ G_2^{a_2} \right) v_i p_l^{l-2} + O_{\prec}(N^{-\frac{1}{2}}). \tag{5.39}
\end{align*}
$$

To see the reduction from (5.38) to (5.39), we notice that the terms absorbed in $O_{\prec}(N^{-\frac{1}{2}})$ always contain some quadratic forms of $X^*G_1^a$ as a factor, for some $a \geq 1$. Then the isotropic local law (2.8) can be applied to show that these terms are bounded by $O_{\prec}(N^{-\frac{1}{2}})$. For instance, we have

$$
\begin{align*}
& N^{-\frac{1}{2}} \sum_{q,k} y_{q,k} \left( \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s+1} \left( X^*G_1^{s_1} \circ G_2^{s_2} v_i \right)_k \right) \left( \frac{d^2 P}{dx_{qk}} \right) p_l^{l-2} \\
& \prec N^{-\frac{1}{2}} \left( \sum_{q,k} y_{q,k} \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s+1} \left( X^*G_1^{s_1} \circ G_2^{s_2} v_i \right)_k \right) \left( \frac{d^2 P}{dx_{qk}} \right) \\
& \prec N^{-1} \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s+1} \left( \sum_{q} \left| y_{q,k} \right| \right) \left( \left| X^*G_1^{s_1} \circ G_2^{s_2} v_i \right| \right) k = O_{\prec}(N^{-\frac{1}{2}}).
\end{align*}
$$

In the first and second steps above, we used the bound $|P| \prec 1$ and (A.9), respectively. In the last step, we used the isotropic local law (2.8) and also the fact $\sum_{q} \left| y_{q,k} \right| \prec \sqrt{N}$. The other negligible terms can be estimated similarly. We omit the details.
Plugging the definitions in (2.17) into (5.39) yields
\[ J_1 = \frac{1}{N} \sum_{q,k} y_q \left( (G_1^q v_i)_q - \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s + 1} (X^* G_1^{s_1} X)_{kk} (G_1^{s_2} v_i)_q \right) \]
\[ \times \sum_{b=1}^2 \left( \sum_{b_1, b_2, b_3 \geq 1 \atop b_1 + b_2 + b_3 = b + 2} (y_b G_1^{b_1})_q (X^* G_1^{b_2} X)_{kk} (G_1^{b_3} v_i)_q - \sum_{b_1, b_2 \geq 1 \atop b_1 + b_2 = b + 1} (y_b G_1^{b_1})_q (G_1^{b_2} v_i)_q \right) \mathcal{P}^{l-2} + O_\prec(N^{-\frac{3}{2}}). \]

Again, applying the identities in Lemma 2.7, the isotropic local laws (2.7), and (2.9), we see
\[ J_1 = \frac{m_1^{(s-1)}}{(s-1)!} \left( \sum_{q} y_q y_q y_q q q q \right) (z m_2 m_1^2) + \left( \sum_{q} y_q y_q y_q q q q \right) (z m_2 m_1^2) \mathcal{P}^{l-2} + O_\prec(N^{-\frac{3}{2}}) \]
\[ = \frac{(z m_2 m_1^{(s-1)})}{(s-1)!} \sum_{b=0}^1 s_{1,1,2} (y_1, y_{b+1}, v_i) (z m_2 m_1^{(s)}) \mathcal{P}^{l-2} + O_\prec(N^{-\frac{3}{2}}). \] (5.40)

Next, we show that
\[ J_2 = \frac{1}{2 N^2} \sum_{q,k} y_q \frac{\partial (X^* G_1^q v_i)_k}{\partial x_{qk}} \left( \frac{\partial \mathcal{P}}{\partial x_{qk}} \right)^2 \mathcal{P}^{l-3} = O_\prec(N^{-\frac{3}{2}}). \] (5.41)

With (A.2), we write \( J_2 \) as
\[ J_2 = \frac{1}{2 N^2} \sum_{q,k} y_q \left( (G_1^q v_i)_q - \sum_{a=1}^2 \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s + 1} (X^* G_1^{s_1} G_2^{s_2} v_i)_k \right) \left( \frac{\partial \mathcal{P}}{\partial x_{qk}} \right)^2 \mathcal{P}^{l-3} \]
\[ = \frac{1}{2 N^2} \sum_{q,k} y_q \left( (G_1^q v_i)_q - \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s + 1} (X^* G_1^{s_1} X)_{kk} (G_1^{s_2} v_i)_q \right) \left( \frac{\partial \mathcal{P}}{\partial x_{qk}} \right)^2 \mathcal{P}^{l-3} + O_\prec(N^{-\frac{3}{2}}), \] (5.42)

where in the last step we bounded the \( a = 1 \) terms by \( O_\prec(N^{-\frac{3}{2}}) \) since
\[ \left| \frac{1}{2 N^2} \sum_{q,k} y_q \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s + 1} (X^* G_1^{s_1} G_2^{s_2} v_i)_k \left( \frac{\partial \mathcal{P}}{\partial x_{qk}} \right)^2 \mathcal{P}^{l-3} \right| \]
\[ \ll N^{-\frac{3}{2}} \sum_{s_1, s_2 \geq 1 \atop s_1 + s_2 = s + 1} \sum_{q,k} \left| (X^* G_1^{s_1} G_2^{s_2} v_i)_k \right| \left| (X^* G_1^{s_1} G_2^{s_2} v_i)_q \right| = O_\prec(N^{-\frac{3}{2}}). \]

Here we used the \( O_\prec(1) \) bound for both \( \mathcal{P} \) and \( \partial \mathcal{P}/\partial x_{qk} \) (c.f., (A.7)) for the first step and (2.8) for the second step.

Further, we have
\[ \left| N^{-\frac{3}{2}} \sum_{q,k} y_q \left( (X^* G_1^{s_1} X)_{kk} \right)^a (G_1^{s_2} v_i)_q \left( \frac{\partial \mathcal{P}}{\partial x_{qk}} \right)^2 \mathcal{P}^{l-3} \right| \]
\[ \ll N^{-\frac{3}{2}} \sum_{a=0, 1} \sum_{q,k} \left| y_q (G_1^{s_2} v_i)_q \right| = O_\prec(N^{-\frac{3}{2}}), \quad a = 0, 1. \] (5.43)

Here, in the first step we used \( O_\prec(1) \) bounds for \( \mathcal{P} \), \( \partial \mathcal{P}/\partial x_{qk} \) (c.f., (A.7)), and also \( (X^* G_1^{s_1} X)_{kk} \) whose bound follows from (2.16) and the local law, and in the second step we use Cauchy-Schwarz inequality and the local law. With (5.43), we can now conclude (5.41) from (5.42). Then (5.37), (5.40) and (5.41) imply (5.14).

In the sequel, we prove (2) of Lemma 5.1, i.e., we show that except for (5.12)-(5.14) all the other terms \( h_{t,a}(\alpha_1, \alpha_2) \) with \( \alpha_1 + \alpha_2 \leq 3 \) can be bounded by \( O_\prec(N^{-\frac{3}{2}}) \). We start with the case when \( \alpha_1 + \alpha_2 = 2 \,
i.e. \((\alpha_1, \alpha_2) = (2,0), (0,2), (1,1)\). Recall the notation \(\kappa_3\) for the common 3rd cumulant of all \(\sqrt{N}x_{ij}\)’s from Assumption 1.1 (iii). First, by (A.3), we have

\[
h_{t,s}(2, 0) = \frac{\kappa_3}{2N} \sum_{q,k} y_{tq} \left( \frac{\partial^2 (X^* G_1^q v_i)_k}{\partial x_{qk}^2} \right) P^{l-1}
\]

\[
= \frac{\kappa_3}{N} \sum_{q,k} y_{tq} \left( \sum_{a_1,a_2=1}^2 \sum_{s_1,s_2 \geq 1} \left( X^* G_1^{s_1} \frac{\partial G_1^{s_2}}{\partial x_{qk}} G_1^{s_2} v_i \right)_k - \sum_{a_1,a_2=1}^2 \left( X^* G_1^{s_1} \frac{\partial G_1^{s_2}}{\partial x_{qk}} G_1^{s_2} v_i \right)_k \right) P^{l-1}. \tag{5.44}
\]

Note that all terms above contain at least one quadratic form of \(X^* G_1^a\) as a factor, for some \(a \geq 1\). This fact eventually leads to the \(O_{\prec}(N^{-\frac{7}{2}})\) bound for all terms above, by the isotropic local law. More specifically, plugging the definitions in (2.17) into (5.44) and taking the sums, we can see that the RHS of (5.44) is a linear combination of the terms of the following forms

\[
N^{-1} \sum_{q,k} y_{tq} (X^* G_1^{s_1})_{kk} (X^* G_1^{s_2})_{kk} (X^* G_1^{s_3})_{kk} P^{l-1} \tag{5.45}
\]

\[
N^{-1} \sum_{q,k} y_{tq} ((X^* G_1^{s_1} X)_{kk})^a (X^* G_1^{s_2})_{kk} (X^* G_1^{s_3})_{kk} P^{l-1}, \tag{5.46}
\]

\[
N^{-1} \sum_{q,k} y_{tq} ((X^* G_1^{s_1} X)_{kk})^a (X^* G_1^{s_3})_{kk} (X^* G_1^{s_3})_{kk} P^{l-1}, \quad a = 1, 2. \tag{5.47}
\]

First, by simply using the \(O_{\prec}(1)\) bound for \(P^{l-1}\) and the \(O_{\prec}(N^{-\frac{7}{2}})\) bound for \((X^* G_1^{s_1})_{kk}, (X^* G_1^{s_2})_{kk},\) and \((X^* G_1^{s_3})_{kk}\) one can get the \(O_{\prec}(N^{-\frac{7}{2}})\) bound for the term in (5.45). Second, using the \(O_{\prec}(1)\) bound for \(P^{l-1}\) and \(((X^* G_1^{s_1} X)_{kk})^a\), and also the \(O_{\prec}(N^{-\frac{7}{2}})\) bound for \((X^* G_1^{s_2})_{kk}\), we have

\[
(5.46) = O_{\prec} \left( N^{-\frac{7}{2}} \sum_q |y_{tq} (G_1^{s_3})_{kk}| \right) = O_{\prec}(N^{-\frac{7}{2}}), \tag{5.48}
\]

where we used the Cauchy-Schwarz inequality and the isotropic local law in the last step. Third, by Cauchy-Schwarz inequality and (2.7), we have

\[
\left| N^{-1} \sum_{q,k} y_{tq} ((X^* G_1^{s_1} X)_{kk})^a (G_1^{s_3})_{kk} (X^* G_1^{s_3})_{kk} \right| \\
\leq N^{-1} \| h_t \| \left( \sum_q \| G_1^{s_3} \|_{2,qq}^2 \right)^{1/2} \left( \sum_k \left| (X^* G_1^{s_1} X)_{kk} \right|^a \right) \left| (X^* G_1^{s_3})_{kk} \right| \\
< N^{-\frac{7}{2}} \left\| (X^* G_1^{s_1} X)_{kk} \right\|^a \left| (X^* G_1^{s_3})_{kk} \right| < N^{-\frac{7}{2}}. \tag{5.49}
\]

In the last step above, we used (5.27). Hence, we conclude \(h_{t,s}(2, 0) = O_{\prec}(N^{-\frac{7}{2}})\).

Next, in the case of \((\alpha_1, \alpha_2) = (0,2)\), by the definition in (5.10), we have

\[
h_{t,s}(0, 2) = (l - 1)(l - 2) \frac{\kappa_3}{2N} \sum_{q,k} y_{tq} (X^* G_1^{a_1} v_i)_k \left( \frac{\partial P}{\partial x_{qk}} \right)^2 P^{l-3}
\]

\[
+ (l - 1) \frac{\kappa_3}{2N} \sum_{q,k} y_{tq} (X^* G_1^{a_1} v_i)_k \frac{\partial^2 P}{\partial x_{qk}^2} P^{l-2}. \tag{5.50}
\]

We then use the formula in (A.6). After expanding the first term in the RHS of (5.50), one notices that it can be written as a linear combination of the terms of the forms

\[
\sum_q y_{tq} (G_1^{s_1} \eta_1)_q (G_1^{s_2} \psi_1)_q \sum_k (X^* G_1^{a_1} v_i)_k (X^* G_1^{b_1} \eta_2)_k (X^* G_1^{b_2} \psi_2)_k P^{l-3}, \tag{5.51}
\]

where the vectors \(\eta_\alpha, \psi_\alpha (\alpha = 1, 2)\) take \(v_1, y_1\) or \(y_2\) and \(a_1,a_2,b_1,b_2 = 1 \text{ or } 2\). We claim that the general form in (5.51) is \(O_{\prec}(N^{-\frac{7}{2}})\) for all choices of \(\eta_\alpha, \psi_\alpha, a_1,a_2,b_1,b_2\) listed above. To see this, we
first notice that the isotropic local law (2.8) implies
\[
\sum_k (X^* G^1_k v_1)_k (X^* G^b_1 \eta_2)_k (X^* G^b_2 \psi_2)_k = O_\prec(N^{-\frac{1}{2}}).
\] (5.52)

Further, from (5.26), we have
\[
\sum_q y_q (G^b_1 \eta_1)_q (G^b_2 \psi_1)_q = O_\prec(1).
\] (5.53)

Combining (5.52), (5.53), and the fact \(|P| \prec 1\), we conclude that the term in (5.51) is of order \(O_\prec(N^{-\frac{1}{2}})\). This further implies that the first term in the RHS of (5.50) is \(O_\prec(N^{-\frac{1}{2}})\).

Analogously, using the formula in (A.8), it is easy to see that the second term in the RHS of (5.50) is a linear combination of the terms of the following forms
\[
N^{-\frac{1}{2}} \left( \sum_{q,k} y_q (G^b_1 \eta_1)_q (G^b_2 \eta_2)_k \left( \sum_k ((X^* G^b_k X)_kk) \eta_2 (X^* G^b_1 v_1)_k \right) P^{l-2},
\] (5.54)
\[
N^{-\frac{1}{2}} \left( \sum_{q,k} y_q (G^b_1 \eta_1)_q \left( \sum_k (X^* G^b_1 \eta_2)_k (X^* G^b_1 v_1)_k \right) P^{l-2},
\] (5.55)
\[
N^{-\frac{1}{2}} \left( \sum_{q,k} y_q (G^b_1 \eta_1)_q \left( \sum_k (X^* G^b_1 \eta_2)_k (X^* G^b_1 v_1)_k \right) P^{l-2},
\] (5.56)
for \(\eta_1, \eta_2 = v_1, y_1, or y_2, a = 0, 1\) and \(b_1, b_2, b_3 = 1 or 2\). We claim that all of the above terms can be bounded by \(O_\prec(N^{-\frac{1}{2}})\). First, recall the bound \(|P| \prec 1\). The \(O_\prec(N^{-\frac{1}{2}})\) bound for (5.54) follows directly from (5.26) and (5.27). From (5.26) and the isotropic local law (2.8), we see that (5.55) is also bounded by \(O_\prec(N^{-\frac{1}{2}})\). The estimate of (5.56) is similar to (5.49) by using the Cauchy-Schwarz inequality and the isotropic local law (2.8). We thus omit the details. Hence, the second term in the RHS of (5.50) is also of order \(O_\prec(N^{-\frac{1}{2}})\). This together with the same bound for the first term in the RHS of (5.50) leads to the fact that
\[
h_{t,s}(0, 2) = O_\prec(N^{-\frac{1}{2}}).
\]

Next, we turn to \(h_{t,s}(1, 1)\). By the definition in (5.10), we have
\[
h_{t,s}(1, 1) = \frac{\kappa_3}{N} \sum_{q,k} y_q \frac{\partial (X^* G^1_k v_1)}{\partial x_{kq}} \frac{\partial P}{\partial x_{kq}} P^{l-2}.
\] (5.57)

Using (A.2) and (A.6), we can write
\[
h_{t,s}(1, 1) = -N^{-\frac{1}{2}} \kappa_3 \sum_{q,k} y_q \left( (G^1_k v_1)_q - \sum_{s_1, a_2 \geq 1} \right) \left( (X^* G^1_k)_{a_2} (X^* G^2 X)_k X (G^b_1 v_1)_q \right) \times \sum_{b=1}^2 \sum_{b_1, b_2 \geq 1} \left( y_q (G^b_1)_q (X^* G^b_1 v_1)_k + (X^* G^b_1 y_b)_k (G^b_1 v_1)_q \right) P^{l-1}.
\] (5.58)

It is easy to see that the above is a linear combination of the terms of the following forms
\[
N^{-\frac{1}{2}} \left( \sum_{q,k} y_q (G^1_k v_1)_q (G^b_1 \eta_1)_q \left( \sum_k (X^* G^b_2 X)_k \eta_2 (X^* G^b_1 X)_k \right) P^{l-1},
\] Similarly to estimates of (5.54) and (5.55), both terms above can be bounded by \(O_\prec(N^{-\frac{1}{2}})\). Hence, we have \(h_{t,s}(1, 1) = O_\prec(N^{-\frac{1}{2}})\).

Next, we consider the other cases for \(a_1 + a_2 = 3\) except for (5.14), i.e. \((a_1, a_2) = (3, 0), (2, 1), (0, 3)\). We start with the formulas in (A.4) and (A.10). Notice that according to the definition in (A.1), we have \(O_2 = \{(0, 1), (0, 2), (1, 0), (2, 0)\}\) in (A.4) and (A.10).

With (A.4), we can now estimate \(h_{t,s}(3, 0)\). By the definition in (5.10),
\[
h_{t,s}(3, 0) = \frac{\kappa_4}{3! N^2} \sum_{q,k} y_q \frac{\partial^3 (X^* G^b_1 v_1)_k}{\partial x_{kq}^3} P^{l-1}.
\] (5.59)
After plugging in (A.4) and taking the sums, one can check that except for the following type of terms

\[ N^{-\frac{1}{2}} \left( \sum_{q} y_q (G_1^{(s_1)} q_q (G_1^{(s_2)} v_1) q_k) \left( \sum_{k} \left( (X^* G_1^{(s_1)} X)_{kk} \right)^a \left( (X^* G_1^{(s_2)} X)_{kk} \right)^b \right) \right) \mathcal{P}^{l-1} \quad a, b = 0, 1, \quad (5.60) \]

all the other terms of (5.59) contain at least one quadratic form of \( X^* G_1^a \) for some \( a \geq 1 \). Actually, by the isotropic local law (2.8), those terms with at least one quadratic form of \( X^* G_1^a \) can all be bounded by \( O_\prec(N^{-1}) \). For instance,

\[ N^{-\frac{1}{2}} \sum_{q,k} y_q (G_1^{(s_1)} q_q (G_1^{(s_2)} v_1) q_k) \mathcal{P}^{l-1} \]

\[ = N^{-\frac{1}{2}} \sum_{q,k} y_q (G_1^{(s_1)} q_q (X^* G_1^{(s_2)})_{kq} (X^* G_1^{(s_2)} v_1) q_k) \mathcal{P}^{l-1} = O_\prec(N^{-1}). \]

The other terms with at least one quadratic form of \( X^* G_1^a \) can be estimated similarly. We omit the details. Further, using (5.26) and also Remark 2.4, one can easily get the \( O_\prec(N^{-\frac{1}{2}}) \) for the terms in (5.60). As a consequence, we get \( h_{t,s}(3,0) = O_\prec(N^{-\frac{1}{2}}) \).

Next, for \( h_{t,s}(2,1) \), by the definition in (5.10), we have

\[ h_{t,s}(2,1) = \frac{(l-1)\kappa_4}{2N^{\frac{1}{2}}} \sum_{q,k} y_q \frac{\partial^2 (X^* G_1^a v_1)_{q_k}}{\partial x_{q_k}^2} \frac{\partial \mathcal{P}}{\partial x_{q_k}} \mathcal{P}^{l-2} \quad (6.51) \]

Using the formula in (A.3) and further the \( O_\prec(N^{-\frac{1}{2}}) \) bound for the quadratic forms of \( X^* G_1^a, a \geq 1 \), it is not difficult to see

\[ \frac{\partial^2 (X^* G_1^a v_1)_{q_k}}{\partial x_{q_k}^2} = O_\prec(N^{-\frac{1}{2}}), \]

similarly to the previous discussion. Then, the above bound together with the \( O_\prec(1) \) bound for \( \partial \mathcal{P}/\partial x_{q_k} \) \((c.f., (A.7)) \) and \( \mathcal{P} \), one can conclude that \( h_{t,s}(2,1) = O_\prec(N^{-\frac{1}{2}}) \).

For \( h_{t,s}(0,3) \), we first write

\[ h_{t,s}(0,3) = \frac{\kappa_4}{3!N^{\frac{1}{2}}} \sum_{q,k} y_q (X^* G_1^a v_1)_{q_k} \frac{\partial^3 \mathcal{P}^{l-1}}{\partial x_{q_k}^3} \]

\[ = \kappa_4 (l-1)(l-2)(l-3) \mathcal{L}_1 + \kappa_4 (l-1)(l-2) \mathcal{L}_2 + \kappa_4 (l-1) \mathcal{L}_3, \]

where

\[ \mathcal{L}_1 := \frac{1}{3!N^{\frac{1}{2}}} \sum_{q,k} y_q (X^* G_1^a v_1)_{q_k} \left( \frac{\partial \mathcal{P}}{\partial x_{q_k}} \right)^3 \mathcal{P}^{l-4}, \]

\[ \mathcal{L}_2 := \frac{1}{2!N^{\frac{1}{2}}} \sum_{q,k} y_q (X^* G_1^a v_1)_{q_k} \frac{\partial \mathcal{P}}{\partial x_{q_k}} \frac{\partial^2 \mathcal{P}}{\partial x_{q_k}^2} \mathcal{P}^{l-3}, \]

\[ \mathcal{L}_3 := \frac{1}{3!N^{\frac{1}{2}}} \sum_{q,k} y_q (X^* G_1^a v_1)_{q_k} \frac{\partial^3 \mathcal{P}}{\partial x_{q_k}^3} \mathcal{P}^{l-2}. \]

First, note that \( \mathcal{L}_1 = O_\prec(N^{-\frac{1}{2}}) \), by using the facts \( |\partial \mathcal{P}/\partial x_{q_k}| \ll 1 \) \((c.f., (A.7)) \) and \( |(X^* G_1^a v_1)_{q_k}| \ll N^{-\frac{1}{2}} \) \((c.f., (2.8)) \), together with the Cauchy-Schwarz inequality.

Second, as for \( \mathcal{L}_2 \), we use the formula of \( \partial^2 \mathcal{P}/\partial x_{q_k}^2 \) in (A.8). Observe that, by the isotropic local laws (2.7) and (2.8), the terms in (A.8) can be bounded by either \( O_\prec(N^{-1/2}) \) or \( O_\prec(\sqrt{N}) \). More precisely, those \( O_\prec(N^{-1/2}) \) terms possess one of the following forms

\[ \sqrt{N} (X^* G_1^{b_1} \eta_1)_q (X^* G_1^{b_2} \eta_2)_q \eta_1 \quad \sqrt{N} (X^* G_1^{b_1} \eta_1)_q (X^* G_1^{b_2})_{q_k} (G_1^{b_3} \eta_2)_q \]

and those \( O_\prec(\sqrt{N}) \) terms possess the common form \( \sqrt{N} (G_1^{b_1} \eta_1)_q (X^* G_1^{b_2} X)_{kk} (G_1^{b_3} \eta_2)_q \). Here, \( \eta_1, \eta_2 = y_1, y_2, \) or \( v_1, \) \( a = 0, 1 \) and \( b_1, b_2, b_3 = 1 \) or 2. The contribution from the \( O_\prec(N^{-1/2}) \) terms can be discussed similarly to \( \mathcal{L}_1 \). We thus omit the details. For the contribution from the those \( O_\prec(\sqrt{N}) \) terms, we notice that it suffices to consider the bound of the following forms

\[ \frac{1}{\sqrt{N}} \sum_{q} y_q (G_1^{b_1} \eta_1)_q (G_1^{b_2})_{q_k} (G_1^{b_3} v_1)_q \left( \sum_{k} (X^* G_1^a v_1)_{q_k} (X^* G_1^{b_1} v_1)_{q_k} ((X^* G_1^{b_3} X)_{kk})^a \right) \mathcal{P}^{l-3}, \quad a = 0, 1 \]

\[ (5.62) \]
which is $O_{\prec}(N^{-\frac{1}{2}})$ by (5.26) and the isotropic local laws (2.7) and (2.8). Hence, $\mathcal{L}_2$ is also bounded by $O_{\prec}(N^{-\frac{1}{2}})$.

Finally, for $\mathcal{L}_3$, we use the bound in (A.11). Then following the same argument as for $\mathcal{L}_1$, one can prove that $\mathcal{L}_3 = O_{\prec}(N^{-\frac{1}{2}})$. To conclude, we have $h_{t,s}(0,3) = O_{\prec}(N^{-\frac{1}{2}})$.

Hence, we conclude the proof of (2) in Lemma 5.1.

Before we proceed to the proof of the remainder term $\mathcal{R}_{t,s}$, let us comment that, using the same reasoning as we previously did for $h_{t,s}(\alpha_1, \alpha_2)$ with $\alpha_1 + \alpha_2 \leq 3$, one can also get

$$N^{-2} \sum_{q,k} \left| y_t \frac{\partial^4 ((X^*G^*_1 v_i)_k P^{(l-1)})}{\partial x_{qk}^4} \right| = O_{\prec}(N^{-\frac{1}{2}}),$$

(5.63)

which further implies that $h_{t,s}(\alpha_1, \alpha_2) = O_{\prec}(N^{-\frac{1}{2}})$ for $\alpha_1 + \alpha_2 = 4$. The main tools are still Lemma 5.2 and the isotropic local laws (2.7) and (2.8). We omit the details. The necessary formulas for the fourth derivatives of $(X^*G^*_1)_{kj}$ and $P$ are recorded in the Appendix for the readers' convenience.

In the end, we prove (3) of Lemma 5.1, i.e., we show the estimate of $\mathcal{R}_{t,s}$. By Lemma 2.6, we can bound $\mathcal{R}_{t,s}$ by

$$|\mathcal{R}_{t,s}| \leq \sqrt{N} \sum_{q,k} \mathbb{E} \left( N^{-\frac{3}{2}} \sup_{|x_{qk}| \leq N^{-\frac{1}{4}}} \left| y_t \frac{\partial^4 ((X^*G^*_1 v_i)_k P^{(l-1)})}{\partial x_{qk}^4} \right| \right) + N^{-\tilde{K}} \sup_{x_{qk} \in \mathbb{R}} \left| y_t \frac{\partial^4 ((X^*G^*_1 v_i)_k P^{(l-1)})}{\partial x_{qk}^4} \right|, \tag{5.64}$$

for any sufficiently large constant $\tilde{K}$. We evaluate the RHS of (5.64) term by term.

First, we claim that similarly to (5.63) we have

$$\sqrt{N} \mathbb{E} \left( N^{-\frac{3}{2}} \sup_{|x_{qk}| \leq N^{-\frac{1}{4}}} \sum_{q,k} \left| y_t \frac{\partial^4 ((X^*G^*_1 v_i)_k P^{(l-1)})}{\partial x_{qk}^4} \right| \right) = O_{\prec}(N^{-\frac{1}{2}}). \tag{5.65}$$

Differently from (5.63), in (5.65), we actually consider a random matrix $\tilde{X}$ with the $(q,k)$-th entry deterministic while all the other entries random. Using a regular perturbation argument through the resolvent expansion, one can show that replacing one random entry $x_{qk}$ in $X$ by any deterministic number bounded by $N^{-1/2+s}$ while keeping all the other $X$ entries random will not change the isotropic local law. Then the isotropic local law together with the trivial deterministic bounds in (5.1)-(5.3) leads to (5.65).

For the second term of (5.64), we simply use the crude deterministic bounds in (5.1)-(5.3). By choosing $\tilde{K}$ sufficiently large, we can conclude that the second term in (5.64) is negligible.

This completes the proof of Lemma 5.1.

\[ \square \]

**Appendix A. Collection of derivatives**

In this section, we summarize some derivatives that appear in the previous sections. And all these derivatives can be obtained by repeatedly applying the second identity in (2.18) and chain rule. For convenience, we set

$$O_i := \{(a_1, \cdots, a_l) : \exists i \in \{1, \cdots, l\}, \ a_i = 0, \text{and } a_j = 1, 2 \text{ for all } j \neq i\} \tag{A.1}$$

Below, we first collect the derivatives of $(X^*G^*_1 v)_k$ for some deterministic unit vector $v$, which can be derived by using (2.18) and the product rule. The first derivative of $(X^*G^*_1 v)_k$

$$\frac{\partial (X^*G^*_1 v)_k}{\partial x_{qk}} = (G^*_1 v)_q - \sum_{a=1}^{2} \sum_{s_1, s_2 \geq 1; s_1 + s_2 = s + 1} (X^*G^*_1 \mathcal{P}_a^Q G^*_1 v)_k. \tag{A.2}$$

The second derivative of $(X^*G^*_1 v)_k$

$$\frac{\partial^2 (X^*G^*_1 v)_k}{\partial x_{qk}^2} = -2 \left( \sum_{a=1}^{2} \sum_{s_1, s_2 \geq 1; s_1 + s_2 = s + 1} (G^*_1 \mathcal{P}_a^Q G^*_1 v)_q + \sum_{a_1, a_2=1}^{2} \sum_{s_1, s_2, s_3 \geq 1; \sum_{i=1}^{2} s_i = s + 2} (X^*G^*_1 \mathcal{P}_{a_1}^Q G^*_1 \mathcal{P}_{a_2}^Q G^*_1 v)_k \right)$$

$$- \sum_{s_1, s_2 \geq 1; s_1 + s_2 = s + 1} (X^*G^*_1 \mathcal{P}_0^Q G^*_1 v)_k. \tag{A.3}$$
The third derivative of \((X^*G^*_1v)_k\)

\[ \frac{\partial^3 (X^*G^*_1v)_k}{\partial x^r_{qk}} = 6 \left( \sum_{a_1,a_2=1}^{2} \sum_{s_1,s_2,s_3 \geq 1}^{3} \left( G^*_{1a_1} P^q_{a_1} G^*_{1a_2} P^q_{a_2} G^*_{1} v \right)_q - \sum_{s_1, s_2 = s+1}^{3} \left( G^*_{1a_1} P^q_{a_1} G^*_{1} v \right)_q \right) \]

\[ - \sum_{a_1,a_2,a_3=1}^{2} \sum_{s_1, s_2, s_3 \geq 1}^{3} \left( X^* \left( \prod_{i=1}^{3} (G^*_{1}) \right) G^*_{1} v \right)_k \]

\[ + \sum_{(a_1,a_2) \in \mathbb{O}_2} \sum_{s_1, s_2 \geq 1}^{3} \left( X^* \left( \prod_{i=1}^{2} (G^*_{1}) \right) G^*_{1} v \right)_k. \]  

(A.4)

The fourth derivative of \((X^*G^*_1v)_k\)

\[ \frac{\partial^4 (X^*G^*_1v)_k}{\partial x^r_{qk}} = 4! \left( \sum_{a_1,a_2,a_3=1}^{2} \sum_{s_1, s_2, s_3 \geq 1}^{3} \left( \left( \prod_{i=1}^{2} (G^*_{1}) \right) G^*_{1} v \right)_q \right) \]

\[ + \sum_{(a_1,a_2) \in \mathbb{O}_2} \sum_{s_1, s_2 \geq 1}^{3} \left( \left( \prod_{i=1}^{2} (G^*_{1}) \right) G^*_{1} v \right)_k \]

\[ + \sum_{a_1, \ldots, a_4=1}^{2} \sum_{s_1, \ldots, s_4 \geq 1}^{3} \left( X^* \left( \prod_{i=1}^{3} (G^*_{1}) \right) G^*_{1} v \right)_k \]

\[ - \sum_{(a_1,a_2,a_3) \in \mathbb{O}_3} \sum_{s_1, s_2, s_3 \geq 1}^{3} \left( X^* \left( \prod_{i=1}^{2} (G^*_{1}) \right) G^*_{1} v \right)_k \]

\[ + \sum_{s_1, s_2 \geq 1}^{3} \left( X^* \left( \prod_{i=1}^{2} (G^*_{1}) \right) G^*_{1} v \right)_k. \]  

(A.5)

Next, for \(P\) defined in (5.5), we collect its derivatives

\[ \frac{\partial^s P}{\partial x^r_{qk}} = \sqrt{N} \sum_{b=1}^{2} y^*_b \frac{\partial^s G^*_b}{\partial x^r_{qk}} v_i \]

for \(1 \leq s \leq 4\). For the first derivative, we have

\[ \frac{\partial P}{\partial x_{qk}} = -\sqrt{N} \sum_{b=1}^{2} b_n \sum_{b_1, b_2 \geq 1}^{2} \left( (y^*_b G^*_b) y_q (X^* G^*_2 v_i)_k + (X^* G^*_1 y_q) (G^*_1 v_i)_q \right). \]  

(A.6)

By (2.8) and Remark 2.4, it is easy to see that

\[ \left| \frac{\partial P}{\partial x_{qk}} \right| \prec 1. \]  

(A.7)

The second derivative of \(P\) is

\[ \frac{\partial^2 P}{\partial x_{qk}} = 2\sqrt{N} \sum_{b=1}^{2} \left( \sum_{a_1,a_2=1}^{2} \sum_{b_1, b_2 \geq 1}^{2} \sum_{s_1, s_2 \geq 1}^{3} y^*_b \left( \prod_{j=1}^{2} (G^*_b P^{qk}) \right) G^*_b v_i - \sum_{b_1, b_2 \geq 1}^{2} y^*_b G^*_b (G^*_1 P^{qk} G^*_2 v_i) \right). \]  

(A.8)

Recalling the definition of \(P^{qk}\) for \(i = 0, 1, 2\) in (2.17), one observes that all terms in the parenthesis admit one of the following forms

\[ (X^* G^*_1 \eta_1)_k (X^* G^*_1 \eta_2)_q (G^*_2 \eta_1) \]

\[ (X^* G^*_1 \eta_1)_k (G^*_1 \eta_2)_q (X^* G^*_1 \eta_2)_k \]

\[ (G^*_1 \eta_1)_q (X^* G^*_1 X) G^*_k (G^*_2 \eta_2)_q \]
for η₁, η₂ = y₁, y₂, vᵢ, a = 0, 1 and b₁, b₂, b₃ = 1, 2, which are bounded by O₂(N⁻²), O₂(N⁻⁴) and O₂(1) respectively, in light of (2.8) and Remark 2.4. Therefore, combining with the prefactor √N in (A.8), we get the bound

\[ \frac{\partial^2 P}{\partial x_{qk}^2} \sim \sqrt{N}. \] (A.9)

The third derivative of P is

\[ \frac{\partial^3 P}{\partial x_{qk}^3} = -6\sqrt{N} \sum_{b=1}^{2} \left( \sum_{a₁, a₂, a₃ = 1}^{2} \sum_{b₁ \cdots b₄ \geq 1 ; \sum_{i=1}^{3} b_i = b+3} \left( y_i^a \left( \prod_{j=1}^{3} (G^b_j \tilde{\mathcal{P}}^k_j) \right) G^b_i v_i \right) \right) \]

\[ - \sum_{(a₁, a₂) \in \mathcal{O}_2} \sum_{b₁, b₂, b₃ \geq 1 ; \sum_{i=1}^{3} b_i = b+2} \left( y_i^a \left( \prod_{j=1}^{3} (G^b_j \tilde{\mathcal{P}}^k_j) \right) G^b_i v_i \right). \] (A.10)

By plugging the definition of Ψ₂ₚₚ in (2.17), one can see that all summands above contain at least one quadratic form of \((X^* G^a_i)\) for some \(a \geq 1\), which by (2.8) will contribute a \(O₂(N^{-2})\) factor. Using this fact, one can easily show the crude bound

\[ \left| \frac{\partial^3 P}{\partial x_{qk}^3} \right| < 1. \] (A.11)

The fourth derivative of P is

\[ \frac{\partial^4 P}{\partial x_{qk}^4} = 4! \sqrt{N} \sum_{b=1}^{2} \left( \sum_{a₁, \cdots, a₄ = 1}^{2} \sum_{b₁ \cdots b₄ \geq 1 ; \sum_{i=1}^{4} b_i = b+4} \left( y_i^a \left( \prod_{j=1}^{4} (G^b_j \tilde{\mathcal{P}}^k_j) \right) G^b_i v_i \right) \right) \]

\[ - \sum_{(a₁, a₂, a₃) \in \mathcal{O}_3} \sum_{b₁, b₂, b₃ \geq 1 ; \sum_{i=1}^{3} b_i = b+3} \left( y_i^a \left( \prod_{j=1}^{3} (G^b_j \tilde{\mathcal{P}}^k_j) \right) G^b_i v_i \right) \]

\[ + \sum_{b₁, b₂, b₃ \geq 1 ; \sum_{i=1}^{3} b_i = b+2} \left( y_i^a \left( \prod_{j=1}^{2} (G^b_j \tilde{\mathcal{P}}^k_j) \right) G^b_i v_i \right). \] (A.12)

**References**

[1] Z.D. Bai, J.F. Yao. Central limit theorems for eigenvalues in a spiked population model. *Annales de l'IHP Probabilités et statistiques* 44(3), 447–474, 2008.

[2] Z.D. Bai, J.F. Yao. On sample eigenvalues in a generalized spiked population model. *Journal of Multivariate Analysis*, 106, 167–177, 2012.

[3] J. Baik, G. Ben Arous, and S. Péché. Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *The Annals of Probability*, 33(5), 1643–1697, 2005.

[4] J. Baik, J.W. Silverstein. Eigenvalues of large sample covariance matrices of spiked population models. *Journal of Multivariate analysis*, 97(6), 1382–1408, 2006.

[5] Z.G. Bao, X.C. Ding, and K. Wang. Singular vector and singular subspace distribution for the matrix denoising model. *arXiv:1809.10476*, 2018.

[6] S. Belinschi, H. Bercovici, M. Capitaine. On the outlying eigenvalues of a polynomial in large independent random matrices. *arXiv:1703.08102*, 2017.

[7] S. Belinschi, H. Bercovici, M. Capitaine, and M. Février. Outliers in the spectrum of large deformed unitarily invariant models. *The Annals of Probability*, 45(6A), 3571–3625, 2017.

[8] F. Benaych-Georges, A. Guionnet, and M. Maïda. Fluctuations of the extreme eigenvalues of finite rank deformations of random matrices. *Electronic Journal of Probability*, 16, 1621–1662, 2011.

[9] F. Benaych-Georges, R. R. Nadakuditi. The singular values and vectors of low rank perturbations of large rectangular random matrices. *Journal of Multivariate Analysis*, 111, 120–135, 2012.

[10] F. Benaych-Georges, R. R. Nadakuditi. The eigenvalues and eigenvectors of finite, low rank perturbations of large random matrices. *Advances in Mathematics*, 227(1), 494–521, 2011.

[11] A. Bloemendaal, A. Knowles, H.-T. Yau, and J. Yin. On the principal components of sample covariance matrices. *Probability theory and related fields*, 164(1-2):459–552, 2016.

[12] A. Bloemendaal, B. Virág. Limits of spiked random matrices I. *Probability Theory and Related Fields*, 156(3-4), 795–825, 2013.

[13] A. Bloemendaal, B. Virág. Limits of spiked random matrices II. *The Annals of Probability*, 44(4), 2726–2769, 2016.
A. Bloemendal, L. Erdos, A. Knowles, H.-T. Yau, and J. Yin. Isotropic local laws for sample covariance and generalized wigner matrices. *Electron. J. Probab.*, 19(33):1–53, 2014.

M. Capitaine. Limiting eigenvectors of outliers for Spiked Information-Plus-Noise type matrices. *Séminaire de Probabilités ALIX* 119–164, Springer, Cham, 2018.

M. Capitaine, C. Donati-Martin. Spectrum of deformed random matrices and free probability. *arXiv:1607.05560*, 2016.

M. Capitaine, C. Donati-Martin. Non universality of fluctuations of outlier eigenvectors for block diagonal deformations of Wigner matrices. *arXiv:1807.07773*, 2018.

M. Capitaine, C. Donati-Martin, and D. Féral. The largest eigenvalues of finite rank deformation of large Wigner matrices: convergence and nonuniversality of the fluctuations. *The Annals of Probability*, 37(1), 1–47, 2009.

M. Capitaine, C. Donati-Martin, and D. Féral. Central limit theorems for eigenvalues of deformations of Wigner matrices. *Annales de l'IHP Probabilités et statistiques* 48(1), 107–133, 2012.

X.C. Ding. High dimensional deformed rectangular matrices with applications in matrix denoising. *Bernoulli (to appear)*, 2017.

L. Erdős, A. Knowles, and H.-T. Yau. Averaging fluctuations in resolvents of random band matrices. *Ann. Henri Poincaré*, 14(8):1837–1926, 2013.

J. Fan, Y. Fan, X. Han, and J. Lv. Asymptotic theory of eigenvectors for large random matrices. *arXiv:1902.06846*, 2019.

D. Féral, S. Péché. The largest eigenvalue of rank one deformation of large Wigner matrices. *Communications in mathematical physics*, 272(1), 185–228, 2007.

Y. He, A. Knowles. Mesoscopic eigenvalue statistics of Wigner matrices. *The Annals of Applied Probability*, 27(3), 1510–1550, 2017.

I. M. Johnstone. On the distribution of the largest eigenvalue in principal components analysis. *The Annals of statistics*, 29(2): 295–327, 2001.

I. M. Johnstone, J. Yang. Notes on asymptotics of sample eigenstructure for spiked covariance models with non-Gaussian data. *arXiv:1810.10427*, 2018.

A.M. Khorunzhy, B.A. Khoruzhenko, and L.A. Pastur. Asymptotic properties of large random matrices with independent entries. *Journal of Mathematical Physics*, 37(10):5033–5060, 1996.

A. Knowles, J. Yin. The isotropic semicircle law and deformation of Wigner matrices. *Communications on Pure and Applied Mathematics*, 66(11), 1663–1749, 2013.

A. Knowles, J. Yin. The outliers of a deformed Wigner matrix. *The Annals of Probability*, 42(5), 1980–2031, 2014.

A. Knowles, J. Yin. Anisotropic local laws for random matrices. *Probability Theory and Related Fields*, 169(1-2):257–352, 2017.

J. O. Lee, K. Schnelli. Local law and Tracy-Widom limit for sparse random matrices. *Probability Theory and Related Fields*, 171(1-2), 543-616, 2018.

P. Loubaton, P. Vallet. Almost sure localization of the eigenvalues in a Gaussian information plus noise model. Application to the spiked models. *Electronic Journal of Probability*, 16, 1934–1959, 2011.

A. Lytova and L. Pastur. Central limit theorem for linear eigenvalue statistics of random matrices with independent entries. *Ann. Probab.*, 37(5):1778–1840, 2009.

V.A. Marčenko, L.A. Pastur. Distribution of eigenvalues for some sets of random matrices. *Mathematics of the USSR-Sbornik*, 1(4):457, 1967.

D. Morales-Jimenez, I. M. Johnstone, M. R. McKay, and J. Yang. Asymptotics of eigenstructure of sample correlation matrices for high-dimensional spiked models. *arXiv:1810.10214*, 2018.

D. Paul. Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica*, 1617–1642, 2007.

S. Péché. The largest eigenvalue of small rank perturbations of Hermitian random matrices. *Probability Theory and Related Fields*, 134(1), 127–173, 2006.

N. S. Pillai, J. Yin. Universality of covariance matrices. *The Annals of Applied Probability*, 24(3), 935-1001, 2014.

A. Pizzo, D. Renfrew, and A. Soshnikov. On finite rank deformations of Wigner matrices. *Annales de l'IHP Probabilités et statistiques* 49(1), 64–94, 2013.