EIGENVALUES IN MULTIVARIATE RANDOM EFFECTS MODELS

A DISSERTATION
SUBMITTED TO THE DEPARTMENT OF STATISTICS
AND THE COMMITTEE ON GRADUATE STUDIES
OF STANFORD UNIVERSITY
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

Zhou Fan
June 2018

Preface

We study principal component analyses in multivariate random and mixed effects linear models. These models are commonly used in quantitative genetics to decompose the variation of phenotypic traits into consistuent variance components. Applications arising in evolutionary biology require understanding the eigenvalues and eigenvectors of these components in high-dimensional multivariate settings. However, these quantities may be difficult to estimate from limited samples when the number of traits is large.

We describe several phenomena concerning sample eigenvalues and eigenvectors of classical MANOVA estimators in the presence of high-dimensional noise, including dispersion of the bulk eigenvalue distribution, bias and aliasing of outlier eigenvalues and eigenvectors, and Tracy-Widom fluctuations at the spectral edges. A common theme is that the spectral properties of the MANOVA estimate for one component may be influenced by the other components. In the setting of a simple spiked covariance model, we introduce alternative estimators for the leading eigenvalues and eigenvectors that correct for this problem in a high-dimensional asymptotic regime.

The contents of this thesis are drawn from three manuscripts. Section 2.2, Chapter 3, and Appendix A are drawn, with minor modification, from the manuscript "Tracy-Widom at each edge of real covariance estimators," jointly authored with Iain M. Johnstone [FJ17]. Sections 2.1, 2.3, 2.4, (parts of) 2.6, and Chapter 4 are drawn, with minor modification, from a manuscript "Spiked covariances and principal components analysis in high-dimensional random effects models," in preparation and jointly authored with Iain M. Johnstone and Yi Sun. Sections 2.5, (parts of) 2.6, Chapter 5, and Appendix B are drawn, with minor modification, from a manuscript "Eigenvalue distributions of variance components estimators in high-dimensional random effects models," jointly authored with Iain M. Johnstone [FJ16].

Acknowledgments

This thesis is the product of the support of many people. First and foremost among them are my Ph.D. advisors Andrea Montanari and Iain Johnstone. Working with Andrea has shown me the excitement of exploring the unknown and taught me to have courage in asking questions which I do not know how to begin to answer. Working with Iain has taught me the importance of understanding, and that the process by which this occurs takes continuous dedication, revisiting, and perseverance. Without both of their support, encouragement, kindness, and mentorship, the work in this thesis would not have been possible.

I am deeply grateful to Mark Blows, for introducing me to the questions addressed in this thesis, his patience in teaching me quantitative genetics, and his continued encouragement of this research. I am also extremely grateful to Yi Sun, for embarking on the latter parts of this project together with me, and for being a wonderful and supportive friend over the years.

Thanks to Emmanuel Candès for his support throughout my Ph.D. studies; to Ron Dror for encouraging me to embark on this path; to Lester Mackey, Amir Dembo, Rob Tibshirani, David Siegmund, and Hua Tang for their advice and mentorship; and to Chiara Sabatti and Lexing Ying for volunteering their time and energy to be on my thesis committee. Thanks to the Fannie & John Hertz Foundation and the NDSEG Fellowship for supporting my graduate studies, and also for exposing me to a broader academic community.

I am fortunate to have met Lexi here at Stanford, whose love and optimism and playful spirit have carried me through these years. I hope that we may learn and laugh and grow together in the many years to come.

Thanks to many friends at Stanford—Ashok, Emma, Janet, Jessy, and Keli for weekends of Chinese food, bubble tea, and 80 points. David, Jessy, Jiyao, Joey, Junyang, Kris, Nan, Rakesh, Snigdha, and Subhabrata for their rapport in the first year. Alex, Andy, Edgar, Emily, Gene, Jong, Keli, Mona, Pragya, Rakesh, and Wenfei for many exciting adventures. Cyrus, Dennis, Jacob, Jelena, Naftali, Nike, Ruby, Song, Xiaoying, and Yash for their friendship and support. Thanks also to friends back home—Benny, Charles, Diana, Marion, Richard, Yi, and many others—for their encouragement.

Finally, thanks to my parents, for their faith in whatever it is that I choose to do.

Contents

Chapter 1

Introduction

We study multivariate random and mixed effects linear models. As a simple example, consider a twin study measuring p quantitative traits in n individuals, consisting of $n/2$ pairs of identical twins. We may model the observed traits of the j^{th} individual in the i^{th} pair as

$$\mathbf{y}_{i,j} = \boldsymbol{\mu} + \boldsymbol{\alpha}_i + \boldsymbol{\varepsilon}_{i,j} \in \mathbb{R}^p. \tag{1.1}$$

Here, $\boldsymbol{\mu}$ is a deterministic vector of mean trait values in the population, and

$$\boldsymbol{\alpha}_i \overset{iid}{\sim} (0, \Sigma_1), \qquad \boldsymbol{\varepsilon}_{i,j} \overset{iid}{\sim} (0, \Sigma_2)$$

are unobserved, independent random vectors modeling trait variation at the pair and individual levels. Assuming the absence of shared environment, the covariance matrices $\Sigma_1, \Sigma_2 \in \mathbb{R}^{p \times p}$ may be interpreted as the genetic and environmental components of variance.

Since the pioneering work of R. A. Fisher [Fis18], such models have been widely used to decompose the variation of quantitative traits into constituent variance components. The genetic variance is commonly further decomposed into that of additive effects from individual alleles, dominance effects between alleles at the same locus, and epistatic effects between alleles at different loci [Wri35]. Environmental components of variance may be individual-specific, as above, or potentially also shared within families or batches of an experimental protocol. In many applications, for example measuring the heritability of traits, predicting evolutionary response to selection, and correcting for confounding variation from experimental procedures, it is of interest to estimate the individual variance components [FM96, LW98, VHW08].

Classically, variance components may be estimated by examining the resemblance between relatives [Fis18]. In plant and animal populations, this is commonly performed using breeding designs. For example, the additive genetic variance may be estimated via a "half-sib" design corresponding to the one-way model (1.1). Each group i consists of individuals j bearing a half-sibling relationship, and $4\,\Sigma_1$ corresponds to the additive genetic variance in the absence of shared environment and epistatis [LW98]. Additional variance due to dominance may be estimated using more complex designs: In the North Carolina I design corresponding to the two-way nested model

$$\mathbf{y}_{i,j,k} = \boldsymbol{\mu} + \boldsymbol{\alpha}_i + \boldsymbol{\beta}_{i,j} + \boldsymbol{\varepsilon}_{i,j,k}, \qquad \boldsymbol{\alpha}_i \overset{iid}{\sim} (0, \Sigma_1), \qquad \boldsymbol{\beta}_{i,j} \overset{iid}{\sim} (0, \Sigma_2), \qquad \boldsymbol{\varepsilon}_{i,j,k} \overset{iid}{\sim} (0, \Sigma_3), \tag{1.2}$$

groups i consist of half-siblings (sharing the father) which are further divided into sub-groups j of full-siblings (sharing also the mother). Comparing Σ_1 and Σ_2 provides a measure of variance due to dominance plus shared maternal environment. Variance due to these two effects may, in turn, be disentangled using the North Carolina II design corresponding to the crossed model

$$\mathbf{y}_{j,k,l} = \boldsymbol{\mu} + \boldsymbol{\beta}_j + \boldsymbol{\gamma}_k + \boldsymbol{\delta}_{j,k} + \boldsymbol{\varepsilon}_{j,k,l}, \tag{1.3}$$

where fathers j are cross-bred to mothers k, and $\mathbf{y}_{j,k,l}$ are the traits in the l^{th} offspring of the mating pair (j, k) [CR48].

The modern era of genome-wide association studies has witnessed a resurgence of mixed effects modeling, where contributions of single-nucleotide polymorphisms (SNPs) to highly polygenic traits are modeled as independent and unobserved random effects [YLGV11, ZCS13, MLH$^+$15, LTBS$^+$15]. Letting $\mathbf{y}_i$ denote the observed traits of individual i with genotypes $(u_{i1}, \ldots, u_{im})$ at m measured SNPs, the basic infinitesimal model represents $\mathbf{y}_i$ as

$$\mathbf{y}_i = \boldsymbol{\mu} + \sum_{j=1}^{m} u_{ij} \boldsymbol{\alpha}_j + \boldsymbol{\varepsilon}_i, \qquad \boldsymbol{\alpha}_j \overset{iid}{\sim} (0, \Sigma_1), \qquad \boldsymbol{\varepsilon}_i \overset{iid}{\sim} (0, \Sigma_2), \tag{1.4}$$

where Σ_1 determines the genetic contribution to trait variation from the measured SNPs. Extensions of this model may divide the SNPs into functional categories, for example corresponding to coding regions or various histone methylation states, and attribute a different covariance Σ_r to the effects of SNPs in each category [FBSG$^+$15].

These types of mixed effects models are often applied in univariate contexts, $p = 1$, to study variation and heritability of individual traits. However, certain questions arising in evolutionary biology require an understanding of the joint variation of multiple, and oftentimes many, phenotypic traits. For example, the evolutionary response of a population to selection is predicted by the breeder's equation [Lus37, Lan79, LA83]

$$\Delta\boldsymbol{\mu} = G(\Sigma^{-1}\mathbf{s}). \tag{1.5}$$

Here, $\mathbf{s} \in \mathbb{R}^p$ is the selection differential quantifying the effect of selection on each trait in the current generation, $\Delta\boldsymbol{\mu} \in \mathbb{R}^p$ is the change in mean trait values inherited in the next generation, Σ is the total population trait covariance, and G is its additive genetic component. Correlation between traits is common at both the genetic and environmental levels [Bar90, WB09], indicating that G and Σ are often not diagonal. Hence selection on one trait may cause a response in a correlated trait, and a full understanding of the evolutionary process will likely require an understanding of the variation of high-dimensional multivariate phenotypes [Blo07, Hou10, HGO10]. For studies involving gene-expression phenotypes, trait dimensionality in the several thousands is common [MCM$^+$14, CMA$^+$18].

In settings of large p, important properties of the variance component matrices Σ_r in the above models are dictated by their spectral structure, and it is often natural to interpret these matrices in terms of their principal component decompositions [Blo07, BM15]. For example, the largest eigenvalues and effective rank of the additive genetic component of covariance indicate the extent to which evolutionary response to natural selection is genetically constrained to a lower dimensional phenotypic subspace, and the principal eigenvectors indicate likely directions of phenotypic response [MH05, HB06, WB09, HMB14, BAC$^+$15]. Similar interpretations apply to the spectral structure of variance components that capture variation due to genetic mutation [MAB15, CMA$^+$18].

Contributions

We study a general multivariate mixed effects linear model with k variance components $\Sigma_1, \ldots, \Sigma_k$. Classical procedures for estimating these components may be unbiased and asymptotically consistent entrywise as an estimate for the variance of each trait and covariance of each trait pair. However, this does not imply desirable properties for the estimated eigenvalues and eigenvectors when p is large.

To illustrate the problems that may arise, Figure 1.1 depicts the eigenvalues and principal eigenvector of the multivariate analysis of variance (MANOVA) [SR74, SCM09] and multivariate restricted maximum likelihood (REML) [KP69, Mey91] estimates of Σ_1 in the balanced one-way model (1.1). REML estimates were computed by the post-processing procedure described in [Ame85]. In this example, the true group covariance Σ_1 has rank one, representing a single direction of variation. The true error covariance Σ_2 also represents a single true direction of variation which is partially aligned with that of Σ_1, plus additional isotropic noise. Partial alignment of eigenvectors of Σ_2 with those of Σ_1 may be common, for example, in sibling designs where the additive genetic covariance contributes both to Σ_1 and Σ_2. We observe in this setting several problematic phenomena concerning either the MANOVA or REML estimate $\widehat{\Sigma}_1$:

Eigenvalue dispersion. The eigenvalues of $\widehat{\Sigma}_1$ are widely dispersed, even though all but one true eigenvalue of Σ_1 is non-zero. In particular, this dispersion causes the MANOVA estimate $\widehat{\Sigma}_1$ to not be positive semi-definite.

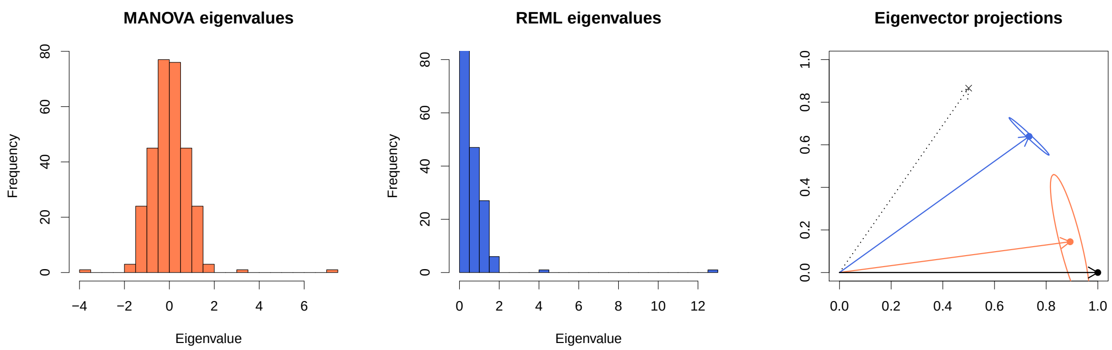

Figure 1.1: Eigenvalues and principal eigenvector of the MANOVA and REML estimates of Σ_1 in a one-way design with $I = 300$ groups of size $J = 2$ and $p = 300$ traits. The true group covariance is $\Sigma_1 = 6\mathbf{e}_1\mathbf{e}_1'$ (rank one), and the true error covariance is $\Sigma_2 = 29\mathbf{v}\mathbf{v}' + \mathrm{Id}$ where $\mathbf{v} = \frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2$. Histograms display eigenvalues averaged across 100 simulations. The rightmost plot displays the empirical mean and 90% ellipsoids for the first two coordinates of the unit-norm principal eigenvector (MANOVA in red and REML in blue), with $\mathbf{e}_1$ and $\mathbf{v}$ shown in black.

Eigenvalue aliasing. The estimate $\widehat{\Sigma}_1$ exhibits multiple outlier eigenvalues which indicate significant directions of variation, even though the true matrix Σ_1 has rank one.

Eigenvalue bias. The largest eigenvalue of $\widehat{\Sigma}_1$ is biased upwards from the true eigenvalue of Σ_1.

Eigenvector aliasing. The principal eigenvector of $\widehat{\Sigma}_1$ is not aligned with the true eigenvector of Σ_1, but rather is biased in the direction of the eigenvector of Σ_2.

Several eigenvalue shrinkage and rank-reduced estimation procedures have been proposed to address some of these shortcomings, with associated simulation studies of their performance in low-to-moderate dimensions [HH81, KM04, MK05, MK08, MK10]. In this thesis, we focus on higher-dimensional applications and study these phenomena theoretically and from an asymptotic viewpoint.

We restrict attention to MANOVA-type estimators, and do not further address REML estimation in this work. We impose throughout an assumption of Gaussianity. As a model for the high-dimensional applications of interest, we study the asymptotic regime where $n, p \to \infty$ proportionally. Motivated by the specific models (1.1–1.4), we assume also that the number of realizations of each random effect increases proportionally with n and p. Our results are summarized in Chapter 2, and the remaining three chapters are dedicated to the mathematical proofs.

We show that in the presense of high-dimensional noise, the eigenvalues of a MANOVA estimator

$\widehat{\Sigma}$ exhibit a dispersion pattern that is well-approximated by a non-degenerate spectral law μ_0. When the noise represented by each variance component is isotropic, a simple reduction to the Marcenko-Pastur model [MP67] shows that μ_0 is characterized by the Marcenko-Pastur equation (cf. Section 2.2). When the noise is non-isotropic, μ_0 may be characterized by the solution of a more general system of fixed-point equations, which we describe in Section 2.5. In both cases, this law μ_0 may depend on variance components other than the one estimated by $\widehat{\Sigma}$.

Assuming isotropic noise, we study in greater detail the spiked covariance model of [Joh01] that encapsulates the example of Figure 1.1. In this model, each true variance component Σ_r may have a small number of spike eigenvalues representing signal directions of variation beyond the isotropic noise. In Section 2.2, we verify that outlier eigenvalues of $\widehat{\Sigma}$ should not appear under the null hypothesis when such signal eigenvalues are absent, and we establish Tracy-Widom asymptotics for the eigenvalues of $\widehat{\Sigma}$ at the edges of the support of μ_0 as a means of testing this null hypothesis.

When signal eigenvalues are present, we show in Section 2.3 that the outlier eigenvalues of the estimate $\widehat{\Sigma}$ may represent a combination of signal eigenvalues and eigenvectors in different variance components. More specifically, each outlier eigenvalue $\hat{\lambda}$ of $\widehat{\Sigma}$ is close to an eigenvalue of a surrogate linear combination of $\Sigma_1, \ldots, \Sigma_k$, and the corresponding eigenvector is partially aligned with the eigenvector of the surrogate. We use this insight in Section 2.4 to develop a novel procedure for estimating the spike eigenvalues and eigenvectors of any component Σ_r, by identifying alternative matrices $\widehat{\Sigma}$ where the surrogate depends only on the single component Σ_r. We prove that the resulting eigenvalue estimates are asymptotically consistent, while the eigenvector estimates are asymptotically void of aliasing effects.

Our results pertain to general mixed effects models, although we focus special attention on the classical setting of balanced classification designs. This encompasses the models (1.1), (1.2), and (1.3) when group sizes are equal. In such designs, MANOVA estimators are canonically defined, and they coincide with REML estimators if the likelihood is maximized over symmetric matrices $\Sigma_1, \ldots, \Sigma_k$ without positive definite constraints. Our results and assumptions are more explicit in this setting, and we discuss these specializations in Section 2.6.

Proof techniques and related literature

Chapters 3, 4, and 5 are devoted to the mathematical proofs of these results, and each may be read independently. Our analyses use techniques of asymptotic random matrix theory, and we provide a necessarily partial summary of related literature here.

In the setting of a global sphericity null hypothesis, Section 2.2 and Chapter 3, our model is closely related to the sample covariance model with a general population covariance matrix Σ. The eigenvalue distribution of this matrix model in the regime $n, p \to \infty$ has been studied by many authors, including [MP67, Yin86, Sil95, SB95]. When $\Sigma = \mathrm{Id}$, the limiting eigenvalue law is commonly called the Marcenko-Pastur distribution. For purposes of hypothesis testing, we focus attention on the extreme eigenvalues at the edges of the spectrum, which were shown to converge to the endpoints of the limiting spectral support for $\Sigma = \mathrm{Id}$ in [Gem80, YBK88, BY93] and for general positive semi-definite Σ in [BS98]. For $\Sigma = \mathrm{Id}$ and complex and real Gaussian data, respectively, [Joh00] and [Joh01] showed that the largest eigenvalue exhibits fluctuations described by the GUE and GOE Tracy-Widom laws of [TW94, TW96]. Generalizations to non-Gaussian data and to the smallest eigenvalue were established in [Sos02, Péc09, FS10, PY14]. For $\Sigma \neq \mathrm{Id}$, the works [Kar07, Ona08] established GUE Tracy-Widom fluctuations of the largest eigenvalue in the complex Gaussian case, under a regularity condition for the rightmost edge introduced in [Kar07]. This was extended to each regular edge of the support in [HHN16]. GOE Tracy-Widom fluctuations for the largest eigenvalue in the real Gaussian setting was proven in [LS16], using techniques different from those of [Kar07, Ona08, HHN16] and based on earlier work for the deformed Wigner model in [LS15]. Universality of these results with respect to the Gaussian assumptions was proven in [BPZ15, KY17]. We generalize the result of [LS16] to establish GOE Tracy-Widom fluctuations at each regular edge of the spectral support, extending the proof to use a discrete Lindeberg swapping argument in place of a continuous flow. We also extend the notion of edge regularity and associated analysis to a model where the analogue of Σ may not be positive semi-definite.

In settings where variance components have a spiked structure, Sections 2.3, 2.4, and Chapter 4, our probabilistic results are analogous to those regarding outlier eigenvalues and eigenvectors for the spiked sample covariance model, studied in [BBP05, BS06, Pau07, Nad08, BY08], and our proofs use the matrix perturbation approach of [Pau07] which is related also to the approaches of [BGN11, BGGM11, BY12]. An extra ingredient needed in our proof is a deterministic approximation for arbitrary linear and quadratic functions of entries of the resolvent in the Marcenko-Pastur model. We establish this for spectral arguments separated from the limiting support, building on the local laws for this setting in [BEK$^+$14, KY17] and using a fluctuation averaging idea inspired by [EYY11, EYY12, EKYY13a, EKYY13b]. We note that new qualitative phenomena emerge in our model which are not present in the setting of spiked sample covariance matrices—outliers may depend on the alignments between population spike eigenvectors in different variance components, and a single spike may generate multiple outliers. This latter phenomenon was observed in a different context in [BBC$^+$17], which studied sums and products of independent unitarily invariant matrices in spiked settings. Our predictions for outlier eigenvalue locations and eigenvector alignments may be shown to coincide with those of [BBC$^+$17] in certain scenarios where the spike eigenvectors of $\Sigma_1, \ldots, \Sigma_k$ are asymptotically unaligned.

Finally, for general variance components $\Sigma_1, \ldots, \Sigma_k$, our matrix model is similar to the model of MIMO channels studied in [MS07, DL11] and also has some points of contact with the models studied in [Lix06, CDS11]. We extend the convergence in mean of the empirical spectral measure in [DL11] to almost-sure convergence, and the fixed-point equations which we derive may be shown to coincide with those of [Lix06, MS07, CDS11, DL11] in common special cases. We formulate our result in terms of a deterministic equivalent spectral law, following [HLN07, CDS11]. However, our proof deviates from the analytical proofs in these works and instead employs a free probability argument inspired by [SV12], which separates the asymptotic approximation from the computation of the fixed-point equations. The approximation argument follows a long line of work establishing asymptotic freeness of large random matrices [Voi91, Dyk95, Voi98, HP00, Col03, CŚ06], in particular in a context of conditional freeness for rectangular matrix models [BG09]. We extend the results of [BG09, SV12] to an asymptotic freeness theorem required for the study of our model. Our computation of the fixed-point equations uses relations between conditional moments, free cumulants, and Cauchy and $\mathcal{R}$-transforms over various sub-algebras, developed in [Spe98, NSS02, SV12].

Notational conventions

For a square matrix X, $\operatorname{spec}(X)$ is its multiset of eigenvalues (counting multiplicity). For a law μ_0 on $\mathbb{R}$, we denote its closed support

$$\operatorname{supp}(\mu_0) = \{x \in \mathbb{R} : \mu_0([x-\varepsilon, x+\varepsilon]) > 0 \text{ for all } \varepsilon > 0\}.$$

$\mathbf{e}_i$ is the i^{th} standard basis vector, Id is the identity matrix, and $\mathbf{1}$ is the all-1's column vector, where dimensions are understood from context. We use Id_n and $\mathbf{1}_n$ to explicitly emphasize the dimension n.

$\|\cdot\|$ is the Euclidean norm for vectors and the Euclidean operator norm for matrices. $\|\cdot\|_{\text{HS}}$ is the matrix Hilbert-Schmidt norm. X' and X^* are the transpose and conjugate-transpose of X. $\operatorname{col}(X)$ is the column span of X, and $\ker(X)$ is its kernel or null space.

$A \otimes B$ is the matrix tensor product. When Y and M are matrices, $Y \sim \mathcal{N}(M, A \otimes B)$ is shorthand for $\operatorname{vec}(Y') \sim \mathcal{N}(\operatorname{vec}(M'), A \otimes B)$, where $\operatorname{vec}(Y')$ and $\operatorname{vec}(M')$ are the row-wise vectorizations of Y and M. $\operatorname{diag}(A_1, \ldots, A_k)$ is the block-diagonal matrix with diagonal blocks $A_1, \ldots, A_k$.

For subspaces U and V, $\dim(U)$ is the dimension of U, $U \oplus V$ is the orthogonal direct sum, and $V \ominus U$ is the orthogonal complement of U in V.

$\mathbb{C}^+$ and $\overline{\mathbb{C}^+}$ are the open and closed upper-half complex planes. For $z \in \mathbb{C}$, $\operatorname{Im} z$ and $\operatorname{Re} z$ are the real and imaginary parts of z. We typically write $z = E + i\eta$ where $E = \operatorname{Re} z$ and $\eta = \operatorname{Im} z$. For $A \subset \mathbb{C}$, $\operatorname{dist}(z, A) = \inf\{|y - z| \colon y \in A\}$ is the distance from z to A.

Chapter 2

Main results

2.1 Model

We consider observations $Y \in \mathbb{R}^{n \times p}$ of p traits in n individuals, modeled by a Gaussian mixed effects linear model

$$Y = X\beta + U_1\alpha_1 + \ldots + U_k\alpha_k, \qquad \alpha_r \sim \mathcal{N}(0, \mathrm{Id}_{m_r} \otimes \Sigma_r) \quad \text{for } r = 1, \ldots, k. \tag{2.1}$$

The matrices $\alpha_1, \ldots, \alpha_k$ are independent, with each matrix $\alpha_r \in \mathbb{R}^{m_r \times p}$ having independent rows, representing m_r (unobserved) realizations of a p-dimensional random effect with distribution $\mathcal{N}(0, \Sigma_r)$. The incidence matrix $U_r \in \mathbb{R}^{n \times m_r}$, which is known from the experimental protocol, determines how the random effect contributes to the observations Y. The first term $X\beta$ models possible additional fixed effects, where $X \in \mathbb{R}^{n \times q}$ is a known design matrix of q regressors and $\beta \in \mathbb{R}^{q \times p}$ contains the corresponding regression coefficients.

This model is usually written with an additional residual error term $\varepsilon \in \mathbb{R}^{n \times p}$. We incorporate this by allowing the last random effect to be $\alpha_k = \varepsilon$ and $U_k = \mathrm{Id}_n$. For example, the one-way model (1.1) corresponds to (2.1) where $k = 2$. Supposing there are I groups of equal size J, we set $m_1 = I$, $m_2 = n = IJ$, stack the vectors $\mathbf{y}_{i,j}$, $\boldsymbol{\alpha}_i$, and $\boldsymbol{\varepsilon}_{i,j}$ as the rows of Y, α_1, and α_2, and identify

$$X = \mathbf{1}_n, \qquad \beta = \boldsymbol{\mu}', \qquad U_1 = \mathrm{Id}_I \otimes \mathbf{1}_J = \begin{pmatrix} \mathbf{1}_J & & \\ & \ddots & \\ & & \mathbf{1}_J \end{pmatrix}, \qquad U_2 = \mathrm{Id}_n\,. \tag{2.2}$$

Here, X is a single all-1's regressor, and U_1 has I columns indicating the I groups. Similarly, the SNP model (1.4) is an example where $k = 2$ and $U_1 \in \mathbb{R}^{n \times m}$ contains the genotype values. The models (1.2) and (1.3), and extensions of (1.4) to different functional categories for SNPs, correspond to examples where $k \geq 3$.

Under the general model (2.1), Y has the multivariate normal distribution

$$Y \sim \mathcal{N}(X\beta,\ U_1U_1' \otimes \Sigma_1 + \ldots + U_kU_k' \otimes \Sigma_k). \tag{2.3}$$

The unknown parameters of the model are $(\beta, \Sigma_1, \ldots, \Sigma_k)$. We study estimators of $\Sigma_1, \ldots, \Sigma_k$ which are invariant to β and take the form

$$\widehat{\Sigma} = Y'BY, \tag{2.4}$$

where the estimation matrix $B \in \mathbb{R}^{n\times n}$ is symmetric and satisfies $BX = 0$. To obtain an estimate of Σ_r, observe that $\mathbb{E}[\alpha_r' M \alpha_r] = (\operatorname{Tr} M)\Sigma_r$ for any matrix M. Then, as $\alpha_1, \ldots, \alpha_k$ are independent with mean 0,

$$\mathbb{E}[Y'BY] = \sum_{r=1}^{k} \mathbb{E}[\alpha_r' U_r' B U_r \alpha_r] = \sum_{r=1}^{k} \operatorname{Tr}(U_r' B U_r)\Sigma_r. \tag{2.5}$$

So $\widehat{\Sigma}$ is an unbiased estimate of Σ_r when B satisfies $\operatorname{Tr} U_r' B U_r = 1$ and $\operatorname{Tr} U_s' B U_s = 0$ for all $s \neq r$.

In balanced classification designs, discussed in greater detail in Section 2.6, the classical MANOVA estimators are obtained by setting B to be combinations of projections onto subspaces of $\mathbb{R}^n$. For example, in the one-way model corresponding to (2.2), defining $\pi_1, \pi_2 \in \mathbb{R}^{n\times n}$ as the orthogonal projections onto $\operatorname{col}(U_1) \ominus \operatorname{col}(\mathbf{1}_n)$ and $\mathbb{R}^n \ominus \operatorname{col}(U_1)$, the MANOVA estimators of Σ_1 and Σ_2 are given by

$$\widehat{\Sigma}_1 = Y' \left(\frac{1}{J} \cdot \frac{\pi_1}{I-1} - \frac{1}{J} \cdot \frac{\pi_2}{n-I} \right) Y, \qquad \widehat{\Sigma}_2 = Y' \frac{\pi_2}{n-I} Y. \tag{2.6}$$

In unbalanced designs and more general models, various alternative choices of B lead to estimators in the generalized MANOVA [SCM09] and MINQUE/MIVQUE families [Rao72, LaM73, SS78].

Motivated by the applications discussed in the introduction, we study spectral properties of the matrix (2.4) in a high-dimensional asymptotic regime.

Assumption 2.1. The number of effects k is fixed while $n, p, m_1, \ldots, m_k \to \infty$. There are constants $C, c > 0$ such that

(a) (Number of traits) $c < p/n < C$.

(b) (Model design) $c < m_r/n < C$ and $\|U_r\| < C$ for each $r = 1, \ldots, k$.

(c) (Estimation matrix) $B = B'$, $BX = 0$, and $\|B\| < C/n$.

(d) (Covariance) $0 \leq \|\Sigma_r\| < C$ for each $r = 1, \ldots, k$.

Assumption 2.1(a) models the high-dimensional setting of interest. In classification designs, Assumption 2.1(b) holds when the number of outer-most groups is proportional to n, and groups (and sub-groups) are bounded in size. This encompasses usual implementations of (1.1) and (1.2) for reasons of optimal experimental design [Rob59a, Rob59b], as well as usual implementations of the crossed design (1.3) where the numbers of fathers, mothers, and offspring in each cross are kept small and n is increased by performing independent replicates (see Example 2.23). In models such as (1.4) where U_r is a matrix of genotype values at m_r SNPs, Assumption 2.1(b) holds if $m_r \asymp n$ and U_r is entrywise bounded by $C/\sqrt{n}$. This latter condition is satisfied if genotypes at each SNP are normalized to mean 0 and variance $1/n$, and SNPs with minor allele frequency below a constant threshold are removed. Under Assumption 2.1(b), the scaling $\|B\| < 1/n$ in Assumption 2.1(c) is then natural to ensure $\operatorname{Tr} U_r' B U_r$ is bounded for each $r = 1, \ldots, k$, and hence $\mathbb{E}[Y'BY]$ is on the same scale as $\Sigma_1, \ldots, \Sigma_k$. Assumption 2.1(d) fixes the global scaling of the model.

In Sections 2.2–2.5, we discuss results under various further structural assumptions for $\Sigma_1, \ldots, \Sigma_k$.

2.2 Edge fluctuations under sphericity

Consider first the following null hypothesis of "global sphericity", in which each random effect is distributed as isotropic Gaussian noise.

Assumption 2.2. There is a constant $C > 0$ such that for each $r = 1, \ldots, k$,

$$\Sigma_r = \sigma_r^2 \operatorname{Id}, \qquad 0 \leq \sigma_r^2 < C.$$

In this setting, by a simple observation, the eigenvalue distribution of $\widehat{\Sigma}$ is well-approximated by a law μ_0 satisfying the Marcenko-Pastur equation. We show that, under a regularity condition which guarantees uniform square-root density decay at an edge of μ_0, the extremal eigenvalue of $\widehat{\Sigma}$ near that edge exhibits real Tracy-Widom fluctuations. This is depicted for an example of the one-way design in Figure 2.1.

The observed eigenvalue near a regular edge may be compared with the quantiles of the Tracy-Widom law to yield a significance test of the above null hypothesis of global sphericity. Such a test may be performed either for the simple null hypothesis where $\sigma_1^2, \ldots, \sigma_k^2$ are fixed and known, or for a composite hypothesis by substituting a $1/n$-consistent estimate $\hat{\sigma}_r^2$ for any unknown σ_r^2. To yield power against non-isotropic alternatives for a particular covariance Σ_r, we suggest performing the test based on the largest eigenvalue (at the rightmost edge) of the MANOVA estimator for Σ_r.

The study of $\widehat{\Sigma}$ under Assumption 2.2 is simplified by the following observation. Set $N = p$ and $M = m_1 + \ldots + m_k$, and define

$$F_{rs} = N\sigma_r\sigma_s U_r' B U_s \in \mathbb{R}^{m_r \times m_s}, \qquad F = \begin{pmatrix} F_{11} & \cdots & F_{1k} \\ \vdots & \ddots & \vdots \\ F_{k1} & \cdots & F_{kk} \end{pmatrix} \in \mathbb{R}^{M \times M}. \tag{2.7}$$

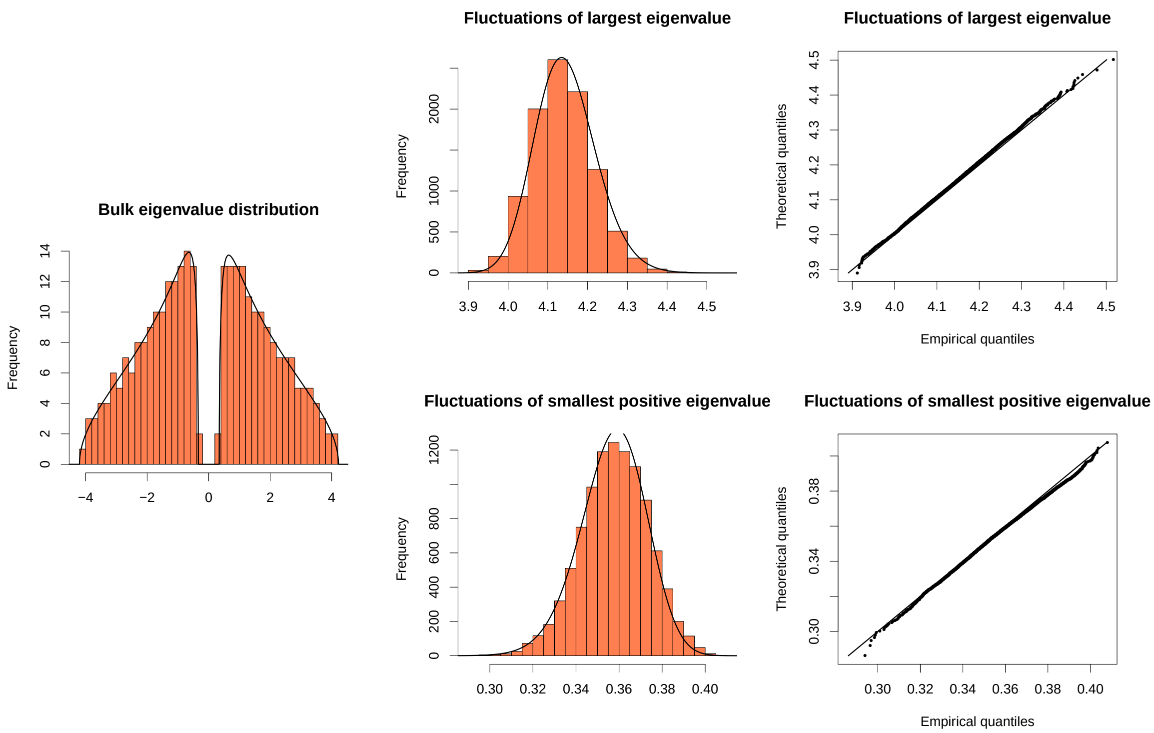

Figure 2.1: Eigenvalue fluctuations at the edges of the spectrum for a one-way design. Left: Empirical non-zero eigenvalues of the MANOVA estimate $\widehat{\Sigma}_1$, overlaid with the density of the law μ_0 (with the point mass at 0 removed). Right: Fluctuations of the largest eigenvalue and smallest positive eigenvalue of $\widehat{\Sigma}_1$ across 10000 simulations, compared with the density function and quantiles of the Tracy-Widom law. Center and scale for the Tracy-Widom law are computed as in Theorem 2.6. The setting is $I = 150$ groups of size $J = 2$ and $p = 600$ traits, with $\Sigma_1 = 0$ and $\Sigma_2 = \mathrm{Id}$.

Proposition 2.3. Under Assumption 2.2, $\widehat{\Sigma} \overset{L}{=} X'FX$ where $X \in \mathbb{R}^{M\times N}$ has i.i.d. $\mathcal{N}(0, 1/N)$ entries.

Proof. We may represent $\alpha_r = \sqrt{N}\sigma_r X_r$, where $X_r \in \mathbb{R}^{m_r\times N}$ has i.i.d. $\mathcal{N}(0, 1/N)$ entries. Then, applying $BX = 0$,

$$\widehat{\Sigma} = Y'BY = \sum_{r,s=1}^{k} \alpha_r' U_r' BU_s \alpha_s = \sum_{r,s=1}^{k} X_r'(N\sigma_r\sigma_s U_r' BU_s)X_s = \sum_{r,s=1}^{k} X_r' F_{rs} X_s.$$

The result follows upon stacking $X_1, \ldots, X_k$ row-wise as $X \in \mathbb{R}^{M\times N}$. □

Let us call $\widehat{\Sigma} = X'FX$ the "Marcenko-Pastur model" [MP67]. If F were positive semi-definite, then $\widehat{\Sigma}$ would have the same non-zero eigenvalues as the sample covariance matrix $F^{1/2}XX'F^{1/2}$, where F represents the population covariance. The matrices B and F in (2.7) may not be positive semi-definite. However, many spectral properties of this model are nonetheless well-understood—we review this in greater detail in Chapter 3.

It is known that the asymptotic spectrum of $\widehat{\Sigma}$ is described by the Marcenko-Pastur equation:

Theorem 2.4. Let $F \in \mathbb{R}^{M \times M}$ be symmetric, and suppose there are constants $C, c > 0$ such that $c < M/N < C$ and $\|F\| < C$. Let $\widehat{\Sigma} = X'FX$ where $X \in \mathbb{R}^{M \times N}$ has i.i.d. $\mathcal{N}(0, 1/N)$ entries. Let $\mu_{\widehat{\Sigma}} = N^{-1} \sum_{i=1}^{N} \delta_{\lambda_i(\widehat{\Sigma})}$ be its empirical spectral distribution.

Then for each $z \in \mathbb{C}^+$, there is a unique value $m_0(z) \in \mathbb{C}^+$ which satisfies

$$z = -\frac{1}{m_0(z)} + \frac{1}{N} \operatorname{Tr} \Big(F[\operatorname{Id} + m_0(z)F]^{-1} \Big). \tag{2.8}$$

This function $m_0 : \mathbb{C}^+ \to \mathbb{C}^+$ defines the Stieltjes transform of a probability distribution μ_0 on $\mathbb{R}$. As $N, M \to \infty$, $\mu_{\widehat{\Sigma}} - \mu_0 \to 0$ weakly almost surely.

Proof. See [MP67, Sil95, SB95] in the setting where M/N converges to a positive constant and the spectral distribution of F converges to a limit distribution. The above formulation follows from Prohorov's theorem and a subsequence argument. □

Denote the δ-neighborhood of the support of μ_0 by

$$\operatorname{supp}(\mu_0)_\delta = \{x \in \mathbb{R} : \operatorname{dist}(x, \operatorname{supp}(\mu_0)) < \delta\}.$$

(Let us emphasize that μ_0 and its support depend on N, M, F, although we suppress this dependence notationally.) Then all eigenvalues of $\widehat{\Sigma}$ fall within $\operatorname{supp}(\mu_0)_\delta$ with high probability:

Theorem 2.5. Fix any constants $\delta, D > 0$. Under the assumptions of Theorem 2.4, for a constant $N_0(\delta, D) > 0$ and all $N \geq N_0(\delta, D)$,

$$\mathbb{P}[\operatorname{spec}(\widehat{\Sigma}) \subset \operatorname{supp}(\mu_0)_\delta] > 1 - N^{-D}.$$

Proof. See [BS98, KY17] for positive definite F, and Appendix A for an extension of the proof to general F. □

Call $E_* \in \mathbb{R}$ a (left or right) edge of μ_0 if it is a (left or right) boundary point of $\operatorname{supp}(\mu_0)$. Under a certain regularity condition, quantified by a constant $\tau > 0$ and stated precisely in Definition 3.5, E_* has uniform separation from other edges of μ_0, and μ_0 admits a density $f_0(x)$ in a neighborhood of E_* which exhibits uniform square-root decay. For such an edge E_*, there is a value $\gamma > 0$ such that $f_0(x) \sim (\gamma/\pi)\sqrt{(E_* - x)_+}$ as $x \to E_*$ if E_* is a right edge, or $f_0(x) \sim (\gamma/\pi)\sqrt{(x - E_*)_+}$ if E_* is a left edge. We call γ the associated scale of E_*. In this setting, we prove the following result, where μ_{TW} is the GOE Tracy-Widom law [TW96].

Theorem 2.6. Under the assumptions of Theorem 2.4, suppose E_* is an edge of μ_0 that is τ-regular in the sense of Definition 3.5 for a constant $\tau > 0$. Let γ be the scale of E_*. Then there exists a (τ-dependent) constant δ such that as $N, M \to \infty$,

(a) If E_* is a right edge and $\lambda_{\max}$ is the largest eigenvalue of $\widehat{\Sigma}$ in $[E_* - \delta, E_* + \delta]$, then

$$(\gamma N)^{2/3}(\lambda_{\max} - E_*) \xrightarrow{L} \mu_{TW}.$$

(b) If E_* is a left edge and $\lambda_{\min}$ is the smallest eigenvalue of $\widehat{\Sigma}$ in $[E_* - \delta, E_* + \delta]$, then

$$(\gamma N)^{2/3}(E_* - \lambda_{\min}) \xrightarrow{L} \mu_{TW}.$$

Chapter 3 is devoted to the proof of this result. Convergence in law here is interpreted as follows: Let F_1 denote the cumulative distribution function of μ_{TW}, and fix $x \in \mathbb{R}$. Then

$$\left|\mathbb{P}[(\gamma N)^{2/3}(\lambda_{\max} - E_*) \leq x] - F_1(x)\right| \leq o(1),$$

where $o(1)$ denotes an (x, τ)-dependent error term which vanishes to 0 as $N, M \to \infty$.

Theorem 2.6 provides a method of testing the global sphericity null hypothesis in Assumption 2.2 using the observed eigenvalues of $\widehat{\Sigma} = Y'BY$, for any fixed estimation matrix B. In detail, a test based on the largest eigenvalue of $\widehat{\Sigma}$ may be performed as follows:

1. Construct the matrix F in (2.7), where $N = p$.
2. Plot the function
$$z_0(m) = -\frac{1}{m} + \frac{1}{N} \operatorname{Tr}\left(F[\mathrm{Id} + mF]^{-1}\right) \tag{2.9}$$
over $m \in \mathbb{R}$, and locate the value m_* closest to 0 such that $z_0'(m_*) = 0$ and $m_* < 0$.
3. Compute E_* and γ as $E_* = z_0(m_*)$ and $\gamma = \sqrt{2/z_0''(m_*)}$.
4. Reject the sphericity null hypothesis at level α if $(\gamma N)^{2/3}(\lambda_{\max} - E_*)$ exceeds the $1 - \alpha$ quantile of the real Tracy-Widom law μ_{TW}.

Proposition 3.3 in Chapter 3 verifies that E_* and γ are the rightmost edge of μ_0 and its associated scale. Regularity of this edge is a mild assumption, which holds, for example, under the following condition.

Proposition 2.7. Under the assumptions of Theorem 2.4, suppose there exists a constant $c > 0$ such that the largest eigenvalue of F is at least c and has multiplicity at least cM. Then the rightmost edge E_* of μ_0 is τ-regular for a constant $\tau > 0$.

We will verify this condition for balanced classification designs in Section 2.6. In more general settings, a diagnostic check of edge regularity may be performed by visual inspection of the plot of $z_0(m)$, and we refer to Definition 3.5 for details.

Example 2.8. The below table displays the accuracy of the Tracy-Widom approximation for several instances of the one-way design with $n = IJ$ individuals and J individuals per group, in the setting $\sigma_1^2 = 0$ and $\sigma_2^2 = 1$.

	F_1	$n = p$			$n = 4 \times p$			
		$J = 2$	$J = 5$	$J = 10$	$J = 2$	$J = 5$	$J = 10$	$2 \times$ SE
	0.90	0.941	0.949	0.959	0.931	0.934	0.940	(0.005)
$p = 20$	0.95	0.973	0.977	0.983	0.968	0.969	0.971	(0.003)
	0.99	0.995	0.997	0.997	0.994	0.994	0.993	(0.002)
	0.90	0.926	0.928	0.934	0.920	0.916	0.919	(0.005)
$p = 100$	0.95	0.964	0.967	0.968	0.960	0.958	0.961	(0.004)
	0.99	0.993	0.995	0.995	0.992	0.991	0.992	(0.002)
	0.90	0.914	0.920	0.919	0.916	0.915	0.921	(0.006)
$p = 500$	0.95	0.958	0.961	0.960	0.957	0.957	0.962	(0.004)
	0.99	0.992	0.993	0.993	0.992	0.992	0.993	(0.002)

Displayed are the empirical cumulative probabilities for $(\gamma N)^{2/3}(\lambda_{\max} - E_*)$ at the theoretical 90th, 95th, and 99th percentiles of the Tracy-Widom law, estimated across 10000 simulations. Here, $\lambda_{\max}$ is the largest eigenvalue of the MANOVA estimate $\widehat{\Sigma}_1$, and E_* and γ are the center and scale for the rightmost edge of μ_0. The final column gives approximate standard errors based on binomial sampling. We observe a conservative bias, particularly at small values of n and p.

Constructing F and computing $z_0(m)$ requires knowledge of $\sigma_1^2, \ldots, \sigma_k^2$. To test a composite hypothesis in which any σ_r^2 is unknown, it may be replaced by a $1/n$-consistent estimate $\hat{\sigma}_r^2$:

Proposition 2.9. Fix $r \in \{1, \ldots, k\}$ and let $\widehat{\Sigma} = Y'BY$ be an unbiased estimator for Σ_r. Let $\hat{\sigma}^2 = p^{-1} \operatorname{Tr} \widehat{\Sigma}$. Then under Assumptions 2.1 and 2.2, for any $\varepsilon, D > 0$ and all $n \geq n_0(\varepsilon, D)$,

$$\mathbb{P}[|\hat{\sigma}^2 - \sigma_r^2| > n^{-1+\varepsilon}] < n^{-D}.$$

Proof. Note that $\mathbb{E}[\hat{\sigma}^2] = \sigma_r^2$. Writing $\widehat{\Sigma} = X'FX$ where X has $\mathcal{N}(0, 1/N)$ entries and F is defined by (2.7), we have

$$\hat{\sigma}^2 = N^{-1} \operatorname{Tr} X'FX = \operatorname{vec}(X)' A \operatorname{vec}(X)$$

where $A = N^{-1} \operatorname{Id}_N \otimes F$ and $\operatorname{vec}(X)$ is the column-wise vectorization of X. The condition $\mathbb{E}[\hat{\sigma}^2] = \sigma_r^2$ implies $N^{-1} \operatorname{Tr} A = \sigma_r^2$. We have $\|A\|_{\mathrm{HS}}^2 = N^{-1} \|F\|_{\mathrm{HS}}^2 < C$ for a constant $C > 0$, so the result follows from the Hanson-Wright inequality (see Lemma 4.6). □

Consequently, letting $\widehat{E}_*$ and $\hat{\gamma}$ be the rightmost edge and associated scale of the law $\hat{\mu}_0$ defined by replacing any of $\sigma_1^2, \ldots, \sigma_k^2$ by $\hat{\sigma}_1^2, \ldots, \hat{\sigma}_k^2$, one may check that when E_* is regular,

$$\mathbb{P}[|\widehat{E}_* - E_*|> n^{-1+\varepsilon}] < n^{-D}, \qquad \mathbb{P}[|\hat{\gamma} - \gamma|> n^{-1+\varepsilon}] < n^{-D}.$$

Then the conclusion of Theorem 2.6 remains asymptotically valid using $\widehat{E}_*$ and $\hat{\gamma}$.

2.3 Outliers in the spiked model

We next consider spiked perturbations of the sphericity null hypothesis in Assumption 2.2.

Assumption 2.10. There are constants $C, \bar{C} > 0$ such that for each $r = 1, \ldots, k$,

$$\Sigma_r = \sigma_r^2 \operatorname{Id} + V_r \Theta_r V_r',$$

where $V_r \in \mathbb{R}^{p \times l_r}$ has orthonormal columns, $\Theta_r \in \mathbb{R}^{l_r \times l_r}$ is diagonal, $0 \leq \sigma_r^2 < C$, $0 \leq l_r < C$, and $\|\Theta_r\|< \bar{C}$. (We set $V_r \Theta_r V_r' = 0$ when $l_r = 0$.)

Hence each Σ_r has an isotropic noise level σ_r^2 (possibly 0 if Σ_r is low-rank) and a bounded number of signal eigenvalues greater than this noise level. We allow σ_r^2, l_r, V_r, and Θ_r to vary with n and p. We will be primarily interested in scenarios where at least one variance $\sigma_1^2, \ldots, \sigma_k^2$ is of size $O(1)$, although let us remark that setting $\sigma_1^2 = \ldots = \sigma_k^2 = 0$ also recovers the classical low-dimensional asymptotic regime where the true dimension of the data is bounded as $n \to \infty$.

In this setting, Theorem 2.5 implies that only a constant number of eigenvalues of $\widehat{\Sigma}$ should fall far from $\operatorname{supp}(\mu_0)$. Let us call these eigenvalues the outliers. We show that there is a family of matrices

$$t(\lambda) \cdot \Sigma = t_1(\lambda)\Sigma_1 + \ldots + t_k(\lambda)\Sigma_k \tag{2.10}$$

such that each outlier eigenvalue $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma})$ is close to a value λ that is an eigenvalue of $t(\lambda) \cdot \Sigma$. When $\widehat{\Sigma}$ is the MANOVA estimator of a variance component Σ_r, we may interpret this matrix as a "surrogate" for the true matrix Σ_r of interest. If $\hat{\lambda}$ is separated from other eigenvalues of $\widehat{\Sigma}$, we show furthermore that its eigenvector $\hat{\mathbf{v}}$ is partially aligned with the eigenvector of $t(\lambda) \cdot \Sigma$, and $\hat{\lambda}$ has asymptotic Gaussian fluctuations on the scale $n^{-1/2}$. Proofs of these results are contained in Chapter 4.

Let $\mathcal{S} \subset \mathbb{R}^p$ be the combined column span of $V_1, \ldots, V_k$, where $\mathcal{S} = \emptyset$ if $l_1 = \ldots = l_k = 0$. Set

$$L = \dim \mathcal{S}, \qquad N = p - L, \qquad M = m_1 + \ldots + m_k,$$

and define F as in (2.7) with the above values N and M. Let $m_0(z)$ be the Stieltjes transform of the law μ_0 in Theorem 2.4, defined for all $z \in \mathbb{C} \setminus \operatorname{supp}(\mu_0)$ via

$$m_0(z) = \int_{\mathbb{R}} \frac{1}{x-z}\,\mu_0(dx). \tag{2.11}$$

Let Tr_r denote the trace of the (r,r) block in the $k \times k$ block decomposition of $\mathbb{C}^{M\times M}$ corresponding to $M = m_1 + \ldots + m_k$. For $z \in \mathbb{C} \setminus \operatorname{supp}(\mu_0)$, define

$$T(z) = z\operatorname{Id} - \sum_{r=1}^{k} t_r(z)\Sigma_r, \qquad t_r(z) = \frac{1}{N\sigma_r^2}\operatorname{Tr}_r\Big(F[\operatorname{Id} + m_0(z)F]^{-1}\Big). \tag{2.12}$$

Here, if $\sigma_r^2 = 0$, then $t_r(z)$ remains well-defined by the identity

$$F[\operatorname{Id} + m_0(z)F]^{-1} = -m_0(z)F[\operatorname{Id} + m_0(z)F]^{-1}F + F \tag{2.13}$$

and the definition of F in (2.7). Let

$$\Lambda_0 = [\ \lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0) :\ 0 = \det(T(\lambda))\ ] \tag{2.14}$$

be the multiset of real roots of the function $z \mapsto \det(T(z))$, counted with their analytic multiplicities. We record here the following alternative definition of $T(z)$, and properties of $T(z)$ and Λ_0.

Proposition 2.11 (Properties of $T(z)$)**.**

(a) The matrix $T(z)$ is equivalently defined as

$$T(z) = -\frac{1}{m_0(z)}\operatorname{Id} - \sum_{r=1}^{k} t_r(z)V_r\Theta_r V_r'. \tag{2.15}$$

(b) For each $z \in \mathbb{C} \setminus \operatorname{supp}(\mu_0)$, $\ker T(z) \subseteq \mathcal{S}$.

(c) For $\lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0)$, $\partial_\lambda T(\lambda) - \operatorname{Id}$ is positive semi-definite.

(d) For $\lambda \in \Lambda_0$, its multiplicity as a root of $0 = \det(T(\lambda))$ is equal to $\dim\ker T(\lambda)$.

Proof. By conjugation symmetry and continuity, the Marcenko-Pastur identity (2.8) holds for each $z \in \mathbb{C} \setminus \operatorname{supp}(\mu_0)$. Part (a) then follows from substituting $\Sigma_r = \sigma_r^2\operatorname{Id} + V_r\Theta_r V_r'$ and applying (2.8). Part (b) follows from (a), as $T(z)$ is the direct sum of an operator on $\mathcal{S}$ and a non-zero multiple of Id on the orthogonal complement $\mathcal{S}^\perp$. Differentiating (2.11), $\partial_\lambda m_0(\lambda) > 0$ for each $\lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0)$, so $\partial_\lambda t_r = -(N\sigma_r^2)^{-1}(\partial_\lambda m_0)\operatorname{Tr}_r F(\operatorname{Id} + m_0F)^{-2}F \leq 0$. Then part (c) follows from (2.12). For $\lambda \in \Lambda_0$, this implies each eigenvalue $\mu_i(\lambda)$ of $T(\lambda)$ satisfies $\mu_i(\lambda) - \mu_i(\lambda') \asymp (\lambda - \lambda')$ as $\lambda' \to \lambda$, so $|\det T(\lambda')| \asymp |\lambda - \lambda'|^d$ for $d = \dim\ker T(\lambda)$. This yields (d). $\square$

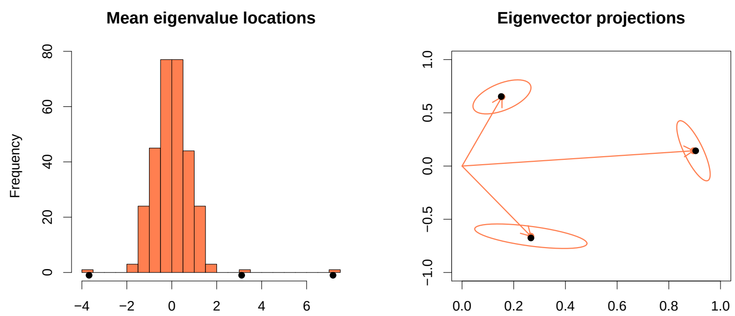

Figure 2.2: Outlier predictions for the MANOVA estimate $\widehat{\Sigma}_1$ in a one-way design. The population covariances are $\Sigma_1 = 6\mathbf{e}_1\mathbf{e}_1'$ and $\Sigma_2 = 29\mathbf{v}\mathbf{v}' + \mathrm{Id}$, where $\mathbf{v} = \frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2$. Left: Mean eigenvalue locations of $\widehat{\Sigma}_1$ across 10000 simulations, with black dots on the axis indicating the predicted values $\lambda \in \Lambda_0$. Right: Means and 90% ellipsoids for the projections of the three outlier eigenvectors onto $\mathcal{S} = \mathrm{col}(\mathbf{e}_1, \mathbf{e}_2)$, with black dots indicating the predictions of Theorem 2.13. The simulated setting is $I = 300$ groups of size $J = 2$, and $p = 300$ traits.

For two finite multisets $A, B \subset \mathbb{R}$, define

$$\text{ordered-dist}(A, B) = \begin{cases} \infty & \text{if } |A| \neq |B| \\ \max_i(|a_{(i)} - b_{(i)}|) & \text{if } |A| = |B|, \end{cases}$$

where $a_{(i)}$ and $b_{(i)}$ are the ordered values of A and B counting multiplicity. The following shows that the outlier eigenvalues of $\widehat{\Sigma}$ are close to the elements of Λ_0. Note that by (2.12), each $\lambda \in \Lambda_0$ is an eigenvalue of the surrogate matrix $t_1(\lambda)\Sigma_1 + \ldots + t_k(\lambda)\Sigma_k$.

Theorem 2.12 (Outlier locations)**.** Fix constants $\delta, \varepsilon, D > 0$. Then under Assumptions 2.1 and 2.10, for a constant $n_0(\delta, \varepsilon, D) > 0$ and all $n \geq n_0(\delta, \varepsilon, D)$, with probability at least $1 - n^{-D}$ there exist $\Lambda_\delta \subseteq \Lambda_0$ and $\hat{\Lambda}_\delta \subseteq \mathrm{spec}(\widehat{\Sigma})$, containing all elements of these multisets outside $\mathrm{supp}(\mu_0)_\delta$, such that

$$\text{ordered-dist}(\Lambda_\delta, \hat{\Lambda}_\delta) < n^{-1/2+\varepsilon}.$$

The multiset Λ_0 represents a theoretical prediction for the locations of the outlier eigenvalues of $\widehat{\Sigma}$—this is depicted in Figure 2.2 for an example of the one-way design. We clarify that Λ_0 is deterministic but n-dependent, and it may contain values arbitrarily close to $\mathrm{supp}(\mu_0)$. Hence we state the result as a matching between two sets Λ_δ and $\widehat{\Lambda}_\delta$ rather than the convergence of outlier eigenvalues of $\widehat{\Sigma}$ to a fixed set Λ_0. We allow Λ_δ and $\widehat{\Lambda}_\delta$ to contain values within $\mathrm{supp}(\mu_0)_\delta$ so as to match values of the other set close to the boundaries of $\mathrm{supp}(\mu_0)_\delta$.

Remark. In the setting of sample covariance matrices $\widehat{\Sigma}$ for i.i.d. multivariate samples, there is a phase transition phenomenon in which spike values greater than a certain threshold yield outlier eigenvalues in $\widehat{\Sigma}$, while spike values less than this threshold do not [BBP05, BS06, Pau07]. This phenomenon occurs also in our setting and is implicitly captured by the cardinality $|\Lambda_0|$, which represents the number of predicted outlier eigenvalues of $\widehat{\Sigma}$. In particular, Λ_0 will be empty if the spike values of $\Theta_1, \ldots, \Theta_k$ are sufficiently small. However, the phase transition thresholds and predicted outlier eigenvalue locations in our setting are defined jointly by $\Theta_1, \ldots, \Theta_k$ and the alignments between $V_1, \ldots, V_k$, rather than by the individual spectra of $\Sigma_1, \ldots, \Sigma_k$.

We next describe eigenvector alignments and eigenvalue fluctuations for isolated outliers $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma})$. Let $P_{\mathcal{S}}$ and $P_{\mathcal{S}^\perp}$ denote the orthogonal projections onto $\mathcal{S}$ and its orthogonal complement.

Theorem 2.13 (Eigenvector alignments)**.** Fix constants $\delta, \varepsilon, D > 0$. Suppose $\lambda \in \Lambda_0 \setminus \operatorname{supp}(\mu_0)_\delta$ has multiplicity one, and $|\lambda - \lambda'| \geq \delta$ for all other $\lambda' \in \Lambda_0$. Let $\mathbf{v}$ be the unit vector in $\ker T(\lambda)$, and let $\hat{\mathbf{v}}$ be the unit eigenvector of the eigenvalue $\hat{\lambda}$ of $\widehat{\Sigma}$ closest to λ. Then, under Assumptions 2.1 and 2.10,

(a) For all $n \geq n_0(\delta, \varepsilon, D)$ and some choice of sign for $\mathbf{v}$, with probability at least $1 - n^{-D}$,

$$\|P_{\mathcal{S}}\hat{\mathbf{v}} - (\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})^{-1/2}\mathbf{v}\| < n^{-1/2+\varepsilon}.$$

(b) $P_{\mathcal{S}^\perp}\hat{\mathbf{v}}/\|P_{\mathcal{S}^\perp}\hat{\mathbf{v}}\|$ is uniformly distributed over unit vectors in $\mathcal{S}^\perp$ and is independent of $P_{\mathcal{S}}\hat{\mathbf{v}}$.

Thus $(\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})^{-1/2}\mathbf{v}$ represents a theoretical prediction for the projection of the sample eigenvector $\hat{\mathbf{v}}$ onto the subspace $\mathcal{S}$—this is also displayed in Figure 2.2 for the one-way design. Here, $(\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})^{-1/2}$ is the predicted inner-product alignment between $\mathbf{v}$ and $\hat{\mathbf{v}}$, which by Proposition 2.11(c) is at most 1.

Next, let $\|\cdot\|_{rs}$ denote the Hilbert-Schmidt norm of the (r, s) block in the $k \times k$ block decomposition of $\mathbb{C}^{M \times M}$. Define

$$w_{rs}(z) = \frac{\|F(\operatorname{Id} + m_0(z)F)^{-1}\|_{rs}^2}{N\sigma_r^2\sigma_s^2}, \tag{2.16}$$

where this is again well-defined by (2.13) even if $\sigma_r^2 = 0$ and/or $\sigma_s^2 = 0$.

Theorem 2.14 (Gaussian fluctuations)**.** Fix $\delta > 0$. Suppose $\lambda \in \Lambda_0 \setminus \operatorname{supp}(\mu_0)_\delta$ has multiplicity one, and $|\lambda - \lambda'| \geq \delta$ for all other $\lambda' \in \Lambda_0$. Let $\mathbf{v}$ be the unit vector in $\ker T(\lambda)$, and let $\hat{\lambda}$ be the eigenvalue of $\widehat{\Sigma}$ closest to λ. Then under Assumptions 2.1 and 2.10,

$$\nu(\lambda)^{-1/2}(\hat{\lambda} - \lambda) \to \mathcal{N}(0, 1)$$

where

$$\nu(\lambda) = \frac{2}{N(\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})^2}\left(\frac{(\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v} - 1)^2}{\partial_\lambda m_0(\lambda)} + \sum_{r,s=1}^{k} w_{rs}(\lambda)(\mathbf{v}'\Sigma_r\mathbf{v})(\mathbf{v}'\Sigma_s\mathbf{v})\right).$$

Furthermore, $\nu(\lambda) > c/n$ for a constant $c > 0$.

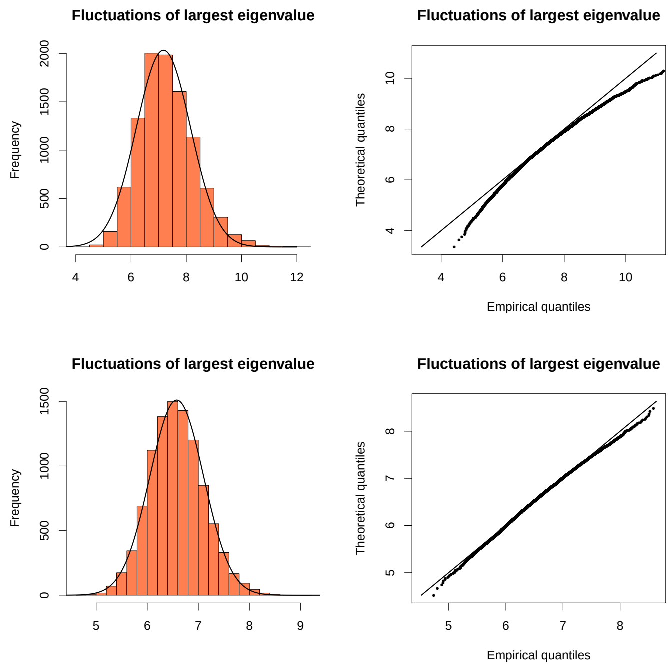

Figure 2.3: Outlier eigenvalue fluctuations in a one-way design. Displayed are fluctuations of the largest outlier eigenvalue of $\widehat{\Sigma}_1$ across 10000 simulations, compared with the density function and quantiles of the Gaussian distribution with mean and variance given in Theorem 2.14. The simulated setting is $I = 300$ groups of size $J = 2$, $p = 300$ traits, and (top) $\Sigma_1 = 6\mathbf{e}_1\mathbf{e}_1'$ and $\Sigma_2 = 29\mathbf{v}\mathbf{v}' + \mathrm{Id}$ where $\mathbf{v} = \frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2$, or (bottom) $\Sigma_1 = 6\mathbf{e}_1\mathbf{e}_1'$ and $\Sigma_2 = \mathrm{Id}$.

Figure 2.3 illustrates the accuracy of this Gaussian approximation for two settings of the one-way design. We observe that the approximation is fairly accurate in a setting with a single outlier, but (in the simulated sample sizes $n = 600$ and $p = 300$) does not adequately capture a skew in the outlier distribution in a setting with an additional positive outlier produced by a large spike in Σ_2. This skew is reduced in examples where there is increased separation between these two positive outliers.

Example 2.15. In the setting of large population spike eigenvalues, it is illustrative to understand the predictions of Theorem 2.12 using a Taylor expansion. Let us carry this out for the MANOVA estimator $\widehat{\Sigma}_1$ for a balanced one-way design (1.1) with I groups of J individuals.

Recalling the form (2.6) for $\widehat{\Sigma}_1$, the computation in Proposition 2.24(b) for general balanced designs will yield, in this setting, the explicit expressions

$$t_1(\lambda) = \frac{(I-1)J}{(I-1)J + N(J\sigma_1^2 + \sigma_2^2)m_0(\lambda)},$$

$$t_2(\lambda) = \frac{I-1}{(I-1)J + N(J\sigma_1^2 + \sigma_2^2)m_0(\lambda)} - \frac{n-I}{(n-I)J - N\sigma_2^2 m_0(\lambda)}.$$

Suppose first that there is a single large spike eigenvalue $\mu = \theta + \sigma_1^2$ in Σ_1, and no spike eigenvalues in Σ_2. Theorem 2.12 and the form (2.15) for $T(\lambda)$ indicate that outlier eigenvalues should appear near the locations

$$\Lambda_0 = [\ \lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0) : m_0(\lambda)t_1(\lambda) = -1/\theta\ ].$$

Proposition A.2 verifies that m_0 is injective on $\mathbb{R} \setminus \operatorname{supp}(\mu_0)$. Hence $m_0(\lambda)t_1(\lambda)$ is also injective, so $|\Lambda_0| \leq 1$. Applying a Taylor expansion around $\lambda = \infty$, we obtain from (2.8)

$$\begin{aligned} m_0(\lambda) &= -\frac{1}{\lambda} - \frac{1}{\lambda^2} \cdot \frac{1}{N} \operatorname{Tr} F + O(1/\lambda^3) = -\frac{1}{\lambda} - \frac{\sigma_1^2}{\lambda^2} + O(1/\lambda^3), \\ m_0(\lambda)t_1(\lambda) &= -\frac{1}{\lambda} - \frac{1}{\lambda^2}\left(\sigma_1^2 + \frac{N}{(I-1)J}(J\sigma_1^2 + \sigma_2^2)\right) + O(1/\lambda^3), \end{aligned}$$

where $N = p - 1$. For large θ and μ, solving $m_0(\lambda)t_1(\lambda) = -1/\theta$ yields

$$\lambda \approx \theta + \sigma_1^2 + c_1 = \mu + c_1, \qquad c_1 = \frac{N}{(I-1)J}(J\sigma_1^2 + \sigma_2^2).$$

So we expect to observe one outlier with an approximate upward bias of c_1.

Next, suppose there is a single large spike eigenvalue $\mu = \theta + \sigma_2^2$ in Σ_2, and no spike eigenvalues in Σ_1. Then we expect outlier eigenvalues near the locations

$$\Lambda_0 = [\ \lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0) : m_0(\lambda)t_2(\lambda) = -1/\theta\ ].$$

Since $m_0(\lambda)$ is injective and the condition $m_0(\lambda)t_2(\lambda) = -1/\theta$ is quadratic in $m_0(\lambda)$, we obtain $|\Lambda_0| \leq 2$. Taylor expanding around $|\lambda| = \infty$, we have after some simplification

$$m_0(\lambda)t_2(\lambda) = -\frac{1}{\lambda^2} \cdot \frac{N}{(I-1)J}\left(\sigma_1^2 + \frac{n-1}{n(J-1)}\sigma_2^2\right) + O(1/|\lambda|^3).$$

Then for large θ, solving $m_0(\lambda)t_2(\lambda) = -1/\theta$ yields two predicted outlier eigenvalues near

$$\lambda \approx \pm\sqrt{c_2\theta}, \qquad c_2 = \frac{N}{(I-1)J}\left(\sigma_1^2 + \frac{n-1}{n(J-1)}\sigma_2^2\right).$$

Let us emphasize that these predictions are in the asymptotic regime where $n, N \to \infty$ and λ is a large but fixed constant, rather than $\lambda \to \infty$ jointly with n, N.

Finally, consider a single spike $\mu_1 = \theta_1 + \sigma_1^2$ in Σ_1 and a single spike $\mu_2 = \theta_2 + \sigma_2^2$ in Σ_2. Letting the corresponding spike eigenvectors have inner-product ρ, we expect outliers near

$$\Lambda_0 = \left[\lambda : 0 = \det\left(-\frac{1}{m_0(\lambda)} \operatorname{Id}_2 - t_1(\lambda)\theta_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - t_2(\lambda)\theta_2 \begin{pmatrix} \rho^2 & \rho\sqrt{1-\rho^2} \\ \rho\sqrt{1-\rho^2} & 1-\rho^2 \end{pmatrix} \right) \right]$$
$$= \left[\lambda : 0 = 1 + m_0(\lambda)\Big(t_1(\lambda)\theta_1 + t_2(\lambda)\theta_2\Big) + m_0(\lambda)^2 t_1(\lambda) t_2(\lambda)\theta_1\theta_2(1-\rho^2) \right].$$

This is a cubic condition in $m_0(\lambda)$, so $|\Lambda_0| \leq 3$. Applying the above Taylor expansions around $\lambda = \infty$, this condition becomes

$$0 = 1 - \frac{\theta_1}{\lambda} - \frac{\theta_1(\sigma_1^2 + c_1)}{\lambda^2} - \frac{\theta_2 c_2}{\lambda^2} + \frac{\theta_1\theta_2(1-\rho^2)c_2}{\lambda^3} + O\left(\frac{\theta_1+\theta_2}{\lambda^3} + \frac{\theta_1\theta_2}{\lambda^4}\right).$$

In a setting where θ_1 and θ_2 are large and of comparable size, there is a predicted outlier λ near θ_1. More precisely, expanding the above around $\lambda = \theta_1$, the location of this outlier is

$$\lambda \approx \theta_1 + \sigma_1^2 + c_1 + (\theta_2/\theta_1)\rho^2 c_2 = \mu_1 + c_1 + (\theta_2/\theta_1)\rho^2 c_2.$$

Thus the upward bias of this outlier is increased from c_1, when there are no spikes in Σ_2, to $c_1 + (\theta_2/\theta_1)\rho^2 c_2$.

2.4 Estimation in the spiked model

The results of the preceding section indicate that under Assumption 2.10, each outlier eigenvalue/eigenvector of $\widehat{\Sigma}$ may be interpreted as estimating an eigenvalue/eigenvector of a surrogate matrix (2.10). When there is no high-dimensional noise, $\sigma_1^2 = \ldots = \sigma_k^2 = 0$, we may verify that $t_r(\lambda) = \operatorname{Tr} U_r' B U_r$ for each $r = 1, \ldots, k$ and any λ. In this setting, if $\widehat{\Sigma}$ is an unbiased MANOVA estimate of a single component Σ_r, then (2.5) implies that the surrogate matrix is also simply Σ_r.

In the presence of high-dimensional noise, this is no longer true. Even for the MANOVA estimate $\widehat{\Sigma}$ of Σ_r, the surrogate matrix may depend on multiple variance components $\Sigma_1, \ldots, \Sigma_k$, so the MANOVA eigenvalues and eigenvectors may exhibit aliasing effects from the other components. We propose an alternative algorithm based on the idea of searching for matrices $\widehat{\Sigma} = Y'BY$ where this surrogate depends only on Σ_r. We show that in our high-dimensional asymptotic setting, this can yield $n^{-1/2}$-consistent estimates of sufficiently large signal eigenvalues, as well as eigenvector estimates which asymptotically do not exhibit this aliasing phenomenon. Figure 2.4 depicts differences between the MANOVA eigenvector and our estimated eigenvector in several examples for the one-way model.

We implement this algorithmic idea as follows: Fix k symmetric matrices $B_1, \ldots, B_k \in \mathbb{R}^{n \times n}$

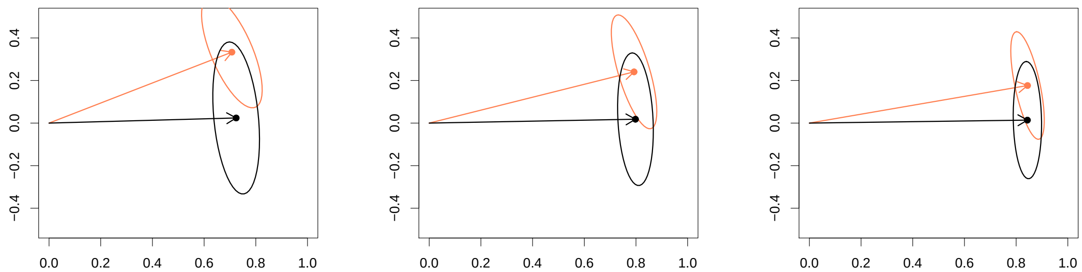

Figure 2.4: Estimates of the principal eigenvector of Σ_1 in a one-way design. The population covariances are $\Sigma_1 = \mu \mathbf{e}_1 \mathbf{e}_1'$ and $\Sigma_2 = 29\mathbf{v}\mathbf{v}' + \mathrm{Id}$, where $\mathbf{v} = \frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2$ and (left) $\mu = 6$, (middle) $\mu = 8$, or (right) $\mu = 10$. Means and 90% ellipsoids across 100 simulations are shown for the first two coordinates of the unit-norm leading MANOVA eigenvector (red) and of the unit-norm estimate of Algorithm 1 (black). The design is $I = 150$ groups of size $J = 2$ with $p = 600$ traits.

satisfying Assumption 2.1(c). For $\mathbf{a} = (a_1, \ldots, a_k) \in \mathbb{R}^k$, denote

$$B(\mathbf{a}) = \sum_{r=1}^{k} a_r B_r.$$

Let $F(\mathbf{a})$ be the matrix defined in (2.7) for $B = B(\mathbf{a})$, let $\widehat{\Sigma}(\mathbf{a}) = Y'B(\mathbf{a})Y$, and let $\mu_0(\mathbf{a})$, $m_0(z, \mathbf{a})$, and $t_r(z, \mathbf{a})$ be the law μ_0 and the functions $m_0(z)$ and $t_r(z)$ defined with $F = F(\mathbf{a})$. We search for coefficients $\mathbf{a} \in \mathbb{R}^k$ where $\widehat{\Sigma}(\mathbf{a})$ has an outlier eigenvalue $\hat{\lambda}$ satisfying $t_s(\hat{\lambda}, \mathbf{a}) = 0$ for all $s \neq r$. At any such pair $(\hat{\lambda}, \mathbf{a})$, the surrogate matrix $t(\hat{\lambda}) \cdot \Sigma$ depends only on Σ_r, and we have $T(\hat{\lambda}, \mathbf{a}) = \hat{\lambda}\,\mathrm{Id} - t_r(\hat{\lambda}, \mathbf{a})\Sigma_r$ by (2.12). By Theorem 2.12, we expect $\hat{\lambda}$ to be close to a value λ where

$$0 = \det T(\lambda, \mathbf{a}) \approx \det(\hat{\lambda}\,\mathrm{Id} - t_r(\hat{\lambda}, \mathbf{a})\Sigma_r). \tag{2.17}$$

Thus, we estimate an eigenvalue μ of Σ_r by $\hat{\mu} = \hat{\lambda}/t_r(\hat{\lambda}, \mathbf{a})$. Furthermore, by Theorem 2.13, we expect the eigenvector $\hat{\mathbf{v}}$ of $\widehat{\Sigma}(\mathbf{a})$ corresponding to $\hat{\lambda}$ to satisfy

$$P_{\mathcal{S}}\hat{\mathbf{v}} \approx (\mathbf{w}'\partial_\lambda T(\lambda, \mathbf{a})\mathbf{w})^{-1/2}\mathbf{w},$$

where $\mathbf{w}$ is the null vector of $T(\lambda, \mathbf{a})$. By (2.17), we expect $\mathbf{w} \approx \mathbf{v}$ where $\mathbf{v}$ is the eigenvector of Σ_r corresponding to μ. Thus, we estimate $\mathbf{v}$ by $\hat{\mathbf{v}}$.

The procedure is summarized in Algorithm 1. We note that the combinations $\mathbf{a}$ where $t_s(\lambda, \mathbf{a}) \approx 0$ for $s \neq r$ are not known a priori—in particular, they depend on the unknown spike eigenvalues and eigenvectors to be estimated. Hence we search for such values $\mathbf{a} \in \mathbb{R}^k$. By scale invariance, we

Algorithm 1 Algorithm for estimating eigenvalues and eigenvectors of Σ_r

Initialize $\mathcal{M} = \emptyset$. Fix $\delta > 0$ a small constant.
for each $\mathbf{a} \in S^{k-1}$ and each $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a})) \cap \mathcal{I}_\delta(\mathbf{a})$ **do**
  if $t_s(\hat{\lambda}, \mathbf{a}) = 0$ for all $s \in \{1, \ldots, k\} \setminus \{r\}$ **then**
    Add $(\hat{\mu}, \hat{\mathbf{v}})$ to $\mathcal{M}$, where $\hat{\mu} = \hat{\lambda}/t_r(\hat{\lambda}, \mathbf{a})$ and $\hat{\mathbf{v}}$ is the unit eigenvector such that $\widehat{\Sigma}(\mathbf{a})\hat{\mathbf{v}} = \hat{\lambda}\hat{\mathbf{v}}$.
  end if
end for
Return $\mathcal{M}$

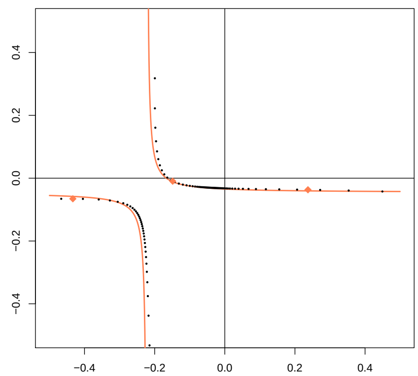

Figure 2.5: Illustration of Algorithm 1 for the one-way design, where $k = 2$. The setting is the same as in Figure 2.2. The red curve depicts the locus $\mathcal{L}$ from (2.19) on the (s_1, s_2) plane, which has one s_1-intercept at $(-1/6, 0)$ and one s_2-intercept at $(0, -1/29)$. Black points show values of $\widehat{\mathcal{L}}$ corresponding to (a_1, a_2) in a grid of 100 equispaced points on the unit circle, from a single data simulation. The three points of $\widehat{\mathcal{L}}$ corresponding to the three outliers of the MANOVA estimate $\widehat{\Sigma}_1$, where $(a_1, a_2) = \pm(1/J, -1/J)$, are depicted in red.

restrict to $\mathbf{a}$ on the unit sphere

$$S^{k-1} = \{\mathbf{a} \in \mathbb{R}^k : \|\mathbf{a}\| = 1\}.$$

We further restrict to outlier eigenvalues $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}))$ which fall above $\operatorname{supp}(\mu_0)$, belonging to

$$\mathcal{I}_\delta(\mathbf{a}) = \{x \in \mathbb{R} : x \geq y + \delta \text{ for all } y \in \operatorname{supp}(\mu_0(\mathbf{a}))\}.$$

We note that outliers falling below $\operatorname{supp}(\mu_0)$ will be identified as corresponding to $-\mathbf{a} \in S^{k-1}$, and for simplicity of the procedure, we ignore any outliers that fall between intervals of $\operatorname{supp}(\mu_0(\mathbf{a}))$.

One may understand the behavior of Algorithm 1 by plotting the values

$$\widehat{\mathcal{L}} = \left\{ m_0(\hat{\lambda}, \mathbf{a}) \cdot (t_1(\hat{\lambda}, \mathbf{a}), \ldots, t_k(\hat{\lambda}, \mathbf{a})) : \ \mathbf{a} \in S^{k-1}, \ \hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a})) \cap \mathcal{I}_\delta(\mathbf{a}) \right\}. \tag{2.18}$$

This is illustrated for an example of the one-way design in Figure 2.5. By Theorem 2.12, we expect these values to fall close to

$$m_0(\lambda, \mathbf{a}) \cdot (t_1(\lambda, \mathbf{a}), \ldots, t_k(\lambda, \mathbf{a})),$$

where λ is the deterministic prediction for the location of $\hat{\lambda}$, satisfying $0 = \det T(\lambda, \mathbf{a})$. By this condition and the form (2.15) for T, these values belong to the locus

$$\mathcal{L} = \left\{ (s_1, \ldots, s_k) \in \mathbb{R}^k : 0 = \det \left(\mathrm{Id} + \sum_{r=1}^{k} s_r V_r \Theta_r V_r' \right) \right\}, \tag{2.19}$$

which does not depend on $\mathbf{a}$ and is defined solely by the spike parameters $\Theta_1, \ldots, \Theta_k$ and $V_1, \ldots, V_k$. This is depicted also in Figure 2.5. (We have picked a simulation to display in Figure 2.5 where $\widehat{\mathcal{L}}$ and $\mathcal{L}$ are particularly close, for purposes of illustration.) The spike values θ on the diagonal of Θ_r are in 1-to-1 correspondence with the points $(0, \ldots, 0, -1/\theta, 0, \ldots, 0) \in \mathcal{L}$ which fall on the r^{th} coordinate axis. Algorithm 1 may be understood as estimating these intercepts by the intercepts of the observed locus $\widehat{\mathcal{L}}$.

We have written Algorithm 1 in the idealized setting where we search over all $\mathbf{a} \in S^{k-1}$. In practice, we discretize S^{k-1} as in Figure 2.5 and search over this discretization for pairs $(\hat{\lambda}, \mathbf{a})$ where $t_s(\hat{\lambda}, \mathbf{a}) \approx 0$ for all $s \neq r$. We then numerically refine each located pair $(\hat{\lambda}, \mathbf{a})$. Computing the values $t_r(\hat{\lambda}, \mathbf{a})$ and the lower endpoint of $\mathcal{I}_\delta(\mathbf{a})$ requires knowledge of the noise variances $\sigma_1^2, \ldots, \sigma_k^2$. These computations are particularly simple in balanced classification designs, and we discuss this in Section 2.6. If $\sigma_1^2, \ldots, \sigma_k^2$ are unknown, they may be replaced by $1/n$-consistent estimates as in Proposition 2.9. (In practice, large outliers of $\widehat{\Sigma}_1, \ldots, \widehat{\Sigma}_k$ may be removed before computing the trace.) The unknown quantity $N = p - L$ may be replaced by the dimension p.

We prove the following theoretical guarantee for this procedure, for simplicity in the setting where Σ_r has separated eigenvalues. Define $s : \mathbb{R}^k \to \mathbb{R}^k$ by

$$s(\mathbf{a}) = (s_1(\mathbf{a}), \ldots, s_k(\mathbf{a})), \qquad s_r(\mathbf{a}) = \frac{1}{N\sigma_r^2} \operatorname{Tr}_r \Big(F(\mathbf{a})[\mathrm{Id} + F(\mathbf{a})]^{-1} \Big). \tag{2.20}$$

As $F(m_0 \cdot \mathbf{a}) = m_0 \cdot F(\mathbf{a})$, this function satisfies $s(m_0(\lambda, \mathbf{a}) \cdot \mathbf{a}) = m_0(\lambda, \mathbf{a}) \cdot (t_1(\lambda, \mathbf{a}), \ldots, t_k(\lambda, \mathbf{a}))$. To guarantee that the algorithm does not make duplicate estimates for each individual spike eigenvalue of Σ_r, we require $B_1, \ldots, B_k$ to be chosen such that s is injective in the following quantitative sense.

Assumption 2.16. There exists a constant $c > 0$ such that for any $\mathbf{a}_1, \mathbf{a}_2 \in \mathbb{R}^k$ where $\mathrm{Id} + F(\mathbf{a}_1)$ and $\mathrm{Id} + F(\mathbf{a}_2)$ are invertible,

$$\|s(\mathbf{a}_1) - s(\mathbf{a}_2)\| \geq c \, \frac{\|\mathbf{a}_1 - \mathbf{a}_2\|}{(1 + \|\mathbf{a}_1\|)(1 + \|\mathbf{a}_2\|)}.$$

We will verify in Section 2.6 that this condition holds for balanced classification designs, where $B_1, \ldots, B_k$ are the projections corresponding to the canonical mean-squares.

Theorem 2.17 (Spike estimation)**.** Fix $\delta, \tau > 0$ and $r \in \{1, \ldots, k\}$. Suppose Assumptions 2.1 and 2.16 hold for $B_1, \ldots, B_k$. Suppose furthermore that the diagonal values θ_i of Θ_r satisfy $\theta_i \geq \tau$ and $|\theta_i - \theta_j| \geq \tau$ for all $1 \leq i \neq j \leq l_r$. Then there exists a constant $c_0 > 0$ (not depending on $\bar{C}$ in Assumption 2.1) such that the following holds:

Let $\mathcal{M}$ be the output of Algorithm 1 with parameter δ for estimating the spikes of Σ_r. Let $\widehat{\mathcal{E}} = [\hat{\mu} : (\hat{\mu}, \hat{\mathbf{v}}) \in \mathcal{M}]$ and $\widehat{\mathcal{V}} = [\hat{\mathbf{v}} : (\hat{\mu}, \hat{\mathbf{v}}) \in \mathcal{M}]$ be the estimated eigenvalues and eigenvectors. Then, for any $\varepsilon, D > 0$ and all $n \geq n_0(\delta, \tau, \varepsilon, D)$,

(a) With probability at least $1 - n^{-D}$, there is a subset $\mathcal{E} \subset \operatorname{spec}(\Sigma_r)$ containing all eigenvalues greater than c_0 such that
$$\text{ordered-dist}(\widehat{\mathcal{E}}, \mathcal{E}) < n^{-1/2+\varepsilon}.$$

(b) On the event of part (a), for any $\mu \in \mathcal{E}$, let $\mathbf{v}$ be the unit eigenvector where $\Sigma_r \mathbf{v} = \mu \mathbf{v}$, and let $(\hat{\mu}, \hat{\mathbf{v}}) \in \mathcal{M}$ be such that $|\hat{\mu} - \mu| < n^{-1/2+\varepsilon}$. Then for some scalar value $\alpha \in (0, 1]$ and choice of sign for $\mathbf{v}$,
$$\|P_{\mathcal{S}} \hat{\mathbf{v}} - \alpha \mathbf{v}\| < n^{-1/2+\varepsilon}.$$

(c) For each $\hat{\mathbf{v}} \in \widehat{\mathcal{V}}$, $P_{\mathcal{S}^\perp} \hat{\mathbf{v}} / \|P_{\mathcal{S}^\perp} \hat{\mathbf{v}}\|$ is independent of $P_{\mathcal{S}} \hat{\mathbf{v}}$ and uniformly distributed over unit vectors in $\mathcal{S}^\perp$.

In the presence of high-dimensional noise, the eigenvector estimate $\hat{\mathbf{v}}$ remains inconsistent for $\mathbf{v}$. However, asymptotically as $n, p \to \infty$, parts (b) and (c) indicate that $\hat{\mathbf{v}}$ is not biased in a particular direction away from $\mathbf{v}$. Note that in part (a), some lower bound c_0 for the size of the population spike eigenvalue is necessary to guarantee estimation of this spike, as otherwise it might not produce an outlier in any matrix $\widehat{\Sigma}(\mathbf{a})$. (In this case, a portion of the true locus $\mathcal{L}$ in (2.19) may not be tracked by the observed locus $\widehat{\mathcal{L}}$.)

Example 2.18. We explore in simulations the accuracy of this procedure for estimating eigenvalues and eigenvectors of Σ_1 in two finite-sample settings of the one-way model (1.1), corresponding to the designs

$$D_1 : \; n = 600, \; p = 300, \; I = 300, \; J = 2$$
$$D_2 : \; n = 300, \; p = 600, \; I = 150, \; J = 2$$

In all simulations, we take $\sigma_1^2 = 0$ and $\sigma_2^2 = 1$. In particular, Σ_1 is low-rank, as hypothesized for genetic covariances of high-dimensional trait sets [WB09, BAC$^+$15]. For both designs, we fix the tuning parameter $\delta = 0.5$.

We first consider a rank-one matrix $\Sigma_1 = \mu \mathbf{e}_1 \mathbf{e}_1'$ for various settings of μ between 2 and 10, and $\Sigma_2 = \mathrm{Id}$ with no spike. The following tables display the mean and standard error of $\hat{\mu}$ estimated by Algorithm 1, and of the alignment $\hat{\mathbf{v}}' \mathbf{e}_1$ of the estimated eigenvector. Displayed also are the corresponding quantities for the leading eigenvalue/eigenvector of the MANOVA estimate $\widehat{\Sigma}_1$. We observe in all cases that Algorithm 1 corrects a bias in the MANOVA eigenvalue, and the alignment $\hat{\mathbf{v}}'\mathbf{e}_1$ is approximately the same as for the MANOVA eigenvector. Algorithm 1 never estimates more than one spike for Σ_1 in this setting; however, if μ is small, it may sometimes estimate 0 spikes. We display also the percentage of simulations in which a spike was estimated. For $\mu = 2$ under Design D_2, the predicted outlier is less than $\delta = 0.5$ away from the edge of the spectrum, and Algorithm 1 never estimated this spike.

Design D_1

	$\mu = 2$	$\mu = 4$	$\mu = 6$	$\mu = 8$	$\mu = 10$
Eigenvalue, MANOVA	2.70 (0.19)	4.60 (0.36)	6.56 (0.52)	8.53 (0.69)	10.51 (0.85)
Alignment $\mathbf{e}_1$, MANOVA	0.85 (0.02)	0.93 (0.01)	0.96 (0.01)	0.97 (0.00)	0.97 (0.00)
Eigenvalue, estimated	2.00 (0.20)	3.98 (0.37)	5.98 (0.53)	7.97 (0.69)	9.96 (0.85)
Alignment $\mathbf{e}_1$, estimated	0.84 (0.02)	0.93 (0.01)	0.95 (0.01)	0.97 (0.00)	0.97 (0.00)
Percent estimated	98	100	100	100	100

Design D_2

	$\mu = 2$	$\mu = 4$	$\mu = 6$	$\mu = 8$	$\mu = 10$
Eigenvalue, MANOVA	4.65 (0.23)	6.31 (0.49)	8.18 (0.72)	10.10 (0.95)	12.04 (1.19)
Alignment $\mathbf{e}_1$, MANOVA	0.58 (0.07)	0.78 (0.03)	0.85 (0.02)	0.88 (0.02)	0.90 (0.01)
Eigenvalue, estimated	NA	4.02 (0.46)	5.89 (0.75)	7.87 (0.98)	9.84 (1.20)
Alignment $\mathbf{e}_1$, estimated	NA	0.76 (0.03)	0.84 (0.02)	0.88 (0.02)	0.90 (0.01)
Percent estimated	0	87	100	100	100

Next, we consider $\Sigma_1 = 0$ and $\Sigma_2 = \theta\mathbf{v}\mathbf{v}' + \mathrm{Id}$ for a unit vector $\mathbf{v}$ and for $\mu = \theta + 1 \in \{10, 20, 30\}$. In both designs D_1 and D_2, this produces one positive and one negative outlier eigenvalue in the MANOVA estimate $\widehat{\Sigma}_1$. The tables below show the percentages of simulations in which a spurious spike eigenvalue is estimated by Algorithm 1 for Σ_1. In such cases, there is enough deviation of the observed locus $\widehat{\mathcal{L}}$ from the true locus $\mathcal{L}$ (which is the horizontal line $s_2 = -1/\theta$) to produce a spurious intercept where $t_2(\hat{\lambda}, \mathbf{a}) = 0$, and the algorithm interprets this as an alignment of the spike in Σ_2 with a small spike in Σ_1. We find that the spurious points $(\hat{\lambda}, \mathbf{a})$ where $t_2(\hat{\lambda}, \mathbf{a}) = 0$ occur for $\hat{\lambda}$ close to the edges of $\mathrm{supp}(\mu_0(\mathbf{a}))$, and this error percentage may be reduced in finite samples by setting a more conservative choice of δ, if desired.

Design D_1

	$\mu = 10$	$\mu = 20$	$\mu = 30$
Percent spurious	2	8	18

Design D_2

	$\mu = 10$	$\mu = 20$	$\mu = 30$
Percent spurious	0	8	15

Next, we consider $\Sigma_1 = \mu \mathbf{e}_1\mathbf{e}_1'$ and $\Sigma_2 = 29\mathbf{v}\mathbf{v}' + \mathrm{Id}$ for $\mathbf{v} = \frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2$, which forms a 60-degree alignment angle with $\mathbf{e}_1$. Displayed are the statistics for the largest estimated eigenvalue/eigenvector and largest MANOVA eigenvalue/eigenvector. Displayed also are the inner-product alignments with the direction $\mathbf{e}_2$ (where signs are chosen so that the estimated eigenvectors have positive $\mathbf{e}_1$ coordinate). The spike in Σ_2 causes the MANOVA eigenvector to be biased towards $\mathbf{v}$, and it also increases the bias and standard error of the MANOVA eigenvalue. In settings of small μ when Algorithm 1 does not always estimate a spike, the values $\hat{\mu}$ and $\hat{\mathbf{v}}'\mathbf{e}_2$ have a selection bias among the simulations where estimation occurs. For the remaining settings, $\hat{\mu}$ and $\hat{\mathbf{v}}'\mathbf{e}_2$ are nearly unbiased for the true values μ and 0, and the alignments $\hat{\mathbf{v}}'\mathbf{e}_1$ are similar to those of the MANOVA eigenvectors.

Design D_1

	$\mu = 2$	$\mu = 4$	$\mu = 6$	$\mu = 8$	$\mu = 10$
Eigenvalue, MANOVA	4.59 (1.14)	5.70 (1.14)	7.28 (1.15)	9.07 (1.22)	10.93 (1.33)
Alignment $\mathbf{e}_1$, MANOVA	0.57 (0.07)	0.80 (0.06)	0.89 (0.04)	0.93 (0.02)	0.95 (0.01)
Alignment $\mathbf{e}_2$, MANOVA	0.47 (0.11)	0.26 (0.16)	0.14 (0.15)	0.09 (0.12)	0.06 (0.10)
Eigenvalue, estimated	2.67 (1.09)	4.18 (1.01)	6.11 (1.07)	8.06 (1.17)	10.03 (1.30)
Alignment $\mathbf{e}_1$, estimated	0.63 (0.10)	0.83 (0.04)	0.90 (0.02)	0.93 (0.02)	0.95 (0.01)
Alignment $\mathbf{e}_2$, estimated	0.10 (0.25)	0.01 (0.19)	0.01 (0.15)	0.00 (0.12)	0.00 (0.10)
Percent estimated	70	100	100	100	100

Design D_2

	$\mu = 2$	$\mu = 4$	$\mu = 6$	$\mu = 8$	$\mu = 10$
Eigenvalue, MANOVA	8.79 (1.52)	9.49 (1.64)	10.57 (1.74)	11.98 (1.85)	13.59 (1.99)
Alignment $\mathbf{e}_1$, MANOVA	0.44 (0.06)	0.58 (0.06)	0.71 (0.05)	0.79 (0.04)	0.84 (0.03)
Alignment $\mathbf{e}_2$, MANOVA	0.53 (0.07)	0.44 (0.10)	0.33 (0.12)	0.24 (0.12)	0.18 (0.12)
Eigenvalue, estimated	5.15 (1.37)	4.84 (1.41)	6.28 (1.56)	8.21 (1.72)	10.15 (1.91)
Alignment $\mathbf{e}_1$, estimated	0.39 (0.05)	0.60 (0.06)	0.72 (0.04)	0.80 (0.03)	0.84 (0.03)
Alignment $\mathbf{e}_2$, estimated	0.34 (0.11)	0.09 (0.17)	0.02 (0.16)	0.02 (0.14)	0.01 (0.13)
Percent estimated	22	77	100	100	100

Finally, we consider a setting with multiple spikes. We set Σ_1 to be of rank 5, with eigenvalues $(10, 8, 6, 4, 2)$. We set Σ_2 to have 5 eigenvalues equal to 30 and remaining eigenvalues equal to 1, with the former 5-dimensional subspace having a 60-degree alignment angle with each spike eigenvector of Σ_1. The tables below display statistics for the five largest estimated and MANOVA eigenvalues in this setting. We observe that Algorithm 1 reduces the bias of the MANOVA eigenvalues, although a positive bias persists at these sample sizes.

Design D_1

	$\mu = 10$	$\mu = 8$	$\mu = 6$	$\mu = 4$	$\mu = 2$
Eigenvalue, MANOVA	12.06 (1.10)	9.70 (1.01)	7.60 (0.96)	5.87 (0.74)	4.53 (0.55)
Eigenvalue, estimated	11.08 (1.12)	8.65 (1.01)	6.38 (0.95)	4.36 (0.76)	2.80 (0.57)
Percent estimated	100	100	100	100	97

Design D_2

	$\mu = 10$	$\mu = 8$	$\mu = 6$	$\mu = 4$	$\mu = 2$
Eigenvalue, MANOVA	15.79 (1.61)	12.94 (1.15)	11.06 (1.00)	9.21 (0.82)	7.80 (0.73)
Eigenvalue, estimated	12.07 (1.68)	8.95 (1.19)	6.77 (1.03)	4.74 (0.86)	3.94 (0.53)
Percent estimated	100	100	100	98	37

2.5 General bulk eigenvalue law

Finally, we consider the general setting of Assumption 2.1 without any additional structure on $\Sigma_1, \ldots, \Sigma_k$. We establish an analogue of Theorem 2.4, showing that the empirical eigenvalue distribution of $\widehat{\Sigma}$ remains well-approximated by a deterministic law μ_0. This law μ_0 is no longer described by the Marcenko-Pastur equation, but it may be analogously described by a more general system of fixed point equations. We show that this system of equations admits a unique fixed point in the appropriate complex domains, and this fixed point may be computed by a simple iterative algorithm.

With a small abuse of previous notation, let us define in this context

$$F_{rs} = \sqrt{m_r m_s} U_r' B U_s \in \mathbb{R}^{m_r \times m_s}, \qquad F = \begin{pmatrix} F_{11} & \cdots & F_{1k} \\ \vdots & \ddots & \vdots \\ F_{k1} & \cdots & F_{kk} \end{pmatrix} \in \mathbb{R}^{M \times M}. \tag{2.21}$$

For $\mathbf{x} = (x_1, \ldots, x_k)$ and $\mathbf{y} = (y_1, \ldots, y_k)$, define

$$D(\mathbf{x}) = \operatorname{diag}(x_1 \operatorname{Id}_{m_1}, \ldots, x_k \operatorname{Id}_{m_k}) \in \mathbb{C}^{M \times M}, \qquad \mathbf{y} \cdot \Sigma = y_1 \Sigma_1 + \ldots + y_k \Sigma_k. \tag{2.22}$$

Theorem 2.19. Suppose Assumption 2.1 holds. For each $z \in \mathbb{C}^+$, there exist unique z-dependent values $x_1, \ldots, x_k \in \mathbb{C}^+ \cup \{0\}$ and $y_1, \ldots, y_k \in \overline{\mathbb{C}^+}$ that satisfy, for $r = 1, \ldots, k$, the equations

$$x_r = -\frac{1}{m_r} \operatorname{Tr}\left((z \operatorname{Id}_p + \mathbf{y} \cdot \Sigma)^{-1} \Sigma_r\right), \tag{2.23}$$

$$y_r = -\frac{1}{m_r} \operatorname{Tr}_r \left([\operatorname{Id}_M + F D(\mathbf{x})]^{-1} F\right). \tag{2.24}$$

The function $m_0 : \mathbb{C}^+ \to \mathbb{C}^+$ defined by

$$m_0(z) = -\frac{1}{p} \operatorname{Tr}\left((z \operatorname{Id}_p + \mathbf{y} \cdot \Sigma)^{-1}\right) \tag{2.25}$$

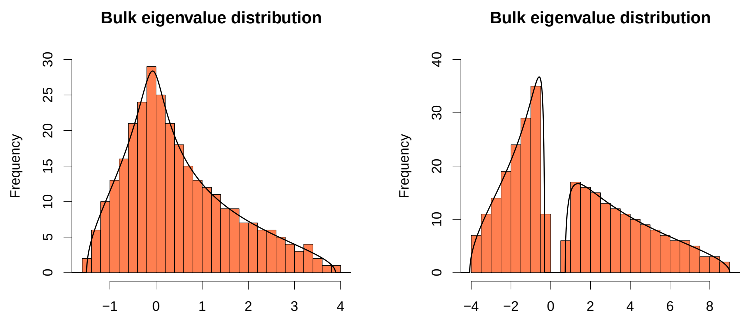

Figure 2.6: Eigenvalues of the MANOVA estimate $\widehat{\Sigma}_1$ in a one-way design with full-rank, non-isotropic Σ_1. The group covariance Σ_1 has uniform eigenvalues between 0 and 1, and the error covariance is $\Sigma_2 = \mathrm{Id}$. Histograms show average eigenvalue locations across 100 simulations, superimposed with the density of the convolution measure $\mu_0 \star \mathrm{Cauchy}(0, 10^{-4})$ computed by the iterative procedure of Theorem 2.20. The left shows $I = 300$ groups of size $J = 2$ and $p = 300$ traits; the right shows $I = 150$ groups of size $J = 2$ and $p = 600$ traits, with eigenvalues of $\widehat{\Sigma}$ equal to 0 and the point mass of μ_0 at 0 both removed.

is the Stieltjes transform of a probability distribution μ_0 on $\mathbb{R}$. Letting $\mu_{\widehat{\Sigma}}$ be the empirical eigenvalue distribution of $\widehat{\Sigma}$, $\mu_{\widehat{\Sigma}} - \mu_0 \to 0$ weakly almost surely.

In most cases, (2.23–2.25) do not admit a closed-form solution in $x_1, \ldots, x_k$, $y_1, \ldots, y_k$, and $m_0(z)$. However, these equations may be solved numerically:

Theorem 2.20. For each $z \in \mathbb{C}^+$, the values x_r and y_r in Theorem 2.19 are the limits, as $t \to \infty$, of the iterative procedure which arbitrarily initializes $y_1^{(0)}, \ldots, y_k^{(0)} \in \overline{\mathbb{C}^+}$ and iteratively computes (for $t = 0, 1, 2, \ldots$) $x_r^{(t)}$ from $y_r^{(t)}$ using (2.23) and $y_r^{(t+1)}$ from $x_r^{(t)}$ using (2.24).

These results are proven in Chapter 5. Note that by (2.11), the value $\pi^{-1} \operatorname{Im} m_0(E + i\eta)$ is the density of the convolution $\mu_0 \star \mathrm{Cauchy}(0, \eta)$ at E. This iterative procedure may be used to numerically compute this density over $E \in \mathbb{R}$, which approximates the law μ_0 for small η. This is depicted in Figure 2.6 for two examples of the one-way design.

2.6 Balanced classification designs

We consider the special example of model (2.1) corresponding to balanced classification designs. In these designs, by considerations of sufficiency, there is a canonical family of matrices B to use in (2.4), and also a canonical choice of matrices $B_1, \ldots, B_k$ for Algorithm 1 corresponding to the classical mean-squares. For such B, quantities such as $z_0(m)$ and $t_r(z)$ in (2.9) and (2.12) have explicit forms, which we record here to facilitate numerical implementations of the preceding procedures.

The technical conditions of edge regularity and injectivity of the map s in (2.20) may also be explicitly checked.

To motivate the general discussion, we first give several examples.

Example 2.21. Consider the one-way model (1.1) in the balanced setting with I groups of equal size J. We assume $J \geq 2$ is a fixed constant. The canonical mean-square matrices of this model are defined by

$$\mathrm{MS}_1 = \frac{1}{I-1}\sum_{i=1}^{I}\sum_{j=1}^{J}(\bar{\mathbf{y}}_i - \bar{\mathbf{y}})(\bar{\mathbf{y}}_i - \bar{\mathbf{y}})', \qquad \mathrm{MS}_2 = \frac{1}{n-I}\sum_{i=1}^{I}\sum_{j=1}^{J}(\mathbf{y}_{i,j} - \bar{\mathbf{y}}_i)(\mathbf{y}_{i,j} - \bar{\mathbf{y}}_i)',$$

where $\bar{\mathbf{y}}_i \in \mathbb{R}^p$ and $\bar{\mathbf{y}} \in \mathbb{R}^p$ denote the sample means in group i and across all groups. The MANOVA estimators are [SCM09]

$$\widehat{\Sigma}_1 = \frac{1}{J}\mathrm{MS}_1 - \frac{1}{J}\mathrm{MS}_2, \qquad \widehat{\Sigma}_2 = \mathrm{MS}_2.$$

Recall that the one-way model may be written in the matrix form

$$Y = \mathbf{1}_n\boldsymbol{\mu}' + U_1\alpha_1 + \alpha_2,$$

where U_1 is defined in (2.2). Defining orthogonal projections π_1 and π_2 onto $\mathrm{col}(U_1) \ominus \mathrm{col}(\mathbf{1}_n)$ and $\mathbb{R}^n \ominus \mathrm{col}(U_1)$, the above mean-squares may be written as

$$\mathrm{MS}_1 = Y'\frac{\pi_1}{I-1}Y, \qquad \mathrm{MS}_2 = Y'\frac{\pi_2}{n-I}Y.$$

The MANOVA estimators then take the equivalent form of (2.6).

Example 2.22. Consider the nested two-way model (1.2) with I groups, each group consisting of J subgroups, and each subgroup consisting of K individuals. We assume $J, K \geq 2$ are fixed constants. This model may be written in the matrix form

$$Y = \mathbf{1}_n\boldsymbol{\mu}' + U_1\alpha_1 + U_2\alpha_2 + \alpha_3,$$

where $\mathbf{y}_{i,j,k}$, $\boldsymbol{\alpha}_i$, $\boldsymbol{\beta}_{i,j}$, and $\boldsymbol{\varepsilon}_{i,j,k}$ are stacked as the rows of Y, α_1, α_2, and α_3, and the incidence matrices are given by

$$U_1 = \mathrm{Id}_I \otimes \mathbf{1}_{JK}, \qquad U_2 = \mathrm{Id}_{IJ} \otimes \mathbf{1}_K.$$

Defining orthogonal projections π_1, π_2, and π_3 onto $\mathrm{col}(U_1) \ominus \mathrm{col}(\mathbf{1}_n)$, $\mathrm{col}(U_2) \ominus \mathrm{col}(U_1)$, and $\mathbb{R}^n \ominus \mathrm{col}(U_2)$, the canonical mean-squares are given by

$$\mathrm{MS}_1 = Y'\frac{\pi_1}{I-1}Y, \qquad \mathrm{MS}_2 = Y'\frac{\pi_2}{IJ-I}Y, \qquad \mathrm{MS}_3 = Y'\frac{\pi_3}{n-IJ}Y.$$

The MANOVA estimators are defined as [SCM09]

$$\widehat{\Sigma}_1 = \frac{1}{JK}\mathrm{MS}_1 - \frac{1}{JK}\mathrm{MS}_2, \qquad \widehat{\Sigma}_2 = \frac{1}{K}\mathrm{MS}_2 - \frac{1}{K}\mathrm{MS}_3, \qquad \widehat{\Sigma}_3 = \mathrm{MS}_3.$$

Example 2.23. Consider the crossed two-way model (1.3) in a replicated setting,

$$\mathbf{y}_{i,j,k,l} = \boldsymbol{\mu} + \boldsymbol{\alpha}_i + \boldsymbol{\beta}_{i,j} + \boldsymbol{\gamma}_{i,k} + \boldsymbol{\delta}_{i,j,k} + \boldsymbol{\varepsilon}_{i,j,k,l}.$$

The entire cross-breeding experiment is replicated I times, with each cross involving J distinct fathers and K distinct mothers. Traits are measured in L different offspring for each (i,j,k). We assume $J, K, L \geq 2$ are fixed constants. This model may be written in the matrix form

$$Y = \mathbf{1}_n\boldsymbol{\mu}' + \sum_{r=1}^{4} U_r\alpha_r + \alpha_5,$$

where the incidence matrices are

$$U_1 = \mathrm{Id}_I \otimes \mathbf{1}_{JKL}, \qquad U_2 = \mathrm{Id}_{IJ} \otimes \mathbf{1}_{KL}, \qquad U_3 = \mathrm{Id}_I \otimes \mathbf{1}_J \otimes \mathrm{Id}_K \otimes \mathbf{1}_L, \qquad U_4 = \mathrm{Id}_{IJK} \otimes \mathbf{1}_L.$$

Defining orthogonal projections $\pi_1, \pi_2, \pi_3, \pi_4, \pi_5$ onto $\mathring{S}_1 = \mathrm{col}(U_1) \ominus \mathrm{col}(\mathbf{1}_n)$, $\mathring{S}_2 = \mathrm{col}(U_2) \ominus \mathrm{col}(U_1)$, $\mathring{S}_3 = \mathrm{col}(U_3) \ominus \mathrm{col}(U_1)$, $\mathring{S}_4 = \mathrm{col}(U_4) \ominus (\mathrm{col}(U_1) \oplus \mathring{S}_2 \oplus \mathring{S}_3)$, and $\mathring{S}_5 = \mathbb{R}^n \ominus \mathrm{col}(U_4)$, the canonical mean-squares are

$$\mathrm{MS}_r = Y'\frac{\pi_r}{d_r}Y \qquad \text{for } r = 1, \ldots, 5,$$

where $d_r = \dim(\mathring{S}_r)$. The forms of the classical MANOVA estimators may be deduced from the general discussion below.

To encompass these examples, we consider a general balanced classification design defined by the following properties:

1. For each r, let $c_r = n/m_r$. Then $U_r'U_r = c_r \,\mathrm{Id}_{m_r}$, and $\Pi_r = c_r^{-1}U_rU_r'$ is an orthogonal projection onto a subspace $S_r \subset \mathbb{R}^n$ of dimension m_r.

2. Define $S_0 = \mathrm{col}(X)$. Then $S_0 \subset S_r \subset S_k = \mathbb{R}^n$ for each $r = 1, \ldots, k-1$.

3. Partially order the subspaces S_r by inclusion: $s \preceq r$ if $S_s \subseteq S_r$. Let $\mathring{S}_0 = S_0$, and for $r = 1, \ldots, k$ let $\mathring{S}_r$ denote the orthogonal complement in S_r of all S_s properly contained in S_r. Then for each r,

$$S_r = \bigoplus_{s \preceq r} \mathring{S}_s. \tag{2.26}$$

   In particular, $\mathbb{R}^n = S_k = \oplus_{r=0}^{k}\mathring{S}_r$.

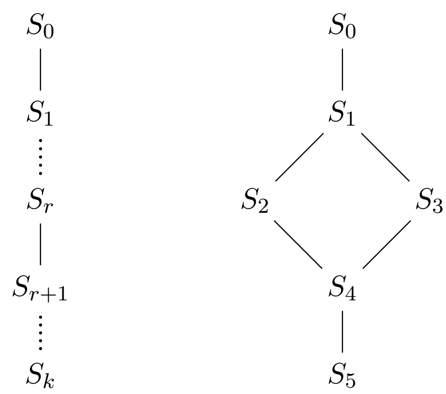

Figure 2.7: Inclusion lattices for the subspaces $\{S_r\}$ determined by the nested (left) and crossed (right) examples.

The subspace inclusion lattices for the nested designs of Examples 2.21 and 2.22 and the crossed design of Example 2.23 are depicted in Figure 2.7.

For each $r = 0, \dots, k$, let $d_r = \dim(\mathring{S}_r)$, let $V_r \in \mathbb{R}^{n \times d_r}$ have orthonormal columns spanning $\mathring{S}_r$, and let $\pi_r = V_r V_r'$ be the orthogonal projection onto $\mathring{S}_r$. (In particular, $d_0 = \dim \operatorname{col}(X)$ is the dimensionality of fixed effects.) Then $\pi_0, \dots, \pi_k$ are mutually orthogonal projections summing to Id_n. Note that the condition (2.26) implies

$$U_r U_r' = c_r \Pi_r = \sum_{s \preceq r} c_r \pi_s.$$

Then the likelihood of Y in (2.3) may be written in the form

$$f(Y) \propto \exp\left(-\frac{1}{2}\sum_{s=0}^{k} \operatorname{Tr}\left[\left(\sum_{r \geq 1:\, r \succeq s} c_r \Sigma_r\right)^{-1} (Y - X\beta)' \pi_s (Y - X\beta)\right]\right)$$

where $\pi_s X = 0$ for $s \geq 1$. Hence the quantities

$$\pi_0 Y, \quad \mathrm{MS}_1 = Y'(\pi_1/d_1)Y, \quad \dots, \quad \mathrm{MS}_k = Y'(\pi_k/d_k)Y$$

form sufficient statistics for this model.

In this setting, we restrict attention to matrices of the form

$$\widehat{\Sigma} = a_1 \mathrm{MS}_1 + \ldots + a_k \mathrm{MS}_k = Y'BY, \qquad B = B(\mathbf{a}) = a_1 \frac{\pi_1}{d_1} + \ldots + a_k \frac{\pi_k}{d_k}, \tag{2.27}$$

and we suggest the choices $B_r = \pi_r / d_r$ for use in Algorithm 1. In particular, the classical MANOVA estimators are of this form: From (2.5), we have

$$\mathbb{E}[\mathrm{MS}_s] = \sum_{r=1}^k d_s^{-1} \operatorname{Tr}(U_r' \pi_s U_r)\Sigma_r = \sum_{r \succeq s} c_r \Sigma_r, \qquad \mathbb{E}[\widehat{\Sigma}] = \sum_{s=1}^k \sum_{r \succeq s} a_s c_r \Sigma_r.$$

The MANOVA estimate of Σ_r is obtained by choosing $\mathbf{a} = (a_1, \ldots, a_k)$ so that $\mathbb{E}[\widehat{\Sigma}] = \Sigma_r$. Denoting

$$H_{rs} = \mathbb{1}\{s \preceq r\} c_r, \qquad H = (H_{rs})_{r,s=1}^k \in \mathbb{R}^{k \times k}, \tag{2.28}$$

this is satisfied by letting $\mathbf{a}$ be the r^{th} column of H^{-1}. (This corresponds to the procedure of Möbius inversion over the subspace inclusion lattice, discussed in greater detail in [Spe83].)

We record the following calculations and properties for this class of models. In particular, part (a) implies that $m_0(z)$ may be computed by solving a polynomial equation of degree $k+1$ in $m_0(z)$. For $z \in \mathbb{C}^+$, the correct root is the unique root $m_0(z) \in \mathbb{C}^+$, while for $z \in \mathbb{R} \setminus \operatorname{supp}(\mu_0)$, the correct root satisfies $z_0'(m_0(z)) > 0$. From this, the quantities $t_r(z)$ and $w_{rs}(z)$ are easily computed in part (b). The edges of $\operatorname{supp}(\mu_0)$ may be found by solving the equation $0 = z_0'(m_*)$, which may be written as a polynomial equation of degree $2k$ in m_*.

Proposition 2.24. Let (2.1) correspond to a balanced classification design, as defined above. Suppose Assumption 2.1(a,b,d) holds for this design, and in addition, $d_r > cn$ for each $r = 1, \ldots, k$ and a constant $c > 0$. Let $\widehat{\Sigma}$ and B be defined by (2.27), where $\mathbf{a} = (a_1, \ldots, a_k) \in \mathbb{R}^k$ satisfies $\|\mathbf{a}\| < C$ for a constant $C > 0$.

(a) Under Assumption 2.2, the Marcenko-Pastur equation (2.8) corresponding to $\widehat{\Sigma}$ takes the form

$$z = -\frac{1}{m_0(z)} + \sum_{s=1}^k C_s b_s(z), \qquad b_s(z) = \frac{a_s}{1 + (N/d_s) a_s C_s m_0(z)}, \qquad C_s = \sum_{r \succeq s} c_r \sigma_r^2. \tag{2.29}$$

If there exist a constant $c > 0$ and indices $s, r \in \{1, \ldots, k\}$ such that $s \preceq r$, $a_s > c$, and $\sigma_r^2 > c$, then the rightmost edge E_* of μ_0 is τ-regular for a constant $\tau > 0$.

(b) Under Assumption 2.10, the functions $t_r(z)$ and $w_{rs}(z)$ from (2.12) and (2.16) take the forms

$$t_r(z) = c_r \sum_{s \geq 1:\, s \preceq r} b_s(z), \qquad w_{rs}(z) = c_r c_s \sum_{t \geq 1:\, t \preceq r,\, t \preceq s} (N/d_t) b_t(z)^2.$$

Furthermore, Assumption 2.16 holds for the estimation matrices $B_r = \pi_r / d_r$.

(c) In the fixed point equations (2.23–2.25), the equation (2.24) takes the explicit form

$$y_r = -c_r \sum_{s \geq 1:\, s \preceq r} \frac{a_s}{1 + (n/d_s) a_s x_{s+}}, \qquad x_{s+} = \sum_{r \succeq s} x_r. \tag{2.30}$$

Proof. We rotate coordinates. Fix $r \in \{1, \ldots, k\}$ and write $\{s : s \preceq r\} = \{s_0, \ldots, s_j\}$ where $s_0 = 0$. We may write the singular value decomposition of U_r as

$$U_r = \sqrt{c_r} \sum_{s \preceq r} V_s W'_{r,s},$$

where the columns of V_s form an orthonormal basis for $\mathring{S}_s$ and where $W_r = [W_{r,s_0} \mid \ldots \mid W_{r,s_j}]$ is orthogonal $m_r \times m_r$. Denote $\check{n} = n - d_0$, $\check{m}_r = m_r - d_0$, $V = [V_1 \mid \ldots \mid V_k] \in \mathbb{R}^{n \times \check{n}}$, and

$$\check{\alpha}_r = \begin{pmatrix} W'_{r,s_1}\alpha_r \\ \vdots \\ W'_{r,s_j}\alpha_r \end{pmatrix} \in \mathbb{R}^{\check{m}_r \times p}, \qquad \check{U}_r = \sqrt{c_r} V' \begin{pmatrix} V_{s_1} & \cdots & V_{s_j} \end{pmatrix} \in \mathbb{R}^{\check{n} \times \check{m}_r}.$$

By rotational invariance, $\check{\alpha}_r$ still has independent rows with distribution $\mathcal{N}(0, \Sigma_r)$. Also, $\check{U}_r$ has a simple form—each $V'V_{s_i} \in \mathbb{R}^{\check{n} \times d_{s_i}}$ has a single block equal to $\mathrm{Id}_{d_{s_i}}$ and remaining blocks 0. Defining

$$\check{Y} = V'Y \in \mathbb{R}^{\check{n} \times p}, \qquad \check{B} = V'BV = \begin{pmatrix} (a_1/d_1)\,\mathrm{Id}_{d_1} & & \\ & \ddots & \\ & & (a_k/d_k)\,\mathrm{Id}_{d_k} \end{pmatrix} \in \mathbb{R}^{\check{n} \times \check{n}}$$

and applying V' to (2.1), we obtain the rotated model

$$\check{Y} = \sum_{r=1}^{k} \check{U}_r \check{\alpha}_r, \qquad \widehat{\Sigma} = \check{Y}'\check{B}\check{Y}. \tag{2.31}$$

For parts (a) and (b), let F be the matrix (2.7) in the model (2.1). Let $\check{M} = \check{m}_1 + \ldots + \check{m}_k$, and denote by $\check{F} \in \mathbb{R}^{\check{M} \times \check{M}}$ this matrix in the rotated model (2.31), with (r,s) block $N\sigma_r\sigma_s\check{U}'_r\check{B}\check{U}_s$. Let $Q = \mathrm{diag}(W_1, \ldots, W_k)$, where W_r is the matrix of right singular vectors of U_r as above. Then observe that $\check{F}$ is the matrix $Q'FQ$ with d_0 rows and d_0 columns of 0's removed from each block. Thus, the law μ_0 and the functions $m_0(z)$, $s_r(\mathbf{a})$, $t_r(z)$, and $w_{rs}(z)$ do not change upon replacing F by $\check{F}$ in their definitions.

For (a), let us further decompose $\check{m}_r = \sum_{s \geq 1:\, s \preceq r} d_s$, and consider $\check{F}$ in the expanded block decomposition corresponding to

$$\check{M} = \sum_{r=1}^{k} \sum_{s \geq 1:\, s \preceq r} d_s.$$

Index a row or column of this decomposition by the pair (r,s) where $s \preceq r$. Then from the forms of $\check{U}_r$ and $\check{B}$, we have

$$\check{F}_{(r,s),(r',s')} = \mathbb{1}\{s = s'\} N \sqrt{c_r c_{r'}} \sigma_r \sigma_{r'} \frac{a_s}{d_s} \mathrm{Id}_{d_s}.$$

For each $s \in \{1, \ldots, k\}$, let E_s be the submatrix formed by the blocks $((r, s), (r', s))$ where $r \succeq s$ and $r' \succeq s$. Note that $\check{F}$ is (upon permuting rows and columns) block-diagonal with blocks $E_1, \ldots, E_k$. We may write $E_s = N(a_s/d_s)R_s' R_s$ where $R_s = (\sqrt{c_r}\sigma_r \operatorname{Id}_{d_s} \;:\; r \succeq s)$. Then E_s has rank d_s, with d_s identical non-zero eigenvalues equal to $N(a_s/d_s)C_s$ where C_s is defined in (2.29). As the eigenvalues of $\check{F}$ are the union of those of $E_1, \ldots, E_k$, writing (2.8) in spectral form establishes (2.29). Under the stated conditions in (a), the largest eigenvalue of $\check{F}$ is positive and bounded away from 0, with multiplicity proportional to n. Then the rightmost edge E_* is regular by Proposition 2.7.

For (b), noting that $R_s R_s' = C_s \operatorname{Id}_{d_s}$, the Woodbury identity yields

$$E_s(\operatorname{Id} + E_s)^{-1} = \frac{Na_s}{d_s} R_s' R_s \left(\operatorname{Id} - \frac{Na_s}{d_s(1 + N(a_s/d_s)C_s)} R_s' R_s \right) = \frac{N(a_s/d_s)}{1 + N(a_s/d_s)C_s} R_s' R_s.$$

Then for all $s \preceq r$ and $s' \preceq r'$,

$$\left(F(\operatorname{Id} + F)^{-1} \right)_{(r,s),(r',s')} = \mathbb{1}\{s = s'\} \sqrt{c_r c_r'} \sigma_r \sigma_{r'} \frac{N(a_s/d_s)}{1 + N(a_s/d_s)C_s} \operatorname{Id}_{d_s}. \tag{2.32}$$

The r^{th} diagonal block trace in the collapsed decomposition $\check{M} = \check{m}_1 + \ldots + \check{m}_k$ is the sum of the trace of the above over $s \preceq r$, $s = s'$, and $r = r'$. Thus

$$s_r(\mathbf{a}) = c_r \sum_{s \preceq r} \frac{a_s}{1 + (N/d_s)a_s C_s} = Hf(\mathbf{a}),$$

where H is defined in (2.28) and

$$f(\mathbf{a}) = \left(\frac{a_1}{1 + (N/d_1)a_1 C_1}, \ldots, \frac{a_k}{1 + (N/d_k)a_k C_k} \right).$$

As $C_1, \ldots, C_k$ and $N/d_1, \ldots, N/d_k$ are bounded above by a constant, we have

$$\|f(\mathbf{a}_1) - f(\mathbf{a}_2)\| \geq \frac{c\,\|\mathbf{a}_1 - \mathbf{a}_2\|}{(1 + \|\mathbf{a}_1\|)(1 + \|\mathbf{a}_2\|)}$$

for a constant $c > 0$. Under a suitable permutation of $1, \ldots, k$, the matrix H is lower-triangular, with all entries bounded above, and with all diagonal entries c_r bounded away from 0. Thus the least singular value of H is bounded away from 0, so Assumption 2.16 holds. Substituting $m_0 a_s$ for a_s in (2.32), we also have

$$\left(F(\operatorname{Id} + m_0 F)^{-1} \right)_{(r,s),(r',s')} = \mathbb{1}\{s = s'\} \sqrt{c_r c_r'} \sigma_r \sigma_{r'} \frac{N(a_s/d_s)}{1 + N(a_s/d_s)C_s m_0} \operatorname{Id}_{d_s}.$$

Taking block traces and Hilbert-Schmidt norms yields the expressions for t_r and w_{rs}.

Finally, for part (c), observe likewise that for F as defined in (2.21),

$$\mathrm{Tr}_r\left([\mathrm{Id}_M + FD(\mathbf{x})]^{-1}F\right) = \mathrm{Tr}_r\left([\mathrm{Id}_{\check{M}} + \check{F}\check{D}(\mathbf{x})]^{-1}\check{F}\right)$$

where $\check{D}(\mathbf{x}) = \mathrm{diag}(x_1 \mathrm{Id}_{\check{m}_1}, \ldots, x_k \mathrm{Id}_{\check{m}_k})$ and $\check{F}$ has blocks $\sqrt{m_r m_s}\check{U}_r'\check{B}\check{U}_s$. Applying again the forms of $\check{U}_r$ and $\check{B}$ and the identity $c_r m_r = n$, we obtain

$$\check{F}_{(r,s),(r',s')} = \mathbb{1}\{s = s'\}\frac{na_s}{d_s}\mathrm{Id}_{d_s}.$$

Fix $s \in \{1, \ldots, k\}$ and consider the submatrix E_s formed by the blocks $((r,s),(r',s))$ where $r \succeq s$ and $r' \succeq s$. Then $E_s = n(a_s/d_s)R_s'R_s$ where $R_s = (\mathrm{Id}_{d_s} \mid \cdots \mid \mathrm{Id}_{d_s})$. The corresponding submatrix of $\check{D}(\mathbf{x})$ is given by $D_s = \mathrm{diag}(x_r \mathrm{Id}_{d_s} : r \succeq s)$. Defining x_{s+} by (2.30) and applying the Woodbury identity, we have

$$(\mathrm{Id} + E_s D_s)^{-1}E_s = \left(\mathrm{Id} - \frac{na_s}{d_s(1 + (n/d_s)a_s x_{s+})}R_s'R_sD_s\right)\frac{na_s}{d_s}R_s'R_s = \frac{na_s}{d_s(1 + (n/d_s)a_s x_{s+})}R_s'R_s.$$

Then for all $s \preceq r$ and $s' \preceq r'$,

$$\left((\mathrm{Id} + FD(\mathbf{x}))^{-1}F\right)_{(r,s),(r',s')} = \mathbb{1}\{s = s'\}\frac{na_s}{d_s(1 + (n/d_s)a_s x_{s+})}\mathrm{Id}_{d_s}.$$

Taking the diagonal block trace in the collapsed decomposition $\check{M} = \check{m}_1 + \ldots + \check{m}_k$ and applying $n/m_r = c_r$, we obtain from (2.24) the explicit form (2.30). □

Chapter 3

Edge fluctuations under sphericity

In this chapter, we discuss in greater detail the edges of the support of the law μ_0 from Theorem 2.4. We then prove Theorem 2.6, which establishes Tracy-Widom fluctuations of the extremal eigenvalue of $\widehat{\Sigma}$ at each regular edge of μ_0 under global sphericity of $\Sigma_1, \ldots, \Sigma_k$.

Our proof generalizes an argument of Lee and Schnelli [LS16], which showed under a similar edge regularity condition that the largest eigenvalue of $\widehat{\Sigma} = X'FX$ exhibits real Tracy-Widom fluctuations for positive definite F. We extend this result in two directions:

1. We show that this holds also for matrices F with negative eigenvalues.
2. The spectrum of the law μ_0 in Theorem 2.4 may have multiple disjoint intervals of support. We establish a Tracy-Widom limit for the extremal eigenvalue at each regular edge of the support, including the internal edges.

When F is positive definite and X has *complex* Gaussian entries, convergence of the largest eigenvalue of $\widehat{\Sigma}$ to the complex Tracy-Widom law was established in [Kar07], and this was extended to each regular edge in [HHN16]. These analyses use the determinantal form of the HCIZ integral over the complex unitary group, which has no known real analogue. The proof of [LS16] in the real setting is different and relies on a universality argument, which we first summarize.

By rotational invariance in law of X, it suffices to consider the case where $F = T$ is diagonal. Let E_* be the rightmost edge of μ_0. The proof of [LS16] considers

$$\widehat{\Sigma}^{(L)} = X'T^{(L)}X$$

for a different matrix $T^{(L)}$, and compares the eigenvalue behavior of $\widehat{\Sigma}$ near E_* with that of $\widehat{\Sigma}^{(L)}$ near its rightmost edge $E_*^{(L)}$. Concretely, the comparison between T and $T^{(L)}$ is achieved by a continuous interpolation over $l \in [0, L]$, where $T^{(0)} = T$ and each $T^{(l)}$ has diagonal entries $\{t_\alpha^{(l)} : \alpha = 1, \ldots, M\}$

given by

$$\frac{1}{t_\alpha^{(l)}} = e^{-l}\frac{1}{t_\alpha^{(0)}} + (1 - e^{-l}). \tag{3.1}$$

(See [LS16, Eq. (6.1)].) For simplicity, each $T^{(l)}$ is then rescaled so that the largest eigenvalue of $\widehat{\Sigma}^{(l)} \equiv X'T^{(l)}X$ fluctuates with identical scale (of order $N^{-2/3}$) for every l. Taking $L = \infty$, $T^{(\infty)}$ is a multiple of the identity, so $\widehat{\Sigma}^{(\infty)}$ is a white Wishart matrix for which the Tracy-Widom distributional limit is known from [Joh01]. Along this interpolation, the upper edge $E_*^{(l)}$ traces a continuous path between $E_*^{(0)}$ and $E_*^{(\infty)}$. Defining

$$\#(E_*^{(l)} + s_1, E_*^{(l)} + s_2) = \text{number of eigenvalues of } \widehat{\Sigma}^{(l)} \text{ in } [E_*^{(l)} + s_1, E_*^{(l)} + s_2],$$

a resolvent approximation idea from [EYY12] establishes the smooth approximation

$$\mathbb{P}\Big[\#(E_*^{(l)} + s_1, E_*^{(l)} + s_2) = 0\Big] \approx \mathbb{E}\left[K(\mathfrak{X}^{(l)}(s_1, s_2))\right], \tag{3.2}$$

where $K(\mathfrak{X}^{(l)}(s_1, s_2))$ is a smoothed indicator of the integrated Stieltjes transform of $\widehat{\Sigma}^{(l)}$ along an interval in $\mathbb{C}^+$ at height $\eta = N^{-2/3-\varepsilon}$ above the corresponding interval on the real axis. The crux of the proof in [LS16] is then to show

$$\left|\frac{d}{dl}\mathbb{E}\left[K(\mathfrak{X}^{(l)}(s_1, s_2))\right]\right| \leq N^{-1/3+\varepsilon} \tag{3.3}$$

for a small constant $\varepsilon > 0$ and s_1, s_2 on the $N^{-2/3}$ scale. This is applied to compare the probability in (3.2) for $l = 0$ and $l = 2\log N$. A simple direct argument compares these probabilities for $l = 2\log N$ and $l = \infty$, concluding the proof.

We extend this argument by showing that the continuous interpolation in (3.1) may be replaced by a discrete interpolating sequence. The resulting extra flexibility permits the extension of this result in the two directions mentioned earlier. Indeed, we note that (3.1) is not well-defined for negative $t_\alpha^{(0)}$, as the right side passes through 0 along the interpolation. More importantly, (3.1) does not allow us to study interior edges of $\widehat{\Sigma}$ when there are multiple disjoint intervals of support, as the support intervals merge and these edges vanish along the interpolation. We instead consider a discrete interpolating sequence $T^{(0)}, T^{(1)}, \ldots, T^{(L)}$ for an integer $L \leq O(N)$, where the diagonal entries $t_\alpha^{(l)}$ satisfy

$$\sum_{\alpha=1}^{M} |t_\alpha^{(l+1)} - t_\alpha^{(l)}| \leq O(1) \tag{3.4}$$

for all $l = 0, \ldots, L-1$. Letting E_* be any regular edge of $\widehat{\Sigma}$, each matrix $\widehat{\Sigma}^{(l)} \equiv X'T^{(l)}X$ will have a corresponding edge $E_*^{(l)}$ such that

$$|E_*^{(l+1)} - E_*^{(l)}| \leq O(1/N). \tag{3.5}$$

Each of these L discrete steps may be thought of as corresponding to a time interval $\Delta l = O(N^{-1})$ in the continuous interpolation (3.1). We show that the above conditions are sufficient to establish a discrete analogue of (3.3),

$$\left|\mathbb{E}\left[K(\mathfrak{X}^{(l+1)}(s_1, s_2))\right] - \mathbb{E}\left[K(\mathfrak{X}^{(l)}(s_1, s_2))\right]\right| \leq N^{-4/3+\varepsilon}. \tag{3.6}$$

As $L \leq O(N)$, summing over $l = 0, \ldots, L-1$ establishes the desired comparison between $T^{(0)}$ and $T^{(L)}$. Importantly, the requirement (3.4) is sufficiently weak to allow a Lindeberg swapping scheme, where each $T^{(l+1)}$ makes a single $O(1)$ perturbation to a single entry of $T^{(l)}$. Hence we may move the diagonal entries of T from one interval of support to another, without continuously evolving them between such intervals. This allows us to preserve the edge E_* as in (3.5) along the entire interpolating sequence, even as the other intervals of support disappear.

Section 3.1 discusses properties of the matrix model $\widehat{\Sigma} = X'TX$ and the law μ_0, including a detailed characterization of its support and edge locations, and introduces our definition of edge regularity. Section 3.2 reviews prerequisite proof ingredients, which are similar to those in [LS16]. These include properties of the limiting Stieltjes transform near regular edges, Schur-complement identities for the resolvent, a local Marcenko-Pastur law as in [BPZ13, KY17], and the resolvent approximation from [EYY12] that formalizes (3.2). The material in these sections are either drawn from existing literature or represent extensions from the positive definite setting. We defer proofs or proof sketches of these extensions to Appendix A.

Section 3.3 constructs an interpolating sequence $T^{(0)}, \ldots, T^{(L)}$ for any starting matrix $T^{(0)} = T$. As in [LS16], we rescale each $T^{(l)}$ so that the eigenvalue of interest fluctuates with identical scale for each l. Consequently, the interpolating sequence will not be exactly Lindeberg, but rather will satisfy $|t_\alpha^{(l+1)} - t_\alpha^{(l)}| \leq O(1)$ for a single entry α and $|t_\beta^{(l+1)} - t_\beta^{(l)}| \leq O(1/N)$ for all remaining entries $\beta \neq \alpha$. The final edge $E_*^{(L)}$ may be either a left or right edge of $\widehat{\Sigma}^{(L)}$, and we conclude the proof by applying either the result of [Joh01] for a positive right edge or [FS10] for a positive left edge of a (real) white Wishart matrix. To ensure that a left edge is not a hard edge at 0, we allow $T^{(L)}$ to have two distinct diagonal entries $\{0, t\}$. Thus, $\widehat{\Sigma}^{(L)}$ may have a different dimensionality ratio from the starting $\widehat{\Sigma}$.

In Section 3.4, we conclude the proof by establishing (3.6). To achieve this, we generalize the "decoupling lemma" of [LS16, Lemma 6.2] to a setting involving two different resolvents G and $\check{G}$, corresponding to $T \equiv T^{(l)}$ and $\check{T} \equiv T^{(l+1)}$. Fortunately, we do not need to perform the same generalization for the "optical theorems" of [LS16, Lemma B.1], as we may apply (3.4) to reduce the higher-order terms arising in the decoupling lemma to involve only G and not $\check{G}$. We will explain this later in the proof.

3.1 Matrix model and edge regularity

By rotational invariance in law of X, it suffices to prove Theorem 2.6 in the case where $F = T$ is diagonal. We record here the assumption of Theorems 2.4, 2.5, and 2.6 in the diagonal case.

Assumption 3.1. $\widehat{\Sigma} = X'TX$, where $T = \operatorname{diag}(t_1, \ldots, t_M) \in \mathbb{R}^{M\times M}$ and $X \in \mathbb{R}^{M\times N}$ has i.i.d. $\mathcal{N}(0, 1/N)$ entries. For a constant $C > 0$, we have $C^{-1} < N/M < C$ and $\|T\| < C$.

As described in Theorem 2.4, in the limit $N, M \to \infty$, the empirical spectrum of $\widehat{\Sigma}$ is well-approximated by a deterministic law μ_0. We note that if T is the identity matrix, then μ_0 is the Marcenko-Pastur law [MP67]. Under our scaling for X, this has density

$$f_0(x) = \frac{1}{2\pi}\frac{\sqrt{(E_+ - x)(x - E_-)}}{x} 1_{(E_-,E_+)}(x), \qquad E_\pm = (1 \pm \sqrt{M/N})^2 \tag{3.7}$$

on the positive real line, and an additional point mass at 0 when $M < N$. More generally, μ_0 is defined by the fixed-point equation (2.8) in its Stieltjes transform, which we may write for diagonal T as

$$z = -\frac{1}{m_0(z)} + \frac{1}{N}\sum_{\alpha=1}^{M} \frac{t_\alpha}{1 + t_\alpha m_0(z)}. \tag{3.8}$$

This law μ_0 admits a continuous density f_0 at each $x \in \mathbb{R}_*$, given by

$$f_0(x) = \lim_{z\in\mathbb{C}^+\to x} \frac{1}{\pi} \operatorname{Im} m_0(z), \tag{3.9}$$

where

$$\mathbb{R}_* = \begin{cases} \mathbb{R} & \text{if } \operatorname{rank}(T) > N \\ \mathbb{R}\setminus\{0\} & \text{if } \operatorname{rank}(T) \le N. \end{cases} \tag{3.10}$$

For $x \neq 0$, this is shown in [SC95]; we extend this to $x = 0$ when $\operatorname{rank}(T) > N$ in Appendix A.1.

The law μ_0 is called the free multiplicative convolution of the empirical distribution of $t_1, \ldots, t_M$ with the Marcenko-Pastur law (3.7). In contrast to the case $T = \mathrm{Id}$, if $t_1, \ldots, t_M$ take more than one distinct value, then μ_0 may have multiple disjoint intervals of support. Two such cases are depicted in Figures 3.1 and 3.2. For each support interval $[E_-, E_+]$ of μ_0, we will call each endpoint E_- and E_+ an *edge*. More formally:

Definition 3.2. $E_* \in \mathbb{R}$ is a **right edge** of μ_0 if $(E_* - \delta, E_*) \subset \operatorname{supp}(\mu_0)$ and $(E_*, E_* + \delta) \subset \mathbb{R}\setminus\operatorname{supp}(\mu_0)$ for some $\delta > 0$. E_* is a **left edge** of μ_0 if this holds with $(E_* - \delta, E_*)$ and $(E_*, E_* + \delta)$ exchanged. When 0 is a point mass of μ_0, we do not consider it an edge.

The support intervals and edge locations of μ_0 are described in a simple way by (3.8): Define

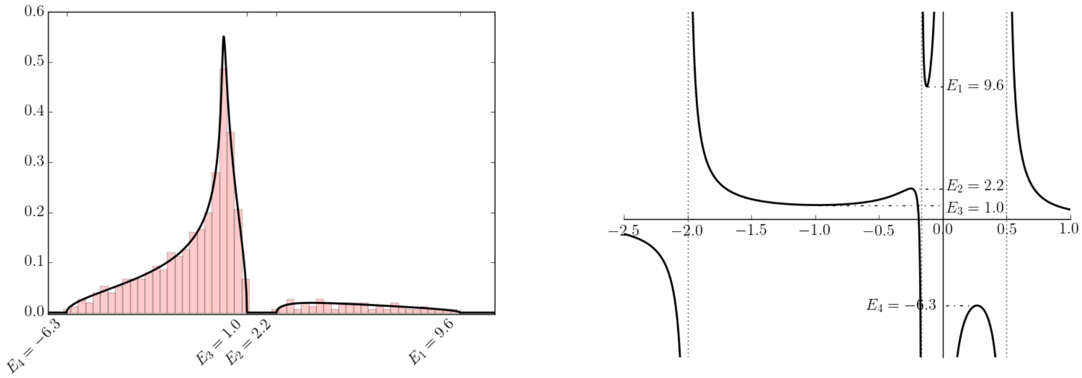

Figure 3.1: Left: Density $f_0(x)$ of μ_0 and simulated eigenvalues of $\widehat{\Sigma}$, for $N = 500$, $M = 700$, and T having 350 eigenvalues at -2, 300 at 0.5, and 50 at 6. The four soft edges of μ_0 are indicated by $E_1, \ldots, E_4$. Right: The function $z_0(m)$, with two local minima and two local maxima corresponding to the four edges of μ_0.

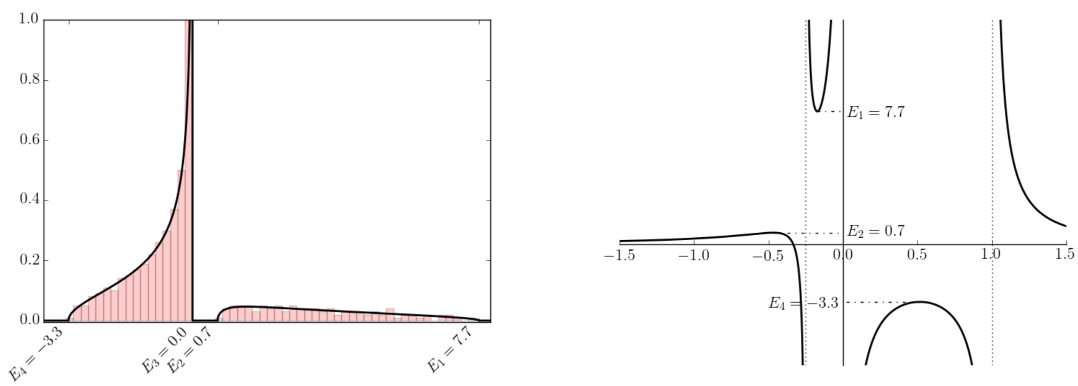

Figure 3.2: Left: Density $f_0(x)$ of μ_0 and simulated eigenvalues of $\widehat{\Sigma}$, for $N = M = 500$, and T having 400 eigenvalues at -1 and 100 at 4. Here, μ_0 has three soft edges E_1, E_2, E_4 and one hard edge $E_3 = 0$. Right: The function $z_0(m)$, with three indicated local extrema, and also a local minimum at $m = \infty$ corresponding to the hard right edge $E_3 = 0$.

$P = \{0\} \cup \{-t_\alpha^{-1} : t_\alpha \neq 0\}$, and consider $\bar{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. Consider the formal inverse of $m_0(z)$,

$$z_0(m) = -\frac{1}{m} + \frac{1}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha}{1 + t_\alpha m}, \tag{3.11}$$

as a real-valued function on $\bar{\mathbb{R}} \setminus P$ with the convention $z_0(\infty) = 0$. Then z_0 is a rational function with poles P—two examples are plotted in Figures 3.1 and 3.2. The following proposition relates the edges of μ_0 to the local extrema of z_0. We indicate its proof in Appendix A.1. (Parts (a), (b), and (d) follow from [SC95], and part (c) was established for positive definite T in [KY17].)

Proposition 3.3. Let $m_1, \ldots, m_n \in \bar{\mathbb{R}} \setminus P$ denote the local minima and local maxima[1] of z_0, ordered such that $0 > m_1 > \ldots > m_k > -\infty$ and $\infty \geq m_{k+1} > \ldots > m_n > 0$. Let $E_j = z_0(m_j)$ for each $j = 1, \ldots, n$. Then:

(a) μ_0 has exactly $n/2$ support intervals and n edges, which are given by $E_1, \ldots, E_n$.

(b) E_j is a right edge if m_j is a local minimum, and a left edge if m_j is a local maximum.

(c) The edges are ordered as

$$E_1 > \ldots > E_k > E_{k+1} > \ldots > E_n.$$

(d) For each E_j where $m_j \neq \infty$, we have $E_j \in \mathbb{R}_*$ and $z_0''(m_j) \neq 0$. Defining $\gamma_j = \sqrt{2/|z_0''(m_j)|}$, the density of μ_0 satisfies $f_0(x) \sim (\gamma_j/\pi)\sqrt{|E_j - x|}$ as $x \to E_j$ with $x \in \operatorname{supp}(\mu_0)$.

Definition 3.4. For each edge E_* of μ_0, the local minimum or maximum m_* of z_0 such that $z_0(m_*) = E_*$ is its ***m*-value**. The edge is **soft** if $m_* \neq \infty$ and **hard** if $m_* = \infty$. For a soft edge, $\gamma = \sqrt{2/|z_0''(m_*)|}$ is its associated **scale**.

Hence the local extrema of z_0 are in 1-to-1 correspondence with the edges of μ_0. Excluding the point mass at 0 when $\operatorname{rank}(T) < N$, $\operatorname{supp}(\mu_0)$ is exactly $[E_n, E_{n-1}] \cup [E_{n-2}, E_{n-3}] \cup \ldots \cup [E_2, E_1]$, where these intervals are disjoint and in increasing order. The density f_0 exhibits square-root decay at each soft edge E_*, with scale inversely related to the curvature of z_0 at m_*.

When T is positive semi-definite, $\operatorname{supp}(\mu_0)$ is nonnegative. In this setting, an edge at 0 is usually called hard and all other edges soft. The above definition generalizes this to non-positive-definite T: A hard edge is always 0 and can occur when $\operatorname{rank}(T) = N$. One example is depicted in Figure 3.2. However, if T has negative eigenvalues, then a soft edge may also be 0 when $\operatorname{rank}(T) > N$.

We now introduce the notion of a "regular" edge of μ_0. For positive definite T, a similar notion was introduced for the rightmost edge in [Kar07] and generalized to all soft edges in [HHN16, KY17].

[1] $m_* \in \bar{\mathbb{R}} \setminus P$ is a local minimum of z_0 if $z_0(m) \geq z_0(m_*)$ for all m in a sufficiently small neighborhood of m_*, with the convention that $m_* = \infty$ is a local minimum if z_0 is positive over $(C, \infty) \cup (-\infty, -C)$ for some $C > 0$. Local maxima are defined similarly.

Definition 3.5. Let $E_* \in \mathbb{R}$ be a soft edge of μ_0 with m-value m_* and scale γ. E_* is **regular** if all of the following hold for a constant $\tau \in (0,1)$:

- $|m_*| < \tau^{-1}$.
- $\gamma < \tau^{-1}$.
- For all $\alpha \in \{1, \ldots, M\}$ such that $t_\alpha \neq 0$, $|m_* + t_\alpha^{-1}| > \tau$.

A smaller constant τ indicates a weaker regularity assumption. We will say E_* is τ-regular if we wish to emphasize the role of τ. All subsequent constants may depend on τ above; we will usually not explicitly state this dependence.

Let us state here, for clarity, that the existence of any regular edge implies T is non-degenerate, in the sense

$$(\text{number of eigenvalues } t_\alpha \text{ such that } |t_\alpha| > c) > cM \tag{3.12}$$

for a constant $c > 0$. (See Proposition 3.11.) Thus the largest and average values of $|t_\alpha|$ are both of constant order.

We discuss implications of edge regularity in Section 3.2.2. One interpretation of this condition is the following, whose proof we defer to Appendix A.2.

Proposition 3.6. Suppose Assumption 3.1 holds and the edge E_* is regular. Then there exist constants $C, c, \delta > 0$ such that

(a) (Separation) The interval $(E_* - \delta, E_* + \delta)$ belongs to $\mathbb{R}_*$ and contains no edge other than E_*.

(b) (Square-root decay) For all $x \in \operatorname{supp}(\mu_0) \cap (E_* - \delta, E_* + \delta)$, the density f_0 of μ_0 satisfies

$$c\sqrt{|E_* - x|} \leq f_0(x) \leq C\sqrt{|E_* - x|}.$$

Whereas Definition 3.2 and Proposition 3.3(d) imply the above for C, c, δ depending on N, edge regularity ensures that the above properties hold uniformly in N.

One may check, via Proposition 3.11 below, that Definition 3.5 is equivalent to the definition of a regular edge in [KY17] when T is positive definite. The condition $|m_*| < \tau^{-1}$ quantifies softness of E_*, so E_* cannot converge to a hard edge at 0. The condition $\gamma < \tau^{-1}$ guarantees non-vanishing curvature of z_0 at m_*, so E_* cannot approach a neighboring interval of support. The condition $|m_* + t_\alpha^{-1}| > \tau$ guarantees separation of m_* from the poles P of z_0; this implies, in particular, that E_* cannot be the edge of a support interval for an outlier eigenvalue of $\widehat{\Sigma}$. This last condition was introduced for the rightmost edge in [Kar07]. In the setting of a simple spiked model [Joh01] where $(t_1, \ldots, t_M) = (\theta, 1, 1, \ldots, 1)$ for fixed $\theta > 1$, if E_* is the rightmost edge, then it is easily verified that this condition is equivalent to θ falling below the phase transition threshold $1 + \sqrt{M/N}$ studied in [BBP05, BS06, Pau07].

Theorem 2.5 guarantees that all eigenvalues of $\widehat{\Sigma}$ fall within a δ-neighborhood of $\operatorname{supp}(\mu_0)$, for any constant $\delta > 0$. Near a regular edge E_*, we have the following strengthening of this guarantee, which shows that the extremal eigenvalue of $\widehat{\Sigma}$ near E_* is typically only at a distance $N^{-2/3}$ from E_*.

Theorem 3.7 ($N^{-2/3}$ concentration at regular edges)**.** Suppose Assumption 3.1 holds, and E_* is a regular right edge. Then there exists a constant $\delta > 0$ such that for any $\varepsilon, D > 0$ and all $N \geq N_0(\varepsilon, D)$,

$$\mathbb{P}\Big[\operatorname{spec}(\widehat{\Sigma}) \cap [E_* + N^{-2/3+\varepsilon}, E_* + \delta] = \emptyset\Big] > 1 - N^{-D}. \tag{3.13}$$

The analogous statement holds if E_* is a regular left edge, with no eigenvalue of $\widehat{\Sigma}$ belonging to $[E_* - \delta, E_* - N^{-2/3+\varepsilon}]$.

This result was established in [KY17] for positive definite T, and we prove in Appendix A.3 its generalization to any T satisfying Assumption 3.1.

3.2 Preliminaries

We collect in this section the requisite ingredients and tools for the proof of Theorem 2.6.

Notation

We denote $\mathcal{I}_M = \{1, \ldots, M\}$ and $\mathcal{I}_N = \{1, \ldots, N\}$. Considering the elements of these index sets as distinct, we define the disjoint union $\mathcal{I} \equiv \mathcal{I}_N \sqcup \mathcal{I}_M$. For a matrix in $\mathbb{C}^{(N+M)\times(N+M)}$, we identify $\{1, 2, \ldots, N+M\} \simeq \mathcal{I}$ and index its rows and columns by $\mathcal{I}$, where $\mathcal{I}_N$ corresponds to the upper left block and $\mathcal{I}_M$ to the lower right block. We consistently use lower-case Roman letters i, j, p, q for indices in $\mathcal{I}_N$, Greek letters $\alpha, \beta, \gamma, \rho$ for indices in $\mathcal{I}_M$, and upper-case Roman letters A, B, C for general indices in $\mathcal{I}$.

Throughout, $C, c > 0$ denote constants that may change from instance to instance. We write $a_N \asymp b_N$ for deterministic non-negative quantities a_N, b_N when $cb_N \leq a_N \leq Ca_N$. The constants C, c may depend on τ in the context of a regular edge.

3.2.1 Stochastic domination

For a non-negative scalar Ψ (either random or deterministic), we write

$$\xi \prec \Psi \qquad \text{and} \qquad \xi = O_{\prec}(\Psi)$$

if, for any constants $\varepsilon, D > 0$ and all $N \geq N_0(\varepsilon, D)$,

$$\mathbb{P}\left[|\xi| > N^{\varepsilon}\Psi\right] < N^{-D}. \tag{3.14}$$

The constant $N_0(\varepsilon, D)$ may depend only on ε, D, the constant in Assumption 3.1, and τ in the context of a τ-regular edge. If we wish to let $N_0(\varepsilon, D)$ depend on another constant a, we will denote this explicitly by writing $\prec_a$.

We review several properties of this definition from [EKY13].

Lemma 3.8. Let U be any index set, and suppose $\xi(u) \prec \Psi(u)$ for all $u \in U$. Let C be any constant (depending only on Assumption 3.1 and τ).

(a) If $|U| \leq N^C$, then $\sup_{u\in U}|\xi(u)|/\Psi(u) \prec 1$.

(b) If $|U| \leq N^C$, then $\sum_{u\in U} \xi(u) \prec \sum_{u\in U} \Psi(u)$.

(c) If $u_1, u_2 \in U$, then $\xi(u_1)\xi(u_2) \prec \Psi(u_1)\Psi(u_2)$.

Proof. All three parts follow from a union bound, as $\varepsilon, D > 0$ in (3.14) are arbitrary. □

Lemma 3.9. Suppose $\xi \prec \Psi$ and Ψ is deterministic. Suppose furthermore that there are constants $C, C_1, C_2, \ldots > 0$ (depending only on Assumption 3.1 and τ) such that $\Psi > N^{-C}$ and $\mathbb{E}[|\xi|^\ell] < N^{C_\ell}$ for each integer $\ell > 0$. Then $\mathbb{E}[\xi|\mathcal{G}] \prec \Psi$ for any sub-σ-field $\mathcal{G}$.

Proof. If $\mathcal{G}$ is trivial so $\mathbb{E}[\xi|\mathcal{G}] = \mathbb{E}[\xi]$, then this follows from Cauchy-Schwarz: For any $\varepsilon > 0$ and all $N \geq N_0(\varepsilon)$,

$$|\mathbb{E}\xi| \leq \mathbb{E}\left[|\xi|\mathbb{1}\{|\xi| \leq N^{\varepsilon/2}\Psi\}\right] + \mathbb{E}\left[|\xi|\mathbb{1}\{|\xi| > N^{\varepsilon/2}\Psi\}\right] \leq N^{\varepsilon/2}\Psi + \mathbb{E}[|\xi|^2]^{1/2}\mathbb{P}[|\xi| > N^{\varepsilon/2}\Psi]^{1/2} < N^\varepsilon \Psi,$$

where the last inequality applies $\xi \prec \Psi$. For general $\mathcal{G}$, consider any $\varepsilon, D > 0$ and fix an integer $k > (D + \varepsilon)/\varepsilon$. Then the above argument yields $\mathbb{E}[|\xi|^k] < N^\varepsilon \Psi^k$ for all $N \geq N_0(\varepsilon, D)$, so

$$\mathbb{P}\Big[|\mathbb{E}[\xi|\mathcal{G}]| > N^\varepsilon \Psi\Big] \leq \frac{\mathbb{E}[|\mathbb{E}[\xi|\mathcal{G}]|^k]}{N^{k\varepsilon}\Psi^k} \leq \frac{\mathbb{E}[|\xi|^k]}{N^{k\varepsilon}\Psi^k} < N^{\varepsilon - k\varepsilon} < N^{-D}.$$

□

When U is a bounded domain of $\mathbb{C}$, part (a) of Lemma 3.8 does not directly apply, but we may oftentimes take the union bound by Lipschitz continuity:

Lemma 3.10. Suppose $\xi(z) \prec \Psi(z)$ for all $z \in U$, where $U \subset \mathbb{C}$ is uniformly bounded in N. Suppose that for any $D > 0$, there exists $C \equiv C(D) > 0$ and an event of probability $1 - N^{-D}$ on which

- $\Psi(z) > N^{-C}$ for all $z \in U$.
- $|\xi(z_1) - \xi(z_2)| \leq N^C|z_1 - z_2|$ and $|\Psi(z_1) - \Psi(z_2)| \leq N^C|z_1 - z_2|$ for all $z_1, z_2 \in U$.

Then $\sup_{z\in U}|\xi(z)|/\Psi(z) \prec 1$.

Proof. For any $\varepsilon, D > 0$, set $C = C(D)$ and $\Delta = N^{-3C}$. Take a net $\mathcal{N} \subset U$ with $|\mathcal{N}| \leq N^{6C+1}$ such that for every $z \in U$, there exists $z' \in \mathcal{N}$ with $|z - z'| < \Delta$. By Lemma 3.8(a), $|\xi(z')| < N^\varepsilon \Psi(z')$ for all $z' \in \mathcal{N}$ with probability $1 - N^{-D}$. Then with probability $1 - 2N^{-D}$, for all $z \in U$,

$$|\xi(z)| \leq |\xi(z')| + \Delta N^C < N^\varepsilon \Psi(z') + \Delta N^C \leq N^\varepsilon \Psi(z) + 2\Delta N^{\varepsilon + C} < 3N^\varepsilon \Psi(z).$$

□

3.2.2 Edge regularity

Let us prove here the sufficient condition of Proposition 2.7 for regularity of the rightmost edge.

Proof of Proposition 2.7. Let t_1 be the maximum eigenvalue of T, and let K be its multiplicity. The m-value m_* for the rightmost edge satisfies $m_* \in (-t_1^{-1}, 0)$. As $t_1 > c$ for a constant $c > 0$, this implies $|m_*| < 1/c$. Furthermore, we have

$$0 = z_0'(m_*) = \frac{1}{m_*^2} - \frac{1}{N} \sum_{\alpha : t_\alpha \neq 0} \frac{1}{(m_* + t_\alpha^{-1})^2}. \tag{3.15}$$

As $|t_\alpha^{-1}| > c$ for a constant $c > 0$ and each α, this implies $|m_*| > c$ for a constant $c > 0$. The condition (3.15) also implies

$$0 \leq \frac{1}{m_*^2} - \frac{K}{N} \frac{1}{(m_* + t_1^{-1})^2}.$$

As K is proportional to N, this yields $|m_* + t_1^{-1}| > c$ for a constant $c > 0$. Then by the condition $m_* \in (-t_1^{-1}, 0)$, we obtain $|m_* + t_\alpha^{-1}| > \tau$ for all non-zero α and some constant $\tau > 0$. Finally, we have

$$z_0''(m_*) = -\frac{2}{m_*^3} + \frac{2}{N} \sum_{\alpha : t_\alpha \neq 0} \frac{1}{(m_* + t_\alpha^{-1})^3} = \sum_{\alpha : t_\alpha \neq 0} -\frac{2}{m_* N} \cdot \frac{t_\alpha^{-1}}{(m_* + t_\alpha^{-1})^3},$$

where the second equality applies (3.15). Note that $m_* < 0$, and $m_* + t_\alpha^{-1} > 0$ if $t_\alpha > 0$ and $m_* + t_\alpha^{-1} < 0$ if $t_\alpha < 0$. Thus each summand on the right side above is positive, and in particular

$$z_0''(m_*) \geq -\frac{2K}{m_* N} \cdot \frac{t_1^{-1}}{(m_* + t_1^{-1})^3}.$$

Thus $\gamma < \tau^{-1}$ for a constant $\tau > 0$. □

We next record a simple consequence of edge regularity.

Proposition 3.11. Suppose Assumption 3.1 holds, and E_* is a regular edge with m-value m_* and scale γ. Then there exist constants $C, c > 0$ such that

$$c < |m_*| < C, \qquad c < \gamma < C, \qquad |E_*| < C,$$

and for all $\alpha = 1, \ldots, M$,

$$|1 + t_\alpha m_*| > c.$$

Furthermore, if any regular edge E_* exists, then T satisfies (3.12), and if T is positive semi-definite, then also $E_* > c > 0$.

Proof. The bounds $|m_*| < \tau^{-1}$ and $\gamma < \tau^{-1}$ are assumed in Definition 3.5. From (3.15) and the condition $|m_* + t_\alpha^{-1}| > \tau$ for each α, the bound $|m_*| > c$ follows. The bounds $|E_*| < C$ and $\gamma > c$ then follow from the definitions $E_* = z_0(m_*)$ and $\gamma^{-2} = |z_0''(m_*)|/2$. For $|1 + t_\alpha m_*|$, take $C > 0$ such that $|m_*| < C$. If $|t_\alpha| > 1/(2C)$, then $|1 + t_\alpha m_*| > \tau/(2C)$ by the condition $|m_* + t_\alpha^{-1}| > \tau$, whereas if $|t_\alpha| \leq 1/(2C)$, then $|1 + t_\alpha m_*| > 1/2$.

From (3.15) and the conditions $|m_*| < C$ and $|1 + t_\alpha m_*| > c$, we have $M^{-1} \sum_\alpha t_\alpha^2 > c$. Together with the assumption $|t_\alpha| < C$ for all α, this implies (3.12). Finally, note that $0 = z_0'(m_*)$ implies $m_*^{-1} = N^{-1} \sum_\alpha t_\alpha^2 m_*/(1 + t_\alpha m_*)^2$, and hence

$$E_* = z_0(m_*) = \frac{1}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha}{(1 + t_\alpha m_*)^2}.$$

If T is positive semi-definite, then $E_* > c$ follows from $|1 + t_\alpha m_*| < C$ and (3.12). $\square$

The remaining implications of edge regularity heuristically follow from the Taylor expansion

$$z_0(m) - E_* = z_0(m) - z_0(m_*) = \frac{z_0''(m_*)}{2}(m - m_*)^2 + O((m - m_*)^3),$$

where there is no first-order term because $0 = z_0'(m_*)$. Consequently,

$$m_0(z) \approx m_* + \sqrt{\frac{2}{z_0''(m_*)}(z - E_*)}$$

for $z \in \mathbb{C}^+$ near E_* and an appropriate choice of square-root. Edge regularity implies uniform control of the above Taylor expansion; we defer detailed proofs to Appendix A.2. Similar properties were established for positive definite T in [BPZ13, KY17].

Proposition 3.12. Suppose Assumption 3.1 holds and E_* is a regular edge with m-value m_*. Then there exist constants $c, \delta > 0$ such that for all $m \in (m_* - \delta, m_* + \delta)$, if E_* is a right edge then

$$z_0''(m) > c,$$

and if E_* is a left edge then $z_0''(m) < -c$.

Proposition 3.13. Suppose Assumption 3.1 holds and E_* is a regular edge. Then there exist constants $C, c, \delta > 0$ such that the following hold: Define

$$\mathbf{D}_0 = \{z \in \mathbb{C}^+ : \operatorname{Re} z \in (E_* - \delta, E_* + \delta), \operatorname{Im} z \in (0, 1]\}.$$

Then for all $z \in \mathbf{D}_0$ and $\alpha \in \{1, \ldots, M\}$,

$$c < |m_0(z)| < C, \qquad c < |1 + t_\alpha m_0(z)| < C.$$

Furthermore, for all $z \in \mathbf{D}_0$, denoting $z = E + i\eta$ and $\kappa = |E - E_*|$,

$$c\sqrt{\kappa + \eta} \leq |m_0(z) - m_*| \leq C\sqrt{\kappa + \eta}, \qquad cf(z) \leq \operatorname{Im} m_0(z) \leq Cf(z)$$

where

$$f(z) = \begin{cases} \sqrt{\kappa + \eta} & \text{if } E \in \operatorname{supp}(\rho) \\ \frac{\eta}{\sqrt{\kappa+\eta}} & \text{if } E \notin \operatorname{supp}(\rho). \end{cases}$$

3.2.3 Resolvent bounds and identities

For $z \in \mathbb{C}^+$, denote the resolvent and Stieltjes transform of $\widehat{\Sigma}$ by

$$G_N(z) = (\widehat{\Sigma} - z \operatorname{Id})^{-1} \in \mathbb{C}^{N \times N}, \qquad m_N(z) = N^{-1} \operatorname{Tr} G_N(z). \tag{3.16}$$

Lemma 3.14. For any $\eta > 0$ and $z, z' \in \mathbb{C}^+$ with $\operatorname{Im} z \geq \eta$ and $\operatorname{Im} z' \geq \eta$, and for any $i, j \in \mathcal{I}_N$,

$$|m_N(z)| \leq \frac{1}{\eta}, \qquad |G_{ij}(z)| \leq \frac{1}{\eta},$$

$$|m_N(z) - m_N(z')| \leq \frac{|z - z'|}{\eta^2}, \qquad |G_{ij}(z) - G_{ij}(z')| \leq \frac{|z - z'|}{\eta^2}.$$

Proof. Let $\widehat{\Sigma} = \sum_i \lambda_i \mathbf{v}_i \mathbf{v}_i'$ be the spectral decomposition of $\widehat{\Sigma}$. Then $G_N(z) = \sum_i (\lambda_i - z)^{-1} \mathbf{v}_i \mathbf{v}_i'$, so $\|G_N(z)\| \leq 1/\eta$ and $\|\partial_z G_N(z)\| \leq 1/\eta^2$. All four statements follow. □

As in [LS16, KY17], define the linearized resolvent $G(z)$ by

$$H(z) = \begin{pmatrix} -z \operatorname{Id} & X' \\ X & -T^{-1} \end{pmatrix} \in \mathbb{C}^{(N+M)\times(N+M)}, \qquad G(z) = H(z)^{-1}.$$

We index rows and columns of $G(z)$ by $\mathcal{I} \equiv \mathcal{I}_N \sqcup \mathcal{I}_M$. The Schur-complement formula for block matrix inversion yields the alternative form

$$G(z) = \begin{pmatrix} G_N(z) & G_N(z) X' T \\ T X G_N(z) & T X G_N(z) X' T - T \end{pmatrix}, \tag{3.17}$$

which is understood as the definition of $G(z)$ when T is not invertible. We will omit the argument z in m_0, m_N, G_N, G when the meaning is clear.

For any $A \in \mathcal{I}$, define $H^{(A)}$ as the submatrix of H with row and column A removed, and define

$$G^{(A)} = (H^{(A)})^{-1}.$$

When T is not invertible, $G^{(A)}$ is defined by the alternative form analogous to (3.17). We index $G^{(A)}$ by $\mathcal{I} \setminus \{A\}$.

Note that G and $G^{(A)}$ are symmetric, in the sense $G' = G$ and $(G^{(A)})' = G^{(A)}$ without complex conjugation. The entries of G and $G^{(A)}$ are related by the following Schur-complement identities:

Lemma 3.15 (Resolvent identities)**.** Fix $z \in \mathbb{C}^+$.

(a) For any $i \in \mathcal{I}_N$,

$$G_{ii} = -\frac{1}{z + \sum_{\alpha,\beta \in \mathcal{I}_M} G^{(i)}_{\alpha\beta} X_{\alpha i} X_{\beta i}}.$$

For any $\alpha \in \mathcal{I}_M$,

$$G_{\alpha\alpha} = -\frac{t_\alpha}{1 + t_\alpha \sum_{i,j \in \mathcal{I}_N} G^{(\alpha)}_{ij} X_{\alpha i} X_{\alpha j}}.$$

(b) For any $i \neq j \in \mathcal{I}_N$,

$$G_{ij} = -G_{ii} \sum_{\beta \in \mathcal{I}_M} G^{(i)}_{\beta j} X_{\beta i}.$$

For any $\alpha \neq \beta \in \mathcal{I}_M$,

$$G_{\alpha\beta} = -G_{\alpha\alpha} \sum_{j \in \mathcal{I}_N} G^{(\alpha)}_{j\beta} X_{\alpha j}.$$

For any $\alpha \in \mathcal{I}_M$ and $i \in \mathcal{I}_N$,

$$G_{i\alpha} = -G_{ii} \sum_{\beta \in \mathcal{I}_M} G^{(i)}_{\beta\alpha} X_{\beta i} = -G_{\alpha\alpha} \sum_{j \in \mathcal{I}_N} G^{(\alpha)}_{ij} X_{\alpha j}.$$

(c) For any $A, B, C \in \mathcal{I}$ with $A \neq C$ and $B \neq C$,

$$G^{(C)}_{AB} = G_{AB} - \frac{G_{AC} G_{CB}}{G_{CC}}.$$

Proof. This is stated in [KY17, Lemma 4.4]. Let us reproduce the argument here: It suffices to consider T invertible, as the non-invertible case follows by continuity. We apply the Schur complement identity

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}^{-1} = \begin{pmatrix} S & -SA_{12}A_{22}^{-1} \\ -A_{22}^{-1}A_{21}S & A_{22}^{-1} + A_{22}^{-1}A_{21}SA_{12}A_{22}^{-1} \end{pmatrix}$$

where $S = (A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1}$. Parts (a) and (b) follow by applying this identity to $G(z) = H(z)^{-1}$ with A_{11} corresponding to the (i,i) or (α,α) coordinate. For part (c), note that

$$A_{11}^{-1} - S = A_{11}^{-1}(-A_{12}A_{22}^{-1}A_{21})S = (A_{11}^{-1}A_{12})(-A_{22}^{-1}A_{21}S).$$

Applying this with A_{22} corresponding to the (C,C) coordinate, we obtain

$$G_{AB}^{(C)} - G_{AB} = \sum_{I \in \mathcal{I} \setminus \{C\}} G_{AI}^{(C)}(G^{-1})_{IC}G_{CB}.$$

Now applying the Schur complement identity with A_{11} corresponding to the (C,C) coordinate, we obtain

$$\frac{G_{AC}}{G_{CC}} = -\sum_{I \in \mathcal{I} \setminus \{C\}} G_{AI}^{(C)}(G^{-1})_{IC}.$$

Combining these yields part (c). □

3.2.4 Local law

We will require sharp bounds on the entries of $G(z)$ for $z \in \mathbb{C}^+$ close to a regular edge E_*. This type of "local law" is established in [KY17] for positive definite T; see also [BPZ13, LS16] for the rightmost edge. We check in Appendix A.3 that the proof generalizes with minor modifications to the setting of Assumption 3.1.

Theorem 3.16 (Entrywise local law at regular edges)**.** Suppose Assumption 3.1 holds and E_* is a τ-regular edge. Then there exists a τ-dependent constant $\delta > 0$ such that the following holds: Fix any constant $a > 0$ and define

$$\mathbf{D} = \{z \in \mathbb{C}^+ : \operatorname{Re} z \in (E_* - \delta, E_* + \delta),\ \operatorname{Im} z \in [N^{-1+a}, 1]\}. \tag{3.18}$$

For $A \in \mathcal{I}$, denote $t_A = 1$ if $A \in \mathcal{I}_N$ and $t_A = t_\alpha$ if $A = \alpha \in \mathcal{I}_M$. Set

$$\Pi(z) = \begin{pmatrix} m_0(z)\operatorname{Id} & 0 \\ 0 & -T(\operatorname{Id} + m_0(z)T)^{-1} \end{pmatrix} \in \mathbb{C}^{(N+M)\times(N+M)}. \tag{3.19}$$

Then for all $z \equiv E + i\eta \in \mathbf{D}$ and $A, B \in \mathcal{I}$,

$$\frac{G_{AB}(z) - \Pi_{AB}(z)}{t_A t_B} \prec_a \sqrt{\frac{\operatorname{Im} m_0(z)}{N\eta}} + \frac{1}{N\eta}, \tag{3.20}$$

and also

$$m_N(z) - m_0(z) \prec_a (N\eta)^{-1}.$$

It is verified from (3.17) that the quantity on the left of (3.20) is alternatively written as

$$\frac{G_{AB}-\Pi_{AB}}{t_At_B}=\begin{pmatrix} G_N-m_0\,\mathrm{Id} & G_NX' \\ XG_N & XG_NX'-m_0(\mathrm{Id}+m_0T)^{-1}\end{pmatrix}_{AB}. \tag{3.21}$$

This is understood as the definition of this quantity when either t_A and/or t_B is 0.

Corollary 3.17. Under the assumptions of Theorem 3.16, for any $\varepsilon, D>0$ and all $N\geq N_0(\varepsilon, D)$,

$$\mathbb{P}\left[\text{there exist } z\in\mathbf{D} \text{ and } A,B\in\mathcal{I}: \frac{|G_{AB}(z)-\Pi_{AB}(z)|}{|t_At_B|}>N^{\varepsilon}\left(\sqrt{\frac{\operatorname{Im} m_0(z)}{N\eta}}+\frac{1}{N\eta}\right)\right]<N^{-D}.$$

Proof. This follows from Lemmas 3.8(a) and 3.10. For a large enough constant $C>0$ and any $D>0$, on an event of probability $1-N^{-D}$, we have $\|X\|<C$ for all $N\geq N_0(D)$. The required boundedness and Lipschitz continuity properties for Lemma 3.10 then follow from (3.21), Lemma 3.14, and Proposition 3.13. □

3.2.5 Resolvent approximation

We formalize the approximation (3.2), following [EYY12, Corollary 6.2]. Fix a regular edge E_* and define, for $s_1,s_2\in\mathbb{R}$ and $\eta>0$,

$$\mathfrak{X}(s_1,s_2,\eta)=N\int_{E_*+s_1}^{E_*+s_2}\operatorname{Im} m_N(y+i\eta)dy. \tag{3.22}$$

For η much smaller than $N^{-2/3}$ and s_1,s_2 on the $N^{-2/3}$ scale, we expect

$$\#(E_*+s_1,E_*+s_2)\approx\pi^{-1}\mathfrak{X}(s_1,s_2,\eta)$$

where the left side denotes the number of eigenvalues of $\widehat{\Sigma}$ in this interval.

We apply this in the form of the following lemma; for convenience, we reproduce here a self-contained proof. (For simplicity, we state the result only for a right edge.)

Lemma 3.18. Suppose Assumption 3.1 holds, and E_* is a regular right edge. Let $K:\mathbb{R}\to[0,1]$ be such that $K(x)=1$ for all $x\leq 1/3$ and $K(x)=0$ for all $x\geq 2/3$. For all sufficiently small constants $\delta,\varepsilon>0$, the following holds:

Let $\lambda_{\max}$ be the maximum eigenvalue of $\widehat{\Sigma}$ in $(E_*-\delta,E_*+\delta)$. Set $s_+=N^{-2/3+\varepsilon}$, $l=N^{-2/3-\varepsilon}$, and $\eta=N^{-2/3-9\varepsilon}$. Then for any $D>0$, all $N\geq N_0(\varepsilon,D)$, and all $s\in[-s_+,s_+]$,

$$\mathbb{E}\left[K(\pi^{-1}\mathfrak{X}(s-l,s_+,\eta))\right]-N^{-D}\leq\mathbb{P}\left[\lambda_{\max}\leq E_*+s\right]\leq\mathbb{E}\left[K(\pi^{-1}\mathfrak{X}(s+l,s_+,\eta))\right]+N^{-D}.$$

Proof. Denote

$$\#(a,b) = \text{number of eigenvalues of } \widehat{\Sigma} \text{ in } [a,b].$$

For any $E_1 < E_2$, any $m > 0$, and any $\lambda \in \mathbb{R}$, we have the casewise bound

$$\left| \mathbb{1}_{[E_1,E_2]}(\lambda) - \int_{E_1}^{E_2} \frac{1}{\pi} \frac{\eta}{\eta^2 + (x-\lambda)^2} dx \right| \leq \begin{cases} \frac{E_2-E_1}{\pi} \frac{\eta}{\eta^2+(E_1-\lambda)^2} & \text{if } \lambda < E_1 - m \\ 1 & \text{if } E_1 - m \leq \lambda \leq E_1 + m \\ \frac{2}{\pi} \frac{\eta}{m} & \text{if } E_1 + m < \lambda < E_2 - m \\ 1 & \text{if } E_2 - m \leq \lambda \leq E_2 + m \\ \frac{E_2-E_1}{\pi} \frac{\eta}{\eta^2+(\lambda-E_2)^2} & \text{if } \lambda > E_2 + m, \end{cases}$$

where the middle case $E_1 + m < \lambda < E_2 - m$ follows from

$$1 - \int_{E_1}^{E_2} \frac{1}{\pi} \frac{\eta}{\eta^2 + (x-\lambda)^2} dx \leq 1 - \int_{\lambda-m}^{\lambda+m} \frac{1}{\pi} \frac{\eta}{\eta^2 + (x-\lambda)^2} dx = 1 - \frac{2}{\pi} \tan^{-1}\left(\frac{m}{\eta}\right) \leq \frac{2}{\pi} \frac{\eta}{m}.$$

For the first case, we apply also the bound

$$\frac{\eta}{\eta^2 + (E_1-\lambda)^2} \leq \frac{\eta}{(E_1-\lambda)^2} \leq \frac{2\eta}{m} \cdot \frac{m}{m^2 + (E_1-\lambda)^2},$$

and similarly for the last case. Hence, summing over λ as the eigenvalues of $\widehat{\Sigma}$,

$$\left| \#(E_1,E_2) - \frac{N}{\pi} \int_{E_1}^{E_2} \operatorname{Im} m_N(x+i\eta) dx \right| \leq R(E_1,E_2,m) + S(E_1,E_2,m) \tag{3.23}$$

where we set

$$\begin{aligned} R(E_1,E_2,m) &= \#(E_1 - m, E_1 + m) + \#(E_2 - m, E_2 + m), \\ S(E_1,E_2,m) &= \frac{2}{\pi} \frac{\eta}{m} \Big((E_2 - E_1) N \operatorname{Im} m_N(E_1 + im) + (E_2 - E_1) N \operatorname{Im} m_N(E_2 + im) \\ &\qquad + \#(E_1 + m, E_2 - m) \Big). \end{aligned}$$

We apply the above with $E_1, E_2 \in [E_* - 2s_+, E_* + 2s_+]$, and with $m = N^{-2/3-3\varepsilon}$. To bound $S(E_1,E_2,m)$, note that Proposition 3.13 and Theorem 3.16 yield, for $j = 1,2$,

$$\operatorname{Im} m_N(E_j + im) \prec N^{-1/3+3\varepsilon}.$$

For $z = E_* + i(2s_+)$, Proposition 3.13 and Theorem 3.16 also yield $Ns_+ \operatorname{Im} m_N(z) \prec N^{3\varepsilon/2}$. Applying

$\#(E_* - v, E_* + v) \le 2Nv \operatorname{Im} m_N(E_* + iv)$ for any $v > 0$, this yields

$$\#(E_* - 2s_+, E_* + 2s_+) \prec N^{3\varepsilon/2}. \tag{3.24}$$

Then applying $\#(E_1 + m, E_2 - m) \le \#(E_* - 2s_+, E_* + 2s_+)$ and $\eta/m = N^{-6\varepsilon}$, we obtain $S(E_1, E_2, m) \prec N^{-2\varepsilon}$. By Lemmas 3.14 and 3.10, we may take a union bound over all such E_1, E_2: For any $\varepsilon', D > 0$,

$$\mathbb{P}\left[\text{there exist } E_1, E_2 \in [E_* - 2s_+, E_* + 2s_+] \text{ such that } S(E_1, E_2, m) > N^{-2\varepsilon+\varepsilon'}\right] \le N^{-D} \tag{3.25}$$

for all $N \ge N_0(\varepsilon', D)$.

Now let $E = E_* + s$ and $E_+ = E_* + s_+ - l$. Then

$$\begin{aligned}
\#(E, E_+) &\le \frac{1}{l^2} \int_{E-l}^{E} \left(\int_{E_+}^{E_+ + l} \#(E_1, E_2) dE_2 \right) dE_1 \\
&\le \frac{N}{\pi} \int_{E-l}^{E_+ + l} \operatorname{Im} m_N(x + i\eta) dx + \frac{1}{l^2} \int_{E-l}^{E} \int_{E_+}^{E_+ + l} R(E_1, E_2, m) dE_2 \, dE_1 + O_\prec(N^{-2\varepsilon}),
\end{aligned}$$

where we have applied (3.23) and (3.25). The first term is $\pi^{-1}\mathfrak{X}(s - l, s_+, \eta)$. For the second term, we obtain from the definition of $R(E_1, E_2, m)$

$$\frac{1}{l^2} \int_{E-l}^{E} \int_{E_+}^{E_+ + l} R(E_1, E_2, m) dE_2 \, dE_1 \le \frac{2m}{l} \#(E - l - m, E + m) + \frac{2m}{l} \#(E_+ - m, E_+ + l + m).$$

Applying (3.24) to crudely bound $\#(E - l - m, E + m)$ and $\#(E_+ - m, E_+ + l + m)$ by $\#(E_* - 2s_+, E_* + 2s_+)$, and noting $m/l = N^{-2\varepsilon}$, we obtain

$$\#(E, E_+) \le \pi^{-1}\mathfrak{X}(s - l, s_+, \eta) + O_\prec(N^{-\varepsilon/2}).$$

Theorem 3.7 yields $\#(E_+, E_* + \delta) = 0$ with probability $1 - N^{-D}$ for $N \ge N_0(\varepsilon, D)$, so

$$\#(E, E_* + \delta) \le \pi^{-1}\mathfrak{X}(s - l, s_+, \eta) + O_\prec(N^{-\varepsilon/2}). \tag{3.26}$$

Similarly, setting $E_+ = E_* + s_+ + l$, we have

$$\begin{aligned}
\#(E, E_* + \delta) &\ge \frac{1}{l^2} \int_{E}^{E+l} \left(\int_{E_+ - l}^{E_+} \#(E_1, E_2) dE_2 \right) dE_1 \\
&\ge \pi^{-1}\mathfrak{X}(s + l, s_+, \eta) - O_\prec(N^{-\varepsilon/2}).
\end{aligned} \tag{3.27}$$

For any $D > 0$ and all $N \ge N_0(\varepsilon, D)$, (3.26) implies that $\pi^{-1}\mathfrak{X}(s - l, s_+, \eta) \ge 2/3$ whenever

$\#(E_* + s, E_* + \delta) \geq 1$, except possibly on an event of probability N^{-D}. Similarly (3.27) implies $\pi^{-1}\mathfrak{X}(s+l, s_+, \eta) \leq 1/3$ whenever $\#(E_* + s, E_* + \delta) = 0$, except possibly on an event of probability N^{-D}. The result then follows from the definition and boundedness of K. $\square$

3.3 The interpolating sequence

We now construct the interpolating sequence $T^{(0)}, \ldots, T^{(L)}$ described at the start of this chapter. We consider only the case of a right edge; this is without loss of generality, as the edge can have arbitrary sign and we may take the reflection $T \mapsto -T$. For each pair $T \equiv T^{(l)}$ and $\check{T} \equiv T^{(l+1)}$, the following definition captures the relevant property that will be needed in the subsequent computation.

Definition 3.19. Let $T, \check{T} \in \mathbb{R}^{M \times M}$ be two diagonal matrices satisfying Assumption 3.1. Let E_* be a right edge of the law ρ defined by T, and let $\check{E}_*$ be a right edge of $\check{\rho}$ defined by $\check{T}$. (T, E_*) and $(\check{T}, \check{E}_*)$ are **swappable** if, for a constant $\phi > 0$, both of the following hold.

- Letting t_α and $\check{t}_\alpha$ be the diagonal entries of T and $\check{T}$,

$$\sum_{\alpha=1}^{M} |t_\alpha - \check{t}_\alpha| < \phi.$$

- The m-values $m, \check{m}_*$ of $E_*, \check{E}_*$ satisfy

$$|m_* - \check{m}_*| < \phi/N.$$

We will say that (T, E_*) and $(\check{T}, \check{E}_*)$ are ϕ-swappable if we wish to emphasize the role of ϕ. All subsequent constants may implicitly depend on ϕ.

We first establish some basic deterministic properties of a swappable pair, including closeness of the edges $E_*, \check{E}_*$ as claimed in (3.5).

Lemma 3.20. Suppose $T, \check{T}$ are diagonal matrices satisfying Assumption 3.1, $E_*, \check{E}_*$ are regular right edges, and (T, E_*) and $(\check{T}, \check{E}_*)$ are swappable. Let m_*, γ and $\check{m}_*, \check{\gamma}$ be the m-values and scales of $E_*, \check{E}_*$. Denote $s_\alpha = (1 + t_\alpha m_*)^{-1}$ and $\check{s}_\alpha = (1 + \check{t}_\alpha \check{m}_*)^{-1}$. For integers $i, j \geq 0$, define

$$A_{i,j} = \frac{1}{N} \sum_{\alpha=1}^{M} t_\alpha^i s_\alpha^i \check{t}_\alpha^j \check{s}_\alpha^j.$$

Then there exists a constant $C > 0$ such that all of the following hold:

(a) For all i, j satisfying $i + j \leq 4$,

$$|A_{i,j} - A_{i+j,0}| \leq C/N.$$

(b) (Closeness of edge location)

$$|E_* - \check{E}_*| \leq C/N,$$

and

$$\left|(E_* - \check{E}_*) - \frac{1}{N}\sum_{\alpha=1}^{M}(t_\alpha - \check{t}_\alpha)s_\alpha \check{s}_\alpha\right| \leq C/N^2. \tag{3.28}$$

(c) (Closeness of scale)

$$|\gamma - \check{\gamma}| \leq C/N.$$

Proof. By Proposition 3.11, $|t_\alpha|, |s_\alpha|, |m_*|, \gamma \leq C$, and also $|\check{t}_\alpha|, |\check{s}_\alpha|, |\check{m}_*|, \check{\gamma} \leq C$. From the definitions of s_α and $\check{s}_\alpha$, we verify

$$t_\alpha s_\alpha - \check{t}_\alpha \check{s}_\alpha = (t_\alpha - \check{t}_\alpha)s_\alpha \check{s}_\alpha + (\check{m}_* - m_*)t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha.$$

Then swappability implies

$$|A_{i,j} - A_{i+1,j-1}| \leq \frac{1}{N}\sum_{\alpha=1}^{M}|t_\alpha^i s_\alpha^i \check{t}_\alpha^{j-1}\check{s}_\alpha^{j-1}||\check{t}_\alpha \check{s}_\alpha - t_\alpha s_\alpha| \leq C/N.$$

Iteratively applying this yields (a).

For (b), note that

$$\begin{aligned} E_* - \check{E}_* &= -\frac{1}{m_*} + \frac{1}{\check{m}_*} + \frac{1}{N}\sum_{\alpha=1}^{M}(t_\alpha s_\alpha - \check{t}_\alpha \check{s}_\alpha) \\ &= (m_* - \check{m}_*)\left(\frac{1}{m_*\check{m}_*} - A_{1,1}\right) + \frac{1}{N}\sum_{\alpha=1}^{M}(t_\alpha - \check{t}_\alpha)s_\alpha \check{s}_\alpha. \end{aligned}$$

Recall $0 = z_0'(m_*) = m_*^{-2} - A_{2,0}$. Then part (b) follows from the definition of swappability, together with $|A_{1,1} - m_*^{-2}| = |A_{1,1} - A_{2,0}| \leq C/N$ and $|m_*^{-2} - m_*^{-1}\check{m}_*^{-1}| \leq C/N$.

For (c), we have $\gamma^{-2} = z_0''(m_*)/2 = -m_*^{-3} + A_{3,0}$. Then (c) follows from $|\gamma^{-2} - \check{\gamma}^{-2}| \leq |m_*^{-3} - \check{m}_*^{-3}| + |A_{3,0} - A_{0,3}| \leq C/N$. ☐

In the rest of this section, we prove the following lemma:

Lemma 3.21. Suppose T is diagonal and satisfies Assumption 3.1, and E_* is a τ-regular right edge with scale $\gamma = 1$. Then there exist τ-dependent constants $C', \tau', \phi > 0$, a sequence of diagonal matrices $T^{(0)}, T^{(1)}, \ldots, T^{(L)}$ in $\mathbb{R}^{M\times M}$ for $L \leq 2M$, and a sequence of right edges $E_*^{(0)}, E_*^{(1)}, \ldots, E_*^{(L)}$ of the corresponding laws $\mu_0^{(l)}$ defined by $T^{(l)}$, such that:

1. $T^{(0)} = T$ and $E_*^{(0)} = E_*$.

2. $T^{(L)}$ has at most two distinct diagonal entries 0 and t, for some $t \in \mathbb{R}$.

3. Each $T^{(l)}$ satisfies Assumption 3.1 with constant C'.

4. Each $E_*^{(l)}$ is τ'-regular.

5. $(T^{(l)}, E_*^{(l)})$ and $(T^{(l+1)}, E_*^{(l+1)})$ are ϕ-swappable for each $l = 0, \ldots, L-1$.

6. (Scaling) Each $E_*^{(l)}$ has associated scale $\gamma^{(l)} = 1$.

We first ignore the scaling condition, property 6, and construct $T^{(0)}, \ldots, T^{(L)}$ and $E_*^{(0)}, \ldots, E_*^{(L)}$ satisfying properties 1–5. We will use a Lindeberg swapping construction, where each $T^{(l+1)}$ differs from $T^{(l)}$ in only one diagonal entry. It is useful to write z_0' and z_0'' as

$$z_0'(m) = \frac{1}{m^2} - \frac{1}{N} \sum_{\alpha: t_\alpha \neq 0} \frac{1}{(m + t_\alpha^{-1})^2}$$
$$z_0''(m) = -\frac{2}{m^3} + \frac{2}{N} \sum_{\alpha: t_\alpha \neq 0} \frac{1}{(m + t_\alpha^{-1})^3},$$

and to think about swapping entries of T as swapping or removing poles of z_0' and z_0''. In particular, for each fixed $m \in \mathbb{R}$, we can easily deduce from the above whether a given swap increases or decreases the values of z_0' and z_0'' at m.

Upon defining a swap $T \to \check{T}$, the identification of the new right edge $\check{E}_*$ for $\check{T}$ uses the following continuity lemma.

Lemma 3.22. Suppose T is a diagonal matrix satisfying Assumption 3.1, and E_* is a τ-regular right edge with m-value m_*. Let $\check{T}$ be a matrix that replaces a single diagonal entry t_α of T by a value $\check{t}_\alpha$, such that $|\check{t}_\alpha| \leq \|T\|$ and either $\check{t}_\alpha = 0$ or $|m_* + \check{t}_\alpha^{-1}| > \tau$. Let $z_0, \check{z}_0$ denote the function (3.11) defined by $T, \check{T}$. Then there exist τ-dependent constants $N_0, \phi > 0$ such that whenever $N \geq N_0$:

- $\check{T}$ has a right edge $\check{E}_*$ with m-value $\check{m}_*$ satisfying $|m_* - \check{m}_*| < \phi/N$.

- The interval between m_* and $\check{m}_*$ does not contain any pole of z_0 or $\check{z}_0$.

- $\operatorname{sign}(m_* - \check{m}_*) = \operatorname{sign}(\check{z}_0'(m_*))$.

(We define $\operatorname{sign}(x) = 1$ if $x > 0$, -1 if $x < 0$, and 0 if $x = 0$.)

Proof. By Proposition 3.11, $|m_*| > \nu$ for a constant ν. Take $\delta < \min(\tau/2, \nu/2)$. Then the given conditions for $\check{t}_\alpha$ imply that $(m_* - \delta, m_* + \delta)$ does not contain any pole of z_0 or $\check{z}_0$, and

$$|z_0'(m) - \check{z}_0'(m)| < C/N$$

for some $C > 0$ and all $m \in (m_* - \delta, m_* + \delta)$. For sufficiently small δ, Proposition 3.12 also ensures $z_0''(m) > c$ for all $m \in (m_* - \delta, m_* + \delta)$. If $\check{z}_0'(m_*) < 0 = z_0'(m_*)$, this implies $\check{z}_0$ must have a local minimum in $(m_*, m_* + C/N)$, for a constant $C > 0$ and all $N \geq N_0$. Similarly, if $\check{z}_0'(m_*) > 0$, then

$\check{z}_0$ has a local minimum in $(m_* - C/N, m_*)$, and if $\check{z}_0'(m_*) = 0$, then $\check{z}_0$ has a local minimum at m_*. The result follows from Proposition 3.3 upon setting $\check{E}_* = \check{z}_0(\check{m}_*)$. □

The basic idea for proving Lemma 3.21 is to take a Lindeberg sequence $T^{(0)}, \ldots, T^{(L)}$ and apply the above lemma for each swap. We cannot do this naively for any Lindeberg sequence, because in general if $E_*^{(l)}$ is τ_l-regular, then the above lemma only guarantees that $E_*^{(l+1)}$ is τ_{l+1}-regular for $\tau_{l+1} = \tau_l - C/N$ and a τ_l-dependent constant $C > 0$. Thus edge regularity, as well as the edge itself, may vanish after $O(N)$ swaps.

To circumvent this, we consider a specific construction of the Lindeberg sequence, apply Lemma 3.22 inductively along this sequence to identify an edge $\check{E}_*$ for each successive $\check{T}$, and use a separate argument to show that $\check{E}_*$ must be τ'-regular for a fixed constant $\tau' > 0$. Hence we may continue to apply Lemma 3.22 along the whole sequence.

We consider separately the cases $m_* < 0$ and $m_* > 0$.

Lemma 3.23. Suppose (the right edge) E_* has m-value $m_* < 0$. Then for some τ-dependent constant N_0, whenever $N \geq N_0$, Lemma 3.21 holds without the scaling condition, property 6.

Proof. We construct a Lindeberg sequence that first reflects about m_* each pole of z_0 to the right of m_*, and then replaces each pole by the one closest to m_*.

Suppose, first, that there are K_1 non-zero diagonal entries t_α of T (positive or negative) where $-t_\alpha^{-1} > m_*$. Consider a sequence of matrices $T^{(0)}, T^{(1)}, \ldots, T^{(K_1)}$ where $T^{(0)} = T$, and each $T^{(k+1)}$ replaces one such diagonal entry t_α of $T^{(k)}$ by the value $\check{t}_\alpha$ such that $-\check{t}_\alpha^{-1} < m_*$ and $|m_* + \check{t}_\alpha^{-1}| = |m_* + t_\alpha^{-1}|$. For each such swap $T \to \check{T}$, we verify $|\check{t}_\alpha| \leq |t_\alpha| \leq \|T\|$, $\check{z}_0'(m_*) = z_0'(m_*) = 0$, and $\check{z}_0''(m_*) > z_0''(m_*) > 0$. Thus we may take $\check{m}_* = m_*$ in Lemma 3.22, and the new edge $\check{E}_* = \check{z}_0(m_*)$ remains τ-regular for the same constant τ.

All diagonal entries of $T^{(K_1)}$ are now nonnegative. Let $t = \|T^{(K_1)}\|$ be the maximal such entry. By the above construction, $-t^{-1} < m_* < 0$. Since $E_*^{(K_1)}$ is τ-regular, (3.12) implies $t > c$ for a constant $c > 0$. Let K_2 be the number of positive diagonal entries of $T^{(K_1)}$ strictly less than t, and consider a sequence $T^{(K_1+1)}, \ldots, T^{(K_1+K_2)}$ where each $T^{(k+1)}$ replaces one such diagonal entry in $T^{(k)}$ by t. Applying Lemma 3.22 inductively to each such swap $T \to \check{T}$, we verify $\check{z}_0'(m_*) < z_0(m_*) = 0$, so $m_* < \check{m}_* < 0$. Then $|\check{m}_*| < |m_*|$ and $\min_\alpha |\check{m}_* + \check{t}_\alpha^{-1}| > \min_\alpha |m_* + t_\alpha^{-1}|$. Also $\check{m}_* + \check{t}_\alpha^{-1} > 0$ for all $\check{t}_\alpha \neq 0$, so $\check{z}_0''(\check{m}_*) > -2/\check{m}_*^3 > 2t^3$. This verifies $\check{E}_* = \check{z}_0(\check{m}_*)$ is τ'-regular for a fixed constant $\tau' > 0$. (We may take any $\tau' < \min(\tau, t^{3/2})$.)

The total number of swaps $L = K_1 + K_2$ is at most $2M$, and all diagonal entries of $T^{(L)}$ belong to $\{0, t\}$. This concludes the proof, with property 5 verified by Lemma 3.22. □

Lemma 3.24. Lemma 3.23 holds also when (the right edge) E_* has m-value $m_* > 0$.

Proof. Proposition 3.3 implies m_* is a local minimum of z_0. The interval $(0, m_*)$ must contain a pole of z_0—otherwise, by the boundary condition of z_0 at 0, there would exist a local maximum m

of z_0 in $(0, m_*)$ satisfying $z_0(m) > z_0(m_*)$, which would contradict the edge ordering in Proposition 3.3(c). Let $-t^{-1}$ be the pole in $(0, m_*)$ closest to m_*. Note that $t < 0$ and $|t| > |m_*|^{-1} > \tau$. We construct a Lindeberg sequence that first replaces a small but constant fraction of entries of T by t, then replaces all non-zero $t_\alpha > t$ by 0, and finally replaces all $t_\alpha < t$ by 0.

First, fix a small constant $c_0 > 0$, let $K_1 = \lfloor c_0 M \rfloor$, and consider a sequence of matrices $T^{(0)}, T^{(1)}, \ldots, T^{(K_1)}$ where $T^{(0)} = T$ and each $T^{(k+1)}$ replaces a different (arbitrary) diagonal entry of $T^{(k)}$ by t. For c_0 sufficiently small, it is easy to check that we may apply Lemma 3.22 to identify an edge $E_*^{(k)}$ for each $k = 1, \ldots, K_1$, such that each $E_*^{(k)}$ remains $\tau/2$-regular.

$T^{(K_1)}$ now has at least $c_0 M$ diagonal entries equal to t. By the condition in Lemma 3.22 that the swap $m_* \to \check{m}_*$ does not cross any pole of z_0 or $\check{z}_0$, we have that $-t^{-1}$ is still the pole in $(0, m_*^{(K_1)})$ closest to $m_*^{(K_1)}$. Let K_2 be the number of non-zero diagonal entries t_α of $T^{(K_1)}$ (positive or negative) such that $t_\alpha > t$. Consider a sequence $T^{(K_1+1)}, \ldots, T^{(K_1+K_2)}$ where each $T^{(k+1)}$ replaces one such entry in $T^{(k)}$ by 0. Applying Lemma 3.22 inductively to each such swap $T \to \check{T}$, we verify $\check{z}_0'(m_*) > z_0'(m_*) = 0$, so $-t^{-1} < \check{m}_* < m_*$. Then $\min_{\alpha: -\check{t}_\alpha^{-1} > -t^{-1}} |\check{m}_* + \check{t}_\alpha^{-1}| > \min_{\alpha: -t_\alpha^{-1} > -t^{-1}} |m_* + t_\alpha^{-1}| > \tau/2$. The conditions $\check{m}_* > |t|^{-1} > c$ and

$$0 = \check{z}_0'(\check{m}_*) \leq \frac{1}{\check{m}_*^2} - \frac{c_0 M}{N} \frac{1}{(\check{m}_* + t^{-1})^2}$$

ensure that $\check{m}_* + t^{-1} > \nu$ for a constant $\nu > 0$, and hence $\min_\alpha |\check{m}_* + \check{t}_\alpha^{-1}| > \min(\nu, \tau/2)$. To bound $\check{z}_0''(\check{m}_*)$, let us introduce the function

$$f(m) = -\frac{2}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha^2 m^3}{(1 + t_\alpha m)^3}$$

and define analogously $\check{f}(m)$ for $\check{T}$. We verify $f'(m) < 0$ for all m, so $f(\check{m}_*) > f(m_*)$. Furthermore, if the swap $T \to \check{T}$ replaces t_α by 0, then $1 + t_\alpha \check{m}_* > 0$. (This is obvious for positive t_α; for negative t_α, it follows from $\check{m}_* < -t_\alpha^{-1}$.) Then $\check{f}(\check{m}_*) > f(\check{m}_*) > f(m_*)$. Applying the condition $0 = z_0'(m_*)$, we verify $f(m_*) = m_*^4 z_0''(m_*)$. Then

$$\check{z}_0''(\check{m}_*) > \frac{m_*^4}{\check{m}_*^4} z_0''(m_*) > z_0''(m_*) > 0.$$

This shows that $\check{E}_* = \check{z}_0(\check{m}_*)$ is τ'-regular for a fixed constant $\tau' > 0$. (We may take $\tau' = \min(\nu, \tau/2)$ as above.)

Finally, $T^{(K_1+K_2)}$ now has at least $c_0 M$ diagonal entries equal to t, and all non-zero diagonal entries t_α satisfy $t_\alpha < t < 0$. Let K_3 be the number of such entries and consider a sequence $T^{(K_1+K_2+1)}, \ldots, T^{(K_1+K_2+K_3)}$ where each $T^{(k+1)}$ replaces one such entry of $T^{(k)}$ by 0. Applying Lemma 3.22 inductively to each such swap $T \to \check{T}$, we verify $\check{z}_0'(m_*) > z_0'(m_*) = 0$, so $-t^{-1} < \check{m}_* < m_*$. As in the K_2 swaps above, this implies $\min_\alpha |\check{m}_* + \check{t}_\alpha^{-1}| > c$ for a constant $c > 0$. The condition

$\check{t}_\alpha < t$ implies $1 + \check{t}_\alpha \check{m}_* < 0$ for all $\check{t}_\alpha$, so we have

$$\check{f}(\check{m}_*) > -\frac{2c_0 M}{N} \frac{t^2 \check{m}_*^3}{(1 + t\check{m}_*)^3} > c$$

for a constant c. Applying again $\check{f}(\check{m}_*) = \check{m}_*^4 \check{z}_0''(\check{m}_*)$, this yields $\check{z}_0''(\check{m}_*) > c > 0$, so $\check{E}_*$ is τ'-regular for a constant $\tau' > 0$.

The total number of swaps $L = K_1 + K_2 + K_3$ is at most $2M$. All diagonal entries of $T^{(L)}$ belong to $\{0, t\}$, so this concludes the proof. □

Proof of Lemma 3.21. By Lemmas 3.23 and 3.24, there exist $T^{(0)}, \ldots, T^{(L)}$ and $E_*^{(0)}, \ldots, E_*^{(L)}$ satisfying conditions 1–5. By Lemma 3.20, the associated scales $\gamma_0, \ldots, \gamma_L$ satisfy $|\gamma_{l+1} - \gamma_l| \leq C/N$ for a ϕ, τ'-dependent constant $C > 0$ and each $l = 0, \ldots, L-1$.

We verify from the definitions of E_*, m_*, γ that under the rescaling $T \mapsto cT$ for any $c > 0$, we have

$$E_* \mapsto cE_*, \qquad m_* \mapsto c^{-1} m_*, \qquad \gamma \mapsto c^{-3/2}\gamma.$$

Consider then the matrices $\tilde{T}^{(l)} = \gamma_l^{2/3} T^{(l)}$ and edges $\tilde{E}_*^{(l)} = \gamma_l^{2/3} E_*^{(l)}$. We check properties 1–6 for $\tilde{T}^{(l)}$ and $\tilde{E}_*^{(l)}$: Properties 1, 2, and 6 are obvious. Since $T^{(0)}, \ldots, T^{(L)}$ are all τ'-regular, Proposition 3.11 implies $c < \gamma_l < C$ for constants $C, c > 0$ and every l, so properties 3 and 4 hold with adjusted constants. Property 5 also holds with an adjusted constant ϕ, since

$$\sum_\alpha |\gamma^{2/3} t_\alpha - \check{\gamma}^{2/3} \check{t}_\alpha| \leq \gamma^{2/3} \sum_\alpha |t_\alpha - \check{t}_\alpha| + |\gamma^{2/3} - \check{\gamma}^{2/3}| \sum_\alpha |\check{t}_\alpha| < \phi'$$

and

$$|\gamma^{-2/3} m_* - \check{\gamma}^{-2/3} \check{m}_*| \leq \gamma^{-2/3} |m_* - \check{m}_*| + |\gamma^{-2/3} - \check{\gamma}^{-2/3}|\, |\check{m}_*| < \phi'/N$$

for a ϕ, τ'-dependent constant $\phi' > 0$. □

3.4 Resolvent comparison

We will conclude the proof of Theorem 2.6 by establishing the following lemma.

Lemma 3.25 (Resolvent comparison)**.** Fix $\varepsilon > 0$ a sufficiently small constant, and let $s_1, s_2, \eta \in \mathbb{R}$ be such that $|s_1|, |s_2| < N^{-2/3+\varepsilon}$ and $\eta \in [N^{-2/3-\varepsilon}, N^{-2/3}]$. Let $T, \check{T} \in \mathbb{R}^{M \times M}$ be two diagonal matrices and $E_*, \check{E}_*$ two corresponding regular right edges, such that (T, E_*) and $(\check{T}, \check{E}_*)$ are swappable and their scales satisfy $\gamma = \check{\gamma} = 1$. Suppose Assumption 3.1 holds.

Let $m_N, \check{m}_N$ be the Stieltjes transforms as in (3.16) corresponding to $T, \check{T}$, and define

$$\mathfrak{X} = N \int_{E_* + s_1}^{E_* + s_2} \operatorname{Im} m_N(y + i\eta) dy, \qquad \check{\mathfrak{X}} = N \int_{\check{E}_* + s_1}^{\check{E}_* + s_2} \operatorname{Im} \check{m}_N(y + i\eta) dy.$$

Let $K : \mathbb{R} \to \mathbb{R}$ be any function such that K and its first four derivatives are uniformly bounded by a constant. Then

$$\mathbb{E}[K(\mathfrak{X}) - K(\check{\mathfrak{X}})] \prec N^{-4/3+16\varepsilon}. \tag{3.29}$$

Let us first prove Theorem 2.6 assuming this lemma.

Proof of Theorem 2.6. By rotational invariance of X, we may assume that $F = T$ is diagonal and satisfies Assumption 3.1. By symmetry with respect to $T \mapsto -T$, it suffices to consider part (a), the case of a right edge. By rescaling $T \mapsto \gamma^{2/3}T$, it suffices to consider the case where $\gamma = 1$.

Let $T^{(0)}, \ldots, T^{(L)}$ and $E_*^{(0)}, \ldots, E_*^{(L)}$ satisfy Lemma 3.21. Define $\mathfrak{X}^{(k)}(s_1, s_2, \eta)$ as in (3.22) for each $(T^{(k)}, E_*^{(k)})$. For a sufficiently small constant $\varepsilon > 0$, let η, s_+, l and $K : [0,\infty) \to [0,1]$ be as in Lemma 3.18, where K has bounded derivatives of all orders.

Fix $x \in \mathbb{R}$ and let $s = xN^{-2/3}$. Applying Lemma 3.18, we have (for all large N)

$$\mathbb{P}[\lambda_{\max}(\widehat{\Sigma}) \leq E_* + s] \leq \mathbb{E}[K(\pi^{-1}\mathfrak{X}^{(0)}(s + l, s_+, \eta))] + N^{-1}.$$

Setting $\varepsilon' = 9\varepsilon$ and applying Lemma 3.25, we have

$$\mathbb{E}[K(\pi^{-1}\mathfrak{X}^{(k)}(s + l, s_+, \eta))] \leq \mathbb{E}[K(\pi^{-1}\mathfrak{X}^{(k+1)}(s + l, s_+, \eta))] + N^{-4/3+17\varepsilon'}$$

for each $k = 0, \ldots, L-1$. Finally, defining $\widehat{\Sigma}^{(L)} = X'T^{(L)}X$ and $\lambda_{\max}(\widehat{\Sigma}^{(L)})$ as its largest eigenvalue in $(E_*^{(L)} - \delta', E_*^{(L)} + \delta')$ for some $\delta' > 0$, applying Lemma 3.18 again yields

$$\mathbb{E}[K(\pi^{-1}\mathfrak{X}^{(L)}(s + l, s_+, \eta))] \leq \mathbb{P}[\lambda_{\max}(\widehat{\Sigma}^{(L)}) \leq E_*^{(L)} + s + 2l] + N^{-1}.$$

Recalling $L \leq 2M$ and combining the above bounds,

$$\mathbb{P}[N^{2/3}(\lambda_{\max}(\widehat{\Sigma}) - E_*) \leq x] \leq \mathbb{P}[N^{2/3}(\lambda_{\max}(\widehat{\Sigma}^{(L)}) - E_*^{(L)}) \leq x + 2N^{-\varepsilon}] + o(1).$$

The matrix $T^{(L)}$ has all diagonal entries 0 or t, so $\widehat{\Sigma}^{(L)} = t\tilde{X}'\tilde{X}$ for $\tilde{X} \in \mathbb{R}^{\tilde{M}\times N}$ having $\mathcal{N}(0, 1/N)$ entries. The corresponding law $\mu_0^{(L)}$ has a single support interval and a unique right edge, so $E_*^{(L)}$ must be this edge. Regularity of $E_*^{(L)}$ and (3.12) imply $|t| \asymp 1$ and $\tilde{M}/N \asymp 1$. If $E_*^{(L)} > 0$, then $t > 0$. Applying [Joh01, Theorem 1.1] for the largest eigenvalue of a real Wishart matrix, we have

$$\mathbb{P}[N^{2/3}(\lambda_{\max}(\widehat{\Sigma}^{(L)}) - E_*^{(L)}) \leq x + 2N^{-\varepsilon}] = F_1(x) + o(1) \tag{3.30}$$

where F_1 is the distribution function of μ_{TW}. If $E_*^{(L)} < 0$, then $t < 0$, and edge regularity implies $\tilde{M}/N$ is bounded away from 1. Then we also have (3.30) by considering $-\widehat{\Sigma}^{(L)}$ and applying [FS10, Theorem I.1.1] for the smallest eigenvalue of a real Wishart matrix. (If $\tilde{M} < N$, we apply this result to the companion matrix $\tilde{X}\tilde{X}'$.) Combining the above, we obtain

$$\mathbb{P}[N^{2/3}(\lambda_{\max}(\widehat{\Sigma}) - E_*) \leq x] \leq F_1(x) + o(1).$$

The reverse bound is analogous, concluding the proof. □

In the remainder of this section, we prove Lemma 3.25.

3.4.1 Individual resolvent bounds

For diagonal T and for $z = y + i\eta$ as appearing in Lemma 3.25, we record here simple resolvent bounds that follow from the local law. Similar bounds were used in [EYY12, LS16]. We also introduce the shorthand notation that will be used in the computation.

Let E_* be a regular right edge. Fix a small constant $\varepsilon > 0$, and fix s_1, s_2, η such that $|s_1|, |s_2| \leq N^{-2/3+\varepsilon}$ and $\eta \in [N^{-2/3-\varepsilon}, N^{-2/3}]$. Changing variables, we write

$$\mathfrak{X} \equiv \mathfrak{X}(s_1, s_2, \eta) = N \int_{s_1}^{s_2} \operatorname{Im} m_N(y + E_* + i\eta) dy.$$

For $y \in [s_1, s_2]$, we write as shorthand

$$z \equiv z(y) = y + E_* + i\eta, \qquad G \equiv G(z(y)), \qquad m_N \equiv m_N(z(y)),$$

$$G^{(\alpha)} \equiv G^{(\alpha)}(z(y)), \qquad m_N^{(\alpha)} \equiv \frac{1}{N} \sum_{i \in \mathcal{I}_N} G_{ii}^{(\alpha)}, \qquad \mathfrak{X}^{(\alpha)} \equiv N \int_{s_1}^{s_2} \operatorname{Im} m_N^{(\alpha)}(y + E_* + i\eta) dy.$$

The above quantities depend implicitly on y.

We use the simplified summation notation

$$\sum_{i,j} \equiv \sum_{i,j \in \mathcal{I}_N}, \qquad \sum_{\alpha,\beta} \equiv \sum_{\alpha,\beta \in \mathcal{I}_M}$$

where summations over lower-case Roman indices are implicitly over $\mathcal{I}_N$ and summations over Greek indices are implicitly over $\mathcal{I}_M$. We use also the simplified integral notation

$$\int \tilde{G}_{AB} \equiv \int_{s_1}^{s_2} G(z(\tilde{y}))_{AB} d\tilde{y}, \qquad \int \tilde{m}_N \equiv \int_{s_1}^{s_2} m_N(z(\tilde{y})) d\tilde{y},$$

etc., so that integrals are implicitly over $[s_1, s_2]$, and we denote by $\tilde{F}$ the function F evaluated at $F(z(\tilde{y}))$ for $\tilde{y}$ the variable of integration. In this notation, $\mathfrak{X}$ and $\mathfrak{X}^{(\alpha)}$ are simply

$$\mathfrak{X} = \sum_i \operatorname{Im} \int \tilde{G}_{ii}, \qquad \mathfrak{X}^{(\alpha)} = \sum_i \operatorname{Im} \int \tilde{G}_{ii}^{(\alpha)}.$$

We introduce the fundamental small parameter

$$\Psi = N^{-1/3+3\varepsilon}. \tag{3.31}$$

We will eventually bound all quantities in the computation by powers of Ψ. In fact, as shown in Lemmas 3.26 and 3.27 below, non-integrated resolvent entries are controlled by powers of the smaller quantity

$$N^{-1/3+\varepsilon}.$$

However, integrated quantities will require the additional slack of $N^{2\varepsilon}$. We will pass to using Ψ for all bounds after this distinction is no longer needed.

We have the following corollaries of Proposition 3.13 and Theorem 3.16:

Lemma 3.26. Under the assumptions of Lemma 3.25, for all $y \in [s_1, s_2]$, $i \neq j \in \mathcal{I}_N$, and $\alpha \neq \beta \in \mathcal{I}_M$,

$$G_{ii} \prec 1, \qquad \frac{1}{G_{ii}} \prec 1, \qquad \frac{G_{\alpha\alpha}}{t_\alpha} \prec 1, \qquad \frac{t_\alpha}{G_{\alpha\alpha}} \prec 1,$$

$$G_{ij} \prec N^{-1/3+\varepsilon}, \qquad \frac{G_{i\alpha}}{t_\alpha} \prec N^{-1/3+\varepsilon}, \qquad \frac{G_{\alpha\beta}}{t_\alpha t_\beta} \prec N^{-1/3+\varepsilon}, \qquad m_N - m_* \prec N^{-1/3+\varepsilon}.$$

When T is not invertible, these quantities are defined by continuity and the form (3.17) for G.

Proof. Proposition 3.13 implies $\operatorname{Im} m_0(z(y)) \leq C\sqrt{\kappa+\eta} \leq CN^{-1/3+\varepsilon/2}$, while $\eta \geq N^{-2/3-\varepsilon}$ by assumption. Then Theorem 3.16 yields $(t_A t_B)^{-1}(G-\Pi)_{AB} \prec N^{-1/3+\varepsilon}$ for all $A, B \in \mathcal{I}$. Proposition 3.13 also implies $|m_0(z)| \asymp 1$ and $|1+t_\alpha m_0(z)| \asymp 1$, from which all of the entrywise bounds on G follow. The bound on m_N follows from $|m_0 - m_*| \leq C\sqrt{\kappa+\eta} \leq CN^{-1/3+\varepsilon/2}$ and $|m_N - m_0| \prec N^{-1/3+\varepsilon}$. □

Lemma 3.27. Under the assumptions of Lemma 3.25, for all $i \in \mathcal{I}_N$ and $\alpha \in \mathcal{I}_M$,

$$\sum_k G_{ik}^{(\alpha)} X_{\alpha k} \prec N^{-1/3+\varepsilon}, \qquad \sum_{p,q} G_{pq}^{(\alpha)} X_{\alpha p} X_{\alpha q} - m_* \prec N^{-1/3+\varepsilon}.$$

Proof. Applying Lemmas 3.15(b) and 3.26,

$$\sum_k G_{ik}^{(\alpha)} X_{\alpha k} = -G_{i\alpha}/G_{\alpha\alpha} \prec N^{-1/3+\varepsilon}.$$

Similarly, applying Lemma 3.15(a) and Theorem 3.16,

$$\sum_{p,q} G_{pq}^{(\alpha)} X_{\alpha p} X_{\alpha q} - m_* = -\frac{1}{G_{\alpha\alpha}} - \frac{1}{t_\alpha} - m_* = \frac{1}{\Pi_{\alpha\alpha}} - \frac{1}{G_{\alpha\alpha}} + (m_0 - m_*) \prec N^{-1/3+\varepsilon}.$$

(These types of bounds are in fact used in the proof of Theorem 3.16 and may also be derived directly from concentration inequalities and the independence of $X_{\alpha k}$ and $G^{(\alpha)}$.) □

Remark 3.28. All probabilistic bounds used in the proof of Lemma 3.35, such as the above, are derived from Theorem 3.16. Thus they in fact hold in the union bound form of Corollary 3.17. We continue to use the notation $\prec$ for convenience, with the implicit understanding that we may take a union bound over all $y \in [s_1, s_2]$, and in particular integrate such bounds over y.

We record one trivial bound for an integral that will be repeatedly used, and which explains the appearance of Ψ.

Lemma 3.29. Suppose the assumptions of Lemma 3.25 hold, $F(z(y)) \prec N^{a(-1/3+\varepsilon)}$ for some $a \geq 2$, and we may take a union bound of this statement over $y \in [s_1, s_2]$ (in the sense of Lemma 3.10). Then, with $\Psi = N^{-1/3+3\varepsilon}$,

$$N \int \tilde{F} \prec \Psi^{a-1}.$$

Proof. This follows, for $a \geq 2$, from

$$N(s_2 - s_1)N^{a(-1/3+\varepsilon)} \leq 2N^{1/3+\varepsilon}N^{a(-1/3+\varepsilon)} \leq 2\Psi^{a-1}.$$

□

The next lemma will allow us to "remove the superscript" in the computation.

Lemma 3.30. Under the assumptions of Lemma 3.25, for any $y \in [s_1, s_2]$, $i, j \in \mathcal{I}_N$ (possibly equal), and $\alpha \in \mathcal{I}_M$,

$$G_{ij} - G_{ij}^{(\alpha)} \prec N^{2(-1/3+\varepsilon)},$$

$$m_N - m_N^{(\alpha)} \prec N^{2(-1/3+\varepsilon)},$$

$$\mathfrak{X} - \mathfrak{X}^{(\alpha)} \prec \Psi.$$

Proof. Applying the last resolvent identity from Lemma 3.15,

$$G_{ij} - G_{ij}^{(\alpha)} = \frac{G_{i\alpha}G_{j\alpha}}{G_{\alpha\alpha}} = G_{i\alpha}\frac{G_{j\alpha}}{t_\alpha}\frac{t_\alpha}{G_{\alpha\alpha}},$$

so the first statement follows from Lemma 3.26. Taking $i = j$ and averaging over $\mathcal{I}_N$ yields the second statement. The third statement follows from

$$\mathfrak{X} - \mathfrak{X}^{(\alpha)} = \operatorname{Im}\left(N \int \tilde{m}_N - \tilde{m}_N^{(\alpha)}\right)$$

and Lemma 3.29. □

3.4.2 Resolvent bounds for a swappable pair

We now record bounds for a swappable pair (T, E_*) and $(\check{T}, \check{E}_*)$, where $E_*, \check{E}_*$ are both regular. We denote by $\check{m}_N, \check{G}, \check{\mathfrak{X}}$ the analogues of $m_N, G, \mathfrak{X}$ for $\check{T}$. For $\varepsilon, s_1, s_2, \eta$ and $y \in [s_1, s_2]$ as in Section

3.4.1, we write as shorthand

$$\check{z} \equiv \check{z}(y) = y + \check{E}_* + i\eta, \qquad \check{G} \equiv \check{G}(\check{z}(y)), \qquad \check{m}_N \equiv \check{m}_N(\check{z}(y)),$$

where these quantities depend implicitly on y. The results of the preceding section hold equally for $\check{G}$, $\check{m}_N$, and $\check{\mathfrak{X}}$.

The desired bound (3.29) arises from the following identity: Suppose first that T and $\check{T}$ are invertible. Applying $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$,

$$G - \check{G} = G \begin{pmatrix} (-\check{z} + z)\,\mathrm{Id} & 0 \\ 0 & -\check{T}^{-1} + T^{-1} \end{pmatrix} \check{G}.$$

Hence, as $z - \check{z} = E_* - \check{E}_*$,

$$G_{ij} - \check{G}_{ij} = \sum_k G_{ik}\check{G}_{jk}(E_* - \check{E}_*) - \sum_\alpha \frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{j\alpha}}{\check{t}_\alpha}(t_\alpha - \check{t}_\alpha). \tag{3.32}$$

This holds also by continuity when T is not invertible, where $G_{i\alpha}/t_\alpha$ and $\check{G}_{j\alpha}/\check{t}_\alpha$ are well-defined by (3.17).

The following lemma will allow us to "remove the check" in the computation.

Lemma 3.31. Suppose the assumptions of Lemma 3.25 hold. Let $\Psi = N^{-1/3+3\varepsilon}$. Then for any $y \in [s_1, s_2]$, $i, j \in \mathcal{I}_N$ (possibly equal), and $\alpha \in \mathcal{I}_M$,

$$G_{ij} - \check{G}_{ij} \prec N^{2(-1/3+\varepsilon)},$$

$$m_N - \check{m}_N \prec N^{2(-1/3+\varepsilon)},$$

$$\mathfrak{X} - \check{\mathfrak{X}} \prec \Psi.$$

Proof. Applying Lemma 3.26 for both G and $\check{G}$, and also the definition of swappability and Lemma 3.20, we have from (3.32)

$$G_{ij} - \check{G}_{ij} \prec |E_* - \check{E}_*| \cdot N \cdot N^{2(-1/3+\varepsilon)} + \sum_\alpha |t_\alpha - \check{t}_\alpha| N^{2(-1/3+\varepsilon)} \prec N^{2(-1/3+\varepsilon)}.$$

(The contribution from $k = i$ or $k = j$ in the first sum of (3.32) is of lower order.) Taking $i = j$ and averaging over $\mathcal{I}_N$ yields the second statement, and integrating over $y \in [s_1, s_2]$ and applying Lemma 3.29 yields the third. □

In many cases, we may strengthen the above lemma by an additional factor of Ψ if we take an expectation. (This type of idea is an important part of the argument in [EYY12, LS16]. For example, setting $a = 0$ and $Y \equiv Y^{(\alpha)} \equiv 1$ in Lemma 3.33 below yields the second-order bound

$\mathbb{E}[\mathfrak{X}-\check{\mathfrak{X}}] \prec \Psi^2$.) To take expectations of remainder terms, we will invoke Lemma 3.9 combined with the following basic bound:

Lemma 3.32. Under the assumptions of Lemma 3.25, let $P \equiv P(z(y))$ be any polynomial in the entries of X and G with bounded degree, bounded (possibly random) coefficients, and at most N^C terms for a constant $C > 0$. Then for a constant $C' > 0$ and all $y \in [s_1, s_2]$,

$$\mathbb{E}[|P|] \leq N^{C'}.$$

Proof. By the triangle inequality and Holder's inequality, it suffices to consider a bounded power of a single entry of G or X. Then the result follows from Lemma 3.14 and the form (3.17) for G. □

Lemma 3.33. Under the assumptions of Lemma 3.25, let Y be any quantity such that $Y \prec \Psi^a$ for some constant $a \geq 0$. Suppose that for each $\alpha \in \mathcal{I}_M$, there exists a quantity $Y^{(\alpha)}$ such that $Y - Y^{(\alpha)} \prec \Psi^{a+1}$, and $Y^{(\alpha)}$ is independent of row α of X. Suppose furthermore that $\mathbb{E}[|Y|^\ell] \leq N^{C_\ell}$ for each integer $\ell > 0$ and some constants $C_1, C_2, \ldots > 0$.

Then, for all $i, j \in \mathcal{I}_N$ (possibly equal) and $y \in [s_1, s_2]$,

$$\mathbb{E}[(G_{ij} - \check{G}_{ij})Y] \prec N^{2(-1/3+\varepsilon)}\Psi^{a+1} \prec \Psi^{a+3},$$

$$\mathbb{E}[(m_N - \check{m}_N)Y] \prec N^{2(-1/3+\varepsilon)}\Psi^{a+1} \prec \Psi^{a+3}.$$

$$\mathbb{E}[(\mathfrak{X} - \check{\mathfrak{X}})Y] \prec \Psi^{a+2}.$$

Proof. Applying (3.28), the trivial bound $N^{-1} \prec \Psi^3$, and Lemma 3.26 to (3.32),

$$\begin{aligned}(G_{ij} - \check{G}_{ij})Y &= \sum_k G_{ik}\check{G}_{jk}(E_* - \check{E}_*)Y - \sum_\alpha \frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{j\alpha}}{\check{t}_\alpha}(t_\alpha - \check{t}_\alpha)Y \\ &= \sum_\alpha (t_\alpha - \check{t}_\alpha)\left(s_\alpha\check{s}_\alpha \frac{1}{N}\sum_k G_{ik}\check{G}_{jk} - \frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{j\alpha}}{\check{t}_\alpha}\right)Y + O_\prec(\Psi^{a+5}).\end{aligned}$$

By swappability and Lemma 3.26, the explicit term on the right is of size $O_\prec(N^{2(-1/3+\varepsilon)}\Psi^a)$. (The contributions from $k = i$ and $k = j$ in the summation are of lower order.) Applying the assumption $Y - Y^{(\alpha)} \prec \Psi^{a+1}$ as well as Lemma 3.30, we may replace Y with $Y^{(\alpha)}$, G_{ik} with $G_{ik}^{(\alpha)}$, and $\check{G}_{jk}$ with $\check{G}_{jk}^{(\alpha)}$ above while introducing an $O_\prec(N^{2(-1/3+\varepsilon)}\Psi^{a+1})$ error. Hence,

$$(G_{ij} - \check{G}_{ij})Y = \sum_\alpha (t_\alpha - \check{t}_\alpha)\left(s_\alpha\check{s}_\alpha \frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{jk}^{(\alpha)} - \frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{j\alpha}}{\check{t}_\alpha}\right)Y^{(\alpha)} + O_\prec(N^{2(-1/3+\varepsilon)}\Psi^{a+1}). \tag{3.33}$$

Applying the resolvent identities from Lemma 3.15,

$$\frac{G_{i\alpha}}{t_\alpha} = \frac{G_{\alpha\alpha}}{t_\alpha}\sum_k G_{ik}^{(\alpha)} X_{\alpha k} = -\frac{1}{1+t_\alpha \sum_{p,q} G_{pq}^{(\alpha)} X_{\alpha p} X_{\alpha q}} \sum_k G_{ik}^{(\alpha)} X_{\alpha k}.$$

Recalling $s_\alpha = (1+t_\alpha m_*)^{-1}$, and applying Lemma 3.27 and a Taylor expansion of $(1+t_\alpha x)^{-1}$ around $x = m_*$,

$$\frac{G_{i\alpha}}{t_\alpha} = -s_\alpha \sum_k G_{ik}^{(\alpha)} X_{\alpha k} + O_\prec(N^{2(-1/3+\varepsilon)}),$$

where the explicit term on the right is of size $O_\prec(N^{-1/3+\varepsilon}) \prec \Psi$. A similar expansion holds for $\check{G}_{j\alpha}/\check{t}_\alpha$. Substituting into (3.33),

$$\begin{aligned}(G_{ij} - \check{G}_{ij})Y = &\sum_\alpha (t_\alpha - \check{t}_\alpha) s_\alpha \check{s}_\alpha \left(\frac{1}{N}\sum_k G_{ik}^{(\alpha)} \check{G}_{jk}^{(\alpha)} - \sum_{k,l} G_{ik}^{(\alpha)} X_{\alpha k} \check{G}_{jl}^{(\alpha)} X_{\alpha l} \right) Y^{(\alpha)} \\ &+ O_\prec(N^{2(-1/3+\varepsilon)}\Psi^{a+1}).\end{aligned}$$

Denoting by $\mathbb{E}_\alpha$ the partial expectation over only row α of X (i.e. conditional on $X_{\beta j}$ for all $\beta \neq \alpha$), we have

$$\mathbb{E}_\alpha \left[\frac{1}{N}\sum_k G_{ik}^{(\alpha)} \check{G}_{jk}^{(\alpha)} - \sum_{k,l} G_{ik}^{(\alpha)} X_{\alpha k} \check{G}_{jl}^{(\alpha)} X_{\alpha l} \right] = 0,$$

while the remainder term remains $O_\prec(N^{2(-1/3+\varepsilon)}\Psi^{a+1})$ by Lemma 3.9, where the moment condition of Lemma 3.9 is verified by Lemma 3.32, the moment assumption on Y, and Cauchy-Schwarz. Then the first statement follows. The second statement follows from applying this with $i = j$ and averaging over $i \in \mathcal{I}_N$. The third statement follows from integrating over $y \in [s_1, s_2]$ and noting $N^{1/3+\varepsilon} N^{2(-1/3+\varepsilon)} = \Psi$ as in Lemma 3.29. (If Y depends on the spectral parameter $z(y)$, this integration is performed by fixing this parameter for Y, evaluating m_N and $\check{m}_N$ at a different parameter $\tilde{y}$, and integrating over $\tilde{y}$. The preceding arguments do not require Y and $m_N, \check{m}_N$ to depend on the same spectral parameter.) $\square$

Finally, recall the notation $s_\alpha = (1+t_\alpha m_*)^{-1}$ and $A_i = N^{-1}\sum_\alpha t_\alpha^i s_\alpha^i$. (This corresponds to $A_{i,0}$ in Lemma 3.20.) We derive a deterministic consequence of swappability and the scaling condition $\gamma = \check{\gamma} = 1$. In the proof of [LS16] for a continuous interpolation $T^{(l)}$, denoting $\dot{t}_\alpha$ and $\dot{m}_*$ the derivatives with respect to l, the differential analogue of the following lemma is the pair of identities

$$\sum_\alpha \dot{t}_\alpha t_\alpha s_\alpha^3 = N\dot{m}_*, \qquad \sum_\alpha \dot{t}_\alpha t_\alpha^2 s_\alpha^4 = N\dot{m}_*(A_4 - m_*^{-4}).$$

These may be derived by implicitly differentiating $0 = z_0'(m_*)$ and $1 = z_0''(m_*)$ with respect to l. We show that discrete versions of these identities continue to hold, with $O(N^{-1})$ error:

Lemma 3.34. Suppose $T, \check{T}$ satisfy Assumption 3.1, $E_*, \check{E}_*$ are associated regular right edges with scales $\gamma = \check{\gamma} = 1$, and (T, E_*) and $(\check{T}, \check{E}_*)$ are swappable. Define $s_\alpha = (1 + t_\alpha m_*)^{-1}$, $\check{s}_\alpha = (1 + \check{t}_\alpha \check{m}_*)^{-1}$, $A_4 = N^{-1} \sum_\alpha t_\alpha^4 s_\alpha^4$, and

$$\mathcal{P}_\alpha = s_\alpha \check{s}_\alpha (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha), \qquad \mathcal{Q}_\alpha = s_\alpha \check{s}_\alpha (t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2 \check{s}_\alpha^2).$$

Then for some constant $C > 0$, both of the following hold:

$$\left| 2N(m_* - \check{m}_*) - \sum_{\alpha=1}^{M} (t_\alpha - \check{t}_\alpha) \mathcal{P}_\alpha \right| \leq C/N \tag{3.34}$$

$$\left| 3N(m_* - \check{m}_*)(A_4 - m_*^{-4}) - \sum_{\alpha=1}^{M} (t_\alpha - \check{t}_\alpha) \mathcal{Q}_\alpha \right| \leq C/N. \tag{3.35}$$

Proof. For (3.34), we have from the identity $0 = z_0'(m_*)$ applied to T and $\check{T}$

$$m_*^{-2} - \check{m}_*^{-2} = \frac{1}{N} \sum_\alpha t_\alpha^2 s_\alpha^2 - \check{t}_\alpha^2 \check{s}_\alpha^2. \tag{3.36}$$

The left side may be written as

$$m_*^{-2} - \check{m}_*^{-2} = (\check{m}_* - m_*)(\check{m}_* + m_*) m_*^{-2} \check{m}_*^{-2} = 2(\check{m}_* - m_*) m_*^{-3} + O(N^{-2}), \tag{3.37}$$

where the second equality applies $|m_*|, |\check{m}_*| \asymp 1$ and $|\check{m}_* - m_*| \leq C/N$. The right side may be written as

$$\frac{1}{N} \sum_\alpha t_\alpha^2 s_\alpha^2 - \check{t}_\alpha^2 \check{s}_\alpha^2 = \frac{1}{N} \sum_\alpha (t_\alpha - \check{t}_\alpha) t_\alpha s_\alpha^2 + (s_\alpha^2 - \check{s}_\alpha^2) t_\alpha \check{t}_\alpha + (t_\alpha - \check{t}_\alpha) \check{t}_\alpha \check{s}_\alpha^2.$$

Including the identities $(1 + t_\alpha m_*) s_\alpha = 1$ and $(1 + \check{t}_\alpha \check{m}_*) \check{s}_\alpha = 1$,

$$\begin{aligned} \frac{1}{N} \sum_\alpha t_\alpha^2 s_\alpha^2 - \check{t}_\alpha^2 \check{s}_\alpha^2 &= \frac{1}{N} \sum_\alpha (t_\alpha - \check{t}_\alpha)(t_\alpha s_\alpha^2 (1 + \check{t}_\alpha \check{m}_*) \check{s}_\alpha + \check{t}_\alpha \check{s}_\alpha^2 (1 + t_\alpha m_*) s_\alpha) + (s_\alpha^2 - \check{s}_\alpha^2) t_\alpha \check{t}_\alpha \\ &= \frac{1}{N} \sum_\alpha (t_\alpha - \check{t}_\alpha) s_\alpha \check{s}_\alpha (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha + t_\alpha s_\alpha \check{t}_\alpha \check{m}_* + \check{t}_\alpha \check{s}_\alpha t_\alpha m_*) + (s_\alpha^2 - \check{s}_\alpha^2) t_\alpha \check{t}_\alpha \\ &\equiv \frac{1}{N} \sum_\alpha (t_\alpha - \check{t}_\alpha) s_\alpha \check{s}_\alpha (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha) + R_\alpha, \end{aligned} \tag{3.38}$$

where we define R_α as the remainder term. Noting that

$$s_\alpha^2 - \check{s}_\alpha^2 = (s_\alpha - \check{s}_\alpha)(s_\alpha + \check{s}_\alpha) = (\check{t}_\alpha \check{m}_* - t_\alpha m_*) s_\alpha \check{s}_\alpha (s_\alpha + \check{s}_\alpha),$$

we have

$$\begin{aligned}R_\alpha &= t_\alpha \check{t}_\alpha s_\alpha \check{s}_\alpha (t_\alpha s_\alpha \check{m}_* + t_\alpha \check{s}_\alpha m_* - \check{t}_\alpha s_\alpha \check{m}_* - \check{t}_\alpha \check{s}_\alpha m_* + \check{t}_\alpha s_\alpha \check{m}_* + \check{t}_\alpha \check{s}_\alpha \check{m}_* - t_\alpha s_\alpha m_* - t_\alpha \check{s}_\alpha m_*)\\ &= t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha (\check{m}_* - m_*)(t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha).\end{aligned}$$

Then, applying Lemma 3.20(a),

$$\frac{1}{N}\sum_\alpha R_\alpha = (\check{m}_* - m_*)(A_{2,1} + A_{1,2}) = 2(\check{m}_* - m_*)A_{3,0} + O(N^{-2}).$$

By the scaling $\gamma = 1$, we have $A_{3,0} = 1 + m_*^{-3}$. Combining this with (3.36), (3.37), and (3.38) and multiplying by N yields (3.34).

The identity (3.35) follows similarly: The condition $\gamma = \check{\gamma}$ implies

$$m_*^{-3} - \check{m}_*^{-3} = \frac{1}{N}\sum_\alpha t_\alpha^3 s_\alpha^3 - \check{t}_\alpha^3 \check{s}_\alpha^3.$$

The left side is

$$(\check{m}_* - m_*)(m_*^2 + m_*\check{m}_* + \check{m}_*^2)m_*^{-3}\check{m}_*^{-3} = 3(\check{m}_* - m_*)m_*^{-4} + O(N^{-2}),$$

while the right side is

$$\begin{aligned}\frac{1}{N}\sum_\alpha t_\alpha^3 s_\alpha^3 - \check{t}_\alpha^3 \check{s}_\alpha^3 &= \frac{1}{N}\sum_\alpha (t_\alpha - \check{t}_\alpha) t_\alpha^2 s_\alpha^3 + (s_\alpha^2 - \check{s}_\alpha^2) t_\alpha^2 s_\alpha \check{t}_\alpha + (t_\alpha - \check{t}_\alpha) t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha^2\\ &\qquad + (s_\alpha - \check{s}_\alpha) t_\alpha \check{t}_\alpha^2 \check{s}_\alpha^2 + (t_\alpha - \check{t}_\alpha)\check{t}_\alpha^2 \check{s}_\alpha^3\\ &= \frac{1}{N}\sum_\alpha (t_\alpha - \check{t}_\alpha)\Big(t_\alpha^2 s_\alpha^3 (1 + \check{t}_\alpha \check{m}_*)\check{s}_\alpha + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha^2 (1 + t_\alpha m_*) s_\alpha\\ &\qquad + \check{t}_\alpha^2 \check{s}_\alpha^3 (1 + t_\alpha m_*) s_\alpha\Big) + (s_\alpha - \check{s}_\alpha)((s_\alpha + \check{s}_\alpha) t_\alpha^2 s_\alpha \check{t}_\alpha + t_\alpha \check{t}_\alpha^2 \check{s}_\alpha^2)\\ &= \frac{1}{N}\sum_\alpha (t_\alpha - \check{t}_\alpha) s_\alpha \check{s}_\alpha (t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2 \check{s}_\alpha^2)\\ &\qquad + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha (\check{m}_* - m_*)(t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2 \check{s}_\alpha^2)\\ &= \left(\frac{1}{N}\sum_\alpha (t_\alpha - \check{t}_\alpha)\mathcal{Q}_\alpha\right) + 3(\check{m}_* - m_*)A_4 + O(N^{-2}).\end{aligned}$$

Combining the above and multiplying by N yields (3.35). $\square$

3.4.3 Proof of resolvent comparison lemma

We use the notation of Sections 3.4.1 and 3.4.2. Define the following quantities, depending implicitly on a fixed index $i \in \mathcal{I}_N$ and $y \in [s_1, s_2]$:

$$
\begin{aligned}
\mathfrak{X}_{3,12'} &= K'(\mathfrak{X})(m_N - m_*)\frac{1}{N}\sum_k G_{ik}^2 \\
\mathfrak{X}_{3,3} &= K'(\mathfrak{X})\frac{1}{N^2}\sum_{k,l} G_{ik}G_{kl}G_{il} \\
\mathfrak{X}_{3,2\tilde{2}} &= K''(\mathfrak{X})\frac{1}{N^2}\sum_{j,k,l} G_{ik}G_{il}\operatorname{Im}\int \tilde{G}_{jk}\tilde{G}_{jl} \\
\mathfrak{X}_{3,2'\tilde{2}'} &= K''(\mathfrak{X})\frac{1}{N^2}\sum_{j,k,l} G_{ik}^2\operatorname{Im}\int \tilde{G}_{jl}^2 \\
\mathfrak{X}_{4,22'} &= K'(\mathfrak{X})(m_N - m_*)^2\frac{1}{N}\sum_k G_{ik}^2 \\
\mathfrak{X}_{4,13} &= K'(\mathfrak{X})(m_N - m_*)\frac{1}{N^2}\sum_{k,l} G_{ik}G_{kl}G_{il} \\
\mathfrak{X}_{4,4} &= K'(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,l} G_{ij}G_{jk}G_{kl}G_{il} \\
\mathfrak{X}_{4,4'} &= K'(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,l} G_{ik}^2G_{jl}^2 \\
\mathfrak{X}_{4,12\tilde{2}} &= K''(\mathfrak{X})(m_N - m_*)\frac{1}{N^2}\sum_{j,k,l} G_{ik}G_{il}\operatorname{Im}\int \tilde{G}_{jk}\tilde{G}_{jl} \\
\mathfrak{X}_{4,12'\tilde{2}'} &= K''(\mathfrak{X})(m_N - m_*)\frac{1}{N^2}\sum_{j,k,l} G_{ik}^2\operatorname{Im}\int \tilde{G}_{jl}^2 \\
\mathfrak{X}_{4,3\tilde{2}} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{ip}G_{iq}G_{pr}\operatorname{Im}\int \tilde{G}_{jq}\tilde{G}_{jr} \\
\mathfrak{X}_{4,3'\tilde{2}} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{ir}^2G_{pq}\operatorname{Im}\int \tilde{G}_{jp}\tilde{G}_{jq} \\
\mathfrak{X}_{4,3\tilde{2}'} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{iq}G_{ir}G_{qr}\operatorname{Im}\int \tilde{G}_{jp}^2 \\
\mathfrak{X}_{4,2\widetilde{12}} &= K''(\mathfrak{X})\frac{1}{N^2}\sum_{j,k,l} G_{ik}G_{il}\operatorname{Im}\int (\tilde{m}_N - m_*)\tilde{G}_{jk}\tilde{G}_{jl} \\
\mathfrak{X}_{4,2'\widetilde{12}'} &= K''(\mathfrak{X})\frac{1}{N^2}\sum_{j,k,l} G_{il}^2\operatorname{Im}\int (\tilde{m}_N - m_*)\tilde{G}_{jk}^2 \\
\mathfrak{X}_{4,2\tilde{3}} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{ip}G_{iq}\operatorname{Im}\int \tilde{G}_{jp}\tilde{G}_{jr}\tilde{G}_{qr}
\end{aligned}
$$

$$
\begin{aligned}
\mathfrak{X}_{4,2\widetilde{3}'} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{ip}G_{iq}\operatorname{Im}\int \tilde{G}_{jr}^2\tilde{G}_{pq}\\
\mathfrak{X}_{4,2'\widetilde{3}} &= K''(\mathfrak{X})\frac{1}{N^3}\sum_{j,p,q,r} G_{ip}^2\operatorname{Im}\int \tilde{G}_{jq}\tilde{G}_{jr}\tilde{G}_{qr}\\
\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}} &= K'''(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,p,q,r} G_{ip}G_{iq}\left(\operatorname{Im}\int \tilde{G}_{jp}\tilde{G}_{jr}\right)\left(\operatorname{Im}\int \tilde{G}_{kq}\tilde{G}_{kr}\right)\\
\mathfrak{X}_{4,2'\widetilde{2}\widetilde{2}} &= K'''(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,p,q,r} G_{ip}^2\left(\operatorname{Im}\int \tilde{G}_{jq}\tilde{G}_{jr}\right)\left(\operatorname{Im}\int \tilde{G}_{kq}\tilde{G}_{kr}\right)\\
\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}'} &= K'''(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,p,q,r} G_{ip}G_{iq}\left(\operatorname{Im}\int \tilde{G}_{jp}\tilde{G}_{jq}\right)\left(\operatorname{Im}\int \tilde{G}_{kr}^2\right)\\
\mathfrak{X}_{4,2'\widetilde{2}'\widetilde{2}'} &= K'''(\mathfrak{X})\frac{1}{N^3}\sum_{j,k,p,q,r} G_{ip}^2\left(\operatorname{Im}\int \tilde{G}_{jq}^2\right)\left(\operatorname{Im}\int \tilde{G}_{kr}^2\right)
\end{aligned}
$$

Define the aggregate quantities

$$
\begin{aligned}
\mathfrak{X}_3 &= \mathfrak{X}_{3,12}+\mathfrak{X}_{3,3}+\mathfrak{X}_{3,2\widetilde{2}}\\
\mathfrak{X}_4 &= 3\mathfrak{X}_{4,22'}+6\mathfrak{X}_{4,13}+12\mathfrak{X}_{4,4}+3\mathfrak{X}_{4,4'}+4\mathfrak{X}_{4,12\widetilde{2}}+8\mathfrak{X}_{4,3\widetilde{2}}+4\mathfrak{X}_{4,3'\widetilde{2}}\\
&\qquad +2\mathfrak{X}_{4,2\widetilde{12}}+2\mathfrak{X}_{4,2\widetilde{3}'}+4\mathfrak{X}_{4,2\widetilde{3}}+4\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}},\\
\mathfrak{X}_4^- &= \mathfrak{X}_{4,2\widetilde{12}}+\mathfrak{X}_{4,2\widetilde{3}'}+2\mathfrak{X}_{4,2\widetilde{3}}-\mathfrak{X}_{4,12\widetilde{2}}-\mathfrak{X}_{4,3'\widetilde{2}}-2\mathfrak{X}_{4,3\widetilde{2}}.
\end{aligned}
$$

(Not all of the above terms appear in these aggregate quantities; we define them because they appear in intermediate steps of the proof.) The notation signifies that each term $\mathfrak{X}_{3,*}$ is of size at most $O_\prec(\Psi^3)$, and each term $\mathfrak{X}_{4,*}$ is of size at most $O_\prec(\Psi^4)$, as may be verified from Lemmas 3.26 and 3.29. A $\sim$ in the subscript denotes an integrated quantity, and a $'$ in the subscript denotes a squared resolvent entry.

Lemma 3.25 is a consequence of the following two technical results.

Lemma 3.35 (Decoupling)**.** Under the assumptions of Lemma 3.25, denote $\mathfrak{X}_\lambda = \lambda\mathfrak{X} + (1-\lambda)\check{\mathfrak{X}}$ for $\lambda \in [0,1]$. For fixed $i \in \mathcal{I}_N$ and $y \in [s_1, s_2]$, define $\mathfrak{X}_3$, $\mathfrak{X}_4$, and $\mathfrak{X}_4^-$ as above. For fixed $\alpha \in \mathcal{I}_M$, let $s_\alpha = (1 + t_\alpha m_*)$ and $\check{s}_\alpha = (1 + \check{t}_\alpha \check{m}_*)$, and define

$$
\mathcal{P}_\alpha = s_\alpha\check{s}_\alpha(t_\alpha s_\alpha + \check{t}_\alpha\check{s}_\alpha),\quad \mathcal{Q}_\alpha = s_\alpha\check{s}_\alpha(t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha\check{t}_\alpha\check{s}_\alpha + \check{t}_\alpha^2\check{s}_\alpha^2),\quad \mathcal{R}_\alpha = s_\alpha\check{s}_\alpha(t_\alpha s_\alpha - \check{t}_\alpha\check{s}_\alpha)^2.
$$

Then

$$
\begin{aligned}
\int_0^1 \mathbb{E}\left[K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}\right] d\lambda &= s_\alpha\check{s}_\alpha\int_0^1 \mathbb{E}\left[K'(\mathfrak{X}_\lambda)\frac{1}{N}\sum_k G_{ik}\check{G}_{ik}\right] d\lambda\\
&\quad - \mathcal{P}_\alpha\mathbb{E}[\mathfrak{X}_3] + \tfrac{1}{3}\mathcal{Q}_\alpha\mathbb{E}[\mathfrak{X}_4] + \tfrac{1}{3}\mathcal{R}_\alpha\mathbb{E}[\mathfrak{X}_4^-] + O_\prec(\Psi^5).
\end{aligned}
$$

Lemma 3.36 (Optical theorems)**.** Under the assumptions of Lemma 3.25, for fixed $i \in \mathcal{I}_N$ and $y \in [s_1, s_2]$, define $\mathfrak{X}_3$ and $\mathfrak{X}_4$ as above. Let $A_4 = N^{-1}\sum_\alpha t_\alpha^4 s_\alpha^4$. Then

$$2\,\mathrm{Im}\,\mathbb{E}[\mathfrak{X}_3] = (A_4 - m_*^{-4})\,\mathrm{Im}\,\mathbb{E}[\mathfrak{X}_4] + O_\prec(\Psi^5).$$

Lemma 3.35 generalizes [LS16, Lemma 6.2] to a swappable pair. We will present its proof in Section 3.4.4, following similar ideas. We introduce the interpolation $\mathfrak{X}_\lambda = \lambda\mathfrak{X} + (1-\lambda)\check{\mathfrak{X}}$ as a device to bound $K(\mathfrak{X}) - K(\check{\mathfrak{X}})$. (This is different from a continuous interpolation between the entries of T and $\check{T}$.) Let us make several additional remarks:

1. The proof in [LS16] requires this lemma in "differential form", where $T = \check{T}$. In this case, we have $G = \check{G}$, $\mathfrak{X}_\lambda = \mathfrak{X}$ for every $\lambda \in [0,1]$, $s_\alpha = \check{s}_\alpha$, and $t_\alpha = \check{t}_\alpha$. Then the integral over λ is irrelevant, and Lemma 3.35 reduces to the full version of [LS16, Lemma 6.2].

2. There is an additional term $\mathfrak{X}_4^-$ that does not appear in [LS16], and which is not canceled by the optical theorems of Lemma 3.36. (When $T = \check{T}$, we have $\mathcal{R}_\alpha = 0$ so this term is not present.) The cancellation will instead occur by symmetry of its definition, upon integrating over y.

3. The main additional complexity in our proof comes from needing to separately track the terms that arise from resolvent expansions of G and $\check{G}$, and from $\mathfrak{X}$ and $\check{\mathfrak{X}}$ after Taylor expanding $K'(\mathfrak{X}_\lambda)$. An important simplification is that we may use Lemmas 3.31 and 3.33 to convert $O_\prec(\Psi^3)$ and $O_\prec(\Psi^4)$ terms to involve only G and not $\check{G}$—hence $\mathfrak{X}_3, \mathfrak{X}_4, \mathfrak{X}_4^-$ are defined only by T and not $\check{T}$. Swappability of (T, E_*) and $(\check{T}, \check{E}_*)$ is used for this simplification.

The other technical ingredient, Lemma 3.36, is identical to the full version of [LS16, Lemma B.1], as the terms $\mathfrak{X}_3$ and $\mathfrak{X}_4$ depend only on the single matrix T. We briefly discuss the breakdown of its proof in Section 3.4.5.

In [LS16], for expositional clarity, these lemmas were stated and proven only in the special case $K' \equiv 1$. Full proofs were presented for an analogous deformed Wigner model in [LS15]. Although more cumbersome, we will demonstrate the full proof of Lemma 3.35 for a general function K in Section 3.4.4, as much of the additional complexity due to two resolvents G and $\check{G}$ arises from the interpolation $\mathfrak{X}_\lambda$ and the Taylor expansion of K'.

We conclude this section by establishing Lemma 3.25 using the above two results:

Proof of Lemma 3.25. We write

$$K(\mathfrak{X}) - K(\check{\mathfrak{X}}) = \int_0^1 \frac{d}{d\lambda} K(\mathfrak{X}_\lambda) d\lambda = \int_0^1 K'(\mathfrak{X}_\lambda)(\mathfrak{X} - \check{\mathfrak{X}}) d\lambda. \tag{3.39}$$

Recalling

$$\mathfrak{X} = \sum_i \mathrm{Im} \int \tilde{G}_{ii}$$

and applying (3.32),

$$\mathfrak{X} - \check{\mathfrak{X}} = \sum_i \operatorname{Im} \int \left(\sum_k \tilde{G}_{ik} \tilde{\check{G}}_{ik} (E_* - \check{E}_*) - \sum_\alpha \frac{\tilde{G}_{i\alpha}}{t_\alpha} \frac{\tilde{\check{G}}_{i\alpha}}{\check{t}_\alpha} (t_\alpha - \check{t}_\alpha) \right).$$

($\tilde{G}$ and $\tilde{\check{G}}$ denote G and $\check{G}$ evaluated at the variable of integration $\tilde{y}$.) Further applying (3.28), Lemma 3.26, and the trivial bound $N^{-2/3+\varepsilon} \prec \Psi^2$,

$$\mathfrak{X} - \check{\mathfrak{X}} = \sum_i \operatorname{Im} \int \sum_\alpha (t_\alpha - \check{t}_\alpha) \left(s_\alpha \check{s}_\alpha \frac{1}{N} \sum_k \tilde{G}_{ik} \tilde{\check{G}}_{ik} - \frac{\tilde{G}_{i\alpha}}{t_\alpha} \frac{\tilde{\check{G}}_{i\alpha}}{\check{t}_\alpha} \right) + O_\prec(\Psi^4).$$

Applying this to (3.39), taking the expectation, exchanging orders of summation and integration, and noting that $K'(\mathfrak{X}_\lambda)$ is real,

$$\begin{aligned} &\mathbb{E}[K(\mathfrak{X}) - K(\check{\mathfrak{X}})] \\ &= \sum_i \sum_\alpha (t_\alpha - \check{t}_\alpha) \operatorname{Im} \int \int_0^1 \mathbb{E} \left[K'(\mathfrak{X}_\lambda) \left(s_\alpha \check{s}_\alpha \frac{1}{N} \sum_k \tilde{G}_{ik} \tilde{\check{G}}_{ik} - \frac{\tilde{G}_{i\alpha}}{t_\alpha} \frac{\tilde{\check{G}}_{i\alpha}}{\check{t}_\alpha} \right) \right] d\lambda \, d\tilde{y} + O_\prec(\Psi^4), \end{aligned}$$

where the expectation of the remainder term is still $O_\prec(\Psi^4)$ by Lemmas 3.9 and 3.32. Denoting by $\tilde{\mathfrak{X}}_3(i)$, $\tilde{\mathfrak{X}}_4(i)$, and $\tilde{\mathfrak{X}}_4^-(i)$ the quantities $\mathfrak{X}_3$, $\mathfrak{X}_4$, and $\mathfrak{X}_4^-$ defined by $\tilde{y}$ and the outer index of summation i, Lemma 3.35 implies

$$\mathbb{E}[K(\mathfrak{X}) - K(\check{\mathfrak{X}})] = \sum_i \sum_\alpha (t_\alpha - \check{t}_\alpha) \operatorname{Im} \int (\mathcal{P}_\alpha \mathbb{E}[\tilde{\mathfrak{X}}_3(i)] - \tfrac{1}{3} \mathcal{Q}_\alpha \mathbb{E}[\tilde{\mathfrak{X}}_4(i)] - \tfrac{1}{3} \mathcal{R}_\alpha \mathbb{E}[\check{\mathfrak{X}}_4^-(i)]) d\tilde{y} + O_\prec(N^{1/3+\varepsilon} \Psi^5),$$

where the error is $N^{1/3+\varepsilon}\Psi^5$ because $\sum_\alpha |t_\alpha - \check{t}_\alpha| \leq C$ and the range of integration is contained in $[-N^{-2/3+\varepsilon}, N^{-2/3+\varepsilon}]$. We note

$$\operatorname{Im} \int \tilde{\mathfrak{X}}_4^-(i) d\tilde{y} = 0$$

by symmetry of the terms defining $\tilde{\mathfrak{X}}_4^-$, so this term vanishes. Then, applying Lemma 3.36,

$$\mathbb{E}[K(\mathfrak{X}) - K(\check{\mathfrak{X}})] = \sum_i \sum_\alpha (t_\alpha - \check{t}_\alpha) \left(\mathcal{P}_\alpha \frac{A_4 - m_*^{-4}}{2} - \frac{\mathcal{Q}_\alpha}{3} \right) \operatorname{Im} \int \mathbb{E}[\tilde{\mathfrak{X}}_4(i)] d\tilde{y} + O_\prec(N^{1/3+\varepsilon} \Psi^5).$$

Finally, applying Lemma 3.34, we have

$$\sum_\alpha (t_\alpha - \check{t}_\alpha) \left(\mathcal{P}_\alpha \frac{A_4 - m_*^{-4}}{2} - \frac{\mathcal{Q}_\alpha}{3} \right) \leq C/N.$$

Hence $\mathbb{E}[K(\mathfrak{X}) - K(\check{\mathfrak{X}})] \prec N^{1/3+\varepsilon} \Psi^5 = N^{-4/3+16\varepsilon}$. □

3.4.4 Proof of decoupling lemma

In this section, we prove Lemma 3.35. We will implicitly use the resolvent bounds of Lemma 3.26 throughout the proof.

Step 1: Consider first a fixed value $\lambda \in [0,1]$. Let $\mathbb{E}_\alpha$ denote the partial expectation over row α of X (i.e. conditional on all $X_{\beta j}$ for $\beta \neq \alpha$). In anticipation of computing $\mathbb{E}_\alpha$ for the quantity on the left, we expand

$$K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}$$

as a polynomial of entries of row α of X, with coefficients independent of all entries in this row.

Applying the resolvent identities,

$$\frac{G_{i\alpha}}{t_\alpha} = \frac{G_{\alpha\alpha}}{t_\alpha}\sum_k G_{ik}^{(\alpha)}X_{\alpha k} = -\frac{1}{1+t_\alpha\sum_{p,q}G_{pq}^{(\alpha)}X_{\alpha p}X_{\alpha q}}\sum_k G_{ik}^{(\alpha)}X_{\alpha k}.$$

Applying Lemma 3.27 and a Taylor expansion of the function $(1+t_\alpha x)^{-1}$ around $x = m_*$,

$$\begin{aligned}\frac{G_{i\alpha}}{t_\alpha} &= -s_\alpha\sum_k G_{ik}^{(\alpha)}X_{\alpha k} + t_\alpha s_\alpha^2\left(\sum_{p,q}G_{pq}^{(\alpha)}X_{\alpha p}X_{\alpha q} - m_*\right)\sum_k G_{ik}^{(\alpha)}X_{\alpha k}\\ &\quad - t_\alpha^2 s_\alpha^3\left(\sum_{p,q}G_{pq}^{(\alpha)}X_{\alpha p}X_{\alpha q} - m_*\right)^2\sum_k G_{ik}^{(\alpha)}X_{\alpha k} + O_\prec(\Psi^4)\\ &\equiv U_1 + U_2 + U_3 + O_\prec(\Psi^4),\end{aligned} \tag{3.40}$$

where we defined the three explicit terms of sizes $O_\prec(\Psi), O_\prec(\Psi^2), O_\prec(\Psi^3)$ as U_1, U_2, U_3. Similarly

$$\frac{\check{G}_{i\alpha}}{\check{t}_\alpha} = \check{U}_1 + \check{U}_2 + \check{U}_3 + O_\prec(\Psi^4), \tag{3.41}$$

where $\check{U}_i$ are defined analogously with $\check{s}_\alpha, \check{t}_\alpha, \check{m}_*, \check{G}$ in place of $s_\alpha, t_\alpha, m_*, G$.

For $K'(\mathfrak{X}_\lambda)$, define $\mathfrak{X}_\lambda^{(\alpha)} = \lambda\mathfrak{X}^{(\alpha)} + (1-\lambda)\check{\mathfrak{X}}^{(\alpha)}$ and note from Lemma 3.30 that $\mathfrak{X}_\lambda - \mathfrak{X}_\lambda^{(\alpha)} \prec \Psi$. Taylor expanding $K'(x)$ around $x = \mathfrak{X}_\lambda^{(\alpha)}$,

$$K'(\mathfrak{X}_\lambda) = K'(\mathfrak{X}_\lambda^{(\alpha)}) + K''(\mathfrak{X}_\lambda^{(\alpha)})(\mathfrak{X}_\lambda - \mathfrak{X}_\lambda^{(\alpha)}) + \frac{K'''(\mathfrak{X}_\lambda^{(\alpha)})}{2}(\mathfrak{X}_\lambda - \mathfrak{X}_\lambda^{(\alpha)})^2 + O_\prec(\Psi^3). \tag{3.42}$$

Applying the definition of $\mathfrak{X}, \mathfrak{X}^{(\alpha)}$ and the resolvent identities,

$$\mathfrak{X} - \mathfrak{X}^{(\alpha)} = \operatorname{Im}\int\sum_j(\tilde{G}_{jj} - \tilde{G}_{jj}^{(\alpha)}) = \operatorname{Im}\int\sum_j\frac{\tilde{G}_{j\alpha}^2}{\tilde{G}_{\alpha\alpha}} = \operatorname{Im}\int\tilde{G}_{\alpha\alpha}\sum_{j,p,q}\tilde{G}_{jp}^{(\alpha)}X_{\alpha p}\tilde{G}_{jq}^{(\alpha)}X_{\alpha q}.$$

Further applying the resolvent identity for $\tilde{G}_{\alpha\alpha}$, a Taylor expansion as above, and Lemma 3.29,

$$\begin{aligned}\mathfrak{X} - \mathfrak{X}^{(\alpha)} &= -t_\alpha s_\alpha \operatorname{Im} \int \sum_{j,p,q} \tilde{G}^{(\alpha)}_{jp} X_{\alpha p} \tilde{G}^{(\alpha)}_{jq} X_{\alpha q} \\ &\quad + t_\alpha^2 s_\alpha^2 \operatorname{Im} \int \sum_{r,s} \left(\tilde{G}^{(\alpha)}_{rs} X_{\alpha r} X_{\alpha s} - m_* \right) \sum_{j,p,q} \tilde{G}^{(\alpha)}_{jp} X_{\alpha p} \tilde{G}^{(\alpha)}_{jq} X_{\alpha q} + O_\prec(\Psi^3) \\ &\equiv V_1 + V_2 + O_\prec(\Psi^3),\end{aligned} \tag{3.43}$$

where $V_1 \prec \Psi$ and $V_2 \prec \Psi^2$. Analogously we may write

$$\check{\mathfrak{X}} - \check{\mathfrak{X}}^{(\alpha)} = \check{V}_1 + \check{V}_2 + O_\prec(\Psi^3), \tag{3.44}$$

where $\check{V}_1, \check{V}_2$ are defined with $\check{s}_\alpha, \check{t}_\alpha, \check{m}_*, \check{G}$ in place of $s_\alpha, t_\alpha, m_*, G$. Substituting (3.43) and (3.44) into (3.42), and combining with (3.40) and (3.41), we obtain

$$K'(\mathfrak{X}_\lambda) \frac{G_{i\alpha}}{t_\alpha} \frac{\check{G}_{i\alpha}}{\check{t}_\alpha} = W_2 + W_3 + W_4 + O_\prec(\Psi^5) \tag{3.45}$$

where the $O_\prec(\Psi^2)$ term is

$$W_2 = K'(\mathfrak{X}^{(\alpha)}_\lambda) U_1 \check{U}_1,$$

the $O_\prec(\Psi^3)$ term is

$$W_3 = K'(\mathfrak{X}^{(\alpha)}_\lambda)(U_2 \check{U}_1 + U_1 \check{U}_2) + K''(\mathfrak{X}^{(\alpha)}_\lambda)(\lambda V_1 + (1-\lambda)\check{V}_1) U_1 \check{U}_1,$$

and the $O_\prec(\Psi^4)$ term is

$$\begin{aligned}W_4 &= K'(\mathfrak{X}^{(\alpha)}_\lambda)(U_3 \check{U}_1 + U_2 \check{U}_2 + U_1 \check{U}_3) + K''(\mathfrak{X}^{(\alpha)}_\lambda)(\lambda V_1 + (1-\lambda)\check{V}_1)(U_2 \check{U}_1 + U_1 \check{U}_2) \\ &\quad + \left[K''(\mathfrak{X}^{(\alpha)}_\lambda)(\lambda V_2 + (1-\lambda)\check{V}_2) + \frac{K'''(\mathfrak{X}^{(\alpha)}_\lambda)}{2} (\lambda V_1 + (1-\lambda)\check{V}_1)^2 \right] U_1 \check{U}_1.\end{aligned}$$

Step 2: We compute $\mathbb{E}_\alpha$ of W_2, W_3, W_4 above. Note that $\mathfrak{X}^{(\alpha)}, \check{\mathfrak{X}}^{(\alpha)}, G^{(\alpha)}, \check{G}^{(\alpha)}$ are independent of row α of X. Then for W_2, we have

$$\begin{aligned}\mathbb{E}_\alpha[W_2] &= s_\alpha \check{s}_\alpha K'(\mathfrak{X}^{(\alpha)}_\lambda) \sum_{k,l} G^{(\alpha)}_{ik} \check{G}^{(\alpha)}_{il} \mathbb{E}_\alpha[X_{\alpha k} X_{\alpha l}] \\ &= s_\alpha \check{s}_\alpha K'(\mathfrak{X}^{(\alpha)}_\lambda) \frac{1}{N} \sum_k G^{(\alpha)}_{ik} \check{G}^{(\alpha)}_{ik},\end{aligned} \tag{3.46}$$

where we have used $\mathbb{E}[X_{\alpha k} X_{\alpha l}] = 1/N$ if $k = l$ and 0 otherwise.

For W_3, let us introduce

$$\mathfrak{Y}^{(\alpha)}_{3,12'} = K'(\mathfrak{X}^{(\alpha)}_\lambda)(m^{(\alpha)}_N - m_*) \frac{1}{N} \sum_k G^{(\alpha)}_{ik} \check{G}^{(\alpha)}_{ik},$$

$$\begin{aligned}
\mathcal{Z}^{(\alpha)}_{3,12'} &= K'(\mathfrak{X}^{(\alpha)}_\lambda)(\check{m}^{(\alpha)}_N - \check{m}_*)\frac{1}{N}\sum_k G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{ik},\\
\mathfrak{Y}^{(\alpha)}_{3,3} &= K'(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{k,l} G^{(\alpha)}_{ik}G^{(\alpha)}_{kl}\check{G}^{(\alpha)}_{il}\\
\mathcal{Z}^{(\alpha)}_{3,3} &= K'(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{k,l} G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{kl}\check{G}^{(\alpha)}_{il}\\
\mathfrak{Y}^{(\alpha)}_{3,2'\tilde{2}'} &= K''(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{j,k,l} G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{ik}\operatorname{Im}\int (\tilde{G}^{(\alpha)}_{jl})^2\\
\mathcal{Z}^{(\alpha)}_{3,2'\tilde{2}'} &= K''(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{j,k,l} G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{ik}\operatorname{Im}\int (\tilde{\check{G}}^{(\alpha)}_{jl})^2\\
\mathfrak{Y}^{(\alpha)}_{3,2\tilde{2}} &= K''(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{j,k,l} G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{il}\operatorname{Im}\int \tilde{G}^{(\alpha)}_{jk}\tilde{G}^{(\alpha)}_{jl}\\
\mathcal{Z}^{(\alpha)}_{3,2\tilde{2}} &= K''(\mathfrak{X}^{(\alpha)}_\lambda)\frac{1}{N^2}\sum_{j,k,l} G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{il}\operatorname{Im}\int \tilde{\check{G}}^{(\alpha)}_{jk}\tilde{\check{G}}^{(\alpha)}_{jl},
\end{aligned}$$

which are versions of $\mathfrak{X}_{3,*}$ that don't depend on row α of X and with various instances of $m_N, m_*, G, \mathfrak{X}$ replaced by $\check{m}_N, \check{m}_*, \check{G}, \mathfrak{X}_\lambda$. Consider the first term of W_3 and write

$$\begin{aligned}
&\mathbb{E}_\alpha[K'(\mathfrak{X}^{(\alpha)}_\lambda)U_2\check{U}_1]\\
&= \mathbb{E}_\alpha\left[-t_\alpha s_\alpha^2\check{s}_\alpha K'(\mathfrak{X}^{(\alpha)}_\lambda)\left(\sum_{p,q}G^{(\alpha)}_{pq}X_{\alpha p}X_{\alpha q} - m_*\right)\sum_{k,l}G^{(\alpha)}_{ik}X_{\alpha k}\check{G}^{(\alpha)}_{il}X_{\alpha l}\right]\\
&= -t_\alpha s_\alpha^2\check{s}_\alpha K'(\mathfrak{X}^{(\alpha)}_\lambda)\sum_{k,l,p,q}\left(G^{(\alpha)}_{pq}\mathbb{E}_\alpha[X_{\alpha p}X_{\alpha q}X_{\alpha k}X_{\alpha l}] - \frac{1}{N}m_*\mathbb{1}\{p=q\}\mathbb{E}_\alpha[X_{\alpha k}X_{\alpha l}]\right)G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{il}.
\end{aligned}$$

The summand corresponding to (k,l,p,q) is 0 unless each distinct index appears at least twice in (k,l,p,q). Furthermore, the case where all four indices are equal is negligible:

$$\sum_k\left(G^{(\alpha)}_{kk}\mathbb{E}_\alpha[X^4_{\alpha k}] - \frac{1}{N}m_*\mathbb{E}_\alpha[X^2_{\alpha k}]\right)G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{ik} \prec N\cdot N^{-2}\cdot\Psi^2 \prec \Psi^5.$$

(The $k=i$ case of the sum may be bounded separately as $O_\prec(N^{-2})$.) Thus up to $O_\prec(\Psi^5)$, we need only consider summands where each distinct index appears exactly twice. Considering the one case where $k=l$ and the two cases where $k=p$ and $k=q$,

$$\begin{aligned}
\mathbb{E}_\alpha[K'(\mathfrak{X}^{(\alpha)}_\lambda)U_2\check{U}_1] = -t_\alpha s_\alpha^2\check{s}_\alpha K'(\mathfrak{X}^{(\alpha)}_\lambda)\Bigg(&\frac{1}{N^2}\sum_k\sum_p^{(k)}\left(G^{(\alpha)}_{pp} - m_*\right)G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{ik}\\
&+\frac{2}{N^2}\sum_k\sum_l^{(k)}G^{(\alpha)}_{ik}\check{G}^{(\alpha)}_{il}G^{(\alpha)}_{kl}\Bigg) + O_\prec(\Psi^5).
\end{aligned}$$

Re-including $p = k$ and $l = k$ into the double summations introduces an additional $O_\prec(\Psi^5)$ error; hence we obtain for the first term of W_3

$$\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})U_2\check{U}_1] = -t_\alpha s_\alpha^2 \check{s}_\alpha(\mathfrak{Y}_{3,12'}^{(\alpha)} + 2\mathfrak{Y}_{3,3}^{(\alpha)}) + O_\prec(\Psi^5). \tag{3.47}$$

Similar arguments apply for the remaining three terms of W_3. For the terms involving an integral, we may apply Lemma 3.29 and also move $X_{\alpha k}$ outside of the integral and imaginary part because X is real and does not depend on the variable of integration $\tilde{y}$. We obtain

$$\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})U_1\check{U}_2] = -\check{t}_\alpha \check{s}_\alpha^2 s_\alpha(\mathcal{Z}_{3,12'}^{(\alpha)} + 2\mathcal{Z}_{3,3}^{(\alpha)}) + O_\prec(\Psi^5), \tag{3.48}$$

$$\mathbb{E}_\alpha[\lambda K''(\mathfrak{X}_\lambda^{(\alpha)})V_1U_1\check{U}_1] = -\lambda t_\alpha s_\alpha^2 \check{s}_\alpha(\mathfrak{Y}_{3,2'\tilde{2}'}^{(\alpha)} + 2\mathfrak{Y}_{3,2\tilde{2}}^{(\alpha)}) + O_\prec(\Psi^5), \tag{3.49}$$

$$\mathbb{E}_\alpha[(1-\lambda)K''(\mathfrak{X}_\lambda^{(\alpha)})\check{V}_1U_1\check{U}_1] = -(1-\lambda)\check{t}_\alpha \check{s}_\alpha^2 s_\alpha(\mathcal{Z}_{3,2'\tilde{2}'}^{(\alpha)} + 2\mathcal{Z}_{3,2\tilde{2}}^{(\alpha)}) + O_\prec(\Psi^5), \tag{3.50}$$

and $\mathbb{E}_\alpha[W_3]$ is the sum of (3.47–3.50).

For W_4, consider the first term and write

$$\begin{aligned}
\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})U_3\check{U}_1] &= \mathbb{E}_\alpha\left[t_\alpha^2 s_\alpha^3 \check{s}_\alpha K'(\mathfrak{X}_\lambda^{(\alpha)})\left(\sum_{p,q} G_{pq}^{(\alpha)}X_{\alpha p}X_{\alpha q} - m_*\right)^2 \sum_{k,l} G_{ik}^{(\alpha)}X_{\alpha k}\check{G}_{il}^{(\alpha)}X_{\alpha l}\right] \\
&= t_\alpha^2 s_\alpha^3 \check{s}_\alpha K'(\mathfrak{X}_\lambda^{(\alpha)}) \sum_{p,q,r,s,k,l}\Bigg(G_{pq}^{(\alpha)}G_{rs}^{(\alpha)}\mathbb{E}_\alpha[X_{\alpha p}X_{\alpha q}X_{\alpha r}X_{\alpha s}X_{\alpha k}X_{\alpha l}] \\
&\qquad - \frac{1}{N}m_*\mathbb{1}\{p=q\}G_{rs}^{(\alpha)}\mathbb{E}_\alpha[X_{\alpha r}X_{\alpha s}X_{\alpha k}X_{\alpha l}] \\
&\qquad - \frac{1}{N}m_*\mathbb{1}\{r=s\}G_{pq}^{(\alpha)}\mathbb{E}_\alpha[X_{\alpha p}X_{\alpha q}X_{\alpha k}X_{\alpha l}] \\
&\qquad + \frac{1}{N^2}m_*^2\mathbb{1}\{p=q\}\mathbb{1}\{r=s\}\mathbb{E}[X_{\alpha k}X_{\alpha l}]\Bigg)G_{ik}^{(\alpha)}\check{G}_{il}^{(\alpha)}.
\end{aligned}$$

A summand corresponding to (k,l,p,q,r,s) is 0 unless each distinct index in (k,l,p,q,r,s) appears at least twice. Furthermore, as in the computations for W_3 above, all summands for which (k,l,p,q,r,s) do not form three distinct pairs may be omitted and reincluded after taking $\mathbb{E}_\alpha$, introducing an $O_\prec(\Psi^5)$ error. Considering all pairings of these indices,

$$\begin{aligned}
\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})U_3\check{U}_1] &= t_\alpha^2 s_\alpha^3 \check{s}_\alpha K'(\mathfrak{X}_\lambda^{(\alpha)})\Bigg((m_N^{(\alpha)} - m_*)^2\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)} \\
&\qquad + 4(m_N^{(\alpha)} - m_*)\frac{1}{N^2}\sum_{k,l} G_{ik}^{(\alpha)}G_{kl}^{(\alpha)}\check{G}_{il}^{(\alpha)} + 8\frac{1}{N^3}\sum_{j,k,l} G_{ik}^{(\alpha)}G_{jk}^{(\alpha)}G_{jl}^{(\alpha)}\check{G}_{il}^{(\alpha)} \\
&\qquad + 2\frac{1}{N^3}\sum_{j,k,l} G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)}(G_{jl}^{(\alpha)})^2\Bigg) + O_\prec(\Psi^5).
\end{aligned}$$

At this point, let us apply Lemmas 3.30 and 3.31 to remove each superscript (α) above and to convert each $\check{G}$ to G, introducing an $O_\prec(\Psi^5)$ error. (We could not do this naively for W_2 and W_3, because the errors would be $O_\prec(\Psi^3)$ and $O_\prec(\Psi^4)$ respectively.) We may also remove the superscript (α) and convert $\mathfrak{X}_\lambda$ to $\mathfrak{X}$ in $K'(\mathfrak{X}_\lambda^{(\alpha)})$, via the second-derivative bounds

$$K'(\mathfrak{X}_\lambda^{(\alpha)}) - K'(\mathfrak{X}_\lambda) \le \|K''\|_\infty |\mathfrak{X}_\lambda^{(\alpha)} - \mathfrak{X}_\lambda| \prec \Psi.$$

$$K'(\mathfrak{X}_\lambda) - K'(\mathfrak{X}) \le \|K''\|_\infty |\mathfrak{X}_\lambda - \mathfrak{X}| \prec \Psi.$$

We thus obtain

$$\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})U_3\check{U}_1] = t_\alpha^2 s_\alpha^3 \check{s}_\alpha(\mathfrak{X}_{4,22'} + 4\mathfrak{X}_{4,13} + 8\mathfrak{X}_{4,4} + 2\mathfrak{X}_{4,4'}) + O_\prec(\Psi^5).$$

Applying a similar computation to each term of W_4, we obtain

$$\mathbb{E}_\alpha[K'(\mathfrak{X}_\lambda^{(\alpha)})(U_3\check{U}_1 + U_2\check{U}_2 + U_1\check{U}_3)] \tag{3.51}$$

$$= s_\alpha\check{s}_\alpha(t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2\check{s}_\alpha^2)(\mathfrak{X}_{4,22'} + 4\mathfrak{X}_{4,13} + 8\mathfrak{X}_{4,4} + 2\mathfrak{X}_{4,4'}) + O_\prec(\Psi^5), \tag{3.52}$$

$$\begin{aligned}&\mathbb{E}_\alpha[K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1)(U_2\check{U}_1 + U_1\check{U}_2)]\\ &= s_\alpha\check{s}_\alpha(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha\check{s}_\alpha)\times\\ &\qquad (\mathfrak{X}_{4,12'\widetilde{2}'} + 2\mathfrak{X}_{4,12\widetilde{2}} + 2\mathfrak{X}_{4,3\widetilde{2}'} + 2\mathfrak{X}_{4,3'\widetilde{2}} + 8\mathfrak{X}_{4,3\widetilde{2}}) + O_\prec(\Psi^5),\end{aligned} \tag{3.53}$$

$$\begin{aligned}&\mathbb{E}_\alpha[K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_2 + (1-\lambda)\check{V}_2)U_1\check{U}_1]\\ &= s_\alpha\check{s}_\alpha(\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2\check{s}_\alpha^2)(\mathfrak{X}_{4,2'\widetilde{12}'} + 2\mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2'\widetilde{3}} + 2\mathfrak{X}_{4,2\widetilde{3}'} + 8\mathfrak{X}_{4,2\widetilde{3}}) + O_\prec(\Psi^5),\end{aligned} \tag{3.54}$$

$$\begin{aligned}&\mathbb{E}_\alpha\left[\frac{K'''(\mathfrak{X}_\lambda^{(\alpha)})}{2}(\lambda V_1 + (1-\lambda)\check{V}_1)^2 U_1\check{U}_1\right]\\ &= \frac{s_\alpha\check{s}_\alpha}{2}(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)^2(\mathfrak{X}_{4,2'\widetilde{2}'\widetilde{2}'} + 2\mathfrak{X}_{4,2'\widetilde{\widetilde{22}}} + 4\mathfrak{X}_{4,2\widetilde{\widetilde{22}}'} + 8\mathfrak{X}_{4,2\widetilde{\widetilde{22}}}) + O_\prec(\Psi^5),\end{aligned} \tag{3.55}$$

and $\mathbb{E}_\alpha[W_4]$ is the sum of (3.52–3.55).

The $O_\prec(\Psi^5)$ remainder in (3.45) is given by the difference of the left side with W_2, W_3, W_4. As this is an integral over a polynomial of entries of $G^{(\alpha)}$ and X, its partial expectation is still $O_\prec(\Psi^5)$ by Lemmas 3.9 and 3.32.

Summarizing the results of Steps 1 and 2, we collect (3.45), (3.46), (3.47–3.50), and (3.52–3.55):

$$\begin{aligned}&\mathbb{E}_\alpha\left[K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}\right]\\ &= s_\alpha\check{s}_\alpha K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)}\\ &\quad - t_\alpha s_\alpha^2\check{s}_\alpha(\mathfrak{Y}_{3,12'}^{(\alpha)} + 2\mathfrak{Y}_{3,3}^{(\alpha)}) - \check{t}_\alpha\check{s}_\alpha^2 s_\alpha(\mathcal{Z}_{3,12'}^{(\alpha)} + 2\mathcal{Z}_{3,3}^{(\alpha)})\\ &\quad - \lambda t_\alpha s_\alpha^2\check{s}_\alpha(\mathfrak{Y}_{3,2'\widetilde{2}'}^{(\alpha)} + 2\mathfrak{Y}_{3,2\widetilde{2}}^{(\alpha)}) - (1-\lambda)\check{t}_\alpha\check{s}_\alpha^2 s_\alpha(\mathcal{Z}_{3,2'\widetilde{2}'}^{(\alpha)} + 2\mathcal{Z}_{3,2\widetilde{2}}^{(\alpha)})\end{aligned}$$

$$
\begin{aligned}
&+ s_\alpha \check{s}_\alpha (t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2 \check{s}_\alpha^2)(\mathfrak{X}_{4,22'} + 4\mathfrak{X}_{4,13} + 8\mathfrak{X}_{4,4} + 2\mathfrak{X}_{4,4'}) \\
&+ s_\alpha \check{s}_\alpha (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)(\mathfrak{X}_{4,12'\widetilde{2}'} + 2\mathfrak{X}_{4,12\widetilde{2}} + 2\mathfrak{X}_{4,3\widetilde{2}'} + 2\mathfrak{X}_{4,3'\widetilde{2}} + 8\mathfrak{X}_{4,3\widetilde{2}}) \\
&+ s_\alpha \check{s}_\alpha (\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2 \check{s}_\alpha^2)(\mathfrak{X}_{4,2'\widetilde{12}'} + 2\mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2'\widetilde{3}} + 2\mathfrak{X}_{4,2\widetilde{3}'} + 8\mathfrak{X}_{4,2\widetilde{3}}) \\
&+ \frac{s_\alpha \check{s}_\alpha}{2} (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)^2 (\mathfrak{X}_{4,2'\widetilde{2}'\widetilde{2}'} + 2\mathfrak{X}_{4,2'\widetilde{\widetilde{2}2}} + 4\mathfrak{X}_{4,2\widetilde{\widetilde{2}2}'} + 8\mathfrak{X}_{4,2\widetilde{\widetilde{2}2}}) + O_\prec(\Psi^5). \qquad (3.56)
\end{aligned}
$$

Step 3: In (3.56), we consider the first term on the right (of size $O_\prec(\Psi^2)$) and remove the superscripts (α), keeping track of the $O_\prec(\Psi^3)$ and $O_\prec(\Psi^4)$ terms that arise.

Applying the resolvent identities and a Taylor expansion for $G_{\alpha\alpha}$, we write

$$
\begin{aligned}
G_{ik}^{(\alpha)} &= G_{ik} - \frac{G_{i\alpha} G_{k\alpha}}{G_{\alpha\alpha}} \\
&= G_{ik} - G_{\alpha\alpha} \sum_{r,s} G_{ir}^{(\alpha)} X_{\alpha r} G_{ks}^{(\alpha)} X_{\alpha s} \\
&= G_{ik} + t_\alpha s_\alpha \sum_{r,s} G_{ir}^{(\alpha)} X_{\alpha r} G_{ks}^{(\alpha)} X_{\alpha s} - t_\alpha^2 s_\alpha^2 \left(\sum_{p,q} G_{pq}^{(\alpha)} X_{\alpha p} X_{\alpha q} - m_* \right) \sum_{r,s} G_{ir}^{(\alpha)} X_{\alpha r} G_{ks}^{(\alpha)} X_{\alpha s} \\
&\qquad + O_\prec(\Psi^4) \\
&\equiv G_{ik} + R_{2k} + R_{3k} + O_\prec(\Psi^4), \qquad (3.57)
\end{aligned}
$$

where we defined the two remainder terms of sizes $O_\prec(\Psi^2), O_\prec(\Psi^3)$ as R_{2k}, R_{3k}. Similarly we write

$$
\check{G}_{ik}^{(\alpha)} = \check{G}_{ik} + \check{R}_{2k} + \check{R}_{3k} + O_\prec(\Psi^4). \qquad (3.58)
$$

For $K'(\mathfrak{X}_\lambda^{(\alpha)})$, we apply the Taylor expansion (3.42) and recall $V_1, \check{V}_1, V_2, \check{V}_2$ from (3.43,3.44) to obtain

$$
\begin{aligned}
K'(\mathfrak{X}_\lambda^{(\alpha)}) &= K'(\mathfrak{X}_\lambda) - K''(\mathfrak{X}_\lambda^{(\alpha)})(\mathfrak{X}_\lambda - \mathfrak{X}_\lambda^{(\alpha)}) - \frac{K'''(\mathfrak{X}_\lambda^{(\alpha)})}{2}(\mathfrak{X}_\lambda - \mathfrak{X}_\lambda^{(\alpha)})^2 + O_\prec(\Psi^3) \\
&= K'(\mathfrak{X}_\lambda) - K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1) - K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_2 + (1-\lambda)\check{V}_2) \\
&\quad - \frac{K'''(\mathfrak{X}_\lambda^{(\alpha)})}{2}(\lambda V_1 + (1-\lambda)\check{V}_1)^2 + O_\prec(\Psi^3).
\end{aligned} \qquad (3.59)
$$

Taking the product of (3.57), (3.58), and (3.59), applying the identity

$$
xyz = (x - \delta_x)(y - \delta_y)(z - \delta_z) + xy\delta_z + x\delta_y z + \delta_x yz - x\delta_y\delta_z - \delta_x y \delta_z - \delta_x \delta_y z + \delta_x \delta_y \delta_z
$$

(with $x = G_{ik}^{(\alpha)}$, $x - \delta_x = G_{ik}$, and $\delta_x = R_{2k} + R_{3k}$, etc.), and averaging over $k \in \mathcal{I}_N$, we obtain

$$
K'(\mathfrak{X}_\lambda^{(\alpha)}) \frac{1}{N} \sum_k G_{ik}^{(\alpha)} \check{G}_{ik}^{(\alpha)} \equiv S_2 + S_{3,1} + S_{3,2} + S_{4,1} + S_{4,2} + S_{4,3} + S_{4,4} + S_{4,5} + O_\prec(\Psi^5), \qquad (3.60)
$$

where the $O_\prec(\Psi^2)$ term is

$$
S_2 = K'(\mathfrak{X}_\lambda) \frac{1}{N} \sum_k G_{ik} \check{G}_{ik},
$$

the $O_\prec(\Psi^3)$ terms are

$$S_{3,1} = K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{R}_{2k} + K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k R_{2k}\check{G}_{ik}^{(\alpha)},$$
$$S_{3,2} = -K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1)\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)},$$

and the $O_\prec(\Psi^4)$ terms are

$$S_{4,1} = K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{R}_{3k} + K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k R_{3k}\check{G}_{ik}^{(\alpha)},$$
$$S_{4,2} = -K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_2 + (1-\lambda)\check{V}_2)\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)},$$
$$S_{4,3} = -\frac{K'''(\mathfrak{X}_\lambda^{(\alpha)})}{2}(\lambda V_1 + (1-\lambda)\check{V}_1)^2\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)},$$
$$S_{4,4} = -K'(\mathfrak{X}_\lambda^{(\alpha)})\frac{1}{N}\sum_k R_{2k}\check{R}_{2k},$$
$$S_{4,5} = K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1)\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{R}_{2k} + K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1)\frac{1}{N}\sum_k R_{2k}\check{G}_{ik}^{(\alpha)}.$$

Recalling the definition of R_{2k} and applying $\mathbb{E}_\alpha$ to the $O_\prec(\Psi^3)$ terms, we obtain

$$\mathbb{E}_\alpha[S_{3,1}] = t_\alpha s_\alpha \mathfrak{Y}_{3,3}^{(\alpha)} + \check{t}_\alpha \check{s}_\alpha \mathcal{Z}_{3,3}^{(\alpha)},$$
$$\mathbb{E}_\alpha[S_{3,2}] = \lambda t_\alpha s_\alpha \mathfrak{Y}_{3,2'\widetilde{2}'}^{(\alpha)} + (1-\lambda)\check{t}_\alpha \check{s}_\alpha \mathcal{Z}_{3,2'\widetilde{2}'}^{(\alpha)}.$$

Similarly, we apply $\mathbb{E}_\alpha$ to each of the $O_\prec(\Psi^4)$ terms, considering all pairings of the four summation indices as in Step 2. Then applying Lemmas 3.30 and 3.31 to remove superscripts and convert $\check{G}$ to G, we obtain

$$\mathbb{E}_\alpha[S_{4,1}] = -(t_\alpha^2 s_\alpha^2 + \check{t}_\alpha^2 \check{s}_\alpha^2)(\mathfrak{X}_{4,13} + 2\mathfrak{X}_{4,4}) + O_\prec(\Psi^5),$$
$$\mathbb{E}_\alpha[S_{4,2}] = -(\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2 \check{s}_\alpha^2)(\mathfrak{X}_{4,2'\widetilde{12}'} + 2\mathfrak{X}_{4,2'\widetilde{3}}) + O_\prec(\Psi^5),$$
$$\mathbb{E}_\alpha[S_{4,3}] = -\frac{1}{2}(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)^2(\mathfrak{X}_{4,2'\widetilde{2}'\widetilde{2}'} + 2\mathfrak{X}_{4,2'\widetilde{2}\widetilde{2}}) + O_\prec(\Psi^5),$$
$$\mathbb{E}_\alpha[S_{4,4}] = -t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha(\mathfrak{X}_{4,4'} + 2\mathfrak{X}_{4,4}) + O_\prec(\Psi^5),$$
$$\mathbb{E}_\alpha[S_{4,5}] = -(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)(\mathfrak{X}_{4,3\widetilde{2}'} + 2\mathfrak{X}_{4,3\widetilde{2}}) + O_\prec(\Psi^5).$$

Then applying $\mathbb{E}_\alpha$ to (3.60), noting that the remainder is again $O_\prec(\Psi^5)$ by Lemmas 3.9 and 3.32, and substituting into (3.56),

$$
\begin{aligned}
\mathbb{E}_\alpha\left[K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}\right] &= s_\alpha\check{s}_\alpha\mathbb{E}_\alpha\left[K'(\mathfrak{X}_\lambda)\frac{1}{N}\sum_k G_{ik}\check{G}_{ik}\right] - t_\alpha s_\alpha^2\check{s}_\alpha(\mathfrak{Y}_{3,12'}^{(\alpha)} + \mathfrak{Y}_{3,3}^{(\alpha)}) \\
&\quad - \check{t}_\alpha\check{s}_\alpha^2 s_\alpha(\mathcal{Z}_{3,12'}^{(\alpha)} + \mathcal{Z}_{3,3}^{(\alpha)}) - 2\lambda t_\alpha s_\alpha^2\check{s}_\alpha\mathfrak{Y}_{3,2\widetilde{2}}^{(\alpha)} - 2(1-\lambda)\check{t}_\alpha\check{s}_\alpha^2 s_\alpha\mathcal{Z}_{3,2\widetilde{2}}^{(\alpha)} \\
&\quad + s_\alpha\check{s}_\alpha(t_\alpha^2 s_\alpha^2 + \check{t}_\alpha^2\check{s}_\alpha^2)(\mathfrak{X}_{4,22'} + 3\mathfrak{X}_{4,13} + 6\mathfrak{X}_{4,4} + 2\mathfrak{X}_{4,4'}) \\
&\quad + s_\alpha\check{s}_\alpha(t_\alpha s_\alpha\check{t}_\alpha\check{s}_\alpha)(\mathfrak{X}_{4,22'} + 4\mathfrak{X}_{4,13} + 6\mathfrak{X}_{4,4} + \mathfrak{X}_{4,4'}) + s_\alpha\check{s}_\alpha(\lambda t_\alpha s_\alpha \\
&\quad + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha\check{s}_\alpha)(\mathfrak{X}_{4,12'\widetilde{2}'} + 2\mathfrak{X}_{4,12\widetilde{2}} + \mathfrak{X}_{4,3\widetilde{2}'} + 2\mathfrak{X}_{4,3'\widetilde{2}} + 6\mathfrak{X}_{4,3\widetilde{2}}) \\
&\quad + s_\alpha\check{s}_\alpha(\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2\check{s}_\alpha^2)(2\mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2\widetilde{3}'} + 8\mathfrak{X}_{4,2\widetilde{3}}) \\
&\quad + \frac{s_\alpha\check{s}_\alpha}{2}(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)^2(4\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}'} + 8\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}}) + O_\prec(\Psi^5).
\end{aligned}
\tag{3.61}
$$

Step 4: In (3.61), we remove the superscript (α) from $\mathfrak{Y}_{3,*}$ and $\mathcal{Z}_{3,*}$, keeping track of the $O_\prec(\Psi^4)$ errors that arise. For each quantity $\mathfrak{Y}_{3,*}^{(\alpha)}$ or $\mathcal{Z}_{3,*}^{(\alpha)}$, let $\mathfrak{Y}_{3,*}$ or $\mathcal{Z}_{3,*}$ be the analogous quantity with each instance of $m_N^{(\alpha)}, G^{(\alpha)}, \tilde{G}^{(\alpha)}, \mathfrak{X}_\lambda^{(\alpha)}$ replaced by $m_N, G, \tilde{G}, \mathfrak{X}_\lambda$.

For $\mathfrak{Y}_{3,12'}^{(\alpha)}$, recall from (3.57)

$$
G_{ik}^{(\alpha)} = G_{ik} + R_{2k} + O_\prec(\Psi^3),
$$

and from (3.59)

$$
K'(\mathfrak{X}_\lambda^{(\alpha)}) = K'(\mathfrak{X}_\lambda) - K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1) + O_\prec(\Psi^2).
$$

For $m_N^{(\alpha)} - m_*$, we apply the resolvent identities and write

$$
\begin{aligned}
m_N^{(\alpha)} - m_* &= m_N - m_* - \frac{1}{N}\sum_j \frac{G_{j\alpha}^2}{G_{\alpha\alpha}} \\
&= m_N - m_* - G_{\alpha\alpha}\frac{1}{N}\sum_{j,k,l} G_{jk}^{(\alpha)}X_{\alpha k}G_{jl}^{(\alpha)}X_{\alpha l} \\
&= m_N - m_* + t_\alpha s_\alpha\frac{1}{N}\sum_{j,k,l} G_{jk}^{(\alpha)}X_{\alpha k}G_{jl}^{(\alpha)}X_{\alpha l} + O_\prec(\Psi^3) \\
&\equiv m_N - m_* + Q + O_\prec(\Psi^3),
\end{aligned}
$$

where Q is the $O_\prec(\Psi^2)$ term. Multiplying the above and averaging over k yields

$$
\begin{aligned}
\mathfrak{Y}_{3,12'}^{(\alpha)} &= \mathfrak{Y}_{3,12'} + K'(\mathfrak{X}_\lambda^{(\alpha)})(m_N^{(\alpha)} - m_*)\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{R}_{2k} \\
&\quad + K'(\mathfrak{X}_\lambda^{(\alpha)})(m_N^{(\alpha)} - m_*)\frac{1}{N}\sum_k \check{G}_{ik}^{(\alpha)}R_{2k} + K'(\mathfrak{X}_\lambda^{(\alpha)})Q\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)} \\
&\quad - K''(\mathfrak{X}_\lambda^{(\alpha)})(\lambda V_1 + (1-\lambda)\check{V}_1)(m_N^{(\alpha)} - m_*)\frac{1}{N}\sum_k G_{ik}^{(\alpha)}\check{G}_{ik}^{(\alpha)} + O_\prec(\Psi^5),
\end{aligned}
$$

where each term except $\mathfrak{Y}_{3,12'}$ on the right is of size $O_\prec(\Psi^4)$. Taking $\mathbb{E}_\alpha$ and applying Lemmas 3.30 and 3.31 to remove superscripts and checks,

$$\mathfrak{Y}_{3,12'}^{(\alpha)} = \mathbb{E}_\alpha[\mathfrak{Y}_{3,12'}] + (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,13} + t_\alpha s_\alpha \mathfrak{X}_{4,4'} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,12'\widetilde{2}'} + O_\prec(\Psi^5). \quad (3.62)$$

Similar arguments yield

$$\begin{aligned}
\mathcal{Z}_{3,12'}^{(\alpha)} &= \mathbb{E}_\alpha[\mathcal{Z}_{3,12'}] + (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,13} + \check{t}_\alpha \check{s}_\alpha \mathfrak{X}_{4,4'} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,12'\widetilde{2}'} + O_\prec(\Psi^5),\\
\mathfrak{Y}_{3,3}^{(\alpha)} &= \mathbb{E}_\alpha[\mathfrak{Y}_{3,3}] + (2t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,4} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,3\widetilde{2}'} + O_\prec(\Psi^5),\\
\mathcal{Z}_{3,3}^{(\alpha)} &= \mathbb{E}_\alpha[\mathcal{Z}_{3,3}] + (t_\alpha s_\alpha + 2\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,4} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,3\widetilde{2}'} + O_\prec(\Psi^5),\\
\mathfrak{Y}_{3,2\widetilde{2}}^{(\alpha)} &= \mathbb{E}_\alpha[\mathfrak{Y}_{3,2\widetilde{2}}] + (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,3\widetilde{2}} + 2t_\alpha s_\alpha \mathfrak{X}_{4,2\widetilde{3}} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}'} + O_\prec(\Psi^5),\\
\mathcal{Z}_{3,2\widetilde{2}}^{(\alpha)} &= \mathbb{E}_\alpha[\mathcal{Z}_{3,2\widetilde{2}}] + (t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,3\widetilde{2}} + 2\check{t}_\alpha \check{s}_\alpha \mathfrak{X}_{4,2\widetilde{3}} + (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}'} + O_\prec(\Psi^5).
\end{aligned}$$

Substituting into (3.61),

$$\begin{aligned}
\mathbb{E}_\alpha\left[K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}\right] &= s_\alpha \check{s}_\alpha \mathbb{E}_\alpha\left[K'(\mathfrak{X}_\lambda)\frac{1}{N}\sum_k G_{ik}\check{G}_{ik}\right] - t_\alpha s_\alpha^2 \check{s}_\alpha \mathbb{E}_\alpha[\mathfrak{Y}_{3,12'} + \mathfrak{Y}_{3,3}]\\
&\quad - \check{t}_\alpha \check{s}_\alpha^2 s_\alpha \mathbb{E}_\alpha[\mathcal{Z}_{3,12'} + \mathcal{Z}_{3,3}] - 2\lambda t_\alpha s_\alpha^2 \check{s}_\alpha \mathbb{E}_\alpha[\mathfrak{Y}_{3,2\widetilde{2}}] - 2(1-\lambda)\check{t}_\alpha \check{s}_\alpha^2 s_\alpha \mathbb{E}_\alpha[\mathcal{Z}_{3,2\widetilde{2}}]\\
&\quad + s_\alpha \check{s}_\alpha (t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha \check{t}_\alpha \check{s}_\alpha + \check{t}_\alpha^2 \check{s}_\alpha^2)(\mathfrak{X}_{4,22'} + 2\mathfrak{X}_{4,13} + 4\mathfrak{X}_{4,4} + \mathfrak{X}_{4,4'})\\
&\quad + s_\alpha \check{s}_\alpha (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha \check{s}_\alpha)(2\mathfrak{X}_{4,12\widetilde{2}} + 2\mathfrak{X}_{4,3'\widetilde{2}} + 4\mathfrak{X}_{4,3\widetilde{2}})\\
&\quad + s_\alpha \check{s}_\alpha (\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2 \check{s}_\alpha^2)(2\mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2\widetilde{3}'} + 4\mathfrak{X}_{4,2\widetilde{3}})\\
&\quad + 4s_\alpha \check{s}_\alpha (\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha \check{s}_\alpha)^2 \mathfrak{X}_{4,2\widetilde{2}\widetilde{2}} + O_\prec(\Psi^5).
\end{aligned} \quad (3.63)$$

Step 5: We take the full expectation of both sides of (3.63), applying Lemma 3.33 to convert $\mathfrak{Y}_{3,*}$ and $\mathcal{Z}_{3,*}$ into $\mathfrak{X}_{3,*}$. We illustrate the argument for $\mathcal{Z}_{3,12'}$:

For $k \neq i$, denote

$$Y = K'(\mathfrak{X}_\lambda)(\check{m}_N - \check{m}_*)G_{ik}, \qquad Y^{(\alpha)} = K'(\mathfrak{X}_\lambda^{(\alpha)})(\check{m}_N^{(\alpha)} - \check{m}_*)G_{ik}^{(\alpha)}.$$

Then $Y \prec \Psi^2$, and $Y - Y^{(\alpha)} \prec \Psi^3$ for all $\alpha \in \mathcal{I}_M$, the latter from Lemma 3.30 and the second-derivative bound for K. Then applying Lemma 3.33,

$$\mathbb{E}[Y\check{G}_{ik}] = \mathbb{E}[YG_{ik}] + O_\prec(\Psi^5).$$

Hence

$$\mathbb{E}\left[K'(\mathfrak{X}_\lambda)(\check{m}_N - \check{m}_*)\frac{1}{N}\sum_k G_{ik}(\check{G}_{ik} - G_{ik})\right] = O_\prec(\Psi^5), \quad (3.64)$$

where the $k = i$ term is controlled directly by Lemma 3.31. Applying this argument again with $Y = K'(\mathfrak{X}_\lambda)G_{ik}^2$, together with the bound $\check{m}_* - m_* \leq C/N \prec \Psi^3$, we may convert the term

$\check{m}_N - \check{m}_*$:

$$\mathbb{E}\left[K'(\mathfrak{X}_\lambda)(\check{m}_N - \check{m}_* - m_N + m_*)\frac{1}{N}\sum_k G_{ik}^2\right] = O_\prec(\Psi^5). \tag{3.65}$$

Finally, a Taylor expansion of $K'(x)$ around $\mathfrak{X}$ yields

$$K'(\mathfrak{X}_\lambda) = K'(\mathfrak{X}) + (1-\lambda)K''(\mathfrak{X})(\check{\mathfrak{X}} - \mathfrak{X}) + O_\prec(\Psi^2), \tag{3.66}$$

where we have used $\check{\mathfrak{X}} - \mathfrak{X} \prec \Psi$ by Lemma 3.31. Applying the third implication of Lemma 3.33 with $Y = K''(\mathfrak{X})(m_N - m_*)G_{ik}^2 \prec \Psi^3$ for $k \neq i$, we obtain

$$\mathbb{E}\left[K''(\mathfrak{X})(\check{\mathfrak{X}} - \mathfrak{X})(m_N - m_*)\frac{1}{N}\sum_k G_{ik}^2\right] = O_\prec(\Psi^5). \tag{3.67}$$

Then combining (3.64–3.67), we obtain $\mathbb{E}[\mathcal{Z}_{3,12'}] = \mathbb{E}[\mathfrak{X}_{3,12'}] + O_\prec(\Psi^5)$.

The same argument holds for the other terms $\mathfrak{Y}_{3,*}$ and $\mathcal{Z}_{3,*}$. Then taking the full expectation of (3.63),

$$\begin{aligned}
\mathbb{E}\left[K'(\mathfrak{X}_\lambda)\frac{G_{i\alpha}}{t_\alpha}\frac{\check{G}_{i\alpha}}{\check{t}_\alpha}\right] &= s_\alpha\check{s}_\alpha\mathbb{E}\left[K'(\mathfrak{X}_\lambda)\frac{1}{N}\sum_k G_{ik}\check{G}_{ik}\right] - (t_\alpha s_\alpha^2\check{s}_\alpha + \check{t}_\alpha\check{s}_\alpha^2 s_\alpha)\mathbb{E}[\mathfrak{X}_{3,12'} + \mathfrak{X}_{3,3}] \\
&\quad - 2(\lambda t_\alpha s_\alpha^2\check{s}_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha^2 s_\alpha)\mathbb{E}[\mathfrak{X}_{3,2\widetilde{2}}] \\
&\quad + s_\alpha\check{s}_\alpha(t_\alpha^2 s_\alpha^2 + t_\alpha s_\alpha\check{t}_\alpha\check{s}_\alpha + \check{t}_\alpha^2\check{s}_\alpha^2)\mathbb{E}[\mathfrak{X}_{4,22'} + 2\mathfrak{X}_{4,13} + 4\mathfrak{X}_{4,4} + \mathfrak{X}_{4,4'}] \\
&\quad + s_\alpha\check{s}_\alpha(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)(t_\alpha s_\alpha + \check{t}_\alpha\check{s}_\alpha)\mathbb{E}[2\mathfrak{X}_{4,12\widetilde{2}} + 2\mathfrak{X}_{4,3'\widetilde{2}} + 4\mathfrak{X}_{4,3\widetilde{2}}] \\
&\quad + s_\alpha\check{s}_\alpha(\lambda t_\alpha^2 s_\alpha^2 + (1-\lambda)\check{t}_\alpha^2\check{s}_\alpha^2)\mathbb{E}[2\mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2\widetilde{3}'} + 4\mathfrak{X}_{4,2\widetilde{3}}] \\
&\quad + 4s_\alpha\check{s}_\alpha(\lambda t_\alpha s_\alpha + (1-\lambda)\check{t}_\alpha\check{s}_\alpha)^2\mathbb{E}[\mathfrak{X}_{4,2\widetilde{2}\widetilde{2}}] + O_\prec(\Psi^5).
\end{aligned} \tag{3.68}$$

Finally, we integrate (3.68) over $\lambda \in [0,1]$, applying $\int \lambda = \int(1-\lambda) = 1/2$ and $\int \lambda^2 = \int 2\lambda(1-\lambda) = \int(1-\lambda)^2 = 1/3$. Simplifying the result and identifying the terms $\mathfrak{X}_3$, $\mathfrak{X}_4$, $\mathfrak{X}_4^-$, $\mathcal{P}_\alpha$, $\mathcal{Q}_\alpha$, and $\mathcal{R}_\alpha$ concludes the proof of the lemma.

3.4.5 Proof of optical theorems

We discuss briefly the proof of Lemma 3.36. In the setting $K' \equiv 1$, Lemma 3.36 corresponds to [LS16, Lemma B.1] upon taking the imaginary part.

The proof for general K is the same as that of [LS16, Lemma B.1], with additional terms arising from the Taylor expansion of K' as in the proof of Lemma 3.35. The computation may be broken down into the following intermediate identities:

$$\begin{aligned}
&\frac{1}{N}\left(\mathbb{E}[K'(\mathfrak{X})] + 2m_*^{-1}\mathbb{E}[K'(\mathfrak{X})(m_N - m_*)]\right) \\
&\quad = 2\mathbb{E}[\mathfrak{X}_3] - 2m_*^{-1}(z - E_*)\mathbb{E}[\mathfrak{X}_2] - (A_4 - 2m_*^{-1} - m_*^{-4})\mathbb{E}[\mathfrak{X}_4] + O_\prec(\Psi^5),
\end{aligned} \tag{3.69}$$

$$\frac{1}{N}\mathbb{E}[K'(\mathfrak{X})(m_N - m_*)] - 2\mathbb{E}[\mathfrak{X}_{4,22'} + \mathfrak{X}_{4,13} + \mathfrak{X}_{4,4} + \mathfrak{X}_{4,12\widetilde{2}}] = O_{\prec}(\Psi^5), \tag{3.70}$$

$$\mathbb{E}[2\mathfrak{X}_{4,13} + 3\mathfrak{X}_{4,4} + \mathfrak{X}_{4,4'} + 2\mathfrak{X}_{4,3\widetilde{2}}] = O_{\prec}(\Psi^5), \tag{3.71}$$

$$(z - E_*)\mathbb{E}[\mathfrak{X}_2] - \mathbb{E}[\mathfrak{X}_{4,22'} + 4\mathfrak{X}_{4,4} + \mathfrak{X}_{4,4'} + 2\mathfrak{X}_{4,3'\widetilde{2}}] = O_{\prec}(\Psi^5), \tag{3.72}$$

$$\mathbb{E}[\mathfrak{X}_{4,12\widetilde{2}} + 2\mathfrak{X}_{4,3\widetilde{2}} + \mathfrak{X}_{4,3'\widetilde{2}} + \mathfrak{X}_{4,2\widetilde{12}} + 2\mathfrak{X}_{4,2\widetilde{3}} + \mathfrak{X}_{4,2\widetilde{3}'} + 2\mathfrak{X}_{4,2\widetilde{\widetilde{2}}}] = O_{\prec}(\Psi^5), \tag{3.73}$$

where

$$\mathfrak{X}_2 = K'(\mathfrak{X})\frac{1}{N}\sum_k G_{ik}^2.$$

For $K' \equiv 1$, (3.69) reduces to [LS16, (B.29)], (3.70) to [LS16, (B.33)], (3.71) to [LS16, (B.38)], and a linear combination of (3.71) and (3.72) to [LS16, (B.51)]. The last identity (3.73) is trivial for $K' \equiv 1$, as the left side is 0. It is analogous to [LS15, Eq. (C.42)] in the full computation for the deformed Wigner model, and may be derived as an "optical theorem" from $\mathfrak{X}_{3,2\widetilde{2}}$ in the same manner as (3.70) and (3.71). (The derivations of these identities do not require positivity of T or E_*.) We omit further details and refer the reader to [LS16].

Lemma 3.36 follows from substituting (3.70) and (3.72) into (3.69), adding $4m_*^{-1}$ times (3.71) and $4m_*^{-1}$ times (3.73), and taking the imaginary part (noting K' is real-valued). This concludes the proof of Lemma 3.25, and hence of Theorem 2.6.

Chapter 4

Outliers in the spiked model

In this chapter, we prove Theorems 2.12–2.14, which describe the behavior of outlier eigenvalues and eigenvectors of $\widehat{\Sigma}$ under a spiked model for $\Sigma_1, \ldots, \Sigma_k$. We also prove Theorem 2.17, which provides theoretical guarantees for Algorithm 1 for estimating spike eigenvalues and eigenvectors in this setting.

Notation: Throughout, $\delta > 0$ is a fixed constant. $C, c > 0$ denote δ-dependent constants that may change from instance to instance. For random (or deterministic) scalars ξ and ζ, we write

$$\xi \prec \zeta \text{ and } \xi = O_\prec(\zeta)$$

if, for any constants $\varepsilon, D > 0$, we have

$$\mathbb{P}[|\xi| > n^\varepsilon |\zeta|] < n^{-D}$$

for all $n \geq n_0$, where n_0 may depend only on δ, ε, D and the constants of Assumptions 2.1 and 2.10.

4.1 Behavior of outliers

The proofs of Theorems 2.12–2.14 will apply a matrix perturbation approach developed in [Pau07]. Without loss of generality, we may rotate coordinates in $\mathbb{R}^p$ so that $\mathcal{S}$ corresponds to the first L coordinates. Hence for every $r = 1, \ldots, k$,

$$V_r = \begin{pmatrix} \mathring{V}_r \\ 0 \end{pmatrix}$$

where $\mathring{V}_r \in \mathbb{R}^{L\times l_r}$. Recalling $N = p - L$ and assuming momentarily that $\sigma_r^2 > 0$, we may write

$$\Sigma_r = \sigma_r^2 \begin{pmatrix} \Gamma_r & 0 \\ 0 & \mathrm{Id}_N \end{pmatrix}, \qquad \Gamma_r = \mathrm{Id}_L + \sigma_r^{-2} \mathring{V}_r \Theta_r \mathring{V}_r'. \tag{4.1}$$

Letting $\mathring{X}_r \in \mathbb{R}^{m_r\times L}$ and $X_r \in \mathbb{R}^{m_r\times N}$ be independent with i.i.d. $\mathcal{N}(0, 1/N)$ entries, and setting $\Xi_r = \mathring{X}_r \Gamma_r^{1/2}$, we may represent α_r as

$$\alpha_r = \sqrt{N} \begin{pmatrix} \mathring{X}_r & X_r \end{pmatrix} \Sigma_r^{1/2} = \sqrt{N}\sigma_r \begin{pmatrix} \Xi_r & X_r \end{pmatrix}.$$

Recalling $F_{rs} = N\sigma_r\sigma_s U_r' B U_s$ from (2.7), we then have

$$\widehat{\Sigma} = Y'BY = \sum_{r,s=1}^k \alpha_r' U_r' B U_s \alpha_s = \sum_{r,s=1}^k \begin{pmatrix} \Xi_r' \\ X_r' \end{pmatrix} F_{rs} \begin{pmatrix} \Xi_s & X_s \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}, \tag{4.2}$$

where

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} \Xi' F \Xi & \Xi' F X \\ X' F \Xi & X' F X \end{pmatrix}, \qquad \begin{pmatrix} \Xi & X \end{pmatrix} = \begin{pmatrix} \Xi_1 & X_1 \\ \vdots & \vdots \\ \Xi_k & X_k \end{pmatrix}.$$

Note that $\sigma_r^2\Gamma_r$, $\sigma_r\Xi_r$, and $F_{rs}/(\sigma_r\sigma_s)$ are well-defined by continuity even when $\sigma_r^2 = 0$ and/or $\sigma_s^2 = 0$. The above definitions are understood in this sense if $\sigma_r^2 = 0$ for any r.

For any $z \notin \mathrm{spec}(X'FX)$, the Schur complement of the lower-right block of $\widehat{\Sigma} - z\,\mathrm{Id}$ is

$$\widehat{K}(z) = (S_{11} - z\,\mathrm{Id}) - S_{12}(S_{22} - z\,\mathrm{Id})^{-1} S_{21} = -\Xi' G_M(z) \Xi - z\,\mathrm{Id}_L \tag{4.3}$$

where

$$G_M(z) = FXG_N(z)X'F - F, \qquad G_N(z) = (X'FX - z\,\mathrm{Id}_N)^{-1}. \tag{4.4}$$

If $\hat{\lambda}$ is an eigenvalue of $\widehat{\Sigma}$ separated from $\mathrm{supp}(\mu_0)$, then we expect from Theorem 2.5 that $\hat{\lambda} \notin \mathrm{spec}(X'FX)$, so we should have $0 = \det \widehat{K}(\hat{\lambda})$. Defining the complex spectral domain

$$U_\delta = \{z \in \mathbb{C} : \mathrm{dist}(z, \mathrm{supp}(\mu_0)) \geq \delta\},$$

we will show that on U_δ, the matrix $\widehat{K}(z)$ is close to the deterministic approximation

$$K(z) = \sum_{r=1}^k t_r(z)(\sigma_r^2\Gamma_r) - z\,\mathrm{Id}_L\,. \tag{4.5}$$

Recalling (4.1) and comparing (4.5) with (2.12), we observe that $K(z)$ is the upper $L \times L$ submatrix of $-T(z)$. This will yield Theorems 2.12 and 2.13. Studying further the fluctuations of $\widehat{K}(z)$ about

$K(z)$, we will establish Theorem 2.14.

We show in Section 4.3 that $G_M(z)$ and $G_N(z)$ are blocks of a linearized resolvent matrix for $X'FX$. Our proof establishes deterministic approximations for linear and quadratic functions of the entries of $G_M(z)$, which we may state as follows: Recall (2.13), and define a deterministic approximation of G_M as

$$\Pi_M = -F(\mathrm{Id} + m_0 F)^{-1} = m_0 F(\mathrm{Id} + m_0 F)^{-1} F - F.$$

Define

$$\Delta(z) = XG_N(z)X' - m_0(z)(\mathrm{Id} + m_0(z)F)^{-1}. \tag{4.6}$$

Then, omitting the spectral argument z for brevity, we have

$$G_M = \Pi_M + F\Delta F, \qquad t_r = (N\sigma_r^2)^{-1} \operatorname{Tr}_r(-G_M + F\Delta F). \tag{4.7}$$

We prove the following lemmas in Section 4.3.

Lemma 4.1. Fix $\delta, \varepsilon, D > 0$. For any $z \in U_\delta$ and any deterministic matrix $V \in \mathbb{C}^{M\times M}$,

$$\mathbb{P}\Big[|\operatorname{Tr} \Delta V| > n^{-1/2+\varepsilon} \|V\|_{\mathrm{HS}}\Big] < n^{-D}.$$

Lemma 4.2. Fix $\delta, \varepsilon, D > 0$. For any $z \in U_\delta$ and any deterministic matrices $V, W \in \mathbb{C}^{M\times M}$,

$$\mathbb{P}\Big[|\operatorname{Tr} \Delta V \Delta W - N^{-1}(\partial_z m_0) \operatorname{Tr}[V(\mathrm{Id} + m_0 F)^{-2}] \operatorname{Tr}[W(\mathrm{Id} + m_0 F)^{-2}]| > n^{1/2+\varepsilon}\|V\|\,\|W\|\Big] < n^{-D}.$$

We will use Lemma 4.1 to approximate linear functions in $G_M(z)$, and then use Lemma 4.2 to approximate quadratic functions in $G_M(z)$. Note that if $V = \mathbf{w}\mathbf{v}'$ is of rank one, then Lemma 4.1 is an anisotropic local law of the form established in [KY17] for spectral arguments z separated from $\mathrm{supp}(\mu_0)$. For general V, the statement above is stronger than that obtained by expressing V as a sum of rank-one matrices and applying the triangle inequality to the Hilbert-Schmidt norm. We will require this stronger form for the proof of Theorem 2.14.

We record here also the following basic results regarding $\mathrm{supp}(\mu_0)$ and the Stieltjes transform $m_0(z)$ for spectral arguments z separated from this support, which are restatements of Propositions A.3 and A.8 in Appendix A.

Proposition 4.3. Suppose Assumption 2.10 holds, and let μ_0 be the law defined by Theorem 2.4. For a constant $C > 0$, $\mathrm{supp}(\mu_0) \subset [-C, C]$.

Proposition 4.4. Suppose Assumption 2.10 holds, and let $m_0(z)$ be the Stieltjes transform of the law μ_0. Fix any constant $\delta > 0$. Then for some constant $c > 0$, all $z \in U_\delta$, and each eigenvalue t_α

of F,

$$|1 + t_\alpha m_0(z)| > c.$$

4.1.1 First-order behavior

We prove Theorems 2.12 and 2.13. Let us first establish the approximations

$$\sup_{z \in U_\delta} \|\widehat{K}(z) - K(z)\| \prec n^{-1/2}, \tag{4.8}$$

$$\sup_{z \in U_\delta} \|\partial_z \widehat{K}(z) - \partial_z K(z)\| \prec n^{-1/2}. \tag{4.9}$$

Denote by $(G_M)_{rs}$ and $(\Pi_M)_{rs}$ the (r, s) blocks of G_M and Π_M. We record a basic lemma which bounds G_M, Π_M, and the derivatives of K and $\widehat{K}$. Quantities such as $F_{rs}/(\sigma_r\sigma_s)$ are defined by continuity at $\sigma_r^2 = 0$ and/or $\sigma_s^2 = 0$.

Lemma 4.5. There is a constant $C > 0$ such that

(a) For all $z \in U_\delta$ and $r, s = 1, \ldots, k$,

$$\|F_{rs}/(\sigma_r\sigma_s)\|/< C, \qquad \|(\Pi_M)_{rs}/(\sigma_r\sigma_s)\| < C, \qquad \|K(z) + z\,\mathrm{Id}\| < C, \qquad \|\partial_z K(z)\| < C.$$

(b) For any $D > 0$ and all $n \geq n_0(\delta, D)$, with probability at least $1 - n^{-D}$, for all $z \in U_\delta$ and $r, s = 1, \ldots, k$

$$\|(G_M)_{rs}/(\sigma_r\sigma_s)\| < C, \qquad \|\widehat{K}(z) + z\,\mathrm{Id}\| < C, \qquad \|\partial_z \widehat{K}(z)\| < C, \qquad \|\partial_z^2 \widehat{K}(z)\| < C.$$

Proof. For (a), $\|F_{rs}/(\sigma_r\sigma_s)\| < C$ by Assumption 2.1. From Proposition 4.4, we have $\|(\mathrm{Id} + m_0 F)^{-1}\| < C$. Furthermore, $|m_0(z)| \leq 1/\delta$ for $z \in U_\delta$ by (2.11). Then, denoting by P_r the projection onto block r and applying

$$(\Pi_M)_{rs} = m_0 P_r F(\mathrm{Id} + m_0 F)^{-1} F P_s - F_{rs},$$

we obtain

$$\|(\Pi_M)_{rs}/(\sigma_r\sigma_s)\| < C\|P_r F/\sigma_r\|\|F P_s/\sigma_s\| + \|F_{rs}/(\sigma_r\sigma_s)\| < C.$$

This implies also $|t_r(z)| < C$, which together with $\|\sigma_r^2 \Gamma_r\| < C$ yields the bound on K. The bound for $\partial_z K$ follows similarly.

For (b), applying Theorem 2.5 and a standard spectral norm bound for Gaussian matrices, on an event of probability $1 - n^{-D}$ we have $\mathrm{spec}(X'FX) \subset \mathrm{supp}(\mu_0)_{\delta/2}$, $\|X_r\| < C$, and $\|\mathring{X}_r\| < C$ for all $r = 1, \ldots, k$. From the spectral decomposition of G_N, on this event, we have $\|G_N\| < C$,

$\|\partial_z G_N\| < C$, and $\|\partial_z^2 G_N\| < C$ for all $z \in U_\delta$. Then

$$\|(G_M)_{rs}/(\sigma_r\sigma_s)\|,\ \|\partial_z (G_M)_{rs}/(\sigma_r\sigma_s)\|,\ \|\partial_z^2 (G_M)_{rs}/(\sigma_r\sigma_s)\| < C.$$

As $\widehat{K} = -\sum_{r,s} \Xi_r' G_M \Xi_s - z\,\mathrm{Id}$ and $\|\sigma_r \Xi_r\| < C\|\sigma_r^2 \Gamma_r\|^{1/2} < C$, this yields the bounds on $\widehat{K}$ and its derivatives. □

We recall also the following bound for Gaussian quadratic forms.

Lemma 4.6 (Gaussian quadratic forms)**.** Let $\mathbf{x}$ and $\mathbf{y}$ be independent vectors of any dimensions, with i.i.d. $\mathcal{N}(0, 1/N)$ entries. Then for any complex deterministic matrices A and B of the corresponding sizes,

$$\mathbf{x}' A\mathbf{x} - N^{-1} \operatorname{Tr} A \prec N^{-1}\|A\|_{\mathrm{HS}}, \qquad \mathbf{x}' B\mathbf{y} \prec N^{-1}\|B\|_{\mathrm{HS}}.$$

Proof. The first statement follows from the Hanson-Wright inequality, see e.g. [RV13]. The second follows from the first applied to $(\mathbf{x}, \mathbf{y})$, with A a 2×2 block matrix having blocks 0, B, B', 0. □

Applying (4.7), we may write $\widehat{K}(z) - K(z) = E_1(z) + E_2(z)$ where

$$E_1(z) = -\Xi' G_M \Xi + \sum_{r=1}^{k} \Big(N^{-1} \operatorname{Tr}_r G_M\Big)\Gamma_r, \tag{4.10}$$

$$E_2(z) = -\sum_{r=1}^{k} \Big(N^{-1} \operatorname{Tr}_r F\Delta F\Big)\Gamma_r. \tag{4.11}$$

Writing P_r for the projection onto block r, Lemma 4.1 yields

$$(N\sigma_r^2)^{-1} \operatorname{Tr}_r F\Delta F = (N\sigma_r^2)^{-1} \operatorname{Tr} \Delta F P_r F \prec n^{-3/2}\|F P_r F/\sigma_r^2\|_{\mathrm{HS}} \prec n^{-1}. \tag{4.12}$$

Hence $\|E_2(z)\| \prec n^{-1}$. For E_1, we write

$$\Xi' G_M \Xi = \sum_{r,s=1}^{k} \Xi_r' (G_M)_{rs} \Xi_s = \sum_{r,s=1}^{k} (\sigma_r^2 \Gamma_r)^{1/2} \mathring{X}_r' \frac{(G_M)_{rs}}{\sigma_r\sigma_s} \mathring{X}_s (\sigma_s^2 \Gamma_s)^{1/2}.$$

Recall that the matrices $\mathring{X}_r$ are independent of each other and of G_M. Applying Lemma 4.6 conditional on G_M and taking a union bound over the columns of $\mathring{X}_r$ and $\mathring{X}_s$, for all r, s,

$$\left\| \mathring{X}_r' \frac{(G_M)_{rs}}{\sigma_r\sigma_s} \mathring{X}_s - \mathbb{1}\{r = s\}((N\sigma_r^2)^{-1} \operatorname{Tr}_r G_M) \operatorname{Id}_L \right\|_\infty \prec n^{-1}\|(G_M)_{rs}/(\sigma_r\sigma_s)\|_{\mathrm{HS}},$$

where $\|A\|_\infty = \max_{i,j}|A_{ij}|$. As L is at most a constant, this norm is equivalent to the operator norm. By Lemma 4.5, $\|(G_M)_{rs}/(\sigma_r\sigma_s)\|_{\mathrm{HS}} \prec n^{1/2}$, so $\|E_1(z)\| \prec n^{-1/2}$. Then

$$\|\widehat{K}(z) - K(z)\| \prec n^{-1/2}. \tag{4.13}$$

Lipschitz continuity allows us to take a union bound over $z \in U_\delta$: On the event where the conclusions of Lemma 4.5 hold, for any $z, z' \in U_\delta$,

$$\|\widehat{K}(z) - \widehat{K}(z')\| < C|z - z'|, \qquad \|K(z) - K(z')\| < C|z - z'|.$$

Then, taking a union bound of (4.13) over a grid of values in $U_\delta \cap \{|z| \leq n^{1/2}\}$ with spacing $n^{-1/2}$, we obtain

$$\sup_{z \in U_\delta :\, |z| \leq n^{1/2}} \|\widehat{K}(z) - K(z)\| \prec n^{-1/2}. \tag{4.14}$$

For $|z| > n^{1/2}$, we apply a direct argument: By Proposition 4.3 and (2.11), we have $|m_0(z)| < Cn^{-1/2}$. Then $|t_r(z) - (N\sigma_r^2)^{-1} \operatorname{Tr}_r F| < Cn^{-1/2}$. Furthermore, on the high-probability event where $\|X'FX\| < C$ and $\|\mathring{X}_r\| < C$ for each $r = 1, \ldots, k$, we have $\|G_N\| < Cn^{-1/2}$, $\|[(G_M)_{rs} - F_{rs}]/(\sigma_r\sigma_s)\| < Cn^{-1/2}$, and $\|\sigma_r \Xi_r\| < C$. Then, on this event,

$$\sup_{|z| > n^{1/2}} \|\widehat{K}(z) - K(z)\| \leq \left\| \Xi' F \Xi - \sum_{r=1}^{k} (N^{-1} \operatorname{Tr}_r F) \Gamma_r \right\| + Cn^{-1/2}.$$

Applying Lemma 4.6 again yields $\sup_{|z| > n^{1/2}} \|\widehat{K}(z) - K(z)\| \prec n^{-1/2}$. Combining with (4.14) yields (4.8). Note that $D_{ij}(z) \equiv \widehat{K}(z)_{ij} - K(z)_{ij}$ is analytic over $U_{\delta/2}$. Letting γ be the circle around z with radius $\delta/2$, the Cauchy integral formula implies

$$|\partial_z D_{ij}(z)| \leq \frac{1}{2\pi} \int_\gamma \frac{|D_{ij}(w)|}{|z - w|^2} dw \leq \frac{4}{\delta} \max_{w \in \gamma} |D_{ij}(w)|.$$

Then applying (4.8) with $\delta/2$ in place of δ, we obtain also the derivative bound (4.9).

Proof of Theorem 2.12. Let $\mathcal{E}$ be the event where

$$\operatorname{spec}(X'FX) \subset \operatorname{supp}(\mu_0)_{\delta/2},$$

$$\sup_{z \in U_{\delta/2}} \|\widehat{K}(z) - K(z)\| < n^{-1/2 + \varepsilon/2}, \qquad \sup_{z \in U_{\delta/2}} \|\partial_z \widehat{K}(z) - \partial_z K(z)\| < n^{-1/2 + \varepsilon/2},$$

which holds with probability $1 - n^{-D}$ for all $n \geq n_0(\delta, \varepsilon, D)$. On $\mathcal{E}$, by the Schur complement identity

$$\det(\widehat{\Sigma} - \lambda \operatorname{Id}) = \det(X'FX - \lambda \operatorname{Id}) \det(\widehat{K}(\lambda)),$$

the eigenvalues of $\widehat{\Sigma}$ outside $\operatorname{supp}(\mu_0)_{\delta/2}$ are the roots $\hat{\lambda} \in U_{\delta/2} \cap \mathbb{R}$ of $\det(\widehat{K}(\hat{\lambda}))$, counting multiplicity. As $T(z)$ is block diagonal with upper $L \times L$ block equal to $-K(z)$ and lower $N \times N$ block equal to $-m_0(z)^{-1} \operatorname{Id}$, the elements of Λ_0 are the roots $\lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0)$ of $\det(K(\lambda))$, counting multiplicity.

Let $\hat{\mu}_1(\lambda) \leq \ldots \leq \hat{\mu}_L(\lambda)$ be the eigenvalues of $\widehat{K}(\lambda)$, and let $\mu_1(\lambda) \leq \ldots \leq \mu_L(\lambda)$ be those of

$K(\lambda)$. Proposition 2.11 implies that $\partial_\lambda K(\lambda)$ has maximum eigenvalue at most -1, so for any interval I of $\mathbb{R} \setminus \operatorname{supp}(\mu_0)$, any $\lambda, \lambda' \in I$ with $\lambda < \lambda'$, and any $\ell \in \{1, \ldots, L\}$,

$$\mu_\ell(\lambda) - \mu_\ell(\lambda') \geq \lambda' - \lambda.$$

On $\mathcal{E}$, for $\lambda \in I \cap U_{\delta/2}$, we may bound the largest eigenvalue of $\partial_\lambda \widehat{K}(\lambda)$ by $-1/2$. Then similarly

$$\hat{\mu}_\ell(\lambda) - \hat{\mu}_\ell(\lambda') \geq (\lambda' - \lambda)/2.$$

For each (λ, ℓ) with $\lambda \in I \cap U_\delta$ and $\mu_\ell(\lambda) = 0$, we have

$$\mu_\ell(\lambda - n^{-1/2+\varepsilon}) \geq n^{-1/2+\varepsilon}, \qquad \mu_\ell(\lambda + n^{-1/2+\varepsilon}) \leq -n^{-1/2+\varepsilon},$$

and hence on $\mathcal{E}$

$$\hat{\mu}_\ell(\lambda - n^{-1/2+\varepsilon}) > 0, \qquad \hat{\mu}_\ell(\lambda + n^{-1/2+\varepsilon}) < 0.$$

So there is some $\hat{\lambda}$ where $\hat{\mu}_\ell(\hat{\lambda}) = 0$ and $|\hat{\lambda} - \lambda| < n^{-1/2+\varepsilon}$. Conversely, for each $(\hat{\lambda}, \ell)$ with $\hat{\lambda} \in I \cap U_\delta$ and $\hat{\mu}_\ell(\hat{\lambda}) = 0$, there is some λ with $\mu_\ell(\lambda) = 0$ and $|\lambda - \hat{\lambda}| < n^{-1/2+\varepsilon}$. Taking Λ_δ and $\widehat{\Lambda}_\delta$ to be the roots of $\det(K(\lambda))$ and $\det(\widehat{K}(\hat{\lambda}))$ corresponding to these pairs (λ, ℓ) and $(\hat{\lambda}, \ell)$ for each interval I of $\mathbb{R} \setminus \operatorname{supp}(\mu_0)$, we obtain Theorem 2.12. □

Proof of Theorem 2.13. For the given λ and $\hat{\lambda}$, Theorem 2.12 implies $\lambda - \hat{\lambda} \prec n^{-1/2}$. Let us write

$$\widehat{K}(\hat{\lambda}) - K(\lambda) = (\widehat{K}(\hat{\lambda}) - \widehat{K}(\lambda)) + (\widehat{K}(\lambda) - K(\lambda)).$$

The first term on the right has norm $O_\prec(n^{-1/2})$, by the bound on $\partial_\lambda \widehat{K}(\lambda)$ from Lemma 4.5. The second term also has norm $O_\prec(n^{-1/2})$, by (4.8). Hence

$$\|\widehat{K}(\hat{\lambda}) - K(\lambda)\| \prec n^{-1/2}. \tag{4.15}$$

Similarly,

$$\|\partial_\lambda \widehat{K}(\hat{\lambda}) - \partial_\lambda K(\lambda)\| \prec n^{-1/2}. \tag{4.16}$$

For the given $\hat{\mathbf{v}}$, let us write $\hat{\mathbf{v}} = (\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2)$ where $\hat{\mathbf{v}}_1$ consists of the first L coordinates. Then, in the block decomposition of $\widehat{\Sigma}$ from (4.2), the equation $\widehat{\Sigma}\hat{\mathbf{v}} = \hat{\lambda}\hat{\mathbf{v}}$ yields

$$S_{11}\hat{\mathbf{v}}_1 + S_{12}\hat{\mathbf{v}}_2 = \hat{\lambda}\hat{\mathbf{v}}_1, \qquad S_{21}\hat{\mathbf{v}}_1 + S_{22}\hat{\mathbf{v}}_2 = \hat{\lambda}\hat{\mathbf{v}}_2.$$

The second equation yields $\hat{\mathbf{v}}_2 = -(S_{22} - \hat{\lambda}\,\mathrm{Id})^{-1} S_{21}\hat{\mathbf{v}}_1$. Substituting this into the first yields

$\widehat{K}(\hat{\lambda})\hat{\mathbf{v}}_1 = 0$, while substituting it into $1 = \|\hat{\mathbf{v}}\|^2 = \|\hat{\mathbf{v}}_1\|^2 + \|\hat{\mathbf{v}}_2\|^2$ yields

$$1 = \hat{\mathbf{v}}_1'(\mathrm{Id} + S_{12}(S_{22} - \hat{\lambda}\,\mathrm{Id})^{-2}S_{21})\hat{\mathbf{v}}_1 = -\hat{\mathbf{v}}_1'(\partial_\lambda \widehat{K}(\hat{\lambda}))\hat{\mathbf{v}}_1.$$

Applying (4.16), we obtain

$$-\hat{\mathbf{v}}_1'(\partial_\lambda K(\lambda))\hat{\mathbf{v}}_1 = 1 + O_\prec(n^{-1/2}). \tag{4.17}$$

In particular, $\|\hat{\mathbf{v}}_1\| \geq c$ for a constant $c > 0$. Hence $\hat{\mathbf{v}}_1/\|\hat{\mathbf{v}}_1\|$ is a well-defined unit vector in $\ker \widehat{K}(\hat{\lambda})$.

For the given $\mathbf{v}$, let us also write $\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2)$. As $\mathbf{v} \in \mathcal{S}$ by Proposition 2.11, we have $\mathbf{v}_2 = 0$, $\|\mathbf{v}_1\| = 1$, and $\mathbf{v}_1 \in \ker K(\lambda)$. We apply the Davis-Kahan theorem to bound $\|\hat{\mathbf{v}}_1/\|\hat{\mathbf{v}}_1\| - \mathbf{v}_1\|$: Let $\mu_1(\lambda) \leq \ldots \leq \mu_L(\lambda)$ be the eigenvalues of $K(\lambda)$, with $\mu_\ell(\lambda) = 0$. By Proposition 2.11, $\partial_\lambda K(\lambda)$ has maximum eigenvalue at most -1. Thus, if $|\mu_{\ell'}(\lambda)| < \delta$ for another $\ell' \neq \ell$, then $\mu_{\ell'}(\lambda - \delta) > 0$ and $\mu_{\ell'}(\lambda + \delta) < 0$, so $\mu_{\ell'}(\lambda') = 0$ for some $\lambda' \in (\lambda - \delta, \lambda + \delta)$. This contradicts the given condition that λ is separated from other elements of Λ_0 by δ. Hence $|\mu_{\ell'}(\lambda)| \geq \delta$ for all $\ell' \neq \ell$, so the Davis-Kahan Theorem and (4.15) imply

$$\|\hat{\mathbf{v}}_1 - \|\hat{\mathbf{v}}_1\|\mathbf{v}_1\| \prec n^{-1/2} \tag{4.18}$$

for an appropriate choice of sign of $\mathbf{v}_1$. Substituting into (4.17), $-\|\hat{\mathbf{v}}_1\|^2\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1 = 1 + O_\prec(n^{-1/2})$. As $\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1 \leq -1$, this yields

$$\|\hat{\mathbf{v}}_1\| = (-\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1)^{-1/2} + O_\prec(n^{-1/2}).$$

Substituting back into (4.18),

$$\|\hat{\mathbf{v}}_1 - (-\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1)^{-1/2}\mathbf{v}_1\| = \|P_\mathcal{S}\hat{\mathbf{v}} - (\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})^{-1/2}\mathbf{v}\| \prec n^{-1/2},$$

where the equality uses $\mathbf{v} = (\mathbf{v}_1, 0)$, $P_\mathcal{S}\hat{\mathbf{v}} = (\hat{\mathbf{v}}_1, 0)$, and that K is the upper-left block of $-T$. This proves (a).

For (b), note simply that for any $O \in \mathbb{R}^{N \times N}$, the rotation $X \mapsto XO$ induces the mapping $(\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2) \mapsto (\hat{\mathbf{v}}_1, O'\hat{\mathbf{v}}_2)$. As X and $\widehat{\Sigma}$ are invariant in law under such a rotation, $\hat{\mathbf{v}}_2$ must be rotationally invariant in law conditional on $\hat{\mathbf{v}}_1$. $\square$

4.1.2 Fluctuations of outlier eigenvalues

Next, we prove Theorem 2.14. We establish asymptotic normality using the following elementary lemma.

Lemma 4.7. Suppose $\mathbf{z} \in \mathbb{R}^n$ has law $\mathcal{N}(0, VV')$ where $V \in \mathbb{R}^{n \times m}$, and let $A \in \mathbb{R}^{n \times n}$. If $\|V'AV\|/\|V'AV\|_{\mathrm{HS}} \to 0$ as $n \to \infty$, then

$$\|V'AV\|_{\mathrm{HS}}^{-1}(\mathbf{z}'A\mathbf{z} - \mathbb{E}[\mathbf{z}'A\mathbf{z}]) \to \mathcal{N}(0, 2).$$

Proof. Denote the spectral decomposition of $V'AV$ as $O'DO$ where $D = \operatorname{diag}(d_1, \dots, d_m)$, and let $\xi \in \mathbb{R}^m$ have i.i.d. $\mathcal{N}(0,1)$ entries. Then $\mathbf{z}'A\mathbf{z} - \mathbb{E}[\mathbf{z}'A\mathbf{z}]$ is equal in law to

$$\xi' D\xi - \mathbb{E}[\xi' D\xi] = \sum_{i=1}^{m} d_i(\xi_i^2 - 1).$$

As

$$\sum_{i=1}^{m} \mathbb{E}\Big[d_i^2(\xi_i^2-1)^2\Big] = 2\|D\|_{\mathrm{HS}}^2, \qquad \sum_{i=1}^{m} \mathbb{E}\Big[|d_i(\xi_i^2-1)|^3\Big] \le C\|D\|_{\mathrm{HS}}^2 \cdot \|D\|,$$

and $\|D\|/\|D\|_{\mathrm{HS}} \to 0$, the result follows from the Lyapunov central limit theorem. $\square$

Proof of Theorem 2.14. For the given λ and $\mathbf{v}$, we have $\mathbf{v} = (\mathbf{v}_1, 0)$, where $\mathbf{v}_1 \in \mathbb{R}^L$ and $K(\lambda)\mathbf{v}_1 = 0$. Furthermore, recall from the proof of Theorem 2.13 that for the given $\hat{\lambda}$, there is a unit vector $\hat{\mathbf{v}}_1$ where $\widehat{K}(\hat{\lambda})\hat{\mathbf{v}}_1 = 0$ and $\|\hat{\mathbf{v}}_1 - \mathbf{v}_1\| \prec n^{-1/2}$. Lemma 4.5 implies $\|\widehat{K}(\hat{\lambda})\| < C$ with probability $1 - n^{-D}$, so

$$\mathbf{v}_1'\widehat{K}(\hat{\lambda})\mathbf{v}_1 = (\hat{\mathbf{v}}_1 - \mathbf{v}_1)'\widehat{K}(\hat{\lambda})(\hat{\mathbf{v}}_1 - \mathbf{v}_1) \prec n^{-1}.$$

Applying this and $\mathbf{v}_1'K(\lambda)\mathbf{v}_1 = 0$, we obtain

$$\mathbf{v}_1'(\widehat{K}(\hat{\lambda}) - \widehat{K}(\lambda))\mathbf{v}_1 + \mathbf{v}_1'(\widehat{K}(\lambda) - K(\lambda))\mathbf{v}_1 \prec n^{-1}. \tag{4.19}$$

Recall that Theorem 2.12 implies $\lambda - \hat{\lambda} \prec n^{-1/2}$. Applying a second-order Taylor expansion for the first term of (4.19), approximating $\partial_\lambda \widehat{K}(\lambda)$ by $\partial_\lambda K(\lambda)$ using (4.9), and bounding $\partial_\lambda^2 \widehat{K}(\lambda)$ using Lemma 4.5, we get

$$\mathbf{v}_1'(\widehat{K}(\hat{\lambda}) - \widehat{K}(\lambda))\mathbf{v}_1 = (\hat{\lambda} - \lambda)\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1 + O_\prec(n^{-1}). \tag{4.20}$$

For the second term of (4.19), recall $\widehat{K}(\lambda) - K(\lambda) = E_1(\lambda) + E_2(\lambda)$ with E_1 and E_2 as in (4.10–4.11). Recall also from (4.12) that $\|E_2(\lambda)\| \prec n^{-1}$. Then (4.19) becomes

$$(\hat{\lambda} - \lambda)\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1 + \mathbf{v}_1'E_1(\lambda)\mathbf{v}_1 \prec n^{-1}. \tag{4.21}$$

Observe that Ξ is independent of X, and $\mathbf{z} = \Xi\mathbf{v}_1 \in \mathbb{R}^M$ has independent Gaussian entries. The covariance matrix of $\mathbf{z}$ is VV' for the diagonal matrix

$$V = V' = N^{-1/2} \sum_{r=1}^{k} (\mathbf{v}_1'\Gamma_r\mathbf{v}_1)^{1/2} P_r.$$

Then $\mathbf{v}_1'E_1(\lambda)\mathbf{v}_1 = \mathbb{E}[-\mathbf{z}'G_M(\lambda)\mathbf{z} \mid X]$, and we may apply Lemma 4.7 conditional on X: Lemma 4.5 implies, with high probability, $\|(G_M)_{rs}/(\sigma_r\sigma_s)\| < C$ for each r, s, so $\|V'G_M(\lambda)V\| < C/n$. On the other hand, since $\mathbf{v}'T(\lambda)\mathbf{v} = 0$, we have from (2.15) and (2.11)

$$\left|\sum_{r=1}^{k} t_r(\lambda)\mathbf{v}_1'\mathring{V}_r\Theta_r\mathring{V}_r'\mathbf{v}_1\right| = \left|\frac{1}{m_0(\lambda)}\right| \geq \delta.$$

Then for some constant $c > 0$ and some $r \in \{1, \dots, k\}$ we must have

$$|t_r(\lambda)| > c, \qquad |\mathbf{v}_1'\mathring{V}_r\Theta_r\mathring{V}_r'\mathbf{v}_1| > c.$$

The latter implies $\mathbf{v}_1'(\sigma_r^2\Gamma_r)\mathbf{v}_1 > c$. The former implies $(N\sigma_r^2)^{-1}|\mathrm{Tr}_r\, G_M(\lambda)| > c$ on an event of probability $1 - n^{-D}$, by (4.7) and (4.12). Then $\|(G_M)_{rr}/\sigma_r^2\|_{\mathrm{HS}} > c\sqrt{n}$, and for this r

$$\|V'G_M(\lambda)V\|_{\mathrm{HS}} \geq N^{-1}\mathbf{v}_1'(\sigma_r^2\Gamma_r)\mathbf{v}_1\|(G_M)_{rr}/\sigma_r^2\|_{\mathrm{HS}} > cn^{-1/2}. \tag{4.22}$$

Thus, on this high probability event, we have $\|V'G_M(\lambda)V\|/\|V'G_M(\lambda)V\|_{\mathrm{HS}} < Cn^{-1/2}$. Applying Lemma 4.7 conditional on X and this event,

$$\|V'G_M(\lambda)V\|_{\mathrm{HS}}^{-1}(\mathbf{v}_1'E_1(\lambda)\mathbf{v}_1) \to \mathcal{N}(0, 2).$$

As the limit does not depend on X, this convergence holds unconditionally as well. Then, applying this, $\mathbf{v}_1'\partial_\lambda K(\lambda)\mathbf{v}_1 = -\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v}$, and (4.22) to (4.21), we have

$$\frac{(\mathbf{v}'\partial_\lambda T(\lambda)\mathbf{v})}{\sqrt{2}\|V'G_M(\lambda)V\|_{\mathrm{HS}}}(\hat{\lambda} - \lambda) \to \mathcal{N}(0, 1). \tag{4.23}$$

Finally, let us approximate $\|V'G_M(\lambda)V\|_{\mathrm{HS}}$: We have

$$\|V'G_MV\|_{\mathrm{HS}}^2 = \mathrm{Tr}\, G_MVV'G_MVV' = \sum_{r,s=1}^{k} N^{-2}(\mathbf{v}_1'\Gamma_r\mathbf{v}_1)(\mathbf{v}_1'\Gamma_s\mathbf{v}_1)\,\mathrm{Tr}\, G_MP_rG_MP_s.$$

We apply $G_M = \Pi_M + F\Delta F$ from (4.7) and expand the above. Note that Lemma 4.1 implies

$$\frac{\mathrm{Tr}\,\Pi_MP_rF\Delta FP_s}{\sigma_r^2\sigma_s^2} \prec n^{-1/2}\frac{\|FP_s\Pi_MP_rF\|_{\mathrm{HS}}}{\sigma_r^2\sigma_s^2} \prec \|FP_s/\sigma_s\|\cdot\|(\Pi_M)_{sr}/(\sigma_s\sigma_r)\|\cdot\|P_rF/\sigma_r\| \prec 1,$$

so the cross terms of the expansion are negligible, and we have

$$\frac{\mathrm{Tr}\, G_MP_rG_MP_s}{\sigma_r^2\sigma_s^2} = \frac{\mathrm{Tr}\,\Pi_MP_r\Pi_MP_s}{\sigma_r^2\sigma_s^2} + \frac{\mathrm{Tr}\, F\Delta FP_rF\Delta FP_s}{\sigma_r^2\sigma_s^2} + O_\prec(1).$$

The first term on the right may be written as $\mathrm{Tr}(P_s\Pi_MP_r)(P_r\Pi_MP_s)/(\sigma_r^2\sigma_s^2) = \|\Pi_M/(\sigma_r\sigma_s)\|_{rs}^2$.

For the second term, applying Lemma 4.2,

$$\begin{aligned}\frac{\operatorname{Tr}\Delta F P_r F \Delta F P_s F}{\sigma_r^2\sigma_s^2} &= (N\sigma_r^2\sigma_s^2)^{-1}(\partial_\lambda m_0)\operatorname{Tr}_r[F(\operatorname{Id}+m_0F)^{-2}F]\operatorname{Tr}_s[F(\operatorname{Id}+m_0F)^{-2}F]+O_\prec(n^{1/2})\\ &= N(\partial_\lambda t_r)(\partial_\lambda t_s)(\partial_\lambda m_0)^{-1}+O_\prec(n^{1/2}).\end{aligned}$$

Then, recalling w_{rs} from (2.16) and applying $\mathbf{v}_1'(\sigma_r^2\Gamma_r)\mathbf{v}_1=\mathbf{v}'\Sigma_r\mathbf{v}$ by (4.1), we obtain

$$\begin{aligned}\|V'G_MV\|_{\mathrm{HS}}^2 &= N^{-1}\sum_{r,s=1}^k w_{rs}(\lambda)(\mathbf{v}'\Sigma_r\mathbf{v})(\mathbf{v}'\Sigma_s\mathbf{v})+(N\partial_\lambda m_0)^{-1}\left(\sum_{r=1}^k(\partial_\lambda t_r)\mathbf{v}'\Sigma_r\mathbf{v}\right)^2+O_\prec(n^{-3/2})\\ &= N^{-1}\sum_{r,s=1}^k w_{rs}(\lambda)(\mathbf{v}'\Sigma_r\mathbf{v})(\mathbf{v}'\Sigma_s\mathbf{v})+(N\partial_\lambda m_0)^{-1}(\mathbf{v}'\partial_\lambda T\mathbf{v}-1)^2+O_\prec(n^{-3/2}),\end{aligned}$$

where the second line applies (2.12). By (4.22), the $O_\prec(n^{-3/2})$ error above is negligible. Then Theorem 2.14 follows from this and (4.23). □

4.2 Guarantees for spike estimation

In this section, we establish Theorem 2.17. For notational convenience, we assume $r=1$. Part (c) of Theorem 2.17 follows immediately from the observation that Algorithm 1 uses only the eigenvalues/eigenvectors of $\widehat{\Sigma}(\mathbf{a})$, so each estimated eigenvector $\hat{\mathbf{v}}$ is equivariant under orthogonal rotations on $\mathcal{S}^\perp$.

For parts (a) and (b), we may decompose their content into the following three claims.

1. With probability at least $1-n^{-D}$, for each $(\hat{\mu},\hat{\mathbf{v}})\in\mathcal{M}$, there exists a spike eigenvalue and eigenvector $(\mu,\mathbf{v})$ of Σ_1 and a scalar $\alpha\in(0,1]$ such that $|\hat{\mu}-\mu|<n^{-1/2+\varepsilon}$ and $\|P_{\mathcal{S}}\hat{\mathbf{v}}-\alpha\mathbf{v}\|<n^{-1/2+\varepsilon}$.

2. For each spike eigenvalue μ of Σ_1 and a sufficiently small constant $\varepsilon>0$, with probability at least $1-n^{-D}$, there is at most one pair $(\hat{\mu},\hat{\mathbf{v}})\in\mathcal{M}$ where $|\hat{\mu}-\mu|<\varepsilon$.

3. For a constant $c_0>0$ independent of $\bar{C}$ in Assumption 2.1, and for each spike eigenvalue μ of Σ_1 with $\mu>c_0$, with probability at least $1-n^{-D}$, there exists $(\hat{\mu},\hat{\mathbf{v}})\in\mathcal{M}$ such that $|\hat{\mu}-\mu|<n^{-1/2+\varepsilon}$.

The first claim will be straightforward to show from the preceding probabilistic results. The second and third claims require a certain injectivity and surjectivity property of the map $(\hat{\lambda},\mathbf{a})\mapsto(t_1(\hat{\lambda},\mathbf{a}),\ldots,t_k(\hat{\lambda},\mathbf{a}))$ for $\mathbf{a}\in S^{k-1}$ and $\hat{\lambda}\in\operatorname{spec}(\widehat{\Sigma}(\mathbf{a}))$. For this, we will use Assumption 2.16.

Denote by $m_0(\lambda,\mathbf{a})$, $T(\lambda,\mathbf{a})$, etc. these functions defined for $B=B(\mathbf{a})=a_1B_1+\ldots+a_kB_k$. We record the following basic bounds.

Lemma 4.8. There is a constant $C > 0$ such that

(a) For all $\mathbf{a} \in S^{k-1}$, $\lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0(\mathbf{a}))_\delta$, and $r = 1, \ldots, k$,

$$|m_0(\lambda, \mathbf{a})| < C, \quad |\partial_\lambda m_0(\lambda, \mathbf{a})| < C, \quad |\partial_\lambda^2 m_0(\lambda, \mathbf{a})| < C, \quad |m_0(\lambda, \mathbf{a})|^{-1} < C(|\lambda| \vee 1),$$

$$\|\partial_{\mathbf{a}} m_0(\lambda, \mathbf{a})\| < C, \quad \|\partial_\lambda \partial_{\mathbf{a}} m_0(\lambda, \mathbf{a})\| < C, \quad \|\partial_{\mathbf{a}}^2 m_0(\lambda, \mathbf{a})\| < C,$$

$$|t_r(\lambda, \mathbf{a})| < C, \quad |\partial_\lambda t_r(\lambda, \mathbf{a})| < C, \quad |\partial_\lambda^2 t_r(\lambda, \mathbf{a})| < C,$$

$$\|\partial_{\mathbf{a}} t_r(\lambda, \mathbf{a})\| < C, \quad \|\partial_\lambda \partial_{\mathbf{a}} t_r(\lambda, \mathbf{a})\| < C, \quad \|\partial_{\mathbf{a}}^2 t_r(\lambda, \mathbf{a})\| < C.$$

(b) For all $\mathbf{a} \in S^{k-1}$, the roots λ of $0 = \det T(\lambda, \mathbf{a})$ are contained in $[-C, C]$.

(c) For any $D > 0$ and all $n \geq n_0(\delta, D)$, with probability at least $1 - n^{-D}$,

$$\sup_{\mathbf{a} \in S^{k-1}} \|\widehat{\Sigma}(\mathbf{a})\| < C, \qquad \sup_{\mathbf{a} \in \mathbb{R}^k} \sup_{r=1}^{k} \|\partial_{a_r} \widehat{\Sigma}(\mathbf{a})\| < C.$$

Proof. For (a), the upper bounds on m_0, $\partial_\lambda m_0$, and $\partial_\lambda^2 m_0$ follow from (2.11) and the condition $|x - \lambda| \geq \delta$ for all $x \in \operatorname{supp}(\mu_0(\mathbf{a}))_\delta$. The upper bound on m_0^{-1} follows from (2.8) and the bounds $\|F(\mathbf{a})\| < C$ and $\|(\mathrm{Id} + m_0 F(\mathbf{a}))^{-1}\| < C$, the latter holding by Proposition 4.4. For the derivatives in $\mathbf{a}$, fix r and denote $m_0 = m_0(\lambda, \mathbf{a})$, $F = F(\mathbf{a})$, and $\partial = \partial_{a_r}$. We have

$$\begin{aligned} \partial\Big(F(\mathrm{Id} + m_0 F)^{-1}\Big) &= (\partial F)(\mathrm{Id} + m_0 F)^{-1} - F(\mathrm{Id} + m_0 F)^{-1}\Big((\partial m_0) F + m_0 (\partial F)\Big)(\mathrm{Id} + m_0 F)^{-1} \\ &= (\mathrm{Id} + m_0 F)^{-1}(\partial F)(\mathrm{Id} + m_0 F)^{-1} - (\partial m_0) F^2 (\mathrm{Id} + m_0 F)^{-2}. \end{aligned} \tag{4.24}$$

Then, differentiating (2.8) with respect to a_r and also with respect to $z = \lambda$, we obtain the equations

$$\begin{aligned} 0 &= (\partial m_0)(m_0^{-2} - N^{-1} \operatorname{Tr}[F^2 (\mathrm{Id} + m_0 F)^{-2}]) + N^{-1} \operatorname{Tr}[(\partial F)(\mathrm{Id} + m_0 F)^{-2}], \\ 1 &= (\partial_\lambda m_0)(m_0^{-2} - N^{-1} \operatorname{Tr}[F^2 (\mathrm{Id} + m_0 F)^{-2}]). \end{aligned}$$

Applying the second equation to the first,

$$\partial m_0 = -(\partial_\lambda m_0) N^{-1} \operatorname{Tr}[(\partial F)(\mathrm{Id} + m_0 F)^{-2}]. \tag{4.25}$$

The bound $\|\partial_{\mathbf{a}} m_0\| < C$ then follows from $|\partial_\lambda m_0| < C$, $\|F_r\| < C$, and $\|(\mathrm{Id} + m_0 F)^{-1}\| < C$. The bounds $\|\partial_\lambda \partial_{\mathbf{a}} m_0\| < C$ and $\|\partial_{\mathbf{a}}^2 m_0\| < C$ follow from the chain rule. For $t_r(\lambda, \mathbf{a})$, recall from (4.7) that

$$-t_r = (N\sigma_r^2)^{-1} \operatorname{Tr}_r \Pi_M = (N\sigma_r^2)^{-1} \operatorname{Tr}_r(m_0 F (\mathrm{Id} + m_0 F)^{-1} F - F).$$

The bound $|t_r| < C$ then follows from $\|P_r F P_r\| < C\sigma_r^2$ and $\|P_r F\| < C\sigma_r$, where P_r is the projection onto block r. The bounds on the derivatives of t_r follow from the chain rule and those on m_0.

Part (a) implies $\|T(\lambda, \mathbf{a})\| < C$ for all $\lambda \in \mathbb{R} \setminus \operatorname{supp}(\mu_0(\mathbf{a}))_\delta$. As Proposition 2.11(c) shows $\partial_\lambda T(\lambda, \mathbf{a})$ has smallest eigenvalue at least 1, $T(\lambda, \mathbf{a})$ must be non-singular for all λ outside $[-C, C]$ for some $C > 0$, implying part (b). Finally, part (c) follows from $\widehat{\Sigma}(\mathbf{a}) = \sum_r a_r Y' B_r Y$ and the observation that $\|Y' B_r Y\| < C$ for all $r = 1, \ldots, k$ with probability $1 - n^{-D}$. ☐

Next, we verify that for the conclusions of Theorems 2.12 and 2.13(a), we may take a union bound over $\mathbf{a} \in S^{k-1}$.

Lemma 4.9. Under the conditions of Theorem 2.17, for all $n \geq n_0(\delta, \varepsilon, D)$, with probability $1 - n^{-D}$ the conclusions of Theorems 2.12 and 2.13(a) hold simultaneously for all $\mathbf{a} \in S^{k-1}$.

Proof. Consider a covering net $\mathcal{N} \subset S^{k-1}$ with $|\mathcal{N}| \leq n^C$ for some $C = C(k) > 0$, such that for all $\mathbf{a} \in S^{k-1}$ there exists $\mathbf{a}_0 \in \mathcal{N}$ where $\|\mathbf{a}_0 - \mathbf{a}\| < n^{-1/2}$. With probability $1 - n^{-D}$, the conclusions of Theorems 2.12 and 2.13 hold with constants $\delta/2$ and $\varepsilon/2$ simultaneously over $\mathbf{a}_0 \in \mathcal{N}$ by a union bound. Furthermore, by Lemma 4.8, with probability at least $1 - n^{-D}$ we have $\|\widehat{\Sigma}(\mathbf{a}) - \widehat{\Sigma}(\mathbf{a}_0)\| < Cn^{-1/2}$ for all $\mathbf{a} \in S^{k-1}$, where $\mathbf{a}_0$ is the closest point to $\mathbf{a}$ in $\mathcal{N}$. Note that by Theorem 2.5, this implies also $\operatorname{supp}(\mu_0(\mathbf{a})) \subseteq \operatorname{supp}(\mu_0(\mathbf{a}_0))_{\delta/4}$ and $\operatorname{supp}(\mu_0(\mathbf{a}_0)) \subseteq \operatorname{supp}(\mu_0(\mathbf{a}))_{\delta/4}$ for all large n.

On the above event, consider any $\mathbf{a} \in S^{k-1}$ and nearest point $\mathbf{a}_0 \in \mathcal{N}$. Let $\Lambda_{\delta/2}(\mathbf{a}_0)$ and $\widehat{\Lambda}_{\delta/2}(\mathbf{a}_0)$ be the sets guaranteed by Theorem 2.12 at $\mathbf{a}_0$, so

$$\text{ordered-dist}(\Lambda_{\delta/2}(\mathbf{a}_0), \widehat{\Lambda}_{\delta/2}(\mathbf{a}_0)) < n^{-1/2+\varepsilon/2}.$$

The condition $\|\widehat{\Sigma}(\mathbf{a}) - \widehat{\Sigma}(\mathbf{a}_0)\| < Cn^{-1/2}$ implies there is $\widehat{\Lambda}_\delta(\mathbf{a}) \subset \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}))$ such that

$$\text{ordered-dist}(\widehat{\Lambda}_\delta(\mathbf{a}), \widehat{\Lambda}_{\delta/2}(\mathbf{a}_0)) < Cn^{-1/2}.$$

Since $\widehat{\Lambda}_{\delta/2}(\mathbf{a}_0)$ contains all eigenvalues of $\widehat{\Sigma}(\mathbf{a}_0)$ outside $\operatorname{supp}(\mu_0(\mathbf{a}_0))_{\delta/2}$, we have that $\widehat{\Lambda}_\delta(\mathbf{a})$ contains all eigenvalues of $\widehat{\Sigma}(\mathbf{a})$ outside $\operatorname{supp}(\mu_0(\mathbf{a}))_\delta$. On the other hand, $\Lambda_{\delta/2}(\mathbf{a}_0)$ is a subset of roots of $0 = \det(K(\lambda, \mathbf{a}_0))$, where $K(\lambda, \mathbf{a}_0)$ is defined by (4.5) at $B = B(\mathbf{a}_0)$. Letting $\mu_1(\lambda, \mathbf{a}_0) \leq \ldots \leq \mu_L(\lambda, \mathbf{a}_0)$ denote the eigenvalues of $K(\lambda, \mathbf{a}_0)$, the multiset $\Lambda_0(\mathbf{a}_0)$ is in 1-to-1 correspondence with pairs (ℓ, λ_0) where $\mu_\ell(\lambda_0, \mathbf{a}_0) = 0$. For each such (ℓ, λ_0), Lemma 4.8 implies $\|K(\lambda_0, \mathbf{a}) - K(\lambda_0, \mathbf{a}_0)\| < Cn^{-1/2}$, so $|\mu_\ell(\lambda_0, \mathbf{a})| < Cn^{-1/2}$. As $-K$ is the upper $L \times L$ submatrix of T, Proposition 2.11(c) implies μ_ℓ decreases in λ at a rate of at least 1, so $\mu_\ell(\lambda, \mathbf{a}) = 0$ for some λ with $|\lambda - \lambda_0| < Cn^{-1/2}$. Thus there exists $\Lambda_\delta(\mathbf{a}) \subseteq \Lambda_0(\mathbf{a})$ where

$$\text{ordered-dist}(\Lambda_\delta(\mathbf{a}), \Lambda_{\delta/2}(\mathbf{a}_0)) < Cn^{-1/2},$$

and similarly $\Lambda_\delta(\mathbf{a})$ contains all elements of $\Lambda_0(\mathbf{a})$ outside $\operatorname{supp}(\mu_0(\mathbf{a}))_\delta$. Then

$$\text{ordered-dist}(\Lambda_\delta(\mathbf{a}), \widehat{\Lambda}_\delta(\mathbf{a})) < 2Cn^{-1/2} + n^{-1/2+\varepsilon/2} < n^{-1/2+\varepsilon},$$

so the conclusion of Theorem 2.12 holds at each $\mathbf{a} \in S^{k-1}$.

For Theorem 2.13(a), let $\lambda \in \Lambda_0(\mathbf{a})$ be separated from other elements of $\Lambda_0(\mathbf{a})$ by δ. Then Proposition 2.11(c) implies 0 is separated from other eigenvalues of $T(\lambda, \mathbf{a})$ by δ. Letting $\lambda_0 \in \Lambda_0(\mathbf{a}_0)$ be such that $|\lambda_0 - \lambda| < Cn^{-1/2}$, as identified above, Lemma 4.8 implies $\|T(\lambda_0, \mathbf{a}_0) - T(\lambda, \mathbf{a})\| < Cn^{-1/2}$. Thus if $\mathbf{v}$ and $\mathbf{v}_0$ are the null unit eigenvectors of $T(\lambda, \mathbf{a})$ and $T(\lambda_0, \mathbf{a}_0)$, then $\|\mathbf{v} - \mathbf{v}_0\| < Cn^{-1/2}$ for an appropriate choice of sign. Similarly, if $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}))$ and $\hat{\lambda}_0 \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}_0))$ are such that $|\hat{\lambda} - \lambda| < n^{-1/2+\varepsilon}$ and $|\hat{\lambda}_0 - \lambda_0| < n^{-1/2+\varepsilon}$, then $\hat{\lambda}$ is separated from other eigenvalues of $\widehat{\Sigma}(\mathbf{a})$ by $\delta - Cn^{-1/2+\varepsilon}$, and the bound $\|\widehat{\Sigma}(\mathbf{a}) - \widehat{\Sigma}(\mathbf{a}_0)\| < Cn^{-1/2}$ implies that the corresponding eigenvectors $\hat{\mathbf{v}}$ and $\hat{\mathbf{v}}_0$ satisfy $\|\hat{\mathbf{v}} - \hat{\mathbf{v}}_0\| < Cn^{-1/2}$. Lemma 4.8 finally implies $\|\partial_\lambda T(\lambda, \mathbf{a}) - \partial_\lambda T(\lambda_0, \mathbf{a}_0)\| < Cn^{-1/2}$, so the conclusion of Theorem 2.13(a) at $\mathbf{a}$ follows from that at $\mathbf{a}_0$. $\square$

We may now establish the first of the above three claims for Theorem 2.17.

Proof of Claim 1. Consider the event of probability $1 - n^{-D}$ on which the conclusions of Theorems 2.12(a) and 2.13 hold simultaneously over $\mathbf{a} \in S^{k-1}$.

For each $(\hat{\mu}, \hat{\mathbf{v}}) \in \mathcal{M}$, there are $\mathbf{a} \in S^{k-1}$ and $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a})) \cap \mathcal{I}_\delta(\mathbf{a})$ with $\hat{\mu} = \hat{\lambda}/t_1(\hat{\lambda}, \mathbf{a})$ and $t_2(\hat{\lambda}, \mathbf{a}) = \ldots = t_k(\hat{\lambda}, \mathbf{a}) = 0$. On the above event, for each such $(\hat{\lambda}, \mathbf{a})$, there exists λ with $|\hat{\lambda} - \lambda| < n^{-1/2+\varepsilon}$ and $0 = \det T(\lambda, \mathbf{a})$. Then Lemma 4.8 implies

$$\|T(\hat{\lambda}, \mathbf{a}) - T(\lambda, \mathbf{a})\| < Cn^{-1/2+\varepsilon}. \tag{4.26}$$

An eigenvalue of $T(\lambda, \mathbf{a})$ is 0, so an eigenvalue of $T(\hat{\lambda}, \mathbf{a})$ has magnitude at most $Cn^{-1/2+\varepsilon}$. From the two equivalent forms (2.12) and (2.15) of T and the condition $t_2(\hat{\lambda}, \mathbf{a}) = \ldots = t_k(\hat{\lambda}, \mathbf{a}) = 0$,

$$T(\hat{\lambda}, \mathbf{a}) = \hat{\lambda} \operatorname{Id} - t_1(\hat{\lambda}, \mathbf{a})\Sigma_1 = -\frac{1}{m_0(\hat{\lambda}, \mathbf{a})} \operatorname{Id} - t_1(\hat{\lambda}, \mathbf{a}) V_1' \Theta_1 V_1. \tag{4.27}$$

Since $|m_0(\lambda, \mathbf{a})| < C$, the second form above implies that the $O(n^{-1/2+\varepsilon})$ eigenvalue of $T(\hat{\lambda}, \mathbf{a})$ must be $\hat{\lambda} - t_1(\hat{\lambda}, \mathbf{a})\mu = -1/m_0(\hat{\lambda}, \mathbf{a}) - t_1(\hat{\lambda}, \mathbf{a})\theta$ for a spike eigenvalue $\mu = \theta + \sigma_1^2$ of Σ_1. As θ is bounded, the condition $|-1/m_0(\hat{\lambda}, \mathbf{a}) - t_1(\hat{\lambda}, \mathbf{a})\theta| < Cn^{-1/2+\varepsilon}$ implies in particular that $|t_1(\hat{\lambda}, \mathbf{a})| > c$ for a constant $c > 0$. Then dividing $|\hat{\lambda} - t_1(\hat{\lambda}, \mathbf{a})\mu| < Cn^{-1/2+\varepsilon}$ by $t_1(\hat{\lambda}, \mathbf{a})$, $|\hat{\mu} - \mu| < Cn^{-1/2+\varepsilon}$ for a different constant $C > 0$. Furthermore, on the above event, $\|P_{\mathcal{S}}\hat{\mathbf{v}} - \alpha\mathbf{w}\| < n^{-1/2+\varepsilon}$ for the null vector $\mathbf{w}$ of $T(\lambda, \mathbf{a})$ and for $\alpha = (\mathbf{w}'\partial_\lambda T(\lambda, \mathbf{a})\mathbf{w})^{-1/2}$. By the second form in (4.27), the separation of values of Θ_1 by τ, and the above lower bound on $t_1(\hat{\lambda}, \mathbf{a})$, the null eigenvalue of $T(\lambda, \mathbf{a})$ is separated from other eigenvalues by a constant $c > 0$. Then (4.26) implies $\|\mathbf{w} - \mathbf{v}\| < Cn^{-1/2+\varepsilon}$ where $\mathbf{v}$ is the (appropriately signed) eigenvector of $T(\hat{\lambda}, \mathbf{a})$ corresponding to the eigenvalue $\hat{\lambda} - t_1(\hat{\lambda}, \mathbf{a})\mu$. This is exactly the eigenvector of Σ_1 corresponding to μ, and thus $\|P_{\mathcal{S}}\hat{\mathbf{v}} - \alpha\mathbf{v}\| < Cn^{-1/2+\varepsilon}$. $\square$

For the remaining two claims, let us first sketch the argument at a high level: Suppose μ is a spike eigenvalue of Σ_1, and $\mathbf{a}_0 \in S^{k-1}$ and $\hat{\lambda}_0 \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}_0))$ are such that

$$\hat{\lambda}_0/t_1(\hat{\lambda}_0, \mathbf{a}_0) \approx \mu, \qquad t_r(\hat{\lambda}_0, \mathbf{a}_0) \approx 0 \text{ for all } r = 2, \ldots, k.$$

We will show that under Assumption 2.16, this holds for some $(\hat{\lambda}_0, \mathbf{a}_0)$ whenever μ is sufficiently large. The separation of μ from other eigenvalues of Σ_1 will imply that $\hat{\lambda}_0$ is separated from other eigenvalues of $\widehat{\Sigma}(\mathbf{a}_0)$. Then for all $\mathbf{a} \in S^{k-1}$ in a neighborhood of $\mathbf{a}_0$, we may identify an eigenvalue $\hat{\lambda}(\mathbf{a})$ of $\widehat{\Sigma}(\mathbf{a})$ such that $\hat{\lambda}(\mathbf{a}_0) = \hat{\lambda}_0$ and $\hat{\lambda}(\mathbf{a})$ varies analytically in $\mathbf{a}$. Applying a version of the inverse function theorem, we will show that the mapping

$$\mathbf{a} \mapsto (t_2(\hat{\lambda}(\mathbf{a}), \mathbf{a}), \ldots, t_k(\hat{\lambda}(\mathbf{a}), \mathbf{a}))$$

is injective in this neighborhood of $\mathbf{a}_0$, and its image contains 0. This local injectivity, together with Assumption 2.16, will imply Claim 2. The image containing 0 will imply Claim 3.

We use the following quantitative version of the inverse function theorem to carry out this argument.

Lemma 4.10. Fix constants $C, c_0, c_1, m > 0$. Let $\mathbf{x}_0 \in \mathbb{R}^m$, let $U = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x} - \mathbf{x}_0\| < c_0\}$, and let $f : U \to \mathbb{R}^m$ be twice continuously differentiable. Denote by $\mathrm{d}f \in \mathbb{R}^{m \times m}$ the derivative of f, and suppose for all $\mathbf{v} \in \mathbb{R}^m$, $i, j, k \in \{1, \ldots, m\}$, and $\mathbf{x} \in U$ that

$$\|(\mathrm{d}f(\mathbf{x}_0))\mathbf{v}\| \geq c_1 \|\mathbf{v}\|, \qquad |\partial_{x_i} \partial_{x_j} f_k(\mathbf{x})| < C.$$

Then there are constants $\varepsilon_0, \varepsilon_1, c > 0$ such that f is injective on $U_0 = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x} - \mathbf{x}_0\| < \varepsilon_0\}$, $\|f(\mathbf{x}_1) - f(\mathbf{x}_2)\| \geq c\|\mathbf{x}_1 - \mathbf{x}_2\|$ for all $\mathbf{x}_1, \mathbf{x}_2 \in U_0$, and the image $f(U_0)$ contains $\{\mathbf{y} \in \mathbb{R}^m : \|\mathbf{y} - f(\mathbf{x}_0)\| < \varepsilon_1\}$.

Proof. Assume without loss of generality $\mathbf{x}_0 = 0$ and $f(\mathbf{x}_0) = 0$. By Taylor's theorem and the given second derivative bound, for all $\mathbf{x} \in U$ and a constant $C > 0$, $\|\mathrm{d}f(\mathbf{x}) - \mathrm{d}f(0)\| \leq C\|\mathbf{x}\|$. Then for sufficiently small $\varepsilon_0 > 0$, all $\mathbf{x} \in U_0 = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x}\| < \varepsilon_0\}$, and all $\mathbf{v} \in \mathbb{R}^m$,

$$\|(\mathrm{d}f(\mathbf{x}))\mathbf{v}\| \geq \|(\mathrm{d}f(0))\mathbf{v}\| - C\|\mathbf{x}\|\|\mathbf{v}\| \geq (c_1 - C\varepsilon_0)\|\mathbf{v}\| \geq (c_1/2)\|\mathbf{v}\|.$$

Furthermore, for all $\mathbf{x}_1, \mathbf{x}_2 \in U$,

$$\|f(\mathbf{x}_2) - f(\mathbf{x}_1) - (\mathrm{d}f(\mathbf{x}_1))(\mathbf{x}_2 - \mathbf{x}_1)\| \leq C\|\mathbf{x}_2 - \mathbf{x}_1\|^2.$$

Then for sufficiently small $\varepsilon_0 > 0$ and all $\mathbf{x}_1, \mathbf{x}_2 \in U_0$,

$$\|f(\mathbf{x}_2) - f(\mathbf{x}_1)\| \geq (c_1/2)\|\mathbf{x}_2 - \mathbf{x}_1\| - C\|\mathbf{x}_2 - \mathbf{x}_1\|^2 \geq c\|\mathbf{x}_2 - \mathbf{x}_1\| \tag{4.28}$$

for a constant $c > 0$. In particular, f is injective on U_0.

To prove the surjectivity claim, let $K = \{\mathbf{x} \in \mathbb{R}^m : \|\mathbf{x}\| \leq \varepsilon_0/2\} \subset U_0$. For a sufficiently small constant $\varepsilon_1 > 0$, the above applied with $\mathbf{x}_2 = \mathbf{x}$ on the boundary of K and $\mathbf{x}_1 = 0$ implies

$$\|f(\mathbf{x})\| > 2\varepsilon_1 \text{ for all } \mathbf{x} \text{ on the boundary of } K.$$

Fix any $\mathbf{y} \in \mathbb{R}^m$ with $\|\mathbf{y}\| < \varepsilon_1$, and define $h(\mathbf{x}) = \|f(\mathbf{x}) - \mathbf{y}\|^2$ over $\mathbf{x} \in K$. As K is compact, there is $\mathbf{x}_* \in K$ that minimizes h. Since $h(0) = \|\mathbf{y}\|^2 < \varepsilon_1^2$ while $h(\mathbf{x}) > \varepsilon_1^2$ for $\mathbf{x}$ on the boundary of K by the above, $\mathbf{x}_*$ is in the interior of K. Then

$$0 = \mathrm{d}h(\mathbf{x}_*) = 2(f(\mathbf{x}_*) - \mathbf{y})'(\mathrm{d}f(\mathbf{x}_*)).$$

Since $\mathrm{d}f(\mathbf{x}_*)$ is invertible by (4.28), this implies $f(\mathbf{x}_*) = \mathbf{y}$. So $f(U_0)$ contains any such $\mathbf{y}$. $\square$

We now make the above proof sketch for Claims 2 and 3 precise.

Lemma 4.11. Let $\mu = \theta + \sigma_1^2$ be the ℓ^{th} largest spike eigenvalue of Σ_1. Define

$$t_+(\lambda, \mathbf{a}) = (t_2(\lambda, \mathbf{a}), \ldots, t_k(\lambda, \mathbf{a})).$$

Then there exist constants $c, \varepsilon_0, \varepsilon_1 > 0$ such that for any $D > 0$ and all $n \geq n_0(\delta, D)$, under the conditions of Theorem 2.17, the following holds with probability at least $1 - n^{-D}$: For all $\mathbf{a}_0 \in S^{k-1}$, if there exists $\hat{\lambda}_0 \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}_0)) \cap \mathcal{I}_\delta(\mathbf{a}_0)$ which satisfies

$$\left| -\frac{1}{m_0(\hat{\lambda}_0, \mathbf{a}_0)} - t_1(\hat{\lambda}_0, \mathbf{a}_0)\,\theta \right| < \varepsilon_1, \qquad \|t_+(\hat{\lambda}_0, \mathbf{a}_0)\| < \varepsilon_1, \tag{4.29}$$

then:

- $\hat{\lambda}_0$ is the ℓ^{th} largest eigenvalue of $\widehat{\Sigma}(\mathbf{a}_0)$.
- The ℓ^{th} largest eigenvalue $\hat{\lambda}(\mathbf{a})$ of $\widehat{\Sigma}(\mathbf{a})$ is simple over $O = \{\mathbf{a} \in \mathbb{R}^k : \|\mathbf{a} - \mathbf{a}_0\| < \varepsilon_0\}$.
- The map $\hat{f}(\mathbf{a}) = t_+(\hat{\lambda}(\mathbf{a}), \mathbf{a})$ is injective on $U = O \cap S^{k-1}$ and satisfies $\|\hat{f}(\mathbf{a}_1) - \hat{f}(\mathbf{a}_2)\| \geq c\|\mathbf{a}_1 - \mathbf{a}_2\|$ for all $\mathbf{a}_1, \mathbf{a}_2 \in U$. Furthermore, its image $\hat{f}(U)$ contains $\{\mathbf{t} \in \mathbb{R}^{k-1} : \|\mathbf{t}\| < \varepsilon_1\}$.

Proof. Throughout the proof, we use the convention that constants $C, c > 0$ do not depend on $\varepsilon_0, \varepsilon_1$.

Let $\mathcal{N} \subset S^{k-1}$ be a covering net with $|\mathcal{N}| \leq n^C$, such that for each $\mathbf{a} \in S^{k-1}$ there is $\mathbf{a}_0 \in \mathcal{N}$ with $\|\mathbf{a} - \mathbf{a}_0\| < n^{-1/2}$. It suffices to establish the result for each fixed $\mathbf{a}_0 \in \mathcal{N}$ with probability $1 - n^{-D}$. The result then holds simultaneously for all $\mathbf{a}_0 \in S^{k-1}$ by a union bound over $\mathcal{N}$ and the Lipschitz continuity of m_0^{-1}, t_1, and t_+ as established in Lemma 4.8.

Thus, let us fix $\mathbf{a}_0 \in \mathcal{N}$. Consider the good event where the conclusion of Theorem 2.12 holds for $B = B(\mathbf{a}_0)$, and also $\|\widehat{\Sigma}(\mathbf{a}) - \widehat{\Sigma}(\mathbf{a}_0)\| \leq C\|\mathbf{a} - \mathbf{a}_0\|$ and $\|\partial_{a_r}\widehat{\Sigma}(\mathbf{a})\| < C$ for all $r = 1, \ldots, k$ and $\mathbf{a} \in \mathbb{R}^k$.

Consider m_0, t_r, T defined at $\mathbf{a}_0$, and (for notational convenience) suppress their dependence on $\mathbf{a}_0$. On this good event, for each $\hat{\lambda}_0$ satisfying (4.29), there exists λ_0 with $|\lambda_0 - \hat{\lambda}_0| < n^{-1/2+\varepsilon}$ and $0 = \det T(\lambda_0)$. Lemma 4.8 implies $|m_0(\lambda_0)^{-1} - m_0(\hat{\lambda}_0)^{-1}| < Cn^{-1/2+\varepsilon}$ and $|t_r(\lambda_0) - t_r(\hat{\lambda}_0)| < Cn^{-1/2+\varepsilon}$ for each r. Then (2.15), (4.29), and the condition $\theta \geq \tau$ in Theorem 2.17 imply

$$\|T(\lambda_0) + m_0(\lambda_0)^{-1}(\mathrm{Id} - \theta^{-1} V_1 \Theta_1 V_1')\| < C\varepsilon_1. \tag{4.30}$$

Since $\lambda_0 \in \mathcal{I}_\delta(\mathbf{a}_0)$ is greater than $\mathrm{supp}(\mu_0)$, we have $m_0(\lambda_0) < 0$ by (2.11). As θ is the ℓ^{th} largest value of Θ_1, this implies the ℓ^{th} smallest eigenvalue of $-m_0(\lambda_0)^{-1}(\mathrm{Id} - \theta^{-1} V_1 \Theta_1 V_1)$ is 0. Then, denoting by $\mu_1(\lambda) \leq \ldots \leq \mu_p(\lambda)$ the eigenvalues of $T(\lambda)$, (4.30) yields $|\mu_\ell(\lambda_0)| < C\varepsilon_1$. The separation of values of Θ_1 by τ further implies $\mu_{\ell-1}(\lambda_0) < -|m_0(\lambda_0)\theta|^{-1}\tau + C\varepsilon_1$ and $\mu_{\ell+1}(\lambda_0) > |m_0(\lambda_0)\theta|^{-1}\tau - C\varepsilon_1$. As $\theta < C$ and $|m_0(\lambda_0)| < C$, for sufficiently small ε_1 this yields

$$\mu_{\ell+1}(\lambda_0) > c, \qquad \mu_{\ell-1}(\lambda_0) < -c, \qquad \mu_\ell(\lambda_0) = 0$$

for a constant $c > 0$, where the third statement must hold because $0 = \det T(\lambda_0)$. For each $j = 1, \ldots, p$ and all $\lambda < \lambda'$ in $\mathcal{I}_\delta(\mathbf{a}_0)$, note that

$$\lambda' - \lambda \leq \mu_j(\lambda') - \mu_j(\lambda) < C(\lambda' - \lambda),$$

where the lower bound follows from Proposition 2.11(c) and the upper bound follows from $\|\partial_\lambda T(\lambda)\| < C$. Then λ_0 is separated from all other roots of $0 = \det T(\lambda)$ by a constant $c > 0$. Furthermore, there are exactly $\ell - 1$ roots of $0 = \det T(\lambda)$ which are greater than λ_0, one corresponding to each μ_j for $j = 1, \ldots, \ell - 1$. Then on the above good event, there can only be one such $\hat{\lambda}_0$ satisfying (4.29), which is the ℓ^{th} largest eigenvalue of $\widehat{\Sigma}(\mathbf{a}_0)$. Furthermore, it is separated from all other eigenvalues of $\widehat{\Sigma}(\mathbf{a}_0)$ by a constant $c > 0$, and for a sufficiently small constant $\varepsilon_0 > 0$, the ℓ^{th} largest eigenvalue $\hat{\lambda}(\mathbf{a})$ is simple and analytic on $O = \{\mathbf{a} \in \mathbb{R}^k : \|\mathbf{a} - \mathbf{a}_0\| < \varepsilon_0\}$. This verifies the first two statements.

To verify the third statement, consider a chart (V, φ) where $V = \{\mathbf{v} \in \mathbb{R}^{k-1} : \|\mathbf{v}\| < \varepsilon_0\}$, $\varphi : V \to U$ is a smooth, bijective map with bounded first- and second-order derivatives, $\varphi(0) = \mathbf{a}_0$, and $\|\varphi(\mathbf{v}_1) - \varphi(\mathbf{v}_2)\| \geq \|\mathbf{v}_1 - \mathbf{v}_2\|/2$ for all $\mathbf{v}_1, \mathbf{v}_2 \in V$. We apply Lemma 4.10 to the map $\hat{g} = \hat{f} \circ \varphi$. To verify the second-derivative bounds for $\hat{g}$, note that for $\mathbf{a} \in O$, letting $\hat{\mathbf{v}}(\mathbf{a})$ be the unit eigenvector where $\widehat{\Sigma}(\mathbf{a})\hat{\mathbf{v}}(\mathbf{a}) = \hat{\lambda}(\mathbf{a})\hat{\mathbf{v}}(\mathbf{a})$, we have

$$\begin{aligned} \partial_{a_r} \hat{\lambda}(\mathbf{a}) &= \hat{\mathbf{v}}(\mathbf{a})'(\partial_{a_r} \widehat{\Sigma}(\mathbf{a}))\hat{\mathbf{v}}(\mathbf{a}), \\ \partial_{a_r}\partial_{a_s} \hat{\lambda}(\mathbf{a}) &= (\partial_{a_s} \hat{\mathbf{v}}(\mathbf{a}))'(\partial_{a_r} \widehat{\Sigma}(\mathbf{a}))\hat{\mathbf{v}}(\mathbf{a}) + \hat{\mathbf{v}}(\mathbf{a})'(\partial_{a_r} \widehat{\Sigma}(\mathbf{a}))(\partial_{a_s} \hat{\mathbf{v}}(\mathbf{a})) \\ &= 2\hat{\mathbf{v}}(\mathbf{a})'(\partial_{a_r} \widehat{\Sigma}(\mathbf{a}))(\hat{\lambda}(\mathbf{a})\,\mathrm{Id} - \widehat{\Sigma}(\mathbf{a}))^\dagger(\partial_{a_s} \widehat{\Sigma}(\mathbf{a}))\hat{\mathbf{v}}(\mathbf{a}), \end{aligned} \tag{4.31}$$

where $(\hat{\lambda}(\mathbf{a})\,\mathrm{Id} - \widehat{\Sigma}(\mathbf{a}))^\dagger$ is the Moore-Penrose pseudo-inverse. Since $\hat{\lambda}(\mathbf{a})$ is separated from other eigenvalues of $\widehat{\Sigma}(\mathbf{a})$ by a constant, $\|(\hat{\lambda}(\mathbf{a})\operatorname{Id}-\widehat{\Sigma}(\mathbf{a}))^\dagger\|< C$. Then Lemma 4.8 and the chain rule imply that on the above good event, $\hat{g}$ has all second-order derivatives bounded on V. It remains to check the condition $\|(\mathrm{d}\hat{g}(0))\mathbf{v}\|\geq c\|\mathbf{v}\|$ for a constant $c>0$ and all $\mathbf{v}\in\mathbb{R}^{k-1}$. Since $\mathrm{d}\hat{g}(0)=\mathrm{d}\hat{f}(\mathbf{a}_0)\cdot\mathrm{d}\varphi(0)$, and $\mathrm{d}\varphi(0)\mathbf{v}$ is orthogonal to $\mathbf{a}_0$ with $\|\mathrm{d}\varphi(0)\mathbf{v}\|\geq\|\mathbf{v}\|/2$, we must check

$$\|(\mathrm{d}\hat{f}(\mathbf{a}_0))\mathbf{w}\|\geq c\|\mathbf{w}\| \tag{4.32}$$

for a constant $c>0$ and all $\mathbf{w}$ orthogonal to $\mathbf{a}_0$, where $\mathrm{d}\hat{f}$ is the derivative of $\hat{f}:O\to\mathbb{R}^{k-1}$.

For this, let $\lambda_0=\hat{\lambda}_0+O(n^{-1/2+\varepsilon})$ be the root of $0=\det T(\lambda,\mathbf{a}_0)$, and let $\mathbf{v}_0\in\ker T(\lambda_0,\mathbf{a}_0)$. As λ_0 is a simple root, the implicit function theorem implies we may define $\lambda(\mathbf{a})$ analytically on a neighborhood of $\mathbf{a}_0$ such that $\lambda(\mathbf{a}_0)=\lambda_0$ and $0=\det T(\lambda(\mathbf{a}),\mathbf{a})$. As $T(\lambda(\mathbf{a}),\mathbf{a})$ is analytic in $\mathbf{a}$ and 0 is a simple eigenvalue of this matrix at $\mathbf{a}_0$, we may also define the null eigenvector $\mathbf{v}(\mathbf{a})$ analytically on a neighborhood of $\mathbf{a}_0$, so that $\mathbf{v}(\mathbf{a}_0)=\mathbf{v}_0$, $T(\lambda(\mathbf{a}),\mathbf{a})\mathbf{v}(\mathbf{a})=0$, and $\|\mathbf{v}(\mathbf{a})\|^2=1$. We show in Lemma 4.12 below that on an event of probability $1-n^{-D}$, we have

$$\|\mathrm{d}\lambda(\mathbf{a}_0)-\mathrm{d}\hat{\lambda}(\mathbf{a}_0)\|< n^{-1/2+\varepsilon}. \tag{4.33}$$

Assuming (4.33) holds, let us first show that the analogue of (4.32) holds for the function

$$f(\mathbf{a})=t_+(\lambda(\mathbf{a}),\mathbf{a}).$$

Denote $m(\mathbf{a})=m_0(\lambda(\mathbf{a}),\mathbf{a})$, $\mathbf{b}(\mathbf{a})=m(\mathbf{a})\mathbf{a}$, and $s_+(\mathbf{b})=(s_2(\mathbf{b}),\ldots,s_k(\mathbf{b}))$ where s is as in (2.20). Then $m(\mathbf{a})f(\mathbf{a})=s_+(\mathbf{b}(\mathbf{a}))$. Denote $\mathbf{b}_0=\mathbf{b}(\mathbf{a}_0)$ and differentiate this with respect to $\mathbf{a}$ at $\mathbf{a}_0$ to get

$$f(\mathbf{a}_0)(\mathrm{d}m(\mathbf{a}_0))'+m(\mathbf{a}_0)\mathrm{d}f(\mathbf{a}_0)=\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0).$$

Hence for any $\mathbf{w}\in\mathbb{R}^k$,

$$\mathrm{d}f(\mathbf{a}_0)\mathbf{w}=\frac{1}{m(\mathbf{a}_0)}\Big(\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}-f(\mathbf{a}_0)(\mathrm{d}m(\mathbf{a}_0))'\mathbf{w}\Big).$$

Applying $\|f(\mathbf{a}_0)\|=\|t_+(\lambda_0,\mathbf{a}_0)\|<\varepsilon_1$ from (4.29), and $\|\mathrm{d}m(\mathbf{a}_0)\|< C$ and $c<|m(\mathbf{a}_0)|< C$ from the chain rule, (4.33), (4.31), and Lemma 4.8, we have

$$\|\mathrm{d}f(\mathbf{a}_0)\mathbf{w}\|\geq c\|\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\|-C\varepsilon_1\|\mathbf{w}\|. \tag{4.34}$$

To bound the first term on the right, recall (2.15) and multiply the condition $0=\mathbf{v}(\mathbf{a})'T(\lambda(\mathbf{a}),\mathbf{a})\mathbf{v}(\mathbf{a})$ by $m(\mathbf{a})$ to get

$$0=\mathbf{v}(\mathbf{a})'\left(-\operatorname{Id}+\sum_{r=1}^{k}s_r(\mathbf{b}(\mathbf{a}))V_r\Theta_rV_r'\right)\mathbf{v}(\mathbf{a}).$$

Differentiate this with respect to $\mathbf{a}$ at $\mathbf{a}_0$, and set $y_r = \mathbf{v}_0' V_r \Theta_r V_r' \mathbf{v}_0$ and $\mathbf{y} = (y_1, \ldots, y_k)$, to get

$$0 = \sum_{r=1}^{k} \mathrm{d}s_r(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0) \cdot \mathbf{v}_0' V_r \Theta_r V_r' \mathbf{v}_0 = \mathbf{y}' \mathrm{d}s(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0).$$

For any $\mathbf{w} \in \mathbb{R}^k$, letting $\mathbf{y}_+ = (y_2, \ldots, y_k)$, this yields

$$\begin{aligned}
\|\mathbf{y}_+\| \cdot \|\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\| &\geq |\mathbf{y}_+' \mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}| \\
&= |y_1 \mathrm{d}s_1(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}| \\
&\geq |y_1| \cdot \|\mathrm{d}s(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\| - |y_1| \cdot \|\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\|.
\end{aligned}$$

So

$$\|\mathrm{d}s_+(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\| \geq \frac{|y_1| \cdot \|\mathrm{d}s(\mathbf{b}_0)\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\|}{|y_1| + \|\mathbf{y}_+\|}. \tag{4.35}$$

Note that $|y_1| + \|\mathbf{y}_+\| < C$. Applying $\mathbf{v}_0' T(\lambda_0, \mathbf{a}_0)\mathbf{v}_0 = 0$ to (4.30), we have also $|y_1 - \theta| < C\varepsilon_1$, so $|y_1| > \theta - C\varepsilon_1 > c$ for sufficiently small $\varepsilon_1 > 0$. Finally, recall $\mathbf{b}(\mathbf{a}) = m(\mathbf{a})\mathbf{a}$, so $\mathrm{d}\mathbf{b}(\mathbf{a}_0) = m(\mathbf{a}_0)\,\mathrm{Id} + \mathbf{a}_0(\mathrm{d}m(\mathbf{a}_0))'$. If $\mathbf{w}$ is orthogonal to $\mathbf{a}_0$, then

$$\|\mathrm{d}\mathbf{b}(\mathbf{a}_0)\mathbf{w}\| = \|m(\mathbf{a}_0)\mathbf{w} + \mathbf{a}_0(\mathrm{d}m(\mathbf{a}_0))'\mathbf{w}\| \geq \|m(\mathbf{a}_0)\mathbf{w}\| \geq c\|\mathbf{w}\|.$$

As $\|\mathbf{b}_0\| < C$, Assumption 2.16 implies $\|\mathrm{d}s(\mathbf{b}_0)\mathbf{v}\| \geq c\|\mathbf{v}\|$ for any $\mathbf{v} \in \mathbb{R}^k$, so combining these observations with (4.35) and (4.34) yields finally $\|(\mathrm{d}f(\mathbf{a}_0))\mathbf{w}\| \geq c\|\mathbf{w}\|$ for $\mathbf{w}$ orthogonal to $\mathbf{a}_0$.

To conclude the proof, recall $f(\mathbf{a}) = t_+(\lambda(\mathbf{a}), \mathbf{a})$ while $\hat{f}(\mathbf{a}) = t_+(\hat{\lambda}(\mathbf{a}), \mathbf{a})$. Applying (4.33), Lemma 4.8, and the chain rule, we obtain $\|\mathrm{d}f(\mathbf{a}_0) - \mathrm{d}\hat{f}(\mathbf{a}_0)\| < Cn^{-1/2+\varepsilon}$. Hence (4.32) holds, and we may apply Lemma 4.10 to the function $\hat{g} = \hat{f} \circ \varphi$. This shows, for some constants $c, \tilde{\varepsilon}_0, \tilde{\varepsilon}_1 > 0$, that $\hat{f}$ is injective on $\tilde{U} = \{\mathbf{a} \in S^{k-1} : \|\mathbf{a} - \mathbf{a}_0\| < \tilde{\varepsilon}_0\}$, $\hat{f}(\tilde{U})$ contains $\{\mathbf{t} \in \mathbb{R}^{k-1} : \|\mathbf{t} - \hat{f}(\mathbf{a}_0)\| < \tilde{\varepsilon}_1\}$, and $\|\hat{f}(\mathbf{a}_1) - \hat{f}(\mathbf{a}_2)\| \geq c\|\mathbf{a}_1 - \mathbf{a}_2\|$ for $\mathbf{a}_1, \mathbf{a}_2 \in \tilde{U}$. Observe that if $\|\mathbf{t}\| < \varepsilon_1$, then $\|\mathbf{t} - \hat{f}(\mathbf{a}_0)\| < 2\varepsilon_1$ by (4.29). Reducing ε_0 and ε_1 to $\tilde{\varepsilon}_0$ and $\tilde{\varepsilon}_1/2$ concludes the proof. □

Lemma 4.12. Let $\mathbf{a}_0 \in S^{k-1}$, let $U \subset \mathbb{R}^k$ be a neighborhood of $\mathbf{a}_0$, and let $\lambda(\mathbf{a})$ and $\hat{\lambda}(\mathbf{a})$ be analytic functions on U such that $0 = \det T(\lambda(\mathbf{a}), \mathbf{a})$ and $\hat{\lambda}(\mathbf{a}) \in \mathrm{spec}(\widehat{\Sigma}(\mathbf{a}))$ for each $\mathbf{a} \in U$. Suppose $\lambda(\mathbf{a}_0) - \hat{\lambda}(\mathbf{a}_0) \prec n^{-1/2}$, and $\lambda(\mathbf{a}_0)$ is separated from all other roots of $0 = \det T(\lambda, \mathbf{a}_0)$ by a constant $c > 0$. Then

$$\|\mathrm{d}\lambda(\mathbf{a}_0) - \mathrm{d}\hat{\lambda}(\mathbf{a}_0)\| \prec n^{-1/2}.$$

Proof. Let $\lambda_0 = \lambda(\mathbf{a}_0)$ and $\hat{\lambda}_0 = \hat{\lambda}(\mathbf{a}_0)$. Denote by $\widehat{K}(\lambda, \mathbf{a})$ and $K(\lambda, \mathbf{a})$ the functions (4.3) and (4.5) for $F = F(\mathbf{a})$. Let us first establish, for each $r = 1, \ldots, k$,

$$\|\partial_{a_r} K(\lambda_0, \mathbf{a}_0) - \partial_{a_r} \widehat{K}(\lambda_0, \mathbf{a}_0)\| \prec n^{-1/2}. \tag{4.36}$$

The proof is similar to that of (4.8), and we will be brief. For notational convenience, we omit all arguments $(\lambda_0, \mathbf{a}_0)$ and denote $\partial = \partial_{a_r}$. Recalling G_M from (4.4),

$$\begin{aligned}\partial G_M &= (\partial F)XG_NX'F + FX(\partial G_N)X'F + FXG_NX'(\partial F) - \partial F\\ &= (\partial F)XG_NX'F - FXG_NX'(\partial F)XG_NX'F + FXG_NX'(\partial F) - \partial F\\ &= -(FXG_NX' - \mathrm{Id})(\partial F)(XG_NX'F - \mathrm{Id}).\end{aligned} \tag{4.37}$$

Denoting by $(\partial G_M)_{rs}$ the (r,s) block, (4.37) and Lemma 4.5 imply $\|(\partial G_M)_{rs}/(\sigma_r\sigma_s)\|_{\mathrm{HS}} \prec n^{1/2}$, so Lemma 4.6 applied conditionally on X yields

$$\left\|\partial\widehat{K} + \sum_{r=1}^{k}\Big(N^{-1}\operatorname{Tr}_r(\partial G_M)\Big)\Gamma_r\right\| \prec n^{-1/2}. \tag{4.38}$$

Now recall $XG_NX' = \Delta + m_0(\mathrm{Id} + m_0F)^{-1}$ from (4.6), so $XG_NX'F - \mathrm{Id} = \Delta F - (\mathrm{Id} + m_0F)^{-1}$. Substituting this into (4.37) and applying Lemmas 4.1 and 4.2, we obtain after some simplification

$$\begin{aligned}\sigma_r^{-2}\operatorname{Tr}_r(\partial G_M) = -\sigma_r^{-2}\operatorname{Tr}_r\left[(\mathrm{Id} + m_0F)^{-1}(\partial F)(\mathrm{Id} + m_0F)^{-1}\right]&\\ - N^{-1}(\partial_\lambda m_0)\operatorname{Tr}\left[(\partial F)(\mathrm{Id} + m_0F)^{-1}\right]\sigma_r^{-2}\operatorname{Tr}_r\left[F^2(\mathrm{Id} + m_0F)^{-2}\right] + O_\prec(n^{1/2})&.\end{aligned}$$

Applying (4.24) and (4.25),

$$(N\sigma_r^2)^{-1}\operatorname{Tr}_r(\partial G_M) = -(N\sigma_r^2)^{-1}\operatorname{Tr}_r\left[\partial\Big(F(\mathrm{Id} + m_0F)^{-1}\Big)\right] + O_\prec(n^{-1/2}) = -\partial t_r + O_\prec(n^{-1/2}).$$

Applying this to (4.38) and recalling the definition (4.5) of K, we obtain (4.36) as desired.

Note that (4.8), (4.9), $\lambda_0 - \hat{\lambda}_0 \prec n^{-1/2}$, and Lemma 4.5 imply

$$\|K(\lambda_0, \mathbf{a}_0) - \widehat{K}(\hat{\lambda}_0, \mathbf{a}_0)\| \prec n^{-1/2}, \tag{4.39}$$

$$\|\partial_\lambda K(\lambda_0, \mathbf{a}_0) - \partial_\lambda\widehat{K}(\hat{\lambda}_0, \mathbf{a}_0)\| \prec n^{-1/2}. \tag{4.40}$$

From (4.38), we verify that on the high-probability event where $\operatorname{spec}(X'F(\mathbf{a}_0)X) \subset \operatorname{supp}(\mu_0(\mathbf{a}_0))_{\delta/2}$, $\|X_r\| < C$, and $\|\mathring{X}_r\| < C$ for all $r = 1, \ldots, k$, we have

$$\sup_{\lambda \in \mathbb{R}\setminus\operatorname{supp}(\mu_0(\mathbf{a}_0))_\delta}\|\partial_{a_r}\widehat{K}(\lambda, \mathbf{a}_0)\| < C, \qquad \sup_{\lambda \in \mathbb{R}\setminus\operatorname{supp}(\mu_0(\mathbf{a}_0))_\delta}\|\partial_\lambda\partial_{a_r}\widehat{K}(\lambda, \mathbf{a}_0)\| < C.$$

Then this and (4.36) yield similarly

$$\|\partial_{a_r}K(\lambda_0, \mathbf{a}_0) - \partial_{a_r}\widehat{K}(\hat{\lambda}_0, \mathbf{a}_0)\| \prec n^{-1/2}. \tag{4.41}$$

Let $\mu_1(\lambda, \mathbf{a}) \le \ldots \le \mu_L(\lambda, \mathbf{a})$ and $\hat{\mu}_1(\lambda, \mathbf{a}) \le \ldots \le \hat{\mu}_L(\lambda, \mathbf{a})$ be the eigenvalues of $K(\lambda, \mathbf{a})$ and

$\widehat{K}(\lambda, \mathbf{a})$. Then (4.39) implies $\mu_\ell(\lambda_0, \mathbf{a}_0) - \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0) \prec n^{-1/2}$ for each ℓ. Note that $0 = \det K(\lambda(\mathbf{a}), \mathbf{a})$ and $0 = \det \widehat{K}(\hat{\lambda}(\mathbf{a}), \mathbf{a})$ for all $\mathbf{a} \in U$. In particular, $\mu_\ell(\lambda_0, \mathbf{a}_0) = 0$ for some ℓ. As λ_0 is separated from other roots of $0 = \det T(\lambda, \mathbf{a}_0)$ by $c > 0$, Proposition 2.11(c) implies 0 is separated from other eigenvalues of $T(\lambda_0, \mathbf{a}_0)$ by c. Assuming U is sufficiently small, this implies that $\mu_\ell(\lambda(\mathbf{a}), \mathbf{a}) = 0$ and $\hat{\mu}_\ell(\lambda(\mathbf{a}), \mathbf{a}) = 0$ for the same ℓ and all $\mathbf{a} \in U$. Differentiating these identities in $\mathbf{a}$ at $\mathbf{a}_0$, we obtain

$$\mathrm{d}\lambda(\mathbf{a}_0) = -(\partial_\lambda \mu_\ell(\lambda_0, \mathbf{a}_0))^{-1} \partial_{\mathbf{a}} \mu_\ell(\lambda_0, \mathbf{a}_0), \qquad \mathrm{d}\hat{\lambda}(\mathbf{a}_0) = -(\partial_\lambda \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0))^{-1} \partial_{\mathbf{a}} \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0). \tag{4.42}$$

Letting $\mathbf{v}_0 \in \ker K(\lambda_0, \mathbf{a}_0)$ and $\hat{\mathbf{v}}_0 \in \ker \widehat{K}(\hat{\lambda}_0, \mathbf{a}_0)$ be the unit eigenvectors, we have for both $\partial = \partial_\lambda$ and $\partial = \partial_{a_r}$ that

$$\partial \mu_\ell(\lambda_0, \mathbf{a}_0) = \mathbf{v}_0' \partial K(\lambda_0, \mathbf{a}_0) \mathbf{v}_0, \qquad \partial \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0) = \hat{\mathbf{v}}_0' \partial \widehat{K}(\hat{\lambda}_0, \mathbf{a}_0) \hat{\mathbf{v}}_0.$$

The Davis-Kahan theorem yields $\|\mathbf{v}_0 - \hat{\mathbf{v}}_0\| \prec n^{-1/2}$, so (4.40), (4.41), and the bounds $\|\partial K\|, \|\partial \widehat{K}\| \prec 1$ imply

$$\partial \mu_\ell(\lambda_0, \mathbf{a}_0) - \partial \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0) \prec n^{-1/2}, \qquad \partial \mu_\ell(\lambda_0, \mathbf{a}_0) \prec 1, \qquad \partial \hat{\mu}_\ell(\hat{\lambda}_0, \mathbf{a}_0) \prec 1.$$

Applying this and $\partial_\lambda \mu_\ell(\lambda_0, \mathbf{a}_0) \leq -1$ to (4.42), we obtain $\|\mathrm{d}\lambda(\mathbf{a}_0) - \mathrm{d}\hat{\lambda}(\mathbf{a}_0)\| \prec n^{-1/2}$. ☐

We now conclude the proofs of the remaining two claims for Theorem 2.17.

Proof of Claim 2. Suppose $\mu = \theta + \sigma_1^2$ is a spike eigenvalue of Σ_1. Each estimated $\hat{\mu}$ where $|\hat{\mu} - \mu| < \varepsilon$ corresponds to a pair $(\hat{\lambda}, \mathbf{a})$ where $\mathbf{a} \in S^{k-1}$, $\hat{\lambda} \in \mathrm{spec}(\widehat{\Sigma}(\mathbf{a})) \cap \mathcal{I}_\delta(\mathbf{a})$, and

$$|\hat{\lambda}/t_1(\hat{\lambda}, \mathbf{a}) - \mu| < \varepsilon, \qquad t_2(\hat{\lambda}, \mathbf{a}) = \ldots = t_k(\hat{\lambda}, \mathbf{a}) = 0.$$

Then $\hat{\lambda} = -1/m_0(\hat{\lambda}, \mathbf{a}) + \sigma_1^2 t_1(\hat{\lambda}, \mathbf{a})$ by (2.8). Applying this and $|t_1(\hat{\lambda}, \mathbf{a})| < C$ to the above, $(\hat{\lambda}, \mathbf{a})$ satisfies

$$\left| -\frac{1}{m_0(\hat{\lambda}, \mathbf{a})} - t_1(\hat{\lambda}, \mathbf{a})\theta \right| < C\varepsilon, \qquad t_2(\hat{\lambda}, \mathbf{a}) = \ldots = t_k(\hat{\lambda}, \mathbf{a}) = 0. \tag{4.43}$$

By Lemma 4.11, there exist constants $\varepsilon_0, \varepsilon_1 > 0$ such that if $C\varepsilon < \varepsilon_1$, then with probability $1 - n^{-D}$, (4.43) cannot hold for two different pairs $(\hat{\lambda}_0, \mathbf{a}_0)$ and $(\hat{\lambda}_1, \mathbf{a}_1)$ with $\|\mathbf{a}_1 - \mathbf{a}_0\| < \varepsilon_0$. On the other hand, on the event where the conclusion of Theorem 2.12 holds for all $\mathbf{a} \in S^{k-1}$, we have $-C < m_0(\hat{\lambda}_0, \mathbf{a}_0) < -c$ and $-C < m_0(\hat{\lambda}_1, \mathbf{a}_1) < -c$ for constants $C, c > 0$ by Lemma 4.8. On this event, if (4.43) holds for $(\hat{\lambda}_0, \mathbf{a}_0)$ and $(\hat{\lambda}_1, \mathbf{a}_1)$ with $\|\mathbf{a}_1 - \mathbf{a}_0\| \geq \varepsilon_0$, then $\|m_0(\hat{\lambda}_0, \mathbf{a}_0)\mathbf{a}_0 - m_0(\hat{\lambda}_1, \mathbf{a}_1)\mathbf{a}_1\| > c\varepsilon_0$ for some $c > 0$ because both $\mathbf{a}_0$ and $\mathbf{a}_1$ belong to the sphere. Recalling $s : \mathbb{R}^k \to \mathbb{R}^k$ from (2.20), note that $m_0(\hat{\lambda}, \mathbf{a})t(\hat{\lambda}, \mathbf{a}) = s(m_0(\hat{\lambda}, \mathbf{a})\mathbf{a})$. Assumption 2.16 then implies $\|m_0(\hat{\lambda}_0, \mathbf{a}_0)t(\hat{\lambda}_0, \mathbf{a}_0) - m_0(\hat{\lambda}_1, \mathbf{a}_1)t(\hat{\lambda}_1, \mathbf{a}_1)\| > c\varepsilon_0$ for a different $c > 0$. But the first condition of (4.43) implies $|m_0(\hat{\lambda}_0, \mathbf{a}_0)t(\hat{\lambda}_0, \mathbf{a}_0) + 1/\theta| < C\varepsilon$ and similarly for $(\hat{\lambda}_1, \mathbf{a}_1)$, for some $C > 0$. This is a contradiction for ε sufficiently small, so with probability $1 - n^{-D}$, at most one pair $(\hat{\lambda}, \mathbf{a})$ satisfies

(4.43). □

Proof of Claim 3. We first show that for a constant $c_0 > 0$ (independent of $\bar{C}$) and any value $\theta > c_0$, there exist $\mathbf{a}_0 \in S^{k-1}$ and $\lambda_0 \in \mathcal{I}_\delta(\mathbf{a}_0)$ where

$$-\frac{1}{m_0(\lambda_0, \mathbf{a}_0)} - t_1(\lambda_0, \mathbf{a}_0)\theta = 0, \qquad t_2(\lambda_0, \mathbf{a}_0) = \ldots = t_k(\lambda_0, \mathbf{a}_0) = 0. \tag{4.44}$$

Indeed, Proposition 4.3 shows $\operatorname{supp}(\mu_0(\mathbf{a})) \in [-C_1, C_1]$ for a constant $C_1 > 0$ and all $\mathbf{a} \in S^{k-1}$. Then for each $\mathbf{a} \in S^{k-1}$, at the left endpoint λ_+ of $\mathcal{I}_\delta(\mathbf{a})$ we have

$$m_0(\lambda_+, \mathbf{a}) = \int \frac{1}{x - \lambda_+}\, \mu_0(\mathbf{a})(dx) \le -(2C_1 + \delta)^{-1}, \tag{4.45}$$

and $m_0(\lambda, \mathbf{a})$ increases to 0 as λ increases from λ_+ to ∞. We apply Lemma 4.10 to the map s from (2.20): Note that $s(0) = 0$, and Assumption 2.16 guarantees $\|(\mathrm{d}s(0))\mathbf{v}\| \ge c\|\mathbf{v}\|$. Setting $U = \{\mathbf{b} : \|\mathbf{b}\| < \varepsilon\}$ for a sufficiently small constant $\varepsilon > 0$, we have $|\partial_{b_i}\partial_{b_j} s_r(\mathbf{b})| < C$ for all i, j, r and $\mathbf{b} \in U$. We may take $\varepsilon < (2C_1 + \delta)^{-1}$. Then applying Lemma 4.10, for some constant $c_0 > 0$ and any $\theta > c_0$, there exists $\mathbf{b}_0 \in U$ such that $s(\mathbf{b}_0) = (-1/\theta, 0, \ldots, 0)$. Now let $\mathbf{a}_0 = -\mathbf{b}_0/\|\mathbf{b}_0\| \in S^{k-1}$. As $\|\mathbf{b}_0\| < (2C_1 + \delta)^{-1}$, (4.45) implies there exists $\lambda \in \mathcal{I}_\delta(\mathbf{a}_0)$ with $m_0(\lambda, \mathbf{a}_0) = -\|\mathbf{b}_0\|$, and hence $\mathbf{b}_0 = m_0(\lambda_0, \mathbf{a}_0)\mathbf{a}_0$. Noting that $m_0(\lambda_0, \mathbf{a}_0)t(\lambda_0, \mathbf{a}_0) = s(\mathbf{b}_0) = (-1/\theta, 0, \ldots, 0)$, this yields (4.44).

Now let $\mu = \theta + \sigma_1^2$ be a spike eigenvalue of Σ_1, where $\theta > c_0$, and let $(\lambda_0, \mathbf{a}_0)$ be as above. By Theorem 2.12, there exists $\hat{\lambda}_0 \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}_0)) \cap \mathcal{I}_\delta(\mathbf{a}_0)$ with $\hat{\lambda}_0 - \lambda_0 \prec n^{-1/2}$. Applying Lemma 4.8,

$$-\frac{1}{m_0(\hat{\lambda}_0, \mathbf{a}_0)} - t_1(\hat{\lambda}_0, \mathbf{a}_0)\theta \prec n^{-1/2}, \qquad t_r(\hat{\lambda}_0, \mathbf{a}_0) \prec n^{-1/2} \text{ for all } r = 2, \ldots, k.$$

Lemma 4.11 implies there exist $\mathbf{a} \in S^{k-1}$ and $\hat{\lambda} \in \operatorname{spec}(\widehat{\Sigma}(\mathbf{a}))$ with $t_+(\hat{\lambda}, \mathbf{a}) = 0$ and $c\|\mathbf{a} - \mathbf{a}_0\| \le \|t_+(\hat{\lambda}_0, \mathbf{a}_0)\|$. The latter condition implies $\|\mathbf{a} - \mathbf{a}_0\| \prec n^{-1/2}$, so also $\|\widehat{\Sigma}(\mathbf{a}) - \widehat{\Sigma}(\mathbf{a}_0)\| \prec n^{-1/2}$, $\hat{\lambda} - \hat{\lambda}_0 \prec n^{-1/2}$, and $\hat{\lambda} \in \mathcal{I}_\delta(\mathbf{a})$ with probability $1 - n^{-D}$. Applying Lemma 4.8 again, we obtain

$$-\frac{1}{m_0(\hat{\lambda}, \mathbf{a})} - t_1(\hat{\lambda}, \mathbf{a})\theta \prec n^{-1/2}, \qquad t_2(\hat{\lambda}, \mathbf{a}) = \ldots = t_k(\hat{\lambda}, \mathbf{a}) = 0.$$

This and (2.8) imply $\hat{\lambda}/t_1(\hat{\lambda}, \mathbf{a}) - \mu \prec n^{-1/2}$, so with probability $1 - n^{-D}$, there is an estimated eigenvalue $\hat{\mu}$ with $|\hat{\mu} - \mu| < n^{-1/2+\varepsilon}$. □

4.3 Resolvent approximations

We conclude the preceding proofs by establishing Lemmas 4.1 and 4.2.

Both statements rely on a "fluctuation averaging" idea, similar to that in [EYY11, EYY12, EKYY13b, EKYY13a], to control a weighted average of weakly dependent random variables. We introduce a variant of this idea which controls the size of the weighted average by the squared-sum of the weights, rather than the size of the largest weight, and also develop it for sums over double-indexed and quadruple-indexed arrays. We present this abstract result in Section 4.3.1, and then apply it to combinations of resolvent entries and their products in the remainder of the section.

4.3.1 Fluctuation averaging

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be independent random variables in some probability space. For $\mathcal{Y}$ a scalar-valued function of $\mathbf{x}_1, \ldots, \mathbf{x}_n$, denote by $\mathbb{E}_i[\mathcal{Y}]$ its expectation with respect to only $\mathbf{x}_i$, i.e.

$$\mathbb{E}_i[\mathcal{Y}] = \mathbb{E}[\mathcal{Y} \mid \mathbf{x}_1, \ldots, \mathbf{x}_{i-1}, \mathbf{x}_{i+1}, \ldots, \mathbf{x}_n].$$

Define

$$\mathcal{Q}_i[\mathcal{Y}] = \mathcal{Y} - \mathbb{E}_i[\mathcal{Y}].$$

Note that the operators $\{\mathbb{E}_i, \mathcal{Q}_i : i = 1, \ldots, n\}$ all commute. For $S \subset \{1, \ldots, n\}$, define

$$\mathbb{E}_S = \prod_{i \in S} \mathbb{E}_i, \qquad \mathcal{Q}_S = \prod_{i \in S} \mathcal{Q}_i$$

where the products denote operator composition.

We will consider subsets $S \subset \{1, \ldots, n\}$ of size at most a constant $\ell > 0$. For quantities ξ and ζ possibly depending on S, we write

$$\xi \prec_\ell \zeta$$

to mean $\mathbb{P}[|\xi| > n^\varepsilon |\zeta|] < n^{-D}$ for all $|S| \leq \ell$ and all $n \geq n_0(\ell, \varepsilon, D)$, where the constant n_0 is allowed to depend on ℓ (in addition to ε and D).

We will require $\mathcal{Y}$ to satisfy the moment condition of the following lemma.

Lemma 4.13. For constants $\tau, C_1, C_2, \ldots > 0$, suppose $\mathcal{Y} \prec n^{-\tau}$ and $\mathbb{E}[|\mathcal{Y}|^\ell] \leq n^{C_\ell}$ for each integer $\ell > 0$. Then for any sub-σ-algebra $\mathcal{G}$, $\mathbb{E}[\mathcal{Y} \mid \mathcal{G}] \prec n^{-\tau}$.

Proof. See Lemma 3.9. □

A variable $\mathcal{Y}_i$ is centered with respect to $\mathbf{x}_i$ if $\mathbb{E}_i[\mathcal{Y}_i] = 0$. If it is independent of $\mathbf{x}_j$, then $\mathcal{Q}_j[\mathcal{Y}_i] = 0$. We quantify weak dependence of $\mathcal{Y}_i$ on $\mathbf{x}_j$ by requiring $\mathcal{Q}_j[\mathcal{Y}_i]$ to be typically smaller than $\mathcal{Y}_i$ by a factor of $n^{-1/2}$. The following is an abstract fluctuation averaging result for variables that are weakly dependent in this sense.

Lemma 4.14. Let $\tau, C_1, C_2, \ldots > 0$ be fixed constants, and let each $\mathcal{Y}_* \in \{\mathcal{Y}_i, \mathcal{Y}_{ij}, \mathcal{Y}_{ijkl}\}$ below be a scalar-valued function of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ that satisfies $\mathcal{Y}_* \prec n^{-\tau}$ and $\mathbb{E}[|\mathcal{Y}_*|^\ell] \leq N^{C_\ell}$ for each $\ell > 0$.

(a) Suppose $(\mathcal{Y}_i : i = 1, \ldots, n)$ satisfy $\mathbb{E}_i[\mathcal{Y}_i] = 0$ and, for all $S \subset \{1, \ldots, n\}$ with $i \notin S$ and $|S| \leq \ell$,

$$Q_S[\mathcal{Y}_i] \prec_\ell N^{-\tau-|S|/2}. \tag{4.46}$$

Then for any deterministic $(u_i \in \mathbb{C} : i = 1, \ldots, n)$,

$$\sum_i u_i \mathcal{Y}_i \prec N^{-\tau} \left(\sum_i |u_i|^2 \right)^{1/2}.$$

(b) Suppose $(\mathcal{Y}_{ij} : i, j = 1, \ldots, n,\ i \neq j)$ satisfy $\mathbb{E}_i[\mathcal{Y}_{ij}] = \mathbb{E}_j[\mathcal{Y}_{ij}] = 0$ and, for all $S \subset \{1, \ldots, n\}$ with $i, j \notin S$ and $|S| \leq \ell$,

$$Q_S[\mathcal{Y}_{ij}] \prec_\ell N^{-\tau-|S|/2}.$$

Then for any deterministic $(u_{ij} \in \mathbb{C} : i, j = 1, \ldots, n,\ i \neq j)$,

$$\sum_{i \neq j} u_{ij} \mathcal{Y}_{ij} \prec N^{-\tau} \left(\sum_{i \neq j} |u_{ij}|^2 \right)^{1/2}.$$

(c) Suppose $(\mathcal{Y}_{ijkl} : i, j, k, l = 1, \ldots, n \text{ all distinct})$ satisfy $\mathbb{E}_i[\mathcal{Y}_{ijkl}] = \mathbb{E}_j[\mathcal{Y}_{ijkl}] = \mathbb{E}_k[\mathcal{Y}_{ijkl}] = \mathbb{E}_l[\mathcal{Y}_{ijkl}] = 0$ and, for all $S \subset \{1, \ldots, n\}$ with $i, j, k, l \notin S$ and $|S| \leq \ell$,

$$Q_S[\mathcal{Y}_{ijkl}] \prec_\ell N^{-\tau-|S|/2}.$$

Then for any deterministic $(u_{ij} \in \mathbb{C} : i, j = 1, \ldots, n,\ i \neq j)$ and $(v_{kl} \in \mathbb{C} : k, l = 1, \ldots, n,\ k \neq l)$,

$$\sum_{\substack{i,j,k,l \\ \text{all distinct}}} u_{ij} v_{kl} \mathcal{Y}_{ijkl} \prec N^{-\tau} \left(\sum_{i \neq j} |u_{ij}|^2 \right)^{1/2} \left(\sum_{k \neq l} |v_{kl}|^2 \right)^{1/2}.$$

Proof. The proof is similar to the "Alternative proof of Theorem 4.7" presented in [EKYY13a, Appendix B]. Fix any constants $\varepsilon, D > 0$, and choose an even integer ℓ such that $(\ell - 1)\varepsilon > D$. For part (a), let us normalize so that $\sum_i |u_i|^2 = 1$. We apply the moment method and bound the quantity

$$\mathbb{E}\left[\left| \sum_i u_i \mathcal{Y}_i \right|^\ell \right] = \sum_{\mathbf{i}} u_{\mathbf{i}} \mathbb{E}[\mathcal{Y}_{\mathbf{i}}], \tag{4.47}$$

where we denote as shorthand

$$\mathbf{i} = (i_1, \ldots, i_\ell), \qquad \sum_{\mathbf{i}} = \sum_{i_1, \ldots, i_\ell = 1}^n, \qquad u_{\mathbf{i}} = \prod_{a=1}^{\ell/2} u_{i_a} \prod_{a=\ell/2+1}^{\ell} \overline{u_{i_a}}, \qquad \mathcal{Y}_{\mathbf{i}} = \prod_{a=1}^{\ell/2} \mathcal{Y}_{i_a} \prod_{a=\ell/2+1}^{\ell} \overline{\mathcal{Y}_{i_a}}.$$

Fix $\mathbf{i}$, and let $\mathcal{T} = \mathcal{T}(\mathbf{i}) \subset \{1,\ldots,n\}$ be the indices that appear exactly once in $\mathbf{i}$. Applying the identity

$$\mathcal{Y} = \left(\prod_{j\in\mathcal{T}}(\mathbb{E}_j + \mathcal{Q}_j)\right)\mathcal{Y} = \sum_{S\subseteq\mathcal{T}} \mathbb{E}_{\mathcal{T}\setminus S}\mathcal{Q}_S\mathcal{Y}$$

to each $\mathcal{Y}_{i_a}$ and expanding the product of the sums,

$$\mathcal{Y}_{\mathbf{i}} = \sum_{S_1,\ldots,S_\ell\subseteq\mathcal{T}} \mathcal{Y}(S_1,\ldots,S_\ell), \qquad \mathcal{Y}(S_1,\ldots,S_\ell) = \prod_{a=1}^{\ell}\mathbb{E}_{\mathcal{T}\setminus S_a}\mathcal{Q}_{S_a}\tilde{\mathcal{Y}}_{i_a}, \qquad \tilde{\mathcal{Y}}_{i_a} = \begin{cases}\mathcal{Y}_{i_a} & a\le \ell/2\\ \overline{\mathcal{Y}_{i_a}} & a\ge \ell/2+1.\end{cases}$$

Note that $Q_{i_a}\tilde{\mathcal{Y}}_{i_a} = \tilde{\mathcal{Y}}_{i_a}$, so (4.46) and Lemma 4.13 yield

$$\mathbb{E}_{\mathcal{T}\setminus S_a}\mathcal{Q}_{S_a}\tilde{\mathcal{Y}}_{i_a} \prec_\ell \mathcal{Q}_{S_a}\tilde{\mathcal{Y}}_{i_a} \prec_\ell n^{-\tau-(|S_a\setminus\{i_a\}|)/2}.$$

Then, taking the product over all $a = 1,\ldots,\ell$ and applying $\sum_a |S_a\setminus\{i_a\}| \ge -|\mathcal{T}| + \sum_a |S_a|$,

$$\mathcal{Y}(S_1,\ldots,S_\ell) \prec_\ell n^{-\ell\tau + \frac{|\mathcal{T}|}{2} - \sum_{a=1}^{\ell}\frac{|S_a|}{2}}. \tag{4.48}$$

Next, note that if $i_a \in \mathcal{T}$, then $\mathcal{Q}_{S_a}\mathcal{Y}_{i_a} = 0$ and $\mathcal{Y}(S_1,\ldots,S_\ell) = 0$ unless $i_a \in S_a$. Furthermore, if $i_a \in S_a$ but $i_a \notin S_b$ for all $b \ne a$, then $\mathbb{E}_{\mathcal{T}\setminus S_b}\mathcal{Q}_{S_b}\tilde{\mathcal{Y}}_{i_b}$ does not depend on $\mathbf{x}_{i_a}$ for all $b\ne a$, so we have

$$\mathbb{E}_{i_a}[\mathcal{Y}(S_1,\ldots,S_\ell)] = \mathbb{E}_{i_a}\left[\mathbb{E}_{\mathcal{T}\setminus S_a}\mathcal{Q}_{S_a}\tilde{\mathcal{Y}}_{i_a}\right]\prod_{b:b\ne a}(\mathbb{E}_{\mathcal{T}\setminus S_b}\mathcal{Q}_{S_b}\tilde{\mathcal{Y}}_{i_b}) = 0.$$

Thus if $\mathbb{E}[\mathcal{Y}(S_1,\ldots,S_\ell)] \ne 0$, then each $i_a \in \mathcal{T}$ must belong to both S_a and at least one other S_b, so $\sum_a |S_a| \ge 2|\mathcal{T}|$. Then (4.48) and Lemma 4.13 yield $\mathbb{E}[\mathcal{Y}(S_1,\ldots,S_\ell)] \prec_\ell n^{-\ell\tau-|\mathcal{T}|/2}$. As the number of choices of subsets $S_1,\ldots,S_\ell \subseteq \mathcal{T}$ is an ℓ-dependent constant, we arrive at

$$\mathbb{E}[\mathcal{Y}_{\mathbf{i}}] \prec_\ell n^{-\ell\tau-|\mathcal{T}|/2}.$$

Returning to (4.47), we obtain

$$\mathbb{E}\left[\left|\sum_i u_i\mathcal{Y}_i\right|^\ell\right] \prec_\ell \sum_{t=0}^{\ell} n^{-\ell\tau-t/2}\sum_{\mathbf{i}:|\mathcal{T}(\mathbf{i})|=t}|u_{\mathbf{i}}|.$$

We may separate the sum over $\{\mathbf{i} : |\mathcal{T}(\mathbf{i})| = t\}$ as a sum first over groupings of the indices $i_1,\ldots,i_\ell$ that coincide, followed by a sum over distinct values of those indices. Under our normalization,

$$\sum_i |u_i| \le n^{1/2}, \qquad \sum_i |u_i|^k \le 1 \text{ for all } k\ge 2.$$

Furthermore, the number of groupings is an ℓ-dependent constant, so

$$\sum_{\mathbf{i}:|\mathcal{T}(\mathbf{i})|=t} |u_{\mathbf{i}}| \prec_\ell n^{t/2}, \qquad \mathbb{E}\left[\left|\sum_i u_i \mathcal{Y}_i\right|^\ell\right] \prec_\ell n^{-\ell\tau}.$$

The latter statement means that the expectation is (deterministically) at most $n^{-\ell\tau+\varepsilon}$ for all $n \geq n_0(\ell,\varepsilon)$. Then, as ℓ depends only on ε and D, and we chose $(\ell-1)\varepsilon > D$, Markov's inequality yields for all $n \geq n_0(\varepsilon, D)$

$$\mathbb{P}\left[\left|\sum_i u_i \mathcal{Y}_i\right| > n^{-\tau+\varepsilon}\right] \leq \frac{n^{-\ell\tau+\varepsilon}}{(n^{-\tau+\varepsilon})^\ell} < n^{-D}.$$

As $\varepsilon, D > 0$ were arbitrary, this concludes the proof of part (a).

Parts (b) and (c) are similar, except for an additional combinatorial argument encapsulated in Lemma 4.15 below: For (b), normalize so that $\sum_{i\neq j}|u_{ij}|^2 = 1$ and write

$$\mathbb{E}\left[\left|\sum_{i\neq j} u_{ij}\mathcal{Y}_{ij}\right|^\ell\right] = \sum_{\mathbf{i},\mathbf{j}} u_{\mathbf{i},\mathbf{j}}\mathbb{E}[\mathcal{Y}_{\mathbf{i},\mathbf{j}}]$$

where

$$\sum_{\mathbf{i},\mathbf{j}} = \sum_{i_1\neq j_1}\cdots\sum_{i_\ell\neq j_\ell}, \qquad u_{\mathbf{i},\mathbf{j}} = \prod_{a=1}^{\ell/2} u_{i_a j_a} \prod_{a=\ell/2+1}^{\ell} \overline{u_{i_a j_a}}, \qquad \mathcal{Y}_{\mathbf{i},\mathbf{j}} = \prod_{a=1}^{\ell/2} \mathcal{Y}_{i_a j_a} \prod_{a=\ell/2+1}^{\ell} \overline{\mathcal{Y}_{i_a j_a}}.$$

Fixing $\mathbf{i},\mathbf{j}$ and letting $\mathcal{T} = \mathcal{T}(\mathbf{i},\mathbf{j})$ be the indices that appear exactly once in the combined vector $(\mathbf{i},\mathbf{j})$, the same argument yields $\mathbb{E}[\mathcal{Y}_{\mathbf{i},\mathbf{j}}] \prec_\ell n^{-\ell\tau-|\mathcal{T}|/2}$. Applying Lemma 4.15 with $B_a[i,j] = |u_{ij}|$ and $B_a[i,i] = 0$ for all $a = 1,\ldots,\ell$ and $i \neq j$, we get

$$\sum_{\mathbf{i},\mathbf{j}:|\mathcal{T}(\mathbf{i},\mathbf{j})|=t} |u_{\mathbf{i},\mathbf{j}}| \prec_\ell n^{t/2},$$

which concludes the proof in the same way as part (a). For part (c), normalize so that $\sum_{i\neq j}|u_{ij}|^2 = \sum_{k\neq l}|v_{kl}|^2 = 1$, and write analogously

$$\mathbb{E}\left[\left|\sum_{\substack{i,j,k,l\\ \text{distinct}}} u_{ij}v_{kl}\mathcal{Y}_{ijkl}\right|^\ell\right] = \sum_{\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}} u_{\mathbf{i},\mathbf{j}}v_{\mathbf{k},\mathbf{l}}\mathbb{E}[\mathcal{Y}_{\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}}].$$

Letting $\mathcal{T}$ be the indices appearing exactly once in the combined vector $(\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l})$, the bound

$\mathbb{E}[\mathcal{Y}_{\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}}] \prec n^{-\ell\tau-|\mathcal{T}|/2}$ follows as before, and the bound

$$\sum_{\mathbf{i},\mathbf{j},\mathbf{k},\mathbf{l}:|\mathcal{T}|=t} |u_{\mathbf{i},\mathbf{j}} v_{\mathbf{k},\mathbf{l}}| \prec n^{t/2}$$

follows from Lemma 4.15 applied with $B_a[i,j] = |u_{ij}|$ and $B_a[i,i] = 0$ for $a = 1, \ldots, \ell$ and $B_a[i,j] = |v_{ij}|$ and $B_a[i,i] = 0$ for $a = \ell+1, \ldots, 2\ell$. □

Lemma 4.15. Fix $\ell \geq 1$. For each $a = 1, \ldots, \ell$, let $B_a = (B_a[i,j]) \in \mathbb{R}^{n \times n}$ satisfy

$$B_a[i,j] \geq 0, \qquad B_a[i,i] = 0, \qquad \|B_a\|_{\mathrm{HS}} \leq 1$$

for all $i, j \in \{1, \ldots, n\}$. For $(\mathbf{i},\mathbf{j}) = (i_1, \ldots, i_\ell, j_1, \ldots, j_\ell) \in \{1, \ldots, n\}^{2\ell}$, denote by $s(\mathbf{i},\mathbf{j})$ the number of elements of $\{1, \ldots, n\}$ that appear exactly once in $(\mathbf{i},\mathbf{j})$. Then for a constant $C_\ell > 0$ and all $s \in \{0, \ldots, 2\ell\}$,

$$\sum_{\substack{\mathbf{i},\mathbf{j} \in \{1,\ldots,n\}^{2\ell} \\ s(\mathbf{i},\mathbf{j})=s}} \prod_{a=1}^{\ell} B_a[i_a, j_a] \leq C_\ell n^{s/2}.$$

Proof. Define an equivalence relation $(\mathbf{i},\mathbf{j}) \sim (\mathbf{i}',\mathbf{j}')$ if a permutation of $\{1, \ldots, n\}$ maps $(\mathbf{i},\mathbf{j})$ to $(\mathbf{i}',\mathbf{j}')$. For an equivalence class E, define $s(E) = s(\mathbf{i},\mathbf{j})$ for any $(\mathbf{i},\mathbf{j}) \in E$. Let $\mathcal{E}$ be the set of equivalence classes where $i_a \neq j_a$ for all $a = 1, \ldots, \ell$. Then, as B_a has zero diagonal,

$$\sum_{\substack{\mathbf{i},\mathbf{j} \in \{1,\ldots,n\}^{2\ell} \\ s(\mathbf{i},\mathbf{j})=s}} \prod_{a=1}^{\ell} B_a[i_a, j_a] = \sum_{E \in \mathcal{E}:\, s(E)=s} B(E), \qquad B(E) = \sum_{(\mathbf{i},\mathbf{j}) \in E} \prod_{a=1}^{\ell} B_a[i_a, j_a].$$

For $E \in \mathcal{E}$, if $(\mathbf{i},\mathbf{j}) \in E$ has m distinct values, then let $(\mathbf{u},\mathbf{v}) = (u_1, \ldots, u_\ell, v_1, \ldots, v_\ell) \in \{1, \ldots, m\}^{2\ell}$ be the canonical element of E where these values are $\{1, \ldots, m\}$ in sequential order. Identify E with the directed multi-graph on the vertex set $\{1, \ldots, m\}$ with the ℓ edges $\{(u_a, v_a) : a = 1, \ldots, \ell\}$. Writing the summation defining $B(E)$ as a summation over the m possible distinct index values,

$$B(E) = \sum_{\substack{i(1),\ldots,i(m)=1 \\ \text{distinct}}}^{n} \prod_{a=1}^{\ell} B_a[i(u_a), i(v_a)].$$

As B_a has nonnegative entries, we may drop the distinctness condition in the sum to obtain the upper bound

$$B(E) \leq U(E) = \sum_{i(1),\ldots,i(m)=1}^{n} \prod_{a=1}^{\ell} B_a[i(u_a), i(v_a)].$$

The number of equivalence classes in $\mathcal{E}$ is a constant $C_\ell > 0$, so it suffices to show for all $E \in \mathcal{E}$

$$U(E) \leq n^{s(E)/2}. \tag{4.49}$$

Let the degree of a vertex be the total number of its in-edges and out-edges. Then $s(E)$ is the number of degree-1 vertices. Consider first a class E where every vertex has even degree. Then each connected component of the multi-graph may be traversed as an Eulerian cycle, where each edge is traversed exactly once in either its forward or backward direction. Letting $\mathcal{C}$ be the set of connected components, this yields

$$U(E) \leq \prod_{C \in \mathcal{C}} \operatorname{Tr} \left(\prod_{a:(u_a,v_a) \in C} \tilde{B}_a \right),$$

where the second product over edges is taken in the order of the Eulerian cycle of C, and $\tilde{B}_a = B_a$ if (u_a, v_a) is traversed in the forward direction and $\tilde{B}_a = B'_a$ if it is traversed in the backward direction. (This holds because each term of $U(E)$ appears on the right upon expanding the traces, and the extra terms on the right are nonnegative.) Note that for any $k \geq 2$ and any matrices $A_1, \ldots, A_k$,

$$\operatorname{Tr} A_1 \ldots A_k \leq \|A_1\|_{\mathrm{HS}} \cdot \|A_2 \ldots A_k\|_{\mathrm{HS}} \leq \|A_1\|_{\mathrm{HS}} \|A_2\|_{\mathrm{HS}} \cdots \|A_k\|_{\mathrm{HS}}.$$

The multi-graph has no self-loops, so each $C \in \mathcal{C}$ has at least 2 edges. Applying this and $\|\tilde{B}_a\|_{\mathrm{HS}} \leq 1$ for each a, we obtain $U(E) \leq 1$.

Next, consider E where every vertex has degree at least 2, and there is some vertex u of odd degree. Then there is another vertex v of odd degree in the same connected component as u, because the sum of vertex degrees in a connected component is even. We may pick v such that there is a path P from u to v, traversing edges either forwards or backwards, where every intermediary vertex between u and v has degree 2. (Otherwise, replace v by the first such vertex along any path from u to v.) Let us remove the path by summing over the intermediary vertex labels: For notational convenience, suppose the intermediary vertices are $p+1, \ldots, m$. Then, since only edges in the path P touch the vertices $p+1, \ldots, m$, we have

$$U(E) = \sum_{i(1),\ldots,i(p)} \prod_{a:(u_a,v_a) \notin P} B_a[i(u_a), i(v_a)] \left(\sum_{i(p+1),\ldots,i(m)} \prod_{a:(u_a,v_a) \in P} B_a[i(u_a), i(v_a)] \right).$$

Note that the quantity in parentheses is element $[u, v]$ of the matrix

$$\prod_{a:(u_a,v_a) \in P} \tilde{B}_a,$$

where the product is taken in the order of traversal of P, and $\tilde{B}_a = B_a$ or B'_a depending on the direction of traversal of edge a. As the Hilbert-Schmidt norm of this product is at most 1, we obtain

$$U(E) \leq U(E'), \qquad U(E') = \sum_{i(1),\ldots,i(p)} \prod_{a:(u_a,v_a)\notin P} B_a[i(u_a), i(v_a)].$$

Here E' corresponds to the multi-graph with path P and intermediary vertices $p+1,\ldots,m$ removed. Each vertex of this new multi-graph still has degree at least 2—hence we may iteratively apply this procedure until the resulting graph has no vertices of odd degree. Then $U(E) \leq 1$ follows from the first case above.

Finally, consider E where $s(E) = s > 0$. For notational convenience, let $1,\ldots,s$ be the vertices of degree 1. Then, applying the general inequality $\sum_{i=1}^N w_i \leq N^{1/2}(\sum_{i=1}^N w_i^2)^{1/2}$ with $N = n^s$, we have

$$U(E) \leq n^{s/2} U(E')^{1/2}, \qquad U(E') = \sum_{i_1,\ldots,i_s=1}^{n} \left(\sum_{i_{s+1},\ldots,i_m=1}^{n} \prod_{a=1}^{\ell} B_a[i(u_a), i(v_a)] \right)^2.$$

The quantity $U(E')$ corresponds to a multi-graph with $s + 2(m-s)$ vertices and 2ℓ edges, where each vertex $s+1,\ldots,m$ is duplicated into two copies. Each of the original vertices $1,\ldots,s$ now has degree 2, and each copy of $s+1,\ldots,m$ continues to have degree at least 2. Then $U(E') \leq 1$ from the above, so $U(E) \leq n^{s/2}$. This establishes (4.49) in all cases, concluding the proof. $\square$

4.3.2 Preliminaries

We first reduce the proofs of Lemmas 4.1 and 4.2 to the case where F is diagonal and invertible, and z belongs to

$$U_\delta^{\mathbb{C}} = \{z \in U_\delta : |\mathrm{Im}\, z| \geq N^{-2}\}.$$

This latter reduction is for convenience of verifying the moment condition of Lemma 4.13.

Lemma 4.16. Suppose Lemmas 4.1 and 4.2 hold for $z \in U_\delta^{\mathbb{C}}$ and when F is replaced by any invertible diagonal matrix T satisfying $\|T\| \leq C$. Then they hold also for the given matrix F and any $z \in U_\delta$.

Proof. Applying rotational invariance in law of X and the transformations $F \mapsto O'FO$, $X \mapsto O'X$, $V \mapsto O'VO$, and $W \mapsto O'WO$, we may reduce from F to the diagonal matrix T of its eigenvalues.

If T is not invertible and/or $z \notin U_\delta^{\mathbb{C}}$, consider an invertible matrix $\tilde{T}$ with $\|T - \tilde{T}\| \leq N^{-2}$ and $\tilde{z} \in U_\delta^{\mathbb{C}}$ with $|z - \tilde{z}| \leq N^{-2}$. Then, denoting by $\tilde{m}_0$ and $\tilde{\Delta}$ these quantities defined with $\tilde{T}$ and $\tilde{z}$, on the high-probability event where $\mathrm{spec}(X'TX) \subset \mathrm{supp}(\mu_0)_{\delta/2}$ and $\|X\| < C$, we have

$$|m_0 - \tilde{m}_0| < CN^{-2}, \qquad |\partial_z m_0 - \partial_z \tilde{m}_0| < CN^{-2}, \qquad \|\Delta - \tilde{\Delta}\| < CN^{-2}.$$

Here, the first two statements follow from (2.11) and the condition $z \in U_\delta$, and the third applies Proposition 4.4 and the identity $A^{-1} - B^{-1} = A^{-1}(B-A)B^{-1}$. Bounding the trace by M times the operator norm, one may then verify $\operatorname{Tr}\Delta V - \operatorname{Tr}\tilde{\Delta}V \prec N^{-1/2}\|V\|_{\mathrm{HS}}$. Similarly, the quantity on the left of Lemma 4.2 changes by $O_\prec(N^{1/2}\|V\|\|W\|)$ upon replacing m_0 and Δ by $\tilde{m}_0$ and $\tilde{\Delta}$. So it suffices to establish Lemmas 4.1 and 4.2 for $\tilde{T}$ and $\tilde{z}$. $\square$

Thus, in the remainder of this section, we consider a diagonal matrix

$$T = \operatorname{diag}(t_1, \ldots, t_M) \in \mathbb{R}^{M\times M}, \qquad t_\alpha \neq 0 \text{ for all } t_\alpha.$$

Define the $(N+M)\times(N+M)$ linearized resolvent

$$G(z) = \begin{pmatrix} -z\operatorname{Id}_N & X' \\ X & -T^{-1} \end{pmatrix}^{-1} = \begin{pmatrix} G_N(z) & G_o(z)' \\ G_o(z) & G_M(z) \end{pmatrix},$$

where the Schur complement identity yields

$$G_N(z) = (X'TX - z\operatorname{Id}_N)^{-1}, \qquad G_o(z) = TXG_N(z), \qquad G_M(z) = TXG_N(z)X'T - T. \tag{4.50}$$

From (4.7), we have

$$\Delta(z) = T^{-1}(G_M(z) - \Pi_M(z))T^{-1}, \qquad \Pi_M(z) = -T(\operatorname{Id} + m_0(z)T)^{-1}. \tag{4.51}$$

Note that G, G_N, G_M are symmetric, and Π_M is diagonal. We omit the spectral argument z when the meaning is clear.

We use the same index notation as in Chapter 3: Denote $\mathcal{I}_N = \{1, \ldots, N\}$, $\mathcal{I}_M = \{1, \ldots, M\}$, and the disjoint union $\mathcal{I} = \mathcal{I}_N \sqcup \mathcal{I}_M$. We index G_N by $\mathcal{I}_N$, G_M by $\mathcal{I}_M$, and G by $\mathcal{I}$. We use Roman letters i, j, k for indices in $\mathcal{I}_N$, Greek letters α, β, γ for indices in $\mathcal{I}_M$, and capital letters A, B, C for general indices in $\mathcal{I}$. We denote by $\mathbf{x}_i \in \mathbb{R}^M$ and $\mathbf{x}_\alpha \in \mathbb{R}^N$ the i^{th} column and α^{th} row of X, both regarded as column vectors. For any subset $\mathcal{S} \subset \mathcal{I}$, $X^{(\mathcal{S})}$ denotes X with rows in $\mathcal{S} \cap \mathcal{I}_M$ and columns in $\mathcal{S} \cap \mathcal{I}_N$ removed, $T^{(\mathcal{S})}$ denotes T with rows and columns in $\mathcal{S} \cap \mathcal{I}_M$ removed, and $G^{(\mathcal{S})}, G_N^{(\mathcal{S})}$ etc. denote these quantities defined with $X^{(\mathcal{S})}$ and $T^{(\mathcal{S})}$ in place of X and T. We index these matrices by $\mathcal{I}_N \setminus \mathcal{S}$ and $\mathcal{I}_M \setminus \mathcal{S}$.

Lemma 4.17 (Resolvent identities)**.**

(a) For all $i \in \mathcal{I}_N$ and $\alpha \in \mathcal{I}_M$,

$$G_{ii} = -\frac{1}{z + \mathbf{x}_i' G_M^{(i)} \mathbf{x}_i}, \qquad G_{\alpha\alpha} = -\frac{t_\alpha}{1 + t_\alpha \mathbf{x}_\alpha' G_N^{(\alpha)} \mathbf{x}_\alpha}.$$

(b) For all $i \neq j \in \mathcal{I}_N$ and $\alpha \neq \beta \in \mathcal{I}_M$, denoting by $\mathbf{e}_i \in \mathbb{R}^N$ and $\mathbf{e}_\alpha \in \mathbb{R}^M$ the standard basis vectors for coordinates i and α,

$$G_{ij} = -G_{ii}\mathbf{x}_i' G_o^{(i)} \mathbf{e}_j = G_{ii} G_{jj}^{(i)} \mathbf{x}_i' G_M^{(ij)} \mathbf{x}_j,$$
$$G_{i\alpha} = -G_{ii}\mathbf{x}_i' G_M^{(i)} \mathbf{e}_\alpha = -G_{\alpha\alpha}\mathbf{e}_i' G_N^{(\alpha)} \mathbf{x}_\alpha,$$
$$G_{\alpha\beta} = -G_{\alpha\alpha}\mathbf{e}_\beta' G_o^{(\alpha)} \mathbf{x}_\alpha = G_{\alpha\alpha} G_{\beta\beta}^{(\alpha)} \mathbf{x}_\alpha' G_N^{(\alpha\beta)} \mathbf{x}_\beta.$$

(c) For all $C \in \mathcal{I}$ and $A, B \in \mathcal{I} \setminus \{C\}$,

$$G_{AB}^{(C)} = G_{AB} - \frac{G_{AC} G_{CB}}{G_{CC}}.$$

Proof. See Lemma 3.15. The second equalities for G_{ij} and $G_{\alpha\beta}$ follow from applying the identities again to the matrices $G_o^{(\alpha)}$ and $G_o^{(i)}$. □

For $i \neq j \in \mathcal{I}_N$ and $\alpha \neq \beta \in \mathcal{I}_M$, define

$$\mathcal{Z}_i = \mathbf{x}_i' G_M^{(i)} \mathbf{x}_i - N^{-1} \operatorname{Tr} G_M^{(i)}, \qquad \mathcal{Z}_\alpha = \mathbf{x}_\alpha' G_N^{(\alpha)} \mathbf{x}_\alpha - N^{-1} \operatorname{Tr} G_N^{(\alpha)},$$

$$\mathcal{Z}_{ij} = \mathbf{x}_i' G_M^{(ij)} \mathbf{x}_j, \qquad \mathcal{Z}_{\alpha\beta} = \mathbf{x}_\alpha' G_N^{(\alpha\beta)} \mathbf{x}_\beta.$$

We will use the following bounds implicitly throughout the remainder of this section. Note that $(|z| \vee 1)^{-1} \leq 1$ and $t_\alpha \leq C$, so we will omit these factors in the bounds in certain applications.

Lemma 4.18. For all $z \in U_\delta$,

(a) (Norm bounds)

$$\|G_N\| \prec (|z| \vee 1)^{-1}, \qquad \|G_o\| \prec (|z| \vee 1)^{-1}, \qquad \|G_M\| \prec 1.$$

(b) (Diagonal bounds) For all $i \in \mathcal{I}_N$ and $\alpha \in \mathcal{I}_M$,

$$G_{ii} \prec (|z| \vee 1)^{-1}, \qquad G_{ii}^{-1} \prec |z| \vee 1, \qquad G_{\alpha\alpha} \prec t_\alpha, \qquad G_{\alpha\alpha}^{-1} \prec t_\alpha^{-1}.$$

(c) ($\mathcal{Z}$ bounds) For all $i \neq j \in \mathcal{I}_N$ and $\alpha \neq \beta \in \mathcal{I}_M$,

$$\mathcal{Z}_i \prec N^{-1/2}, \qquad \mathcal{Z}_\alpha \prec (|z| \vee 1)^{-1} N^{-1/2}, \qquad \mathcal{Z}_{ij} \prec N^{-1/2}, \qquad \mathcal{Z}_{\alpha\beta} \prec (|z| \vee 1)^{-1} N^{-1/2},$$

$$\mathbf{e}_i' G_N^{(\alpha)} \mathbf{x}_\alpha \prec (|z| \vee 1)^{-1} N^{-1/2}, \qquad \mathbf{x}_i' G_M^{(i)} \mathbf{e}_\alpha \prec t_\alpha N^{-1/2},$$
$$\mathbf{x}_i' G_o^{(i)} \mathbf{e}_j \prec (|z| \vee 1)^{-1} N^{-1/2}, \qquad \mathbf{e}_\beta' G_o^{(\alpha)} \mathbf{x}_\alpha \prec t_\beta (|z| \vee 1)^{-1} N^{-1/2}.$$

(d) (Off-diagonal bounds) For all $i \neq j \in \mathcal{I}_N$ and $\alpha \neq \beta \in \mathcal{I}_M$,

$$G_{ij} \prec (|z| \vee 1)^{-2} N^{-1/2}, \qquad G_{i\alpha} \prec t_\alpha (|z| \vee 1)^{-1} N^{-1/2}, \qquad G_{\alpha\beta} \prec t_\alpha t_\beta (|z| \vee 1)^{-1} N^{-1/2}.$$

Proof. By Theorem 2.5, $\operatorname{spec}(X'TX) \subset \operatorname{supp}(\mu_0)_{\delta/2}$ holds with high probability. On this event, $\|G_N\| \leq C \min(1/\delta, 1/|z|)$. As $\|X\| \prec 1$, part (a) follows from (4.50).

For (b), the bounds on G_{ii} and $G_{\alpha\alpha}$ follow from (4.50) and part (a). The bounds on G_{ii}^{-1} and $G_{\alpha\alpha}^{-1}$ follow from Lemma 4.17(a), $\|G_N^{(\alpha)}\| \prec 1$ and $\|G_M^{(i)}\| \prec 1$ in part (a), and $\|\mathbf{x}_i\| \prec 1$ and $\|\mathbf{x}_\alpha\| \prec 1$.

For (c), note that part (a) implies $\|G_M^{(i)}\|_{\mathrm{HS}} \prec N^{1/2}$ and $\|G_N^{(\alpha)}\|_{\mathrm{HS}} \prec (|z| \vee 1)^{-1} N^{1/2}$. Then the bounds for $\mathcal{Z}_i$ and $\mathcal{Z}_\alpha$ follow from Lemma 4.6 applied conditionally on $X^{(i)}$ and $X^{(\alpha)}$. For $\mathcal{Z}_{ij}$, as $\mathbf{x}_i$ is independent of $G_M^{(ij)} \mathbf{x}_j$, we have that $\mathbf{x}_i' G_M^{(ij)} \mathbf{x}_j$ is Gaussian conditional on $X^{(i)}$ and $|\mathbf{x}_i' G_M^{(ij)} \mathbf{x}_j| \prec N^{-1/2} \|G_M^{(ij)} \mathbf{x}_j\| \prec N^{-1/2} \|G_M^{(ij)}\| \prec N^{-1/2}$. The remaining five bounds are similar.

Finally, (d) follows from Lemma 4.17(b) and parts (b) and (c). □

4.3.3 Linear functions of the resolvent

We prove Lemma 4.1. Let $\mathbb{E}_i$ and $\mathbb{E}_\alpha$ be the partial expectations over column $\mathbf{x}_i$ and row $\mathbf{x}_\alpha$ of X. For $S \subset \mathcal{I}_N$ or $S \subset \mathcal{I}_M$, let $\mathbb{E}_S$, $\mathcal{Q}_S$, and $\prec_\ell$ be as in Section 4.3.1. Note that $\mathbb{E}_i[\mathcal{Z}_i] = 0$, $\mathbb{E}_\alpha[\mathcal{Z}_\alpha] = 0$, and $\mathbb{E}_\alpha[\mathcal{Z}_{\alpha\beta}] = \mathbb{E}_\beta[\mathcal{Z}_{\alpha\beta}] = 0$. We verify that these quantities satisfy the conditions of Lemma 4.14.

Lemma 4.19. For $z \in U_\delta^{\mathbb{C}}$, each $\mathcal{Z}_* \in \{\mathcal{Z}_i, \mathcal{Z}_\alpha, \mathcal{Z}_{\alpha\beta}\}$, and some constants $C_1, C_2, \ldots > 0$, we have $\mathbb{E}[|\mathcal{Z}_*|^\ell] \leq N^{C_\ell}$ for each $\ell > 0$. Furthermore, for any constant $\ell > 0$,

(a) For $S \subset \mathcal{I}_N$ with $i \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Z}_i \prec_\ell N^{-1/2-|S|/2}$.

(b) For $S \subset \mathcal{I}_M$ with $\alpha \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Z}_\alpha \prec_\ell N^{-1/2-|S|/2}$.

(c) For $S \subset \mathcal{I}_M$ with $\alpha, \beta \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Z}_{\alpha\beta} \prec_\ell N^{-1/2-|S|/2}$.

Proof. Let $C_\ell > 0$ denote an ℓ-dependent constant that may change from instance to instance. Taking the expectation first over $\mathbf{x}_i$, we have $\mathbb{E}[|\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i|^\ell] \leq \mathbb{E}[\|G_M^{(i)}\|^\ell \|\mathbf{x}_i\|^{2\ell}] \leq C_\ell \mathbb{E}[\|G_M^{(i)}\|^\ell]$. Note that $\|G_N^{(i)}\| \leq 1/|\operatorname{Im} z| \leq N^2$ for $z \in U_\delta^{\mathbb{C}}$, so $\|G_M^{(i)}\| \leq C(N^2 \|X^{(i)}\|^2 + 1)$ by (4.50). Then $\mathbb{E}[|\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i|^\ell] \leq N^{C_\ell}$ follows. Also $\mathbb{E}[|N^{-1} \operatorname{Tr} G_M^{(i)}|^\ell] \leq C_\ell \mathbb{E}[\|G_M^{(i)}\|^\ell] \leq N^{C_\ell}$, so $\mathbb{E}[|\mathcal{Z}_i|^\ell] \leq N^{C_\ell}$. Similar arguments show $\mathbb{E}[|\mathcal{Z}_\alpha|^\ell] \leq N^{C_\ell}$ and $\mathbb{E}[|\mathcal{Z}_{\alpha\beta}|^\ell] \leq N^{C_\ell}$.

For the remaining statements, the argument is similar to the type of resolvent expansion performed in [BEK$^+$14]. We begin with (a): For $S = \emptyset$, this follows from Lemma 4.18. For $|S| \geq 1$, observe that $\mathcal{Z}_i = \mathcal{Q}_i[\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i]$, so $\mathcal{Q}_S[\mathcal{Z}_i] = \mathcal{Q}_{S \cup \{i\}}[\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i]$. Define

$$G_{\mathbf{x}j}^{(i)} = \sum_{\alpha \in \mathcal{I}_M} X_{i\alpha} G_{\alpha j}^{(i)} = \mathbf{x}_i' G_o^{(i)} \mathbf{e}_j.$$

Suppose $j \in S$. We may apply Lemma 4.17(c) to write

$$\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i = \sum_{\alpha,\beta} X_{\alpha i} G_{\alpha\beta}^{(i)} X_{\beta i} = L(\{j\}) + R(\{j\})$$

where

$$L(\{j\}) = \sum_{\alpha,\beta} X_{\alpha i} G_{\alpha\beta}^{(ij)} X_{\beta i} = \mathbf{x}_i' G_M^{(ij)} \mathbf{x}_i, \qquad R(\{j\}) = \sum_{\alpha,\beta} X_{\alpha i} \frac{G_{\alpha j}^{(i)} G_{\beta j}^{(i)}}{G_{jj}^{(i)}} X_{\beta i} = \frac{(G_{\mathbf{x}j}^{(i)})^2}{G_{jj}^{(i)}}.$$

Here, $L(\{j\})$ no longer depends on $\mathbf{x}_j$. Note that Lemma 4.17(c) yields, for $j \neq k$,

$$G_{\mathbf{x}j} = G_{\mathbf{x}j}^{(k)} + \frac{G_{\mathbf{x}k} G_{jk}}{G_{kk}}, \qquad \frac{1}{G_{jj}} = \frac{1}{G_{jj}^{(k)}} - \frac{G_{jk}^2}{G_{jj} G_{jj}^{(k)} G_{kk}}. \tag{4.52}$$

Then if $|S| \geq 2$ and $k \in S$, let us apply these identities to the numerator and denominator of $R(\{j\})$ to further write

$$\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i = L(\{j,k\}) + R(\{j,k\}),$$

where

$$L(\{j,k\}) = L(\{j\}) + \frac{(G_{\mathbf{x}j}^{(ik)})^2}{G_{jj}^{(ik)}}$$

collects terms which no longer depend on at least one of $\mathbf{x}_j$ or $\mathbf{x}_k$, and the remainder is

$$R(\{j,k\}) = -(G_{\mathbf{x}j}^{(ik)})^2 \frac{(G_{jk}^{(i)})^2}{G_{jj}^{(i)} G_{jj}^{(ik)} G_{kk}^{(i)}} + G_{\mathbf{x}j}^{(ik)} \frac{G_{\mathbf{x}k}^{(i)} G_{jk}^{(i)}}{G_{kk}^{(i)}} \frac{1}{G_{jj}^{(i)}} + \frac{G_{\mathbf{x}k}^{(i)} G_{jk}^{(i)}}{G_{kk}^{(i)}} G_{\mathbf{x}j}^{(i)} \frac{1}{G_{jj}^{(i)}}.$$

Recursively using (4.52) to apply this procedure for each index in S, we obtain

$$\mathbf{x}_i' G_M^{(i)} \mathbf{x}_i = L(S) + R(S),$$

where

- Each term of $L(S)$ does not depend on at least one of the columns $(\mathbf{x}_j : j \in S)$.
- $R(S)$ is a sum of at most C_ℓ summands, each summand a product of at most C_ℓ terms, for a constant C_ℓ depending only on ℓ (the maximum size of S).
- Each summand of $R(S)$ is a product of 2 terms of the form $G_{\mathbf{x}j}^{(\mathcal{T})}$, some number $m \geq |S|-1$ of terms of the form $G_{jk}^{(\mathcal{T})}$ for $j \neq k$, and $m+1$ terms of the form $(G_{jj}^{(\mathcal{T})})^{-1}$. Here $i \in \mathcal{T} \subseteq S$.

We observe that $\mathcal{Q}_{S \cup \{i\}}[L(S)] = 0$. Applying $G_{\mathbf{x}j}^{(\mathcal{T})} \prec_\ell (|z| \vee 1)^{-1} N^{-1/2}$, $G_{jk}^{(\mathcal{T})} \prec_\ell (|z| \vee 1)^{-1} N^{-1/2}$, and $(G_{jj}^{(\mathcal{T})})^{-1} \prec_\ell |z| \vee 1$, we have $R(S) \prec_\ell N^{-(|S|+1)/2}$. Then part (a) follows from Lemma 4.13 and the bound

$$\mathcal{Q}_{S\cup\{i\}}[R(S)] = \left(\prod_{j\in S\cup\{i\}}(1-\mathbb{E}_j)\right)[R(S)] \leq \sum_{\mathcal{T}:\mathcal{T}\subseteq S\cup\{i\}} |\mathbb{E}_{\mathcal{T}}[R(S)]| \prec_\ell R(S).$$

The proof of part (b) is similar: Define

$$\check{G}_{\alpha\beta} = \frac{G_{\alpha\beta}}{|t_\alpha t_\beta|^{1/2}}, \qquad \check{G}^{(\alpha)}_{\beta\mathbf{x}} = \sum_{i\in\mathcal{I}_N} \frac{G_{\beta i}}{|t_\beta|^{1/2}} X_{i\alpha} = |t_\beta|^{-1/2}\mathbf{e}'_\beta G_o^{(\alpha)}\mathbf{x}_\alpha.$$

We apply Lemma 4.17(c) in the forms

$$\mathbf{x}'_\alpha G_N^{(\alpha)}\mathbf{x}_\alpha = \mathbf{x}'_\alpha G_N^{(\alpha\beta)}\mathbf{x}_\alpha + \frac{(\check{G}^{(\alpha)}_{\beta\mathbf{x}})^2}{\check{G}^{(\alpha)}_{\beta\beta}}, \qquad \check{G}_{\alpha\beta} = \check{G}^{(\gamma)}_{\alpha\beta} + \frac{\check{G}_{\alpha\gamma}\check{G}_{\beta\gamma}}{\check{G}_{\gamma\gamma}}, \qquad \frac{1}{\check{G}_{\beta\beta}} = \frac{1}{\check{G}^{(\gamma)}_{\beta\beta}} - \frac{(\check{G}_{\beta\gamma})^2}{\check{G}_{\beta\beta}\check{G}^{(\gamma)}_{\beta\beta}\check{G}_{\gamma\gamma}}. \tag{4.53}$$

This allows us to write, for each $S \subset \mathcal{I}_M$ with $|S|\geq 1$ and $\alpha \notin S$,

$$\mathbf{x}'_\alpha G_N^{(\alpha)}\mathbf{x}_\alpha = L(S) + R(S),$$

where $L(S)$ contains terms not depending on at least one row $(\mathbf{x}_\beta : \beta \in S)$, and each summand of $R(S)$ is a product of 2 terms of the form $\check{G}^{(\mathcal{T})}_{\beta\mathbf{x}}$, $m \geq |S|-1$ terms of the form $\check{G}^{(\mathcal{T})}_{\beta\gamma}$ for $\beta \neq \gamma$, and $m+1$ terms of the form $(\check{G}^{(\mathcal{T})}_{\beta\beta})^{-1}$. Applying $\check{G}^{(\mathcal{T})}_{\beta\mathbf{x}} \prec N^{-1/2}$, $\check{G}^{(\mathcal{T})}_{\beta\gamma} \prec N^{-1/2}$, and $(\check{G}^{(\mathcal{T})}_{\beta\beta})^{-1} \prec 1$, we obtain part (b). The argument for part (c) is similar and omitted for brevity. $\square$

Define the empirical Stieltjes transform

$$m_N(z) = N^{-1}\operatorname{Tr} G_N(z) = N^{-1}\operatorname{Tr}(X'TX - z\operatorname{Id})^{-1}.$$

We next establish a bound on $m_N - m_0$ for z separated from $\operatorname{supp}(\mu_0)$. We follow [BEK+14, KY17], although for simplicity we will use the result of Theorem 2.5 to establish "stability" of the Marcenko-Pastur equation, rather than proving this directly using the stochastic continuity argument of [BEK+14].

Lemma 4.20. Let $z \in U_\delta^{\mathbb{C}}$. Then $m_N(z) - m_0(z) \prec N^{-1}$.

Proof. Recall the function

$$z_0(m) = -\frac{1}{m} + \frac{1}{N}\sum_\alpha \frac{t_\alpha}{1+t_\alpha m}.$$

We first establish the following claim: If for all $z \in U_\delta^{\mathbb{C}}$ and a constant $\tau > 0$ we have

$$z - z_0(m_N(z)) \prec N^{-\tau}, \tag{4.54}$$

then also for all $z \in U_\delta^{\mathbb{C}}$ we have

$$m_0(z) - m_N(z) \prec N^{-\tau}. \tag{4.55}$$

Indeed, fix any constants $\varepsilon, D > 0$. Suppose first that $\operatorname{Im} z \geq N^{-\tau+\varepsilon}$. Let $\mathcal{E}$ be the event where $|z - z_0(m_N)| < N^{-\tau+\varepsilon/2}$, which holds with probability at least $1 - N^{-D}$ by (4.54). On $\mathcal{E}$ we have $\operatorname{Im} z_0(m_N) > 0$, so Theorem 2.4 guarantees that $m_0(z_0(m_N))$ is the unique root $m \in \mathbb{C}^+$ to the equation $z_0(m_N) = z_0(m)$. Thus $m_0(z_0(m_N)) = m_N$. Applying $|\partial_z m_0| \leq C$ for all $z \in U_\delta$ and integrating this bound along a path from z to $z_0(m_N)$, we obtain

$$|m_0(z) - m_N(z)| = |m_0(z) - m_0(z_0(m_N))| < CN^{-\tau+\varepsilon/2}.$$

Now suppose $\operatorname{Im} z \in (0, N^{-\tau+\varepsilon})$. Let $\tilde{z}$ be such that $\operatorname{Re} \tilde{z} = \operatorname{Re} z$ and $\operatorname{Im} \tilde{z} = N^{-\tau+\varepsilon}$. By the preceding argument, $|m_0(\tilde{z}) - m_N(\tilde{z})| < CN^{-\tau+\varepsilon/2}$ with probability at least $1 - N^{-D}$. Apply again $|\partial_z m_0| \leq C$, and also $|\partial_z m_N| \leq C$ on the event $\operatorname{spec}(X'TX) \subset \operatorname{supp}(\mu_0)_{\delta/2}$, which holds with probability $1 - N^{-D}$ by Theorem 2.5. Then

$$|m_0(z) - m_N(z)| \leq |m_0(z) - m_0(\tilde{z})| + |m_0(\tilde{z}) - m_N(\tilde{z})| + |m_N(\tilde{z}) - m_N(z)| < CN^{-\tau+\varepsilon/2}$$

with probability $1 - 2N^{-D}$. The same arguments hold by conjugation symmetry for $\operatorname{Im} z < 0$, and hence in all cases we obtain (4.55).

It remains to establish (4.54) for $\tau = 1$. Applying Lemma 4.17(a),

$$G_{ii}^{-1} = -z - \mathbf{x}_i' G_M^{(i)} \mathbf{x}_i = -z - N^{-1} \operatorname{Tr} G_M^{(i)} - \mathcal{Z}_i. \tag{4.56}$$

Next, applying Lemma 4.17(c),

$$N^{-1} \operatorname{Tr} G_M^{(i)} = N^{-1} \sum_\alpha G_{\alpha\alpha}^{(i)} = N^{-1} \sum_\alpha \left(G_{\alpha\alpha} - \frac{G_{i\alpha}^2}{G_{ii}} \right) = N^{-1} \operatorname{Tr} G_M - G_{ii}^{-1} N^{-1} \sum_\alpha G_{i\alpha}^2.$$

Then applying the bounds $G_{ii}^{-1} \prec |z| \vee 1$ and $G_{i\alpha} \prec (|z| \vee 1)^{-1/2} N^{-1/2}$,

$$G_{ii}^{-1} = -z - N^{-1} \operatorname{Tr} G_M - \mathcal{Z}_i + O_\prec(N^{-1}). \tag{4.57}$$

Applying $\mathcal{Z}_i \prec N^{-1/2}$ and $G_{jj} \prec (|z| \vee 1)^{-1}$, this yields $G_{jj}/G_{ii} - 1 = G_{jj}(G_{ii}^{-1} - G_{jj}^{-1}) \prec (|z| \vee 1)^{-1} N^{-1/2}$ for all $i, j \in \mathcal{I}_N$. Then for all $i \in \mathcal{I}_N$, we have $m_N/G_{ii} - 1 \prec (|z| \vee 1)^{-1} N^{-1/2}$, and hence also

$$G_{ii}/m_N - 1 \prec (|z| \vee 1)^{-1} N^{-1/2}. \tag{4.58}$$

Expanding G_{ii}^{-1} around m_N^{-1},

$$\begin{aligned}N^{-1}\sum_i G_{ii}^{-1} &= N^{-1}\sum_i \left(m_N^{-1} - m_N^{-2}(G_{ii}-m_N) + m_N^{-2}G_{ii}^{-1}(G_{ii}-m_N)^2\right)\\ &= m_N^{-1} + N^{-1}m_N^{-2}\sum_i G_{ii}^{-1}(G_{ii}-m_N)^2.\end{aligned}$$

Thus

$$m_N^{-1} = N^{-1}\sum_i G_{ii}^{-1}\left(1-(G_{ii}/m_N-1)^2\right).$$

Applying (4.58), $G_{ii}^{-1} \prec |z|\vee 1$, and (4.57), we obtain

$$m_N^{-1} = N^{-1}\sum_i G_{ii}^{-1} + O_\prec(N^{-1}) = -z - N^{-1}\operatorname{Tr} G_M - N^{-1}\sum_i \mathcal{Z}_i + O_\prec(N^{-1}). \tag{4.59}$$

Next, applying Lemma 4.17 and the bounds $G_{\alpha\alpha}^{-1} \prec t_\alpha^{-1}$ and $G_{i\alpha} \prec t_\alpha N^{-1/2}$, we obtain analogously to (4.57)

$$t_\alpha G_{\alpha\alpha}^{-1} = -1 - t_\alpha \mathbf{x}_\alpha' G_N^{(\alpha)}\mathbf{x}_\alpha = -1 - t_\alpha m_N - t_\alpha \mathcal{Z}_\alpha + O_\prec(t_\alpha N^{-1}). \tag{4.60}$$

Since $G_{\alpha\alpha}/t_\alpha \prec 1$ and $\mathcal{Z}_\alpha \prec N^{-1/2}$, the above implies in particular $(1+t_\alpha m_N)^{-1} \prec 1$ and $(1+t_\alpha m_N + t_\alpha\mathcal{Z}_\alpha)^{-1} \prec 1$. Then multiplying the above by $G_{\alpha\alpha}(1+t_\alpha m_N+t_\alpha\mathcal{Z}_\alpha)^{-1}$, we obtain

$$\begin{aligned}G_{\alpha\alpha} &= -\frac{t_\alpha}{1+t_\alpha m_N + t_\alpha \mathcal{Z}_\alpha} + O_\prec(t_\alpha^2 N^{-1})\\ &= -\frac{t_\alpha}{1+t_\alpha m_N} + \frac{t_\alpha^2\mathcal{Z}_\alpha}{(1+t_\alpha m_N)^2} + O_\prec(t_\alpha^2 N^{-1}).\end{aligned} \tag{4.61}$$

As $\operatorname{Tr} G_M = \sum_\alpha G_{\alpha\alpha}$, combining with (4.59) and recalling the definition of $z_0(m)$, we have

$$z - z_0(m_N) = -N^{-1}\sum_i \mathcal{Z}_i - N^{-1}\sum_\alpha \frac{t_\alpha^2}{(1+t_\alpha m_N)^2}\mathcal{Z}_\alpha + O_\prec(N^{-1}).$$

Applying first the bounds $\mathcal{Z}_i \prec N^{-1/2}$, $\mathcal{Z}_\alpha \prec N^{-1/2}$, and $(1+t_\alpha m_N)^{-1} \prec 1$ to the above, we obtain $z - z_0(m_N) \prec N^{-1/2}$. Then (4.55) yields $m_0 - m_N \prec N^{-1/2}$. This allows us to replace m_N by m_0 with an additional $O_\prec(N^{-1})$ error, yielding

$$z - z_0(m_N) = -N^{-1}\sum_i \mathcal{Z}_i - N^{-1}\sum_\alpha \frac{t_\alpha^2}{(1+t_\alpha m_0)^2}\mathcal{Z}_\alpha + O_\prec(N^{-1}).$$

By Proposition 4.4, $|t_\alpha|^2/|1+t_\alpha m_0|^2 \leq C$ for a constant $C>0$. Then Lemmas 4.14(a) and 4.19(a–b) imply that both sums above are $O_\prec(N^{-1})$. So (4.54) holds with $\tau = 1$. □

We record an estimate from the above proof for future use:

Lemma 4.21. For $z \in U_\delta^{\mathbb{C}}$ and each $\alpha \in \mathcal{I}_M$,

$$\frac{G_{\alpha\alpha} - \Pi_{\alpha\alpha}}{t_\alpha^2} = \frac{1}{(1 + t_\alpha m_0)^2} \mathcal{Z}_\alpha + O_\prec(N^{-1}).$$

Proof. This follows from (4.61), upon applying $m_N - m_0 \prec N^{-1}$ and $|1+t_\alpha m_0| \geq c$ from Proposition 4.4 to yield $-t_\alpha/(1 + t_\alpha m_N) = \Pi_{\alpha\alpha} + O_\prec(t_\alpha^2 N^{-1})$ and $t_\alpha^2 \mathcal{Z}_\alpha/(1 + t_\alpha m_N)^2 = t_\alpha^2 \mathcal{Z}_\alpha/(1 + t_\alpha m_0)^2 + O_\prec(t_\alpha^2 N^{-1})$. $\square$

We now conclude the proof of Lemma 4.1: By Lemma 4.16, we may consider the case where $F = T$ is diagonal and invertible, and $z \in U_\delta^{\mathbb{C}}$. We write

$$\operatorname{Tr} \Delta V = \sum_\alpha \Delta_{\alpha\alpha} V_{\alpha\alpha} + \sum_{\alpha \neq \beta} \Delta_{\alpha\beta} V_{\alpha\beta}.$$

Applying (4.51) and Lemma 4.21,

$$\sum_\alpha \Delta_{\alpha\alpha} V_{\alpha\alpha} = \sum_\alpha \frac{G_{\alpha\alpha} - \Pi_{\alpha\alpha}}{t_\alpha^2} V_{\alpha\alpha} = \sum_\alpha \frac{1}{(1 + t_\alpha m_0)^2} V_{\alpha\alpha} \mathcal{Z}_\alpha + O_\prec(N^{-1/2} \|V\|_{\mathrm{HS}}).$$

As $|1 + t_\alpha m_0| > c$ by Proposition 4.4, we may apply Lemmas 4.14(a) and 4.19(b) to yield

$$\sum_\alpha \Delta_{\alpha\alpha} V_{\alpha\alpha} \prec N^{-1/2} \|V\|_{\mathrm{HS}}.$$

For the off-diagonal contribution, by (4.51) and Lemma 4.17(b) we have

$$\sum_{\alpha \neq \beta} \Delta_{\alpha\beta} V_{\alpha\beta} = \sum_{\alpha \neq \beta} \frac{G_{\alpha\beta}}{t_\alpha t_\beta} V_{\alpha\beta} = \sum_{\alpha \neq \beta} \frac{G_{\alpha\alpha} G_{\beta\beta}^{(\alpha)}}{t_\alpha t_\beta} V_{\alpha\beta} \mathcal{Z}_{\alpha\beta}.$$

As $\mathcal{Z}_{\alpha\beta} \prec N^{-1/2}$ and $\sum_{\alpha \neq \beta} |V_{\alpha\beta}| \leq M (\sum_{\alpha \neq \beta} |V_{\alpha\beta}|^2)^{1/2} \prec N \|V\|_{\mathrm{HS}}$, we may make $O_\prec(N^{-1})$ adjustments of the coefficients of $V_{\alpha\beta} \mathcal{Z}_{\alpha\beta}$ while incurring an $O_\prec(N^{-1/2} \|V\|_{\mathrm{HS}})$ error in the sum. Then, applying $G_{\beta\beta}^{(\alpha)}/t_\beta = G_{\beta\beta}/t_\beta + O_\prec(N^{-1})$ by Lemma 4.17(c), followed by Lemma 4.21, we have

$$\sum_{\alpha \neq \beta} \Delta_{\alpha\beta} V_{\alpha\beta} = \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} + O_\prec(N^{-1/2} \|V\|_{\mathrm{HS}})$$

where

$$\mathrm{I} = \sum_{\alpha \neq \beta} \frac{\Pi_{\alpha\alpha} \Pi_{\beta\beta}}{t_\alpha t_\beta} V_{\alpha\beta} \mathcal{Z}_{\alpha\beta},$$

$$\mathrm{II} = \sum_{\alpha \neq \beta} \frac{t_\alpha}{(1+t_\alpha m_0)^2} \mathcal{Z}_\alpha \frac{\Pi_{\beta\beta}}{t_\beta} V_{\alpha\beta} \mathcal{Z}_{\alpha\beta},$$
$$\mathrm{III} = \sum_{\alpha \neq \beta} \frac{\Pi_{\alpha\alpha}}{t_\alpha} \frac{t_\beta}{(1+t_\beta m_0)^2} \mathcal{Z}_\beta V_{\alpha\beta} \mathcal{Z}_{\alpha\beta},$$
$$\mathrm{IV} = \sum_{\alpha \neq \beta} \frac{t_\alpha}{(1+t_\alpha m_0)^2} \mathcal{Z}_\alpha \frac{t_\beta}{(1+t_\beta m_0)^2} \mathcal{Z}_\beta V_{\alpha\beta} \mathcal{Z}_{\alpha\beta}.$$

Lemmas 4.14(b) and 4.19(c) yield $\mathrm{I} \prec N^{-1/2}\|V\|_{\mathrm{HS}}$. For II, first fixing α and summing over β, Lemmas 4.14(a) and 4.19(c) yield

$$\sum_{\beta \notin \{\alpha\}} \frac{\Pi_{\beta\beta}}{t_\beta} V_{\alpha\beta} \mathcal{Z}_{\alpha\beta} \prec N^{-1/2}\|\mathbf{v}_\alpha\|$$

where $\mathbf{v}_\alpha$ is row α of V. Then, applying $\mathcal{Z}_\alpha \prec N^{-1/2}$,

$$\mathrm{II} \prec \sum_\alpha N^{-1}\|\mathbf{v}_\alpha\| \prec N^{-1/2}\|V\|_{\mathrm{HS}}.$$

Similarly $\mathrm{III} \prec N^{-1/2}\|V\|_{\mathrm{HS}}$. Finally, the direct bounds $\mathcal{Z}_\alpha, \mathcal{Z}_\beta, \mathcal{Z}_{\alpha\beta} \prec N^{-1/2}$ and $\sum_{\alpha \neq \beta}|V_{\alpha\beta}| \prec N\|V\|_{\mathrm{HS}}$ yield $\mathrm{IV} \prec N^{-1/2}\|V\|_{\mathrm{HS}}$. Thus $\operatorname{Tr} \Delta V \prec N^{-1/2}\|V\|_{\mathrm{HS}}$ as desired.

4.3.4 Quadratic functions of the resolvent

We now prove Lemma 4.2. We will apply the fluctuation averaging mechanism, Lemma 4.14, to the quantities

$$\mathcal{Y}_{\alpha\beta\gamma\rho} = (\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\beta)(\mathbf{x}_\gamma' G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\rho), \qquad \mathcal{Y}_{\alpha\beta\gamma} = (\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)} \mathbf{x}_\beta)(\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma),$$
$$\tilde{\mathcal{Y}}_{\alpha\beta\gamma} = G_{\alpha\alpha}^{(\beta\gamma)} (\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)} \mathbf{x}_\beta)(\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma),$$
$$\mathcal{Y}_{\alpha\beta,1} = \mathcal{Z}_{\alpha\beta}^2 - N^{-1}\mathbf{x}_\alpha'(G_N^{(\alpha\beta)})^2\mathbf{x}_\alpha, \qquad \mathcal{Y}_{\alpha\beta,2} = N^{-1}\mathbf{x}_\alpha'(G_N^{(\alpha\beta)})^2\mathbf{x}_\alpha - N^{-2}\operatorname{Tr}[(G_N^{(\alpha\beta)})^2]$$

where $\alpha, \beta, \gamma, \rho$ above are distinct. Note that each $\mathcal{Y}_*$ above satisfies $\mathcal{Y}_* \prec N^{-1}$, and furthermore

$$\mathbb{E}_\alpha[\mathcal{Y}_{\alpha\beta\gamma\rho}] = \mathbb{E}_\beta[\mathcal{Y}_{\alpha\beta\gamma\rho}] = \mathbb{E}_\gamma[\mathcal{Y}_{\alpha\beta\gamma\rho}] = \mathbb{E}_\rho[\mathcal{Y}_{\alpha\beta\gamma\rho}] = 0,$$

$$\mathbb{E}_\beta[\mathcal{Y}_{\alpha\beta\gamma}] = \mathbb{E}_\gamma[\mathcal{Y}_{\alpha\beta\gamma}] = 0, \qquad \mathbb{E}_\beta[\tilde{\mathcal{Y}}_{\alpha\beta\gamma}] = \mathbb{E}_\gamma[\tilde{\mathcal{Y}}_{\alpha\beta\gamma}] = 0, \qquad \mathbb{E}_\beta[\mathcal{Y}_{\alpha\beta,1}] = 0, \qquad \mathbb{E}_\alpha[\mathcal{Y}_{\alpha\beta,2}] = 0.$$

The following verifies the conditions of Lemma 4.14.

Lemma 4.22. For $z \in U_\delta^{\mathbb{C}}$, each $\mathcal{Y}_* \in \{\mathcal{Y}_{\alpha\beta\gamma\rho}, \mathcal{Y}_{\alpha\beta\gamma}, \tilde{\mathcal{Y}}_{\alpha\beta\gamma}, \mathcal{Y}_{\alpha\beta,1}, \mathcal{Y}_{\alpha\beta,2}\}$, and some constants $C_1, C_2, \ldots > 0$, we have $\mathbb{E}[|\mathcal{Y}_*|^\ell] \leq N^{C_\ell}$ for all $\ell > 0$. Furthermore, for any constant $\ell > 0$,

(a) For $S \subset \mathcal{I}_M$ with $\alpha, \beta, \gamma, \rho \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Y}_{\alpha\beta\gamma\rho} \prec_\ell N^{-1-|S|/2}$.

(b) For $S \subset \mathcal{I}_M$ with $\alpha, \beta, \gamma \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Y}_{\alpha\beta\gamma} \prec_\ell N^{-1-|S|/2}$.

(c) For $S \subset \mathcal{I}_M$ with $\alpha, \beta, \gamma \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \tilde{\mathcal{Y}}_{\alpha\beta\gamma} \prec_\ell N^{-1-|S|/2}$.

(d) For $S \subset \mathcal{I}_M$ with $\alpha, \beta \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Y}_{\alpha\beta,1} \prec_\ell N^{-1-|S|/2}$.

(e) For $S \subset \mathcal{I}_M$ with $\alpha, \beta \notin S$ and $|S| \leq \ell$, $\mathcal{Q}_S \mathcal{Y}_{\alpha\beta,2} \prec_\ell N^{-1-|S|/2}$.

Proof. The bound $\mathbb{E}[|\mathcal{Y}_*|^\ell] \leq N^{C_\ell}$ follows from $\|G_N^{(*)}\| \leq 1/|\mathrm{Im}\, z| \leq N^2$ for $z \in U_\delta^{\mathbb{C}}$ and the same arguments as in Lemma 4.19.

The remainder of the proof is also similar to Lemma 4.19(b–c): For (a), define

$$\check{G}_{\alpha\beta} = \frac{G_{\alpha\beta}}{|t_\alpha t_\beta|^{1/2}}, \qquad \check{G}_{\eta\mathbf{x}_\alpha}^{(\alpha\beta\gamma\rho)} = \mathbf{e}_\eta' G_o^{(\alpha\beta\gamma\rho)} \mathbf{x}_\alpha / |t_\eta|^{1/2} = \sum_i \frac{G_{\eta i}^{(\alpha\beta\gamma\rho)}}{|t_\eta|^{1/2}} X_{i\alpha}.$$

We iterate through S and expand both of the terms $\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\beta$ and $\mathbf{x}_\gamma' G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\rho$ simultaneously, using Lemma 4.17(c) in the form

$$\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\beta = \mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma\rho\eta)} \mathbf{x}_\beta + \frac{\check{G}_{\eta\mathbf{x}_\alpha}^{(\alpha\beta\gamma\rho)} \check{G}_{\eta\mathbf{x}_\beta}^{(\alpha\beta\gamma\rho)}}{\check{G}_{\eta\eta}^{(\alpha\beta\gamma\rho)}}$$

together with the latter two identities of (4.53). This yields, for each $S \subset \mathcal{I}_M$ with $|S| \geq 1$ and $\alpha, \beta, \gamma, \rho \notin S$, a decomposition

$$\mathcal{Y}_{\alpha\beta\gamma\rho} = L(S) + R(S)$$

where $L(S)$ collects terms not depending on at least one row $(\mathbf{x}_\eta : \eta \in S)$, and each summand of $R(S)$ is a product of $m \geq |S|+2$ "numerator" terms of the form $\mathbf{x}_\alpha' G_N^{(\mathcal{T})} \mathbf{x}_\beta$, $\check{G}_{\eta\mathbf{x}_\alpha}^{(\mathcal{T})}$, or $\check{G}_{\eta\nu}^{(\mathcal{T})}$ and $m-2$ "denominator" terms of the form $(\check{G}_{\eta\eta}^{(\mathcal{T})})^{-1}$. Each numerator term is $O_\prec(N^{-1/2})$ and each denominator term is $O_\prec(1)$, so $R(S) \prec_\ell N^{-1-|S|/2}$. Then $\mathcal{Q}_S[\mathcal{Y}_{\alpha\beta\gamma\rho}] = \mathcal{Q}_S[R(S)] \prec_\ell N^{-1-|S|/2}$.

The same argument holds for parts (b–e). For (c), we expand also the term $G_{\alpha\alpha}^{(\beta\gamma)}$ together with the other two terms, using the second identity of (4.53). For (d) and (e) we apply this argument separately to

$$\mathcal{Z}_{\alpha\beta}^2 = (\mathbf{x}_\alpha' G_N^{(\alpha\beta)} \mathbf{x}_\beta)^2, \qquad \mathbf{x}_\alpha' (G_N^{(\alpha\beta)})^2 \mathbf{x}_\alpha = \sum_i (\mathbf{x}_\alpha' G_N^{(\alpha\beta)} \mathbf{e}_i)^2, \qquad \mathrm{Tr}[(G_N^{(\alpha\beta)})^2] = \sum_{i,j} (\mathbf{e}_i' G_N^{(\alpha\beta)} \mathbf{e}_j)^2$$

and to each of the above summands. We obtain the additional numerator terms $\mathbf{x}_\alpha' G_N^{(\alpha\beta)} \mathbf{e}_i$, $\mathbf{e}_i' G_N^{(\alpha\beta)} \mathbf{e}_j$, and $\check{G}_{i\eta}^{(\mathcal{T})} = G_{i\eta}^{(\mathcal{T})} / |t_\eta|^{1/2}$ in the expansions, which are still $O_\prec(N^{-1/2})$. $\square$

Using this, we prove Lemma 4.2. By Lemma 4.16, we may consider $F = T$ diagonal and invertible, and $z \in U_\delta^{\mathbb{C}}$. For convenience, let us normalize so that $\|V\|=\|W\|=1$. We write

$$\operatorname{Tr} \Delta V \Delta W = \sum_{\alpha,\beta,\gamma,\rho} \Delta_{\alpha\beta} V_{\beta\gamma} \Delta_{\gamma\rho} W_{\rho\alpha}. \tag{4.62}$$

Fixing α, β, summing over γ, ρ, and applying Lemma 4.1,

$$\sum_{\gamma,\rho \notin \{\alpha,\beta\}} V_{\beta\gamma} \Delta_{\gamma\rho} W_{\rho\alpha} \prec N^{-1/2}. \tag{4.63}$$

Combining with the bound $\Delta_{\alpha\beta} \prec N^{-1/2}$ and then summing over α, β, we see that $\operatorname{Tr} \Delta V \Delta W \prec N$.

We show that the terms where $\alpha = \beta$, $\alpha = \gamma$, $\beta = \rho$, and/or $\gamma = \rho$ are $O_\prec(1)$: Consider first $\alpha = \beta$. Applying again (4.63) and $\Delta_{\alpha\alpha} \prec N^{-1/2}$, we obtain

$$\sum_{\alpha,\gamma,\rho} \Delta_{\alpha\alpha} V_{\alpha\gamma} \Delta_{\gamma\rho} W_{\rho\alpha} \prec \sum_\alpha |\Delta_{\alpha\alpha}| N^{-1/2} \prec 1.$$

Symmetrically, for $\gamma = \rho$,

$$\sum_{\alpha,\beta,\gamma} \Delta_{\alpha\beta} V_{\beta\gamma} \Delta_{\gamma\gamma} W_{\gamma\alpha} \prec 1.$$

For $\alpha = \gamma$, let $\mathbf{v}_\alpha$ and $\mathbf{w}_\alpha$ be columns α of V and W. Summing first over β, ρ, we have by Lemma 4.1

$$\sum_{\alpha,\beta,\rho} \Delta_{\alpha\beta} V_{\beta\alpha} \Delta_{\alpha\rho} W_{\rho\alpha} = \sum_\alpha \mathbf{e}_\alpha' \Delta \mathbf{v}_\alpha \mathbf{e}_\alpha' \Delta \mathbf{w}_\alpha \prec \sum_\alpha N^{-1/2} \cdot N^{-1/2} \prec 1.$$

Symmetrically, for $\beta = \rho$,

$$\sum_{\alpha,\beta,\gamma} \Delta_{\alpha\beta} V_{\beta\gamma} \Delta_{\gamma\beta} W_{\beta\alpha} \prec 1.$$

When two or more of these four cases hold simultaneously, for example $\alpha = \beta = \gamma$ or $\alpha = \gamma,\ \beta = \rho$ or $\alpha = \beta = \gamma = \rho$, we have

$$\begin{aligned}
\sum_{\alpha,\rho} \Delta_{\alpha\alpha} V_{\alpha\alpha} \Delta_{\alpha\rho} W_{\rho\alpha} &\prec \sum_\alpha |\Delta_{\alpha\alpha} V_{\alpha\alpha}| N^{-1/2} \prec 1, \\
\sum_{\alpha,\beta} \Delta_{\alpha\beta} V_{\beta\alpha} \Delta_{\alpha\beta} W_{\beta\alpha} &\prec N^{-1} \sum_{\alpha,\beta} |V_{\beta\alpha} W_{\beta\alpha}| \prec 1, \\
\sum_\alpha \Delta_{\alpha\alpha} V_{\alpha\alpha} \Delta_{\alpha\alpha} W_{\alpha\alpha} &\prec N^{-1} \sum_\alpha |V_{\alpha\alpha} W_{\alpha\alpha}| \prec 1.
\end{aligned}$$

Then we may eliminate all of these cases from the sum (4.62) by inclusion-exclusion.

The remaining cases are when possibly $\alpha = \rho$ and/or $\beta = \gamma$. We write the contributions from these cases as

$$\mathrm{I} = \sum_{\alpha,\beta,\gamma,\rho}^{*} \Delta_{\alpha\beta} V_{\beta\gamma} \Delta_{\gamma\rho} W_{\rho\alpha}, \qquad \mathrm{II} = \sum_{\alpha,\beta,\gamma}^{*} \Delta_{\alpha\beta} V_{\beta\gamma} \Delta_{\gamma\alpha} W_{\alpha\alpha},$$

$$\mathrm{III} = \sum_{\alpha,\beta,\rho}^{*} \Delta_{\alpha\beta} V_{\beta\beta} \Delta_{\beta\rho} W_{\rho\alpha}, \qquad \mathrm{IV} = \sum_{\alpha,\beta}^{*} \Delta_{\alpha\beta} V_{\beta\beta} \Delta_{\beta\alpha} W_{\alpha\alpha},$$

where summations with $*$ denote that all indices are restricted to be distinct.

For I, let us first apply

$$G_{\alpha\alpha}/t_\alpha = \Pi_{\alpha\alpha}/t_\alpha + O_\prec(N^{-1/2}), \qquad G^{(\alpha)}_{\beta\beta}/t_\beta = \Pi_{\beta\beta}/t_\beta + O_\prec(N^{-1/2})$$

from Lemma 4.21. Then, by (4.51) and Lemma 4.17(b), we have

$$\Delta_{\alpha\beta} = \frac{G_{\alpha\beta}}{t_\alpha t_\beta} = \frac{G_{\alpha\alpha} G^{(\alpha)}_{\beta\beta}}{t_\alpha t_\beta} \mathcal{Z}_{\alpha\beta} = \frac{\Pi_{\alpha\alpha}}{t_\alpha} \frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta} + O_\prec(N^{-1}). \tag{4.64}$$

Note that (4.63) holds also with the summation further restricted to $\gamma \neq \rho$, by Lemma 4.1. Then, as the $O_\prec(N^{-1})$ remainder term in (4.64) does not depend on γ and ρ,

$$\mathrm{I} = \sum_{\alpha,\beta,\gamma,\rho}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha} \frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta} \right) V_{\beta\gamma} \Delta_{\gamma\rho} W_{\rho\alpha} + O_\prec(N^{1/2}). \tag{4.65}$$

For fixed γ and ρ, applying Lemma 4.14(b) and Lemma 4.19(c), we also have

$$\sum_{\alpha,\beta \notin \{\gamma,\rho\}}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha} \frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta} \right) V_{\beta\gamma} W_{\rho\alpha} \prec N^{-1/2}.$$

Then we may apply the approximation (4.64) to $\Delta_{\gamma\rho}$ in (4.65), yielding

$$\mathrm{I} = \sum_{\alpha,\beta,\gamma,\rho}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha} \frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta} \right) V_{\beta\gamma} \left(\frac{\Pi_{\gamma\gamma}}{t_\gamma} \frac{\Pi_{\rho\rho}}{t_\rho} \mathcal{Z}_{\gamma\rho} \right) W_{\rho\alpha} + O_\prec(N^{1/2}). \tag{4.66}$$

Next, let us apply Lemma 4.17(b–c) and write

$$\begin{aligned} \mathcal{Z}_{\alpha\beta} &= \mathbf{x}'_\alpha G_N^{(\alpha\beta)} \mathbf{x}_\beta \\ &= \sum_{i,j} X_{\alpha i} X_{\beta j} \left(G^{(\alpha\beta\gamma)}_{ij} + \frac{G^{(\alpha\beta)}_{i\gamma} G^{(\alpha\beta)}_{j\gamma}}{G^{(\alpha\beta)}_{\gamma\gamma}} \right) \\ &= \sum_{i,j} X_{\alpha i} X_{\beta j} \left(G^{(\alpha\beta\gamma)}_{ij} + G^{(\alpha\beta)}_{\gamma\gamma} (\mathbf{e}'_i G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma)(\mathbf{e}'_j G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma) \right) \\ &= \mathbf{x}'_\alpha G_N^{(\alpha\beta\gamma)} \mathbf{x}_\beta + G^{(\alpha\beta)}_{\gamma\gamma} (\mathbf{x}'_\alpha G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma)(\mathbf{x}'_\beta G_N^{(\alpha\beta\gamma)} \mathbf{x}_\gamma). \end{aligned} \tag{4.67}$$

Applying these steps again to the first term of (4.67), we obtain $\mathcal{Z}_{\alpha\beta} = \mathcal{Z}^{(\gamma\rho)}_{\alpha\beta} + R_{\alpha\beta\gamma\rho}$ where

$$\mathcal{Z}^{(\gamma\rho)}_{\alpha\beta} = \mathbf{x}'_\alpha G_N^{(\alpha\beta\gamma\rho)} \mathbf{x}_\beta,$$

$$R_{\alpha\beta\gamma\rho} = G_{\gamma\gamma}^{(\alpha\beta)}(\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)}\mathbf{x}_\gamma)(\mathbf{x}_\beta' G_N^{(\alpha\beta\gamma)}\mathbf{x}_\gamma) + G_{\rho\rho}^{(\alpha\beta\gamma)}(\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma\rho)}\mathbf{x}_\rho)(\mathbf{x}_\beta' G_N^{(\alpha\beta\gamma\rho)}\mathbf{x}_\rho).$$

By Lemmas 4.14(b) and 4.22(c), for fixed γ and ρ, we have

$$\sum_{\alpha,\beta\notin\{\gamma,\rho\}}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta} R_{\alpha\beta\gamma\rho}\right) V_{\beta\gamma} W_{\rho\alpha} \prec N^{-1}.$$

Then, applying this and $\mathcal{Z}_{\gamma\rho} \prec N^{-1/2}$, (4.66) holds with $\mathcal{Z}_{\alpha\beta}$ replaced by $\mathcal{Z}_{\alpha\beta}^{(\gamma\rho)}$. Applying the symmetric argument to replace $\mathcal{Z}_{\gamma\rho}$ by $\mathcal{Z}_{\gamma\rho}^{(\alpha\beta)}$, we obtain

$$\mathrm{I} = \sum_{\alpha,\beta,\gamma,\rho}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta}^{(\gamma\rho)}\right) V_{\beta\gamma} \left(\frac{\Pi_{\gamma\gamma}}{t_\gamma}\frac{\Pi_{\rho\rho}}{t_\rho} \mathcal{Z}_{\gamma\rho}^{(\alpha\beta)}\right) W_{\rho\alpha} + O_\prec(N^{1/2}).$$

Recognizing $\mathcal{Z}_{\alpha\beta}^{(\gamma\rho)}\mathcal{Z}_{\gamma\rho}^{(\alpha\beta)} = \mathcal{Y}_{\alpha\beta\gamma\rho}$ and applying Lemmas 4.14(c) and 4.22(a), the summation above is $O_\prec(1)$. Then $\mathrm{I} \prec N^{1/2}$.

A similar argument holds for II: Lemma 4.1 yields for fixed α, β

$$\sum_{\gamma\notin\{\alpha,\beta\}} V_{\beta\gamma}\Delta_{\gamma\alpha}W_{\alpha\alpha} \prec N^{-1/2}.$$

Then applying (4.64),

$$\mathrm{II} = \sum_{\alpha,\beta,\gamma}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta}\right) V_{\beta\gamma}\Delta_{\gamma\alpha}W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

For fixed α, γ, Lemmas 4.14(a) and Lemma 4.19(c) then yield

$$\sum_{\beta\notin\{\alpha,\gamma\}} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta}\right) V_{\beta\gamma}W_{\alpha\alpha} \prec N^{-1/2},$$

so applying (4.64) again to approximate $\Delta_{\gamma\alpha}$ yields

$$\mathrm{II} = \sum_{\alpha,\beta,\gamma}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta} \mathcal{Z}_{\alpha\beta}\right) V_{\beta\gamma} \left(\frac{\Pi_{\gamma\gamma}}{t_\gamma}\frac{\Pi_{\alpha\alpha}}{t_\alpha} \mathcal{Z}_{\alpha\gamma}\right) W_{\alpha\alpha} + O_\prec(N^{1/2}). \tag{4.68}$$

Note that

$$\sum_{\beta\notin\{\alpha,\gamma\}} \frac{\Pi_{\beta\beta}}{t_\beta} G_{\gamma\gamma}^{(\alpha\beta)}(\mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)}\mathbf{x}_\gamma)(\mathbf{x}_\beta' G_N^{(\alpha\beta\gamma)}\mathbf{x}_\gamma) V_{\beta\gamma} \prec N^{-1}$$

by Lemmas 4.14(a) and 4.22(c). Then applying (4.67) and $\mathcal{Z}_{\alpha\gamma} \prec N^{-1/2}$, we may replace $\mathcal{Z}_{\alpha\beta}$ by

$\mathcal{Z}_{\alpha\beta}^{(\gamma)} = \mathbf{x}_\alpha' G_N^{(\alpha\beta\gamma)} \mathbf{x}_\beta$ in (4.68). Applying the symmetric argument to replace $\mathcal{Z}_{\alpha\gamma}$ by $\mathcal{Z}_{\alpha\gamma}^{(\beta)}$, we obtain

$$\mathrm{II} = \sum_{\alpha,\beta,\gamma}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\mathcal{Z}_{\alpha\beta}^{(\gamma)}\right) V_{\beta\gamma} \left(\frac{\Pi_{\gamma\gamma}}{t_\gamma}\frac{\Pi_{\alpha\alpha}}{t_\alpha}\mathcal{Z}_{\alpha\gamma}^{(\beta)}\right) W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

Recognizing $\mathcal{Z}_{\alpha\beta}^{(\gamma)}\mathcal{Z}_{\alpha\gamma}^{(\beta)} = \mathcal{Y}_{\alpha\beta\gamma}$ and applying Lemmas 4.14(b) and 4.22(b),

$$\sum_{\beta,\gamma\notin\{\alpha\}}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\mathcal{Z}_{\alpha\beta}^{(\gamma)}\right) V_{\beta\gamma} \left(\frac{\Pi_{\gamma\gamma}}{t_\gamma}\frac{\Pi_{\alpha\alpha}}{t_\alpha}\mathcal{Z}_{\alpha\gamma}^{(\beta)}\right) \prec N^{-1}\|V\|_{\mathrm{HS}} \prec N^{-1/2}.$$

Then $\mathrm{II} \prec N^{1/2}$. By symmetry, $\mathrm{III} \prec N^{1/2}$ also.

For IV, a direct bound using (4.64), $|V_{\beta\beta}| \leq 1$, and $|W_{\alpha\alpha}| \leq 1$ yields

$$\mathrm{IV} = \sum_{\alpha,\beta}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\mathcal{Z}_{\alpha\beta}\right)^2 V_{\beta\beta} W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

Summing first over β, Lemmas 4.14(a) and 4.22(d) yield

$$\sum_{\beta\notin\{\alpha\}} \left(\frac{\Pi_{\beta\beta}}{t_\beta}\right)^2 V_{\beta\beta}\left(\mathcal{Z}_{\alpha\beta}^2 - \mathbb{E}_\beta[\mathcal{Z}_{\alpha\beta}^2]\right) \prec N^{-1/2}.$$

Then summing over α and applying $|W_{\alpha\alpha}| \leq 1$,

$$\mathrm{IV} = \sum_{\alpha,\beta}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\right)^2 \mathbb{E}_\beta[\mathcal{Z}_{\alpha\beta}^2] V_{\beta\beta} W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

Next, summing first over α, Lemmas 4.14(a) and 4.22(e) yield

$$\sum_{\alpha\notin\{\beta\}} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\right)^2 W_{\alpha\alpha}\left(\mathbb{E}_\beta[\mathcal{Z}_{\alpha\beta}^2] - \mathbb{E}_{\alpha\beta}[\mathcal{Z}_{\alpha\beta}^2]\right) \prec N^{-1/2}.$$

Summing over β and applying $|V_{\beta\beta}| \leq 1$,

$$\mathrm{IV} = \sum_{\alpha,\beta}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\right)^2 \mathbb{E}_{\alpha\beta}[\mathcal{Z}_{\alpha\beta}^2] V_{\beta\beta} W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

Finally, let us verify

$$\mathbb{E}_{\alpha\beta}[\mathcal{Z}_{\alpha\beta}^2] = N^{-1}\partial_z m_0 + O_\prec(N^{-3/2}). \tag{4.69}$$

First note that $\mathbb{E}_{\alpha\beta}[\mathcal{Z}_{\alpha\beta}^2] = N^{-2}\,\mathrm{Tr}[(G_N^{(\alpha\beta)})^2]$. Writing $G_N^{(\alpha\beta)} = G_N + R$, Lemma 4.17(c) implies that each entry of R is $O_\prec(N^{-1})$. Then $\operatorname{Tr}[(G_N^{(\alpha\beta)})^2] = \operatorname{Tr} G_N^2 + 2\operatorname{Tr} G_N R + \operatorname{Tr} R^2$. We have

$$\operatorname{Tr} G_N R = \sum_i G_{ii}R_{ii} + \sum_{i\neq j} G_{ij}R_{ij} \prec \sum_i 1\cdot N^{-1} + \sum_{i\neq j} N^{-1/2}\cdot N^{-1} \prec N^{1/2}, \qquad \operatorname{Tr} R^2 = \sum_{i,j} R_{ij}^2 \prec 1.$$

Hence $\mathbb{E}_{\alpha\beta}[\mathcal{Z}_{\alpha\beta}^2] = N^{-2}\operatorname{Tr} G_N^2 + O_\prec(N^{-3/2})$. Next, note that $N^{-1}\operatorname{Tr} G_N^2 = \partial_z m_N$ by the spectral representation of G_N. From Lemma 4.20, $m_N - m_0 \prec N^{-1}$. Applying the same Lipschitz continuity and Cauchy integral argument as in Section 4.1.1, we obtain $\partial_z m_N - \partial_z m_0 \prec N^{-1}$, and hence (4.69).

Combining these arguments,

$$\operatorname{Tr} \Delta V \Delta W = \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} + O_\prec(1) = N^{-1}(\partial_z m_0) \sum_{\alpha,\beta}^{*} \left(\frac{\Pi_{\alpha\alpha}}{t_\alpha}\frac{\Pi_{\beta\beta}}{t_\beta}\right)^2 V_{\beta\beta}W_{\alpha\alpha} + O_\prec(N^{1/2}).$$

Including the $\alpha = \beta$ case into the sum introduces an $O_\prec(1)$ error. Then writing $\sum_\beta V_{\beta\beta}(\Pi_{\beta\beta}/t_\beta)^2 = \operatorname{Tr}(V[\mathrm{Id} + m_0 T]^{-2})$ and similarly for W concludes the proof.

Chapter 5

General bulk eigenvalue law

In this chapter, we prove Theorems 2.19 and 2.20, which establish fixed-point equations for the bulk eigenvalue distribution of $\widehat{\Sigma}$ for general, unstructured covariances $\Sigma_1, \ldots, \Sigma_k$. Our proof uses the tools of operator-valued free probability theory, in particular rectangular probability spaces and their connection to operator-valued freeness developed in [BG09], and the free deterministic equivalents approach of [SV12]. We first provide an overview of the proof strategy.

Let us write α_r in (2.1) as $\alpha_r = \sqrt{m_r} G_r \Sigma_r^{1/2}$, where $G_r \in \mathbb{R}^{m_r \times p}$ has i.i.d. $\mathcal{N}(0, 1/m_r)$ entries. Then $\widehat{\Sigma} = Y'BY$ takes the form

$$\widehat{\Sigma} = \sum_{r,s=1}^{k} \Sigma_r^{1/2} G_r' (\sqrt{m_r m_s} U_r' B U_s) G_s \Sigma_s^{1/2}.$$

We observe the following: If $O_0, O_1, \ldots, O_k \in \mathbb{R}^{p \times p}$ and $O_{k+r} \in \mathbb{R}^{m_r \times m_r}$ for each $r = 1, \ldots, k$ are real orthogonal matrices, then by rotational invariance of G_r, the eigenvalue measure $\mu_{\widehat{\Sigma}}$ remains invariant in law under the transformations

$$\Sigma_r^{1/2} \mapsto H_r := O_r' \Sigma_r^{1/2} O_0, \quad \sqrt{m_r m_s} U_r' B U_s \mapsto F_{rs} := O_{k+r}' (\sqrt{m_r m_s} U_r' B U_s) O_{k+s}.$$

Hence we may equivalently consider the matrix

$$W = \sum_{r,s=1}^{k} H_r' G_r' F_{rs} G_s H_s \tag{5.1}$$

for $O_0, \ldots, O_{2k}$ independent and Haar-distributed. The families $\{F_{rs}\}$, $\{G_r\}$, $\{H_r\}$ are independent of each other, with each family satisfying a certain joint orthogonal invariance in law (formalized in Section 5.1).

Following [BG09], we embed the matrices $\{F_{rs}\}$, $\{G_r\}$, $\{H_r\}$ into a square matrix space $\mathbb{C}^{N \times N}$.

We then consider deterministic elements $\{f_{rs}\}$, $\{g_r\}$, $\{h_r\}$ in a von Neumann algebra $\mathcal{A}$ with tracial state τ, such that these elements model the embedded matrices, and $\{f_{rs}\}$, $\{g_r\}$, and $\{h_r\}$ are free with amalgamation over a diagonal sub-algebra of projections in $\mathcal{A}$. We follow the deterministic equivalents approach of [SV12] and allow $(\mathcal{A},\tau)$ and $\{f_{rs}\},\{g_r\},\{h_r\}$ to also depend on n and p.

Our proof of Theorem 2.19 consists of two steps:

1. For independent, jointly orthogonally-invariant families of random matrices, we formalize the notion of a free deterministic equivalent and prove an asymptotic freeness result establishing validity of this approximation.

2. For our specific model of interest, we show that the Stieltjes transform of $w := \sum_{r,s} h_r^* g_r^* f_{rs} g_s h_s$ in the free model satisfies the equations (2.23–2.25).

We establish separately the existence and uniqueness of the fixed point to (2.23–2.24) using a contractive mapping argument and uniqueness of analytic continuation. This implies that the Stieltjes transform of w in step 2 is uniquely determined by (2.23–2.25), which implies by step 1 that (2.23–2.25) asymptotically determine the Stieltjes transform of W.

Notation

For a $*$-algebra $\mathcal{A}$ and elements $(a_i)_{i\in\mathcal{I}}$ of $\mathcal{A}$, $\langle a_i : i \in \mathcal{I}\rangle$ denotes the sub-$*$-algebra generated by $(a_i)_{i\in\mathcal{I}}$. We write $\langle\{a_i\}\rangle$ if the index set $\mathcal{I}$ is clear from context. If $\mathcal{A}$ is a von Neumann algebra, $\langle\{a_i\}\rangle_{W^*}$ denotes the generated von Neumann sub-algebra, i.e. the ultraweak closure of $\langle\{a_i\}\rangle$, and $\|a_i\|$ denotes the C^*-norm.

5.1 Operator-valued free probability

5.1.1 Background

We review definitions from operator-valued free probability theory and its application to rectangular random matrices, drawn from [VDN92, Voi95, BG09].

Definition. A **non-commutative probability space** $(\mathcal{A},\tau)$ is a unital $*$-algebra $\mathcal{A}$ over $\mathbb{C}$ and a $*$-linear functional $\tau : \mathcal{A} \to \mathbb{C}$ called the **trace** that satisfies, for all $a, b \in \mathcal{A}$ and for $1_{\mathcal{A}} \in \mathcal{A}$ the multiplicative unit,

$$\tau(1_{\mathcal{A}}) = 1, \quad \tau(ab) = \tau(ba).$$

For our purposes, $\mathcal{A}$ will always be a von Neumann algebra having norm $\|\cdot\|$, and τ a positive, faithful, and normal trace. In particular, τ will be norm-continuous with $|\tau(a)| \leq \|a\|$.

Following [BG09], we embed rectangular matrices into a larger square space according to the following structure.

Definition. Let $(\mathcal{A}, \tau)$ be a non-commutative probability space and $d \geq 1$ a positive integer. For $p_1, \ldots, p_d \in \mathcal{A}$, $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ is a **rectangular probability space** if $p_1, \ldots, p_d$ are non-zero pairwise-orthogonal projections summing to 1, i.e. for all $r \neq s \in \{1, \ldots, d\}$,

$$p_r \neq 0, \;\; p_r = p_r^* = p_r^2, \;\; p_r p_s = 0, \;\; p_1 + \ldots + p_d = 1.$$

An element $a \in \mathcal{A}$ is **simple**, or (r,s)-simple, if $p_r a p_s = a$ for some $r, s \in \{1, \ldots, d\}$ (possibly $r = s$).

Example 5.1. Let $N_1, \ldots, N_d \geq 1$ be positive integers and denote $N = N_1 + \ldots + N_d$. Consider the $*$-algebra $\mathcal{A} = \mathbb{C}^{N \times N}$, with the involution $*$ given by the conjugate transpose map $A \mapsto A^*$. For $A \in \mathbb{C}^{N \times N}$, let $\tau(A) = N^{-1} \operatorname{Tr} A$. Then $(\mathcal{A}, \tau) = (\mathbb{C}^{N \times N}, N^{-1} \operatorname{Tr})$ is a non-commutative probability space. Any $A \in \mathbb{C}^{N \times N}$ may be written in block form as

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1d} \\ A_{21} & A_{22} & \cdots & A_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ A_{d1} & A_{d2} & \cdots & A_{dd} \end{pmatrix},$$

where $A_{st} \in \mathbb{C}^{N_s \times N_t}$. For each $r = 1, \ldots, d$, denote by P_r the matrix with (r,r) block equal to Id_{N_r} and (s,t) block equal to 0 for all other s, t. Then P_r is a projection, and $(\mathbb{C}^{N \times N}, N^{-1} \operatorname{Tr}, P_1, \ldots, P_d)$ is a rectangular probability space. $A \in \mathbb{C}^{N \times N}$ is simple if $A_{st} \neq 0$ for at most one block (s,t).

In a rectangular probability space, the projections $p_1, \ldots, p_d$ generate a sub-$*$-algebra

$$\mathcal{D} := \langle p_1, \ldots, p_d \rangle = \left\{ \sum_{r=1}^{d} z_r p_r : z_r \in \mathbb{C} \right\}. \tag{5.2}$$

We may define a $*$-linear map $\mathbf{F}^{\mathcal{D}} : \mathcal{A} \to \mathcal{D}$ by

$$\mathbf{F}^{\mathcal{D}}(a) = \sum_{r=1}^{d} p_r \tau_r(a), \qquad \tau_r(a) = \tau(p_r a p_r)/\tau(p_r), \tag{5.3}$$

which is a projection onto $\mathcal{D}$ in the sense $\mathbf{F}^{\mathcal{D}}(d) = d$ for all $d \in \mathcal{D}$. In Example 5.1, $\mathcal{D}$ consists of matrices $A \in \mathbb{C}^{N \times N}$ for which A_{rr} is a multiple of the identity for each r and $A_{rs} = 0$ for each $r \neq s$. In this example, $\tau_r(A) = N_r^{-1} \operatorname{Tr}_r A$ where $\operatorname{Tr}_r A = \operatorname{Tr} A_{rr}$, so $\mathbf{F}^{\mathcal{D}}$ encodes the trace of each diagonal block.

The tuple $(\mathcal{A}, \mathcal{D}, \mathbf{F}^{\mathcal{D}})$ is an example of the following definition for an operator-valued probability space.

Definition. A **$\mathcal{B}$-valued probability space** $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ is a $*$-algebra $\mathcal{A}$, a sub-$*$-algebra $\mathcal{B} \subseteq \mathcal{A}$ containing $1_{\mathcal{A}}$, and a $*$-linear map $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$ called the **conditional expectation** satisfying, for all $b, b' \in \mathcal{B}$ and $a \in \mathcal{A}$,

$$\mathbf{F}^{\mathcal{B}}(bab') = b\mathbf{F}^{\mathcal{B}}(a)b', \quad \mathbf{F}^{\mathcal{B}}(b) = b.$$

We identify $\mathbb{C} \subset \mathcal{A}$ as a sub-algebra via the inclusion map $z \mapsto z1_{\mathcal{A}}$, and we write 1 for $1_{\mathcal{A}}$ and z for $z1_{\mathcal{A}}$. Then a non-commutative probability space $(\mathcal{A}, \tau)$ is also a $\mathbb{C}$-valued probability space with $\mathcal{B} = \mathbb{C}$ and $\mathbf{F}^{\mathcal{B}} = \tau$.

Definition. Let $(\mathcal{A}, \tau)$ be a non-commutative probability space and $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$ a conditional expectation onto a sub-algebra $\mathcal{B} \subset \mathcal{A}$. $\mathbf{F}^{\mathcal{B}}$ is $\boldsymbol{\tau}$**-invariant** if $\tau \circ \mathbf{F}^{B} = \tau$.

It is verified that $\mathbf{F}^{\mathcal{D}} : \mathcal{A} \to \mathcal{D}$ defined by (5.3) is τ-invariant. When $\mathcal{B}$ is a von Neumann sub-algebra of (a von Neumann algebra) $\mathcal{A}$, there exists a unique τ-invariant conditional expectation $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$, which is norm-continuous and satisfies $\|\mathbf{F}^{\mathcal{B}}(a)\| \leq \|a\|$. If $\mathcal{D} \subseteq \mathcal{B} \subseteq \mathcal{A}$ are nested von Neumann sub-algebras with τ-invariant conditional expectations $\mathbf{F}^{\mathcal{D}} : \mathcal{A} \to \mathcal{D}$, $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$, then we have the analogue of the classical tower property,

$$\mathbf{F}^{\mathcal{D}} = \mathbf{F}^{\mathcal{D}} \circ \mathbf{F}^{\mathcal{B}}. \tag{5.4}$$

We note that $\mathcal{D}$ in (5.2) is a von Neumann sub-algebra of $\mathcal{A}$, as it is finite-dimensional.

In the space $(\mathcal{A}, \tau)$, $a \in \mathcal{A}$ may be thought of as an analogue of a bounded random variable, $\tau(a)$ its expectation, and $\mathbf{F}^{\mathcal{B}}(a)$ its conditional expectation with respect to a sub-sigma-field. The following definitions then provide an analogue of the conditional distribution of a, and more generally of the conditional joint distribution of a collection $(a_i)_{i \in \mathcal{I}}$.

Definition. Let $\mathcal{B}$ be a $*$-algebra and $\mathcal{I}$ be any set. A $*$**-monomial** in the variables $\{x_i : i \in \mathcal{I}\}$ with coefficients in $\mathcal{B}$ is an expression of the form $b_1 y_1 b_2 y_2 \ldots b_{l-1} y_{l-1} b_l$ where $l \geq 1$, $b_1, \ldots, b_l \in \mathcal{B}$, and $y_1, \ldots, y_{l-1} \in \{x_i, x_i^* : i \in \mathcal{I}\}$. A $*$**-polynomial** in $\{x_i : i \in \mathcal{I}\}$ with coefficients in $\mathcal{B}$ is any finite sum of such monomials.

We write $Q(a_i : i \in \mathcal{I})$ as the evaluation of a $*$-polynomial Q at $x_i = a_i$.

Definition. Let $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ be a $\mathcal{B}$-valued probability space, let $(a_i)_{i \in \mathcal{I}}$ be elements of $\mathcal{A}$, and let $\mathcal{Q}$ denote the set of all $*$-polynomials in variables $\{x_i : i \in \mathcal{I}\}$ with coefficients in $\mathcal{B}$. The (joint) $\mathcal{B}$**-law** of $(a_i)_{i \in \mathcal{I}}$ is the collection of values in $\mathcal{B}$

$$\{\mathbf{F}^{\mathcal{B}}[Q(a_i : i \in I)]\}_{Q \in \mathcal{Q}}. \tag{5.5}$$

In the scalar setting where $\mathcal{B} = \mathbb{C}$ and $\mathbf{F}^{\mathcal{B}} = \tau$, a $*$-monomial takes the simpler form $z y_1 y_2 \ldots y_{l-1}$ for $z \in \mathbb{C}$ and $y_1, \ldots, y_{l-1} \in \{x_i, x_i^* : i \in \mathcal{I}\}$ (because $\mathbb{C}$ commutes with $\mathcal{A}$). Then the collection of values (5.5) is determined by the scalar-valued moments $\tau(w)$ for all words w in the letters $\{x_i, x_i^* : i \in \mathcal{I}\}$. This is the analogue of the unconditional joint distribution of a family of bounded random variables, as specified by the joint moments.

Finally, the following definition of operator-valued freeness, introduced in [Voi95], has similarities to the notion of conditional independence of sub-sigma-fields in the classical setting.

Definition. Let $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ be a $\mathcal{B}$-valued probability space and $(\mathcal{A}_i)_{i\in\mathcal{I}}$ a collection of sub-$*$-algebras of $\mathcal{A}$ which contain $\mathcal{B}$. $(\mathcal{A}_i)_{i\in\mathcal{I}}$ are **$\mathcal{B}$-free**, or free with amalgamation over $\mathcal{B}$, if for all $m \geq 1$, for all $i_1, \ldots, i_m \in \mathcal{I}$ with $i_1 \neq i_2$, $i_2 \neq i_3$, ..., $i_{m-1} \neq i_m$, and for all $a_1 \in \mathcal{A}_{i_1}, \ldots, a_m \in \mathcal{A}_{i_m}$, the following implication holds:

$$\mathbf{F}^{\mathcal{B}}(a_1) = \mathbf{F}^{\mathcal{B}}(a_2) = \ldots = \mathbf{F}^{\mathcal{B}}(a_m) = 0 \Rightarrow \mathbf{F}^{\mathcal{B}}(a_1 a_2 \ldots a_m) = 0.$$

Subsets $(S_i)_{i\in\mathcal{I}}$ of $\mathcal{A}$ are $\mathcal{B}$-free if the sub-$*$-algebras $(\langle S_i, \mathcal{B}\rangle)_{i\in\mathcal{I}}$ are.

In the classical setting, the joint law of (conditionally) independent random variables is determined by their marginal (conditional) laws. A similar statement holds for freeness:

Proposition 5.2. Suppose $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ is a $\mathcal{B}$-valued probability space, and subsets $(S_i)_{i\in\mathcal{I}}$ of $\mathcal{A}$ are $\mathcal{B}$-free. Then the $\mathcal{B}$-law of $\bigcup_{i\in\mathcal{I}} S_i$ is determined by the individual $\mathcal{B}$-laws of the S_i's.

Proof. See [Voi95, Proposition 1.3]. □

5.1.2 Free deterministic equivalents and asymptotic freeness

Free deterministic equivalents were introduced in [SV12]. Here, we formalize a bit this definition for independent jointly orthogonally-invariant families of matrices, and we establish closeness of the random matrices and the free approximation in a general setting.

Definition 5.3. For fixed $d \geq 1$, consider two sequences of N-dependent rectangular probability spaces $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ and $(\mathcal{A}', \tau', p'_1, \ldots, p'_d)$ such that for each $r \in \{1, \ldots, d\}$, as $N \to \infty$,

$$|\tau(p_r) - \tau'(p'_r)| \to 0.$$

For a common index set $\mathcal{I}$, consider elements $(a_i)_{i\in\mathcal{I}}$ of $\mathcal{A}$ and $(a'_i)_{i\in\mathcal{I}}$ of $\mathcal{A}'$. Then $(a_i)_{i\in\mathcal{I}}$ and $(a'_i)_{i\in\mathcal{I}}$ are **asymptotically equal in $\mathcal{D}$-law** if the following holds: For any $r \in \{1, \ldots, d\}$ and any $*$-polynomial Q in the variables $\{x_i : i \in \mathcal{I}\}$ with coefficients in $\mathcal{D} = \langle p_1, \ldots, p_d\rangle$, denoting by Q' the corresponding $*$-polynomial with coefficients in $\mathcal{D}' = \langle p'_1, \ldots, p'_d\rangle$, as $N \to \infty$,

$$|\tau_r[Q(a_i : i \in \mathcal{I})] - \tau'_r[Q'(a'_i : i \in \mathcal{I})]| \to 0. \tag{5.6}$$

If $(a_i)_{i\in\mathcal{I}}$ and/or $(a'_i)_{i\in\mathcal{I}}$ are random elements of $\mathcal{A}$ and/or $\mathcal{A}'$, then they are **asymptotically equal in $\mathcal{D}$-law a.s.** if the above holds almost surely for each individual $*$-polynomial Q.

In the above, τ_r and τ'_r are defined by (5.3). "Corresponding" means that Q' is obtained by expressing each coefficient $d \in \mathcal{D}$ of Q in the form (5.2) and replacing $p_1, \ldots, p_d$ by $p'_1, \ldots, p'_d$.

We will apply Definition 5.3 by taking one of the two rectangular spaces to be $(\mathbb{C}^{N\times N}, N^{-1}\operatorname{Tr})$ as in Example 5.1, containing random elements, and the other to be an approximating deterministic model. (We will use "distribution" for random matrices to mean their distribution as random elements of $\mathbb{C}^{N\times N}$ in the usual sense, reserving the term "$\mathcal{B}$-law" for Definition 5.1.1.) Freeness relations in the deterministic model will emerge from the following notion of rotational invariance of the random matrices.

Definition 5.4. Consider $(\mathbb{C}^{N\times N}, N^{-1}\operatorname{Tr}, P_1, \ldots, P_d)$ as in Example 5.1. A family of random matrices $(H_i)_{i\in\mathcal{I}}$ in $\mathbb{C}^{N\times N}$ is **block-orthogonally invariant** if, for any orthogonal matrices $O_r \in \mathbb{R}^{N_r\times N_r}$ for $r = 1, \ldots, d$, denoting $O = \operatorname{diag}(O_1, \ldots, O_d) \in \mathbb{R}^{N\times N}$, the joint distribution of $(H_i)_{i\in\mathcal{I}}$ is equal to that of $(O'H_iO)_{i\in\mathcal{I}}$.

Let us provide several examples. We discuss the constructions of the spaces $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ for these examples in Appendix B.2.

Example 5.5. Fix $r \in \{1, \ldots, d\}$ and let $G \in \mathbb{C}^{N\times N}$ be a simple random matrix such that the diagonal block $G_{rr} \in \mathbb{C}^{N_r\times N_r}$ is distributed as the GUE or GOE, scaled to have entries of variance $1/N_r$. (Simple means $G_{st} = 0$ for all other blocks (s,t).) Let $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ be a rectangular space with $\tau(p_s) = N_s/N$ for each $s = 1, \ldots, d$, such that $\mathcal{A}$ contains a self-adjoint simple element g satisfying $g = g^*$ and $p_r g p_r = g$, with moments given by the semi-circle law:

$$\tau_r(g^l) = \int_{-2}^{2} \frac{x^l}{2\pi}\sqrt{4-x^2}\,dx \qquad \text{for all } l \geq 0.$$

For any corresponding $*$-polynomials Q and q as in Definition 5.3, we may verify $N_r^{-1}\operatorname{Tr}_r Q(G) - \tau_r(q(g)) \to 0$ a.s. by the classical Wigner semi-circle theorem [Wig55]. Then G and g are asymptotically equal in $\mathcal{D}$-law a.s. Furthermore, G is block-orthogonally invariant.

Example 5.6. Fix $r_1 \neq r_2 \in \{1, \ldots, d\}$ and let $G \in \mathbb{C}^{N\times N}$ be a simple random matrix such that the block $G_{r_1 r_2}$ has i.i.d. Gaussian or complex Gaussian entries with variance $1/N_{r_1}$. Let $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ satisfy $\tau(p_s) = N_s/N$ for each s, such that $\mathcal{A}$ contains a simple element g satisfying $p_{r_1} g p_{r_2} = g$, where g^*g has moments given by the Marcenko-Pastur law:

$$\tau_{r_2}((g^*g)^l) = \int x^l \nu_{N_{r_2}/N_{r_1}}(x)dx \qquad \text{for all } l \geq 0$$

where ν_λ is the standard Marcenko-Pastur density

$$\nu_\lambda(x) = \frac{1}{2\pi}\frac{\sqrt{(\lambda_+ - x)(x-\lambda_-)}}{\lambda x}\mathbb{1}_{[\lambda_-,\lambda_+]}(x), \qquad \lambda_\pm = (1 \pm \sqrt{\lambda})^2. \tag{5.7}$$

By definition of τ_r and the cyclic property of τ, we also have

$$\tau_{r_1}((gg^*)^l) = (N_{r_2}/N_{r_1})\tau_{r_2}((g^*g)^l).$$

For any corresponding $*$-polynomials Q and q as in Definition 5.3, we may verify $N_{r_2}^{-1}\operatorname{Tr}_{r_2} Q(G) - \tau_{r_2}(q(g)) \to 0$ and $N_{r_1}^{-1}\operatorname{Tr}_{r_1} Q(G) - \tau_{r_1}(q(g)) \to 0$ a.s. by the classical Marcenko-Pastur theorem [MP67]. Then G and g are asymptotically equal in $\mathcal{D}$-law a.s., and G is block-orthogonally invariant.

Example 5.7. Let $B_1, \ldots, B_k \in \mathbb{C}^{N\times N}$ be deterministic simple matrices, say with $P_{r_i}B_iP_{s_i} = B_i$ for each $i = 1, \ldots, k$ and $r_i, s_i \in \{1, \ldots, d\}$. Let $O_1 \in \mathbb{R}^{N_1\times N_1}, \ldots, O_d \in \mathbb{R}^{N_d\times N_d}$ be independent Haar-distributed orthogonal matrices, define $O = \operatorname{diag}(O_1, \ldots, O_d) \in \mathbb{R}^{N\times N}$, and let $\check{B}_i = O'B_iO$. Let $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ satisfy $\tau(p_s) = N_s/N$ for each s, such that $\mathcal{A}$ contains simple elements $b_1, \ldots, b_k$ satisfying $p_{r_i}b_ip_{s_i} = b_i$ for each $i = 1, \ldots, k$, and

$$N_r^{-1}\operatorname{Tr}_r Q(B_1, \ldots, B_k) = \tau_r(q(b_1, \ldots, b_k)) \tag{5.8}$$

for any corresponding $*$-polynomials Q and q with coefficients in $\langle P_1, \ldots, P_d\rangle$ and $\langle p_1, \ldots, p_d\rangle$. As $\operatorname{Tr}_r Q(B_1, \ldots, B_k)$ is invariant under $B_i \mapsto O'B_iO$, (5.8) holds also with $\check{B}_i$ in place of B_i. Then $(\check{B}_i)_{i\in\{1,\ldots,k\}}$ and $(b_i)_{i\in\{1,\ldots,k\}}$ are exactly (and hence also asymptotically) equal in $\mathcal{D}$-law, and $(\check{B}_i)_{i\in\{1,\ldots,k\}}$ is block-orthogonally invariant by construction.

To study the interaction of several independent and block-orthogonally invariant matrix families, we will take a deterministic model for each family, as in Examples 5.5, 5.6, and 5.7 above, and consider a combined model in which these families are $\mathcal{D}$-free:

Definition 5.8. Consider $(\mathbb{C}^{N\times N}, N^{-1}\operatorname{Tr}, P_1, \ldots, P_d)$ as in Example 5.1. Suppose

$$(H_i)_{i\in\mathcal{I}_1}, \ldots, (H_i)_{i\in\mathcal{I}_J}$$

are finite families of random matrices in $\mathbb{C}^{N\times N}$ such that:

- These families are independent from each other, and
- For each $j = 1, \ldots, J$, $(H_i)_{i\in\mathcal{I}_j}$ is block-orthogonally invariant.

Then a **free deterministic equivalent** for $(H_i)_{i\in\mathcal{I}_1}, \ldots, (H_i)_{i\in\mathcal{I}_J}$ is any (N-dependent) rectangular probability space $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ and families $(h_i)_{i\in\mathcal{I}_1}, \ldots, (h_i)_{i\in\mathcal{I}_J}$ of deterministic elements in $\mathcal{A}$ such that, as $N \to \infty$:

- For each $r = 1, \ldots, d$, $|N^{-1}\operatorname{Tr} P_r - \tau(p_r)| \to 0$,
- For each $j = 1, \ldots, J$, $(H_i)_{i\in\mathcal{I}_j}$ and $(h_i)_{i\in\mathcal{I}_j}$ are asymptotically equal in $\mathcal{D}$-law a.s., and
- $(h_i)_{i\in\mathcal{I}_1}, \ldots, (h_i)_{i\in\mathcal{I}_J}$ are free with amalgamation over $\mathcal{D} = \langle p_1, \ldots, p_d\rangle$.

We then have the following asymptotic freeness theorem, which establishes the validity of this approximation.

Theorem 5.9. In the space $(\mathbb{C}^{N\times N}, N^{-1}\operatorname{Tr}, P_1,\ldots,P_d)$ of Example 5.1, suppose $(H_i)_{i\in\mathcal{I}_1}$, …, $(H_i)_{i\in\mathcal{I}_J}$ are independent, block-orthogonally invariant families of random matrices, and let $(h_i)_{i\in\mathcal{I}_1}$, …, $(h_i)_{i\in\mathcal{I}_J}$ be any free deterministic equivalent in $(\mathcal{A},\tau,p_1,\ldots,p_d)$. If there exist constants $C, c>0$ such that $c<N_r/N$ for all r and $\|H_i\|< C$ a.s. for all $i\in\mathcal{I}_j$, all $\mathcal{I}_j$, and all large N, then $(H_i)_{i\in\mathcal{I}_j, j\in\{1,\ldots,J\}}$ and $(h_i)_{i\in\mathcal{I}_j, j\in\{1,\ldots,J\}}$ are asymptotically equal in $\mathcal{D}$-law a.s.

More informally, if $(h_i)_{i\in\mathcal{I}_j}$ asymptotically models the family $(H_i)_{i\in\mathcal{I}_j}$ for each j, and these matrix families are independent and block-orthogonally invariant, then a system in which $(h_i)_{i\in\mathcal{I}_j}$ are $\mathcal{D}$-free asymptotically models the matrices jointly over j.

The proof of this theorem is contained in Appendix B. The theorem is analogous to [BG09, Theorem 1.6] and [SV12, Theorem 2.7], which establish similar results for complex unitary invariance. It permits multiple matrix families (where matrices within each family are not independent), uses the almost-sure trace $N^{-1}\operatorname{Tr}$ rather than $\mathbb{E}\circ N^{-1}\operatorname{Tr}$, and imposes boundedness rather than joint convergence assumptions. This last point fully embraces the deterministic equivalents approach.

We will apply Theorem 5.9 in the form of the following corollary, whose proof we also defer to Appendix B: Suppose that $w\in\mathcal{A}$ satisfies $|\tau(w^l)|\leq C^l$ for a constant $C>0$ and all $l\geq 1$. We may define its Stieltjes transform by the convergent series

$$m_w(z)=\tau((w-z)^{-1})=-\sum_{l\geq 0}^{\infty} z^{-(l+1)}\tau(w^l) \tag{5.9}$$

for $z\in\mathbb{C}^+$ with $|z|> C$, where we use the convention $w^0=1$ for all $w\in\mathcal{A}$.

Corollary 5.10. Under the assumptions of Theorem 5.9, let Q be a self-adjoint $*$-polynomial (with $\mathbb{C}$-valued coefficients) in $(x_i)_{i\in\mathcal{I}_j, j\in\{1,\ldots,J\}}$, and let

$$W=Q(H_i : i\in\mathcal{I}_j, j\in\{1,\ldots,J\})\in\mathbb{C}^{N\times N},$$
$$w=Q(h_i : i\in\mathcal{I}_j, j\in\{1,\ldots,J\})\in\mathcal{A}.$$

Suppose $|\tau(w^l)|\leq C^l$ for all $N, l\geq 1$ and some $C>0$. Then for a sufficiently large constant $C_0>0$, letting $\mathbb{D}=\{z\in\mathbb{C}^+ : |z|> C_0\}$ and defining $m_W(z)=N^{-1}\operatorname{Tr}(W-z\operatorname{Id}_N)^{-1}$ and $m_w(z)=\tau((w-z)^{-1})$,

$$m_W(z)-m_w(z)\to 0$$

pointwise almost surely over $z\in\mathbb{D}$.

5.1.3 Computational tools

Our computations in the free model will use the tools of free cumulants, $\mathcal{R}$-transforms, and Cauchy transforms discussed in [Spe98, NSS02, SV12]. We review some relevant concepts here.

Let $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ be a $\mathcal{B}$-valued probability space and $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$ a conditional expectation. For $l \geq 1$, the l^{th} order **free cumulant** of $\mathbf{F}^{\mathcal{B}}$ is a map $\kappa_l^{\mathcal{B}} : \mathcal{A}^l \to \mathcal{B}$ defined by $\mathbf{F}^{\mathcal{B}}$ and certain moment-cumulant relations over the non-crossing partition lattice; we refer the reader to [SV12] and [Spe98, Chapters 2 and 3] for details. We will use the properties that $\kappa_l^{\mathcal{B}}$ is linear in each argument and satisfies the relations

$$\kappa_l^{\mathcal{B}}(ba_1, a_2, \ldots, a_{l-1}, a_l b') = b\kappa_l^{\mathcal{B}}(a_1, \ldots, a_l)b', \tag{5.10}$$

$$\kappa_l^{\mathcal{B}}(a_1, \ldots, a_{j-1}, a_j b, a_{j+1}, \ldots, a_l) = \kappa_l^{\mathcal{B}}(a_1, \ldots, a_j, ba_{j+1}, \ldots, a_l) \tag{5.11}$$

for any $b, b' \in \mathcal{B}$ and $a_1, \ldots, a_l \in \mathcal{A}$.

For $a \in \mathcal{A}$, the $\boldsymbol{\mathcal{B}}$**-valued** $\boldsymbol{\mathcal{R}}$**-transform** of a is defined, for $b \in \mathcal{B}$, as

$$\mathcal{R}_a^{\mathcal{B}}(b) = \sum_{l \geq 1} \kappa_l^{\mathcal{B}}(ab, \ldots, ab, a). \tag{5.12}$$

The $\boldsymbol{\mathcal{B}}$**-valued Cauchy transform** of a is defined, for invertible $b \in \mathcal{B}$, as

$$G_a^{\mathcal{B}}(b) = \mathbf{F}^{\mathcal{B}}((b-a)^{-1}) = \sum_{l \geq 0} \mathbf{F}^{\mathcal{B}}(b^{-1}(ab^{-1})^l), \tag{5.13}$$

with the convention $a^0 = 1$ for all $a \in \mathcal{A}$. The moment-cumulant relations imply that $G_a^{\mathcal{B}}(b)$ and $\mathcal{R}_a^{\mathcal{B}}(b) + b^{-1}$ are inverses with respect to composition:

Proposition 5.11. Let $(\mathcal{A}, \mathcal{B}, \mathbf{F}^{\mathcal{B}})$ be a $\mathcal{B}$-valued probability space. For $a \in \mathcal{A}$ and invertible $b \in \mathcal{B}$,

$$G_a^{\mathcal{B}}(b^{-1} + \mathcal{R}_a^{\mathcal{B}}(b)) = b, \tag{5.14}$$

$$G_a^{\mathcal{B}}(b) = \left(b - \mathcal{R}_a^{\mathcal{B}}(G_a^{\mathcal{B}}(b))\right)^{-1}. \tag{5.15}$$

Proof. See [Voi95, Theorem 4.9] and also [Spe98, Theorem 4.1.12]. □

Remark. When $\mathcal{A}$ is a von Neumann algebra, the right sides of (5.12) and (5.13) may be understood as convergent series in $\mathcal{A}$ with respect to the norm $\|\cdot\|$, for sufficiently small $\|b\|$ and $\|b^{-1}\|$ respectively. Indeed, (5.13) defines a convergent series in $\mathcal{B}$ when $\|b^{-1}\| < 1/\|a\|$, with

$$\|G_a^{\mathcal{B}}(b)\| \leq \sum_{l \geq 0} \|b^{-1}\|^{l+1} \|a\|^l = \frac{\|b^{-1}\|}{1 - \|a\|\|b^{-1}\|}. \tag{5.16}$$

Also, explicit inversion of the moment-cumulant relations for the non-crossing partition lattice yields the cumulant bound

$$\|\kappa_l^{\mathcal{B}}(a_1, \ldots, a_l)\| \leq 16^l \prod_{i=1}^{l} \|a_i\| \tag{5.17}$$

(see [NS06, Proposition 13.15]), so (5.12) defines a convergent series in $\mathcal{B}$ when $16\|b\|< 1/\|a\|$, with

$$\|\mathcal{R}_a^{\mathcal{B}}(b)\|\leq \sum_{l\geq 1} 16^l \|a\|^l \|b\|^{l-1}= \frac{16\|a\|}{1-16\|a\|\|b\|}.$$

The identities (5.14) and (5.15) hold as equalities of elements in $\mathcal{B}$ when $\|b\|$ and $\|b^{-1}\|$ are sufficiently small, respectively.

Our computation will pass between $\mathcal{R}$-transforms and Cauchy transforms with respect to nested sub-algebras of $\mathcal{A}$. Central to this approach is the following result from [NSS02] (see also [SV12]):

Proposition 5.12. Let $(\mathcal{A}, \mathcal{D}, \mathbf{F}^{\mathcal{D}})$ be a $\mathcal{D}$-valued probability space, let $\mathcal{B}, \mathcal{H} \subseteq \mathcal{A}$ be sub-$*$-algebras containing $\mathcal{D}$, and let $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$ be a conditional expectation such that $\mathbf{F}^{\mathcal{D}} \circ \mathbf{F}^{\mathcal{B}} = \mathbf{F}^{\mathcal{D}}$. Let $\kappa_l^{\mathcal{B}}$ and $\kappa_l^{\mathcal{D}}$ denote the free cumulants for $\mathbf{F}^{\mathcal{B}}$ and $\mathbf{F}^{\mathcal{D}}$. If $\mathcal{B}$ and $\mathcal{H}$ are $\mathcal{D}$-free, then for all $l \geq 1$, $h_1, \ldots, h_l \in \mathcal{H}$, and $b_1, \ldots, b_{l-1} \in \mathcal{B}$,

$$\kappa_l^{\mathcal{B}}(h_1 b_1, \ldots, h_{l-1} b_{l-1}, h_l) = \kappa_l^{\mathcal{D}}(h_1 \mathbf{F}^{\mathcal{D}}(b_1), \ldots, h_{l-1} \mathbf{F}^{\mathcal{D}}(b_{l-1}), h_l).$$

Proof. See [NSS02, Theorem 3.6]. ☐

For sub-algebras $\mathcal{D} \subseteq \mathcal{B} \subseteq \mathcal{A}$ and conditional expectations $\mathbf{F}^{\mathcal{D}} : \mathcal{A} \to \mathcal{D}$ and $\mathbf{F}^{\mathcal{B}} : \mathcal{A} \to \mathcal{B}$ satisfying (5.4), we also have for any $a \in \mathcal{A}$ and invertible $d \in \mathcal{D}$ (with sufficiently small $\|d^{-1}\|$), by (5.13),

$$G_a^{\mathcal{D}}(d) = \mathbf{F}^{\mathcal{D}} \circ G_a^{\mathcal{B}}(d). \tag{5.18}$$

Finally, note that for $\mathcal{B} = \mathbb{C}$ and $\mathbf{F}^{\mathcal{B}} = \tau$, the scalar-valued Cauchy transform $G_a^{\mathbb{C}}(z)$ is simply $-m_a(z)$ from (5.9). (The minus sign is a difference in sign convention for the Cauchy/Stieltjes transform.)

5.2 Computation in the free model

We will prove analogues of Theorems 2.19 and 2.20 for a slightly more general matrix model: Fix $k \geq 1$, let $p, n_1, \ldots, n_k, m_1, \ldots, m_k \in \mathbb{N}$, and denote $M = \sum_{r=1}^k m_r$. Let $F \in \mathbb{C}^{M \times M}$ be deterministic with $F^* = F$, and denote by $F_{rs} \in \mathbb{C}^{m_r \times m_s}$ its (r, s) submatrix. For $r = 1, \ldots, k$, let $H_r \in \mathbb{C}^{n_r \times p}$ be deterministic, and let G_r be independent random matrices such that either $G_r \in \mathbb{R}^{m_r \times n_r}$ with $(G_r)_{ij} \overset{iid}{\sim} \mathcal{N}(0, m_r^{-1})$ or $G_r \in \mathbb{C}^{m_r \times n_r}$ with $\operatorname{Im}(G_r)_{ij}, \operatorname{Re}(G_r)_{ij} \overset{iid}{\sim} \mathcal{N}(0, (2m_r)^{-1})$. Define

$$W = \sum_{r,s=1}^k H_r^* G_r^* F_{rs} G_s H_s \in \mathbb{C}^{p \times p},$$

with empirical spectral measure μ_W. Denote $\mathbf{y} \cdot H^*H = \sum_{s=1}^k y_s H_s^* H_s$, and let $D(\mathbf{x})$ and Tr_r be as in Theorem 2.19.

Theorem 5.13. Suppose $p, n_1, \ldots, n_k, m_1, \ldots, m_k \to \infty$, such that $c < m_r/p < C$, $c < n_r/p < C$, $\|H_r\| < C$, and $\|F_{rs}\| < C$ for all $r, s = 1, \ldots, k$ and some constants $C, c > 0$. Then:

(a) For each $z \in \mathbb{C}^+$, there exist unique values $x_1, \ldots, x_k \in \mathbb{C}^+ \cup \{0\}$ and $y_1, \ldots, y_k \in \overline{\mathbb{C}^+}$ that satisfy, for $r = 1, \ldots, k$, the equations

$$x_r = -\frac{1}{m_r} \mathrm{Tr}\left((z \,\mathrm{Id}_p + \mathbf{y} \cdot H^*H)^{-1} H_r^* H_r\right), \tag{5.19}$$

$$y_r = -\frac{1}{m_r} \mathrm{Tr}_r\left([\mathrm{Id}_M + FD(\mathbf{x})]^{-1} F\right). \tag{5.20}$$

(b) $\mu_W - \mu_0 \to 0$ weakly a.s. for a probability measure μ_0 on $\mathbb{R}$ with Stieltjes transform

$$m_0(z) = -\frac{1}{p} \mathrm{Tr}\left((z \,\mathrm{Id}_p + \mathbf{y} \cdot H^*H)^{-1}\right). \tag{5.21}$$

(c) For each $z \in \mathbb{C}^+$, the values x_r, y_r in (a) are the limits, as $t \to \infty$, of $x_r^{(t)}, y_r^{(t)}$ computed by iterating (5.19–5.20) in the manner of Theorem 2.20.

Theorems 2.19 and 2.20 follow by specializing this result to $F_{rs} = \sqrt{m_r m_s} U_r' B U_s$, $n_r = p$, and $H_r = \Sigma_r^{1/2}$.

5.2.1 Defining a free deterministic equivalent

Consider the transformations

$$H_r \mapsto O_r' H_r O_0, \qquad F_{rs} \mapsto O_{k+r}' F_{rs} O_{k+s}$$

for independent Haar-distributed orthogonal matrices $O_0, \ldots, O_{2k}$ of the appropriate sizes. The eigenvalue measure μ_W remains invariant in law under these transformations. Hence it suffices to prove Theorem 5.13 with H_r and F_{rs} replaced by these randomly-rotated matrices, which (with a slight abuse of notation) we continue to denote by H_r and F_{rs}.

Let $N = p + \sum_{r=1}^k n_r + \sum_{r=1}^k m_r$, and embed the matrices W, H_r, G_r, F_{rs} as simple elements of $\mathbb{C}^{N \times N}$ in the following regions of the block-matrix decomposition corresponding to $\mathbb{C}^N = \mathbb{C}^p \oplus$

$\mathbb{C}^{n_1} \oplus \cdots \oplus \mathbb{C}^{n_k} \oplus \mathbb{C}^{m_1} \oplus \cdots \oplus \mathbb{C}^{m_k}$:

W	H_1^*	$\cdots$	H_k^*			
H_1				G_1^*		
$\vdots$					$\ddots$	
H_k						G_k^*
	G_1			F_{11}	$\cdots$	F_{1k}
		$\ddots$		$\vdots$	$\ddots$	$\vdots$
			G_k	F_{k1}	$\cdots$	F_{kk}

Denote by $P_0, \ldots, P_{2k}$ the diagonal projections corresponding to the above decomposition, and by $\tilde{W}, \tilde{F}_{rs}, \tilde{G}_r, \tilde{H}_r \in \mathbb{C}^{N \times N}$ the embedded matrices. (For example, $P_0 = \operatorname{diag}(\mathrm{Id}_p, 0, \ldots, 0)$, and $\tilde{W}$ has upper-left block equal to W and remaining blocks 0.) Then $\tilde{W}, \tilde{F}_{rs}, \tilde{G}_r, \tilde{H}_r$ are simple elements of the rectangular space $(\mathbb{C}^{N \times N}, N^{-1} \operatorname{Tr}, P_0, \ldots, P_{2k})$, and the $k+2$ families $\{\tilde{F}_{rs}\}$, $\{\tilde{H}_r\}$, $\tilde{G}_1$, …, $\tilde{G}_k$ are independent of each other and are block-orthogonally invariant.

For the approximating free model, consider a second rectangular space $(\mathcal{A}, \tau, p_0, \ldots, p_{2k})$ with deterministic elements $f_{rs}, g_r, h_r \in \mathcal{A}$, such that the following hold:

1. $p_0, \ldots, p_{2k}$ have traces

$$\tau(p_0) = p/N, \quad \tau(p_r) = n_r/N, \quad \tau(p_{k+r}) = m_r/N \qquad \text{for all } r = 1, \ldots, k.$$

2. f_{rs}, g_r, h_r are simple elements such that for all $r, s \in \{1, \ldots, k\}$,

$$p_{k+r} f_{rs} p_{k+s} = f_{rs}, \qquad p_{k+r} g_r p_r = g_r, \qquad p_r h_r p_0 = h_r.$$

3. $\{f_{rs} : 1 \leq r, s \leq k\}$ has the same joint $\mathcal{D}$-law as $\{\tilde{F}_{rs} : 1 \leq r, s \leq k\}$, and $\{h_r : 1 \leq r \leq k\}$ has the same joint $\mathcal{D}$-law as $\{\tilde{H}_r : 1 \leq r \leq k\}$. I.e., for any $r \in \{0, \ldots, 2k\}$ and any non-commutative $*$-polynomials Q_1, Q_2 with coefficients in $\langle P_0, \ldots, P_{2k} \rangle$, letting q_1, q_2 denote the corresponding $*$-polynomials with coefficients in $\langle p_0, \ldots, p_{2k} \rangle$,

$$\tau_r \left[q_1(f_{st} : s, t \in \{1, \ldots, k\}) \right] = N_r^{-1} \operatorname{Tr}_r Q_1(\tilde{F}_{st} : s, t \in \{1, \ldots, k\}), \tag{5.22}$$

$$\tau_r \left[q_2(h_s : s \in \{1, \ldots, k\}) \right] = N_r^{-1} \operatorname{Tr}_r Q_2(\tilde{H}_s : s \in \{1, \ldots, k\}). \tag{5.23}$$

4. For each r, $g_r^* g_r$ has Marcenko-Pastur law with parameter $\lambda = n_r/m_r$. I.e. for ν_λ as in (5.7),

$$\tau_r((g_r^* g_r)^l) = \int x^l \nu_{n_r/m_r}(x) dx \qquad \text{for all } l \geq 0. \tag{5.24}$$

5. The $k+2$ families $\{f_{rs}\}$, $\{h_r\}$, $g_1,\ldots,g_k$ are free with amalgamation over $\mathcal{D}=\langle p_0,\ldots,p_{2k}\rangle$.

The right sides of (5.22) and (5.23) are deterministic, as they are invariant to the random rotations of F_{rs} and H_r. Also, (5.24) completely specifies $\tau(q(g_r))$ for any $*$-polynomial q with coefficients in $\mathcal{D}$. Then these conditions 1–5 fully specify the joint $\mathcal{D}$-law of all elements $f_{rs}, g_r, h_r \in \mathcal{A}$. These elements are a free deterministic equivalent for $\tilde{F}_{rs}, \tilde{G}_r, \tilde{H}_r \in \mathbb{C}^{N\times N}$ in the sense of Definition 5.8.

The following lemma establishes existence of this model as a von Neumann algebra. We indicate the references that establish this type of construction in Appendix B.

Lemma 5.14. Under the conditions of Theorem 5.13, there exists a (N-dependent) rectangular probability space $(\mathcal{A},\tau,p_0,\ldots,p_{2k})$ such that:

(a) $\mathcal{A}$ is a von Neumann algebra and τ is a positive, faithful, normal trace.

(b) $\mathcal{A}$ contains elements f_{rs}, g_r, h_r for $r,s\in\{1,\ldots,k\}$ that satisfy the above conditions. Furthermore, the von Neumann sub-algebras $\langle\mathcal{D},\{f_{rs}\}\rangle_{W^*}$, $\langle\mathcal{D},\{h_r\}\rangle_{W^*}$, $\langle\mathcal{D},g_1\rangle_{W^*}$, ..., $\langle\mathcal{D},g_k\rangle_{W^*}$ are free over $\mathcal{D}$.

(c) There exists a constant $C>0$ such that $\|f_{rs}\|, \|h_r\|, \|g_r\|\leq C$ for all N and all r,s.

5.2.2 Computing the Stieltjes transform

We will use twice the following intermediary lemma:

Lemma 5.15. Let $(\mathcal{A},\tau,q_0,q_1,\ldots,q_k)$ be a rectangular probability space, where $\mathcal{A}$ is von Neumann and τ is positive, faithful, and normal. Let $\mathcal{D}=\langle q_0,\ldots,q_k\rangle$, let $\mathcal{B},\mathcal{C}\subset\mathcal{A}$ be von Neumann sub-algebras containing $\mathcal{D}$ that are free over $\mathcal{D}$, and let $\mathbf{F}^{\mathcal{D}}:\mathcal{A}\to\mathcal{D}$ and $\mathbf{F}^{\mathcal{C}}:\mathcal{A}\to\mathcal{C}$ be the τ-invariant conditional expectations.

Let $b_{rs}\in\mathcal{B}$ and $c_r\in\mathcal{C}$ for $1\leq r,s\leq k$ be such that $q_r b_{rs} q_s = b_{rs}$, $q_r c_r = c_r$, $\|b_{rs}\|\leq C$, and $\|c_r\|\leq C$ for some constant $C>0$. Define $a=\sum_{r,s=1}^k c_r^* b_{rs} c_s$ and $b=\sum_{r,s=1}^k b_{rs}$. Then for $e\in\mathcal{C}$ with $\|e\|$ sufficiently small,

$$\mathcal{R}_a^{\mathcal{C}}(e)=\sum_{r=1}^k c_r^* c_r \tau_r\left(\mathcal{R}_b^{\mathcal{D}}\left(\sum_{s=1}^k \tau_s(c_s e c_s^*) q_s\right)\right),$$

where $\mathcal{R}_a^{\mathcal{C}}$ and $\mathcal{R}_b^{\mathcal{D}}$ are the $\mathcal{C}$-valued and $\mathcal{D}$-valued $\mathcal{R}$-transforms of a and b.

Proof. We use the computational idea of [SV12]: Denote by $\kappa_l^{\mathcal{C}}$ and $\kappa_l^{\mathcal{D}}$ the $\mathcal{C}$-valued and $\mathcal{D}$-valued free cumulants. For $l\geq 1$ and $e\in\mathcal{C}$,

$$\begin{aligned}&\kappa_l^{\mathcal{C}}(ae,\ldots,ae,a)\\ &=\kappa_l^{\mathcal{C}}\left(\sum_{r,s=1}^k c_r^* b_{rs} c_s e,\ \ldots,\ \sum_{r,s=1}^k c_r^* b_{rs} c_s e, \sum_{r,s=1}^k c_r^* b_{rs} c_s\right)\end{aligned}$$

$$
\begin{aligned}
&= \sum_{r_1,s_1,\ldots,r_l,s_l=1}^{k} \kappa_l^{\mathcal{C}}(c_{r_1}^* b_{r_1 s_1} c_{s_1} e,\ \ldots,\ c_{r_{l-1}}^* b_{r_{l-1}s_{l-1}} c_{s_{l-1}} e,\ c_{r_l}^* b_{r_l s_l} c_{s_l}) \\
&= \sum_{r_1,s_1,\ldots,r_l,s_l=1}^{k} c_{r_1}^* \kappa_l^{\mathcal{C}}(b_{r_1 s_1} c_{s_1} e c_{r_2}^*,\ \ldots,\ b_{r_{l-1}s_{l-1}} c_{s_{l-1}} e c_{r_l}^*,\ b_{r_l s_l})\, c_{s_l} \\
&= \sum_{r_1,s_1,\ldots,r_l,s_l=1}^{k} c_{r_1}^* \kappa_l^{\mathcal{D}}(b_{r_1 s_1} \mathbf{F}^{\mathcal{D}}(c_{s_1} e c_{r_2}^*),\ \ldots,\ b_{r_{l-1}s_{l-1}} \mathbf{F}^{\mathcal{D}}(c_{s_{l-1}} e c_{r_l}^*),\ b_{r_l s_l})\, c_{s_l},
\end{aligned}
$$

where we applied the definition of a, multi-linearity of $\kappa_l^{\mathcal{C}}$, the identities (5.10) and (5.11), and Proposition 5.12 using freeness of $\mathcal{B}$ and $\mathcal{C}$ over $\mathcal{D}$.

By the identity $c_r = q_r c_r$, each $c_s e c_r^*$ is simple, and we have from (5.3)

$$
\mathbf{F}^{\mathcal{D}}(c_s e c_r^*) = \begin{cases} 0 & \text{if } s \neq r \\ \tau_s(c_s e c_s^*) q_s & \text{if } s = r. \end{cases}
$$

Furthermore, for any $d \in \mathcal{D}$, as $d = \tau_0(d) q_0 + \ldots + \tau_k(d) q_k$, we have $c_r^* d c_s = c_r^* c_r \tau_r(d)$ if $r = s$ and 0 otherwise. Hence we may restrict the above sum to $s_1 = r_2,\ s_2 = r_3,\ \ldots,\ s_{l-1} = r_l,\ s_l = r_1$. Then, setting

$$
d = \sum_{r=1}^{k} \tau_r(c_r e c_r^*) q_r \tag{5.25}
$$

and applying the identity $q_r b_{rs} q_s = b_{rs}$,

$$
\kappa_l^{\mathcal{C}}(ae, \ldots, ae, a) = \sum_{r_1,\ldots,r_l=1}^{k} c_{r_1}^* c_{r_1} \tau_{r_1}\left(\kappa_l^{\mathcal{D}}(b_{r_1 r_2} d,\ \ldots,\ b_{r_{l-1} r_l} d,\ b_{r_l r_1})\right). \tag{5.26}
$$

On the other hand, similar arguments yield

$$
\begin{aligned}
&\kappa_l^{\mathcal{D}}(bd, \ldots, bd, b) \\
&= \sum_{r_1,s_1,\ldots,r_l,s_l=1}^{k} \kappa_l^{\mathcal{D}}(b_{r_1 s_1} d,\ \ldots,\ b_{r_{l-1}s_{l-1}} d,\ b_{r_l s_l}) \\
&= \sum_{r_1,s_1,\ldots,r_l,s_l=1}^{k} q_{r_1} \kappa_l^{\mathcal{D}}(b_{r_1 s_1} q_{s_1} d q_{r_2},\ \ldots,\ b_{r_{l-1}s_{l-1}} q_{s_{l-1}} d q_{r_l},\ b_{r_l s_l})\, q_{s_l} \\
&= \sum_{r_1,\ldots,r_l=1}^{k} q_{r_1} \kappa_l^{\mathcal{D}}(b_{r_1 r_2} d,\ \ldots,\ b_{r_{l-1} r_l} d,\ b_{r_l r_1}).
\end{aligned}
$$

Comparing with (5.26), $\kappa_l^{\mathcal{C}}(ae, \ldots, ae, a) = \sum_{r=1}^{k} c_r^* c_r \tau_r\left(\kappa_l^{\mathcal{D}}(bd, \ldots, bd, b)\right)$. Summing over l and recalling (5.12), for $\|e\|$ sufficiently small,

$$\mathcal{R}_a^{\mathcal{C}}(e) = \sum_{l\geq 1}\sum_{r=1}^{k} c_r^* c_r \tau_r \left(\kappa_l^{\mathcal{D}}(bd,\ldots,bd,b)\right).$$

Noting that $\|d\| \leq \sum_{s=1}^{k}\|c_s\|^2\|e\|$ and applying (5.17), we may exchange the order of summations on the right and move the summation over l inside τ_r by linearity and norm-continuity of τ, yielding the desired result. □

We now perform the desired computation of the Stieltjes transform of w.

Lemma 5.16. Under the conditions of Theorem 5.13, let $(\mathcal{A},\tau,p_0,\ldots,p_{2k})$ and f_{rs}, g_r, h_r be as in Lemma 5.14, and let $w = \sum_{r,s=1}^{k} h_r^* g_r^* f_{rs} g_s h_s$. Then for a constant $C_0 > 0$, defining $\mathbb{D} = \{z \in \mathbb{C}^+ : |z| > C_0\}$, there exist analytic functions $x_1,\ldots,x_k : \mathbb{D} \to \mathbb{C}^+ \cup \{0\}$ and $y_1,\ldots,y_k : \mathbb{D} \to \mathbb{C}$ that satisfy, for every $z \in \mathbb{D}$ and for $m_0(z) = \tau_0((w-z)^{-1})$, the equations (5.19–5.21).

Proof. If $H_r = 0$ for some r, then we may set $x_r \equiv 0$, define y_r by (5.20), and reduce to the case $k-1$. Hence, it suffices to consider $H_r \neq 0$ for all r.

Define the von Neumann sub-algebras $\mathcal{D} = \langle p_r : 0 \leq r \leq 2k\rangle$, $\mathcal{F} = \langle \mathcal{D}, \{f_{rs}\}\rangle_{W^*}$, $\mathcal{G} = \langle \mathcal{D}, \{g_r\}\rangle_{W^*}$, and $\mathcal{H} = \langle \mathcal{D}, \{h_r\}\rangle_{W^*}$. Denote by $\mathbf{F}^{\mathcal{D}}$, $\mathcal{R}^{\mathcal{D}}$, and $G^{\mathcal{D}}$ the τ-invariant conditional expectation onto $\mathcal{D}$ and the $\mathcal{D}$-valued $\mathcal{R}$-transform and Cauchy transform, and similarly for $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{H}$.

We first work algebraically (Steps 1–3), assuming that arguments b to Cauchy transforms are invertible with $\|b^{-1}\|$ sufficiently small, arguments b to $\mathcal{R}$-transforms have $\|b\|$ sufficiently small, and applying series expansions for $(b-a)^{-1}$. We will check that these assumptions hold and also establish the desired analyticity properties in Step 4.

Step 1: We first relate the $\mathcal{D}$-valued Cauchy transform of w to that of $v = \sum_{r,s=1}^{k} g_r^* f_{rs} g_s$. We apply Lemma 5.15 with $q_0 = p_0 + \sum_{r=k+1}^{2k} p_r$, $q_r = p_r$ for $r = 1,\ldots,k$, $\mathcal{C} = \mathcal{H}$, and $\mathcal{B} = \langle \mathcal{F},\mathcal{G}\rangle$. Then for $c \in \mathcal{H}$,

$$\mathcal{R}_w^{\mathcal{H}}(c) = \sum_{r=1}^{k} h_r^* h_r \tau_r\left(\mathcal{R}_v^{\mathcal{D}}\Big(\sum_{s=1}^{k} p_s \tau_s(h_s c h_s^*)\Big)\right). \tag{5.27}$$

To rewrite this using Cauchy transforms, for invertible $d \in \mathcal{D}$ and each $r = 1,\ldots,k$, define

$$\alpha_r(d) = \tau_r\left(h_r G_w^{\mathcal{H}}(d) h_r^*\right), \tag{5.28}$$

$$\beta_r(d) = \tau_r\left(\mathcal{R}_v^{\mathcal{D}}\Big(\sum_{s=1}^{k} p_s \alpha_s(d)\Big)\right). \tag{5.29}$$

Then (5.15) and (5.27) with $c = G_w^{\mathcal{H}}(d)$ imply

$$G_w^{\mathcal{H}}(d) = \left(d - \mathcal{R}_w^{\mathcal{H}}\left(G_w^{\mathcal{H}}(d)\right)\right)^{-1} = \Big(d - \sum_{r=1}^{k} h_r^* h_r \beta_r(d)\Big)^{-1}. \tag{5.30}$$

Projecting down to $\mathcal{D}$ using (5.18) yields

$$G_w^{\mathcal{D}}(d) = \mathbf{F}^{\mathcal{D}}\bigg(\Big(d - \sum_{r=1}^{k} h_r^* h_r \beta_r(d)\Big)^{-1}\bigg). \tag{5.31}$$

Applying (5.30) to (5.28),

$$\alpha_r(d) = \tau_r\bigg(h_r\Big(d - \sum_{s=1}^{k} h_s^* h_s \beta_s(d)\Big)^{-1} h_r^*\bigg). \tag{5.32}$$

Noting that $(p_1 + \ldots + p_k)v(p_1 + \ldots + p_k) = v$, (5.12) and (5.10) imply $\mathcal{R}_v^{\mathcal{D}}(d) \in \langle p_1, \ldots, p_k\rangle$ for any $d \in \mathcal{D}$, so we may write (5.29) as

$$\mathcal{R}_v^{\mathcal{D}}\Big(\sum_{r=1}^{k} p_r \alpha_r(d)\Big) = \sum_{r=1}^{k} p_r \beta_r(d).$$

For $r = 0$ and $r \in \{k+1, \ldots, 2k\}$, set $\beta_r(d) = 0$ and define $\alpha_r(d)$ arbitrarily, say by $\alpha_r(d) = \|d^{-1}\|$. Since $vp_r = p_r v = 0$ if $r = 0$ or $r \in \{k+1, \ldots, 2k\}$, applying (5.12) and multi-linearity of $\kappa_l^{\mathcal{D}}$, we may rewrite the above as

$$\mathcal{R}_v^{\mathcal{D}}\Big(\sum_{r=0}^{2k} p_r \alpha_r(d)\Big) = \sum_{r=0}^{2k} p_r \beta_r(d).$$

Applying (5.14) with $b = \sum_{r=0}^{2k} p_r \alpha_r(d)$, we get

$$G_v^{\mathcal{D}}\bigg(\sum_{r=0}^{2k} p_r\Big(\frac{1}{\alpha_r(d)} + \beta_r(d)\Big)\bigg) = \sum_{r=0}^{2k} p_r \alpha_r(d). \tag{5.33}$$

The relation between $G_w^{\mathcal{D}}$ and $G_v^{\mathcal{D}}$ is given by (5.31), (5.32), and (5.33).

Step 2: Next, we relate the $\mathcal{D}$-valued Cauchy transforms of v and $u = \sum_{r,s=1}^{k} f_{rs}$. We apply Lemma 5.15 with $q_0 = \sum_{r=0}^{k} p_r$, $q_r = p_{r+k}$ for $r = 1, \ldots, k$, $\mathcal{C} = \mathcal{G}$, and $\mathcal{B} = \mathcal{F}$. Then for $c \in \mathcal{G}$,

$$\mathcal{R}_v^{\mathcal{G}}(c) = \sum_{r=1}^{k} g_r^* g_r \tau_{r+k}\bigg(\mathcal{R}_u^{\mathcal{D}}\Big(\sum_{s=1}^{k} p_{s+k} \tau_{s+k}(g_s c g_s^*)\Big)\bigg). \tag{5.34}$$

To rewrite this using Cauchy transforms, for invertible $d \in \mathcal{D}$ and all $r = 1, \ldots, k$, define

$$\gamma_{r+k}(d) = \tau_{r+k}(g_r G_v^{\mathcal{G}}(d) g_r^*), \tag{5.35}$$

$$\delta_{r+k}(d) = \tau_{r+k}\left(\mathcal{R}_u^{\mathcal{D}}\Big(\sum_{s=1}^{k} p_{s+k}\gamma_{s+k}(d)\Big)\right). \tag{5.36}$$

As in Step 1, for $r = 0, \ldots, k$ let us also define $\delta_r(d) = 0$ and $\gamma_r(d) = \|d^{-1}\|$. Then, noting $(p_{k+1} + \ldots + p_{2k})u(p_{k+1} + \ldots + p_{2k}) = u$, the same arguments as in Step 1 yield the analogous identities

$$G_v^{\mathcal{D}}(d) = \mathbf{F}^{\mathcal{D}}\left(\Big(d - \sum_{s=1}^{k} g_s^* g_s \delta_{s+k}(d)\Big)^{-1}\right), \tag{5.37}$$

$$\gamma_{r+k}(d) = \tau_{r+k}\left(g_r \Big(d - \sum_{s=1}^{k} g_s^* g_s \delta_{s+k}(d)\Big)^{-1} g_r^*\right), \tag{5.38}$$

$$G_u^{\mathcal{D}}\left(\sum_{r=0}^{2k} p_r \Big(\frac{1}{\gamma_r(d)} + \delta_r(d)\Big)\right) = \sum_{r=0}^{2k} p_r \gamma_r(d). \tag{5.39}$$

As $g_r^* g_r$ has moments given by (5.24), we may write (5.37) and (5.38) explicitly: Denote $d = d_0 p_0 + \ldots + d_{2k} p_{2k}$ for $d_0, \ldots, d_{2k} \in \mathbb{C}$. As d is invertible, we have $d^{-1} = d_0^{-1} p_0 + \ldots + d_{2k}^{-1} p_{2k}$. For any $x \in \mathcal{A}$ that commutes with $\mathcal{D}$,

$$(d - x)^{-1} = \sum_{l \geq 0} d^{-1}(x d^{-1})^l = \sum_{l \geq 0} x^l d^{-l-1}.$$

So for $r = 1, \ldots, k$, noting that $p_r = p_r^2$ and that $\mathcal{D}$ commutes with itself,

$$\begin{aligned}\tau_r\left((d - x)^{-1}\right) &= \frac{N}{n_r} \sum_{l \geq 0} \tau(p_r x^l d^{-l-1} p_r) \\ &= \frac{N}{n_r} \sum_{l \geq 0} \tau((p_r x^l p_r)(p_r d^{-1} p_r)^{l+1}) = \sum_{l \geq 0} \frac{\tau_r(x^l)}{d_r^{l+1}}.\end{aligned}$$

Noting that $g_s^* g_s$ commutes with $\mathcal{D}$, applying the above to (5.37) with $x = \sum_{s=1}^{k} g_s^* g_s \delta_{s+k}(d)$, and recalling (5.24),

$$\begin{aligned}\tau_r(G_v^{\mathcal{D}}(d)) &= \sum_{l \geq 0} \frac{\tau_r((g_r^* g_r)^l)\delta_{r+k}(d)^l}{d_r^{l+1}} \\ &= \int \sum_{l \geq 0} \frac{x^l \delta_{r+k}(d)^l}{d_r^{l+1}} \nu_{n_r/m_r}(x) dx\end{aligned}$$

$$
\begin{aligned}
&= \int \frac{1}{d_r - x\delta_{r+k}(d)} \nu_{n_r/m_r}(x)dx \\
&= \frac{1}{\delta_{r+k}(d)} G^{\mathbb{C}}_{\nu_{n_r/m_r}}(d_r/\delta_{r+k}(d)),
\end{aligned} \tag{5.40}
$$

where $G^{\mathbb{C}}_{\nu_{n_r/m_r}}$ is the Cauchy transform of the Marcenko-Pastur law ν_{n_r/m_r}.

Similarly, we may write (5.38) as

$$
\begin{aligned}
\gamma_{r+k}(d) &= \frac{n_r}{m_r}\tau_r\bigg(\Big(d - \sum_{s=1}^{k} g_s^* g_s \delta_{s+k}(d)\Big)^{-1} g_r^* g_r\bigg) \\
&= \frac{n_r}{m_r}\int \frac{x}{d_r - x\delta_{r+k}(d)} \nu_{n_r/m_r}(x)dx \\
&= \frac{n_r}{m_r}\bigg(-\frac{1}{\delta_{r+k}(d)} + \frac{d_r}{\delta_{r+k}(d)^2} G^{\mathbb{C}}_{\nu_{n_r/m_r}}(d_r/\delta_{r+k}(d))\bigg) \\
&= \frac{n_r}{m_r}\bigg(-\frac{1}{\delta_{r+k}(d)} + \frac{d_r}{\delta_{r+k}(d)} \tau_r(G_v^{\mathcal{D}}(d))\bigg),
\end{aligned} \tag{5.41}
$$

where the first equality applies the cyclic property of τ and the definitions of τ_{r+k} and τ_r, the second applies (5.24) upon passing to a power series and back as above, the third applies the definition of the Cauchy transform, and the last applies (5.40). The relation between $G_v^{\mathcal{D}}$ and $G_u^{\mathcal{D}}$ is given by (5.40), (5.41), and (5.39).

Step 3: We compute $m_0(z)$ for $z \in \mathbb{C}^+$ using (5.31), (5.32), (5.33), (5.40), (5.41), and (5.39). Fixing $z \in \mathbb{C}^+$, let us write

$$
\begin{aligned}
\alpha_r = \alpha_r(z), \quad \beta_r = \beta_r(z), \quad d_r = \frac{1}{\alpha_r} + \beta_r, \quad d = \sum_{r=0}^{2k} d_r p_r, \\
\gamma_r = \gamma_r(d), \quad \delta_r = \delta_r(d), \quad e_r = \frac{1}{\gamma_r} + \delta_r, \quad e = \sum_{r=0}^{2k} e_r p_r.
\end{aligned}
$$

Applying (5.31) and projecting down to $\mathbb{C}$,

$$
m_0(z) = -\tau_0\bigg(\Big(z - \sum_{r=1}^{k} h_r^* h_r \beta_r\Big)^{-1}\bigg).
$$

Note that $h_r^* h_r$ commutes with $\mathcal{D}$ and $p_0 h_r^* h_r p_0 = h_r^* h_r$ for each $r = 1, \ldots, k$. Then, passing to a power series as in Step 2, and then applying (5.23) and the spectral calculus,

$$
m_0(z) = -\sum_{l \geq 0} z^{-(l+1)} \tau_0\bigg(\Big(\sum_{r=1}^{k} h_r^* h_r \beta_r\Big)^{l}\bigg)
$$

$$
\begin{aligned}
&= -\sum_{l\geq 0} z^{-(l+1)} \frac{1}{p} \operatorname{Tr}\left(\Big(\sum_{r=1}^{k} \beta_r H_r^* H_r\Big)^l\right) \\
&= -\frac{1}{p} \operatorname{Tr}\Big(z \operatorname{Id}_p - \sum_{r=1}^{k} \beta_r H_r^* H_r\Big)^{-1}. \qquad (5.42)
\end{aligned}
$$

Similarly, (5.32) implies for each $r = 1, \ldots, k$

$$
\alpha_r = \frac{1}{n_r} \operatorname{Tr}\left(\Big(z \operatorname{Id}_p - \sum_{s=1}^{k} \beta_s H_s^* H_s\Big)^{-1} H_r^* H_r\right). \qquad (5.43)
$$

Now applying (5.40) and recalling (5.33) and the definition of d_r, for each $r = 1, \ldots, k$,

$$
\alpha_r = \tau_r(G_v^{\mathcal{D}}(d)) = \frac{1}{\delta_{r+k}} G^{\mathbb{C}}_{\nu_{n_r/m_r}}\left(\frac{1}{\alpha_r \delta_{r+k}} + \frac{\beta_r}{\delta_{r+k}}\right).
$$

Applying (5.15) and the Marcenko-Pastur $\mathcal{R}$-transform $\mathcal{R}^{\mathbb{C}}_{\nu_\lambda}(z) = (1 - \lambda z)^{-1}$, this is rewritten as

$$
\frac{\beta_r}{\delta_{r+k}} = \mathcal{R}^{\mathbb{C}}_{\nu_{n_r/m_r}}(\alpha_r \delta_{r+k}) = \frac{m_r}{m_r - n_r \alpha_r \delta_{r+k}}. \qquad (5.44)
$$

By (5.41) and (5.33),

$$
\gamma_{r+k} = \frac{n_r}{m_r} \frac{\alpha_r \beta_r}{\delta_{r+k}}. \qquad (5.45)
$$

We derive two consequences of (5.44) and (5.45). First, substituting for β_r in (5.45) using (5.44) and recalling the definition of e_{r+k} yields

$$
e_{r+k} = \frac{m_r}{n_r \alpha_r}. \qquad (5.46)
$$

Second, rearranging (5.44), we get $\beta_r/\delta_{r+k} = 1 + n_r \alpha_r \beta_r / m_r$. Inserting into (5.45) yields this time

$$
\beta_r = \frac{m_r}{n_r^2 \alpha_r^2}(m_r \gamma_{r+k} - n_r \alpha_r). \qquad (5.47)
$$

By (5.39), for each $r = 1, \ldots, k$,

$$
\gamma_{r+k} = \tau_{r+k}(G_u^{\mathcal{D}}(e)) = \tau_{r+k}((e-u)^{-1}).
$$

Passing to a power series for $(e-u)^{-1}$, applying (5.22), and passing back,

$$
\begin{aligned}
\gamma_{r+k} &= \frac{1}{m_r} \operatorname{Tr}_{r+k}\left(\operatorname{diag}(e_0 \operatorname{Id}_p, \ldots, e_{2k} \operatorname{Id}_{m_k}) - \tilde{F}\right)^{-1} \\
&= \frac{1}{m_r} \operatorname{Tr}_r\left(\operatorname{diag}(e_{k+1} \operatorname{Id}_{m_1}, \ldots, e_{2k} \operatorname{Id}_{m_k}) - F\right)^{-1}
\end{aligned}
$$

$$= \frac{1}{m_r} \operatorname{Tr}_r(D^{-1} - F)^{-1} \tag{5.48}$$

where the last line applies (5.46) and sets $D = \operatorname{diag}(D_1 \operatorname{Id}_{m_1}, \ldots, D_k \operatorname{Id}_{m_k})$ for $D_r = n_r\alpha_r/m_r$. Noting $\operatorname{Tr}_r D = n_r\alpha_r$, (5.47) yields

$$\begin{aligned}\beta_r &= \frac{1}{m_r D_r^2} \operatorname{Tr}_r[(D^{-1} - F)^{-1} - D] \\ &= \frac{1}{m_r} \operatorname{Tr}_r[(F^{-1} - D)^{-1}] = \frac{1}{m_r} \operatorname{Tr}_r((\operatorname{Id}_M - FD)^{-1}F) \end{aligned} \tag{5.49}$$

where we used the Woodbury identity and $\operatorname{Tr}_r DAD = D_r^2 \operatorname{Tr} A$. (These equalities hold when F is invertible, and hence for all F by continuity.) Setting $x_r = -n_r\alpha_r/m_r$ and $y_r = -\beta_r$, we obtain (5.19), (5.20), and (5.21) from (5.42), (5.43), and (5.49).

Step 4: Finally, we verify the validity of the preceding calculations when $z \in \mathbb{D} = \{z \in \mathbb{C}^+ : |z| > C_0\}$ and $C_0 > 0$ is sufficiently large. Call a scalar quantity $u = u(N, z)$ "uniformly bounded" if $|u| < C$ for all $z \in \mathbb{D}$, all N, and some constants $C_0, C > 0$. Call u "uniformly small" if for any constant $c > 0$ there exists $C_0 > 0$ such that $|u| < c$ for all $z \in \mathbb{D}$ and all N.

As $\|w\| \leq C$ by Lemma 5.14(c), $c = G_w^{\mathcal{H}}(z)$ is well-defined by the convergent series (5.13) for $z \in \mathbb{D}$. Furthermore by (5.16), $\|c\|$ is uniformly small, so we may apply (5.27). $\alpha_r(z)$ as defined by (5.28) satisfies

$$\begin{aligned}\alpha_r(z) &= \tau_r\left(h_r \sum_{l=0}^{\infty} \mathbf{F}^{\mathcal{H}}\left(z^{-1}(wz^{-1})^l\right) h_r^*\right) \\ &= \sum_{l=0}^{\infty} z^{-(l+1)} \tau(p_r)^{-1} \tau\left(h_r \mathbf{F}^{\mathcal{H}}(w^l) h_r^*\right) = \sum_{l=0}^{\infty} z^{-(l+1)} \frac{N}{n_r} \tau(w^l h_r^* h_r)\end{aligned}$$

for $z \in \mathbb{D}$. Since $|\tau(w^l h_r^* h_r)| \leq \|w\|^l \|h_r\|^2$, α_r defines an analytic function on $\mathbb{D}$ such that $\alpha_r(z) \sim (zn_r)^{-1} \operatorname{Tr}(H_r^* H_r)$ as $|z| \to \infty$. In particular, since H_r is non-zero by our initial assumption, $\alpha_r(z) \neq 0$ and $\operatorname{Im} \alpha_r(z) < 0$ for $z \in \mathbb{D}$. This verifies that $x_r(z) = -n_r\alpha_r(z)/m_r \in \mathbb{C}^+$ and x_r is analytic on $\mathbb{D}$. Furthermore, α_r is uniformly small for each r. Then applying (5.12), multi-linearity of κ_l, and (5.17), it is verified that $\beta_r(z)$ defined by (5.29) is uniformly bounded and analytic on $\mathbb{D}$. So $y_r(z) = -\beta_r(z)$ is analytic on $\mathbb{D}$.

As β_r is uniformly bounded, the formal series leading to (5.42) and (5.43) are convergent for $z \in \mathbb{D}$. Furthermore, $d_r = 1/\alpha_r + \beta_r$ is well-defined as $\alpha_r \neq 0$, and $\|d^{-1}\|$ is uniformly small. Then $c = G_v^{\mathcal{G}}(d)$ is well-defined by (5.13) and also uniformly small, so we may apply (5.34). By the same arguments as above, $\gamma_{r+k}(d)$ as defined by (5.35) is non-zero and uniformly small, and $\delta_{r+k}(d)$ as defined by (5.36) is uniformly bounded. Then the formal series leading to (5.40) and (5.41) are convergent for $z \in \mathbb{D}$. Furthermore, $e_r = 1/\gamma_r + \delta_r$ is well-defined and $\|e^{-1}\|$ is uniformly small, so the formal series leading to (5.48) is convergent for $z \in \mathbb{D}$. This verifies the validity of the preceding calculations and concludes the proof. $\square$

5.3 Analyzing the fixed-point equations

To finish the proof of Theorem 5.13, we show using a contractive mapping argument that (5.19–5.20) have a unique solution in the stated domains, which is the limit of the procedure in Theorem 2.20. The analysis follows arguments similar to those in [CDS11] and [DL11].

Lemma 5.17 ([CL11])**.** Let $\Omega \subseteq \mathbb{C}$ be a connected open set, let $E \subseteq \Omega$ be any set with an accumulation point in Ω, let $a, b \in \mathbb{C}$ be any two distinct fixed values, and let $\{f_n\}_{n=1}^{\infty}$ be a sequence of analytic functions $f_n : \Omega \to \mathbb{C}$. If $f_n(z) \notin \{a, b\}$ for all $z \in \Omega$ and $n \geq 1$, and if $\lim_{n\to\infty} f_n(z)$ exists (and is finite) for each $z \in E$, then $\{f_n\}_{n=1}^{\infty}$ converges uniformly on compact subsets of Ω to an analytic function.

Proof. The result is originally due to [CL11]. It also follows by the theory of normal families: $\{f_n\}_{n=1}^{\infty}$ is a normal family by Montel's fundamental normality test, see e.g. [Sch13, Section 2.7]. Hence every subsequence has a further subsequence that converges uniformly on compact sets to an analytic function. All such analytic functions must coincide on E, hence they coincide on all of Ω by uniqueness of analytic extensions, implying the desired result. $\square$

In the notation of Theorem 5.13, denote $\mathbf{x} = (x_1, \ldots, x_k)$, $\mathbf{y} = (y_1, \ldots, y_k)$,

$$f_r(z, \mathbf{y}) = -\frac{1}{m_r} \operatorname{Tr}\left((z \operatorname{Id}_p + \mathbf{y} \cdot H^* H)^{-1} H_r^* H_r\right),$$
$$g_r(\mathbf{x}) = -\frac{1}{m_r} \operatorname{Tr}_r\left([\operatorname{Id}_M + F D(\mathbf{x})]^{-1} F\right).$$

Lemma 5.18. Under the conditions of Theorem 5.13:

(a) For all $z \in \mathbb{C}^+$ and $\mathbf{y} \in (\overline{\mathbb{C}^+})^k$, $z \operatorname{Id}_p + \mathbf{y} \cdot H^* H$ is invertible, $f_r(z, \mathbf{y}) \in \mathbb{C}^+ \cup \{0\}$, and $m_0(z) \in \mathbb{C}^+$ for m_0 as defined by (5.21).

(b) For all $\mathbf{x} \in (\mathbb{C}^+ \cup \{0\})^k$, $\operatorname{Id}_M + F D(\mathbf{x})$ is invertible and $g_r(\mathbf{x}) \in \overline{\mathbb{C}^+}$.

Proof of Lemma 5.18. For any $\mathbf{v} \in \mathbb{C}^p$,

$$\operatorname{Im}[\mathbf{v}^*(z \operatorname{Id}_p + \mathbf{y} \cdot H^* H)\mathbf{v}] = (\operatorname{Im} z)\mathbf{v}^*\mathbf{v} + \sum_s (\operatorname{Im} y_s)\mathbf{v}^* H_s^* H_s \mathbf{v} > 0.$$

Hence $z \operatorname{Id}_p + \mathbf{y} \cdot H^* H$ is invertible. Letting $T = (z \operatorname{Id}_p + \mathbf{y} \cdot H^* H)^{-1}$,

$$m_r f_r(z, \mathbf{y}) = -\operatorname{Tr} T H_r^* H_r = -\operatorname{Tr} T H_r^* H_r T^* (z \operatorname{Id}_p + \mathbf{y} \cdot H^* H)^*$$

$$= -\overline{z} \operatorname{Tr} TH_r^* H_r T^* - \sum_{s=1}^{k} \overline{y_s} \operatorname{Tr} TH_r^* H_r T^* H_s^* H_s.$$

As $\operatorname{Tr} TRT^* S$ is real and nonnegative for any Hermitian positive-semidefinite matrices R and S, the above implies $\operatorname{Im} f_r(z, \mathbf{y}) \geq 0$. In fact, as $\operatorname{Tr} TH_r^* H_r T^* > 0$ unless $H_r = 0$, either $\operatorname{Im} f_r(z, \mathbf{y}) > 0$ or $f_r(z, \mathbf{y}) = 0$. Similarly,

$$pm_0(z) = -\operatorname{Tr} T = -\overline{z} \operatorname{Tr} TT^* - \sum_{s=1}^{k} \overline{y_s} \operatorname{Tr} TT^* H_s^* H_s,$$

and as $\operatorname{Tr} TT^* > 0$, $\operatorname{Im} m_0(z) > 0$. This establishes (a).

For (b), let us first show $\operatorname{Id}_M + FD(\mathbf{x})$ is invertible. Note if $x_1 = 0$, then by the fact that a block matrix

$$\begin{pmatrix} A & B \\ 0 & C \end{pmatrix}$$

is invertible if and only if A and C are invertible, it suffices to show invertibility of the lower-right $(n_2 + \ldots + n_k) \times (n_2 + \ldots + n_k)$ submatrix. Hence we may reduce to the case where $x_s \neq 0$, i.e. $x_s \in \mathbb{C}^+$, for all s. Suppose $\operatorname{rank}(F) = m$ and let $F^\dagger$ denote the pseudo-inverse of F, so that $FF^\dagger$ is a projection matrix of rank m onto the column span of F. $F^\dagger$ is Hermitian, since F is. Let Q denote the projection orthogonal to $FF^\dagger$, of rank $M - m$. Then

$$\operatorname{Id}_M + FD(\mathbf{x}) = Q + F(F^\dagger + D(\mathbf{x})).$$

For each $s = 1, \ldots, k$, let P_s be the projection of rank m_s such that $D(\mathbf{x}) = \sum_{s=1}^{k} x_s P_s$. Then for any $\mathbf{v} \in \mathbb{C}^M$,

$$\operatorname{Im}[\mathbf{v}^*(F^\dagger + D(\mathbf{x}))\mathbf{v}] = \operatorname{Im}[\mathbf{v}^* D(\mathbf{x})\mathbf{v}] = \sum_s (\operatorname{Im} x_s)\mathbf{v}^* P_s \mathbf{v} > 0,$$

as $\mathbf{v}^* F^\dagger \mathbf{v}$ and $\mathbf{v}^* P_s \mathbf{v}$ are real and $\operatorname{Im} a_s > 0$ for each s. Hence $F^\dagger + D(\mathbf{x})$ is invertible, so $\operatorname{Id}_M + FD(\mathbf{x})$ is of full column rank and thus also invertible.

For the second claim, supposing momentarily that F is invertible and letting $J = (F^{-1} + D(\mathbf{x}))^{-1}$,

$$\begin{aligned} m_r g_r(\mathbf{x}) &= -\operatorname{Tr}_r J = -\operatorname{Tr}_r \left(J \left(F^{-1} + \sum_{s=1}^{k} x_s P_s \right)^* J^* \right) \\ &= -\operatorname{Tr} P_r J F^{-1} J^* - \sum_{s=1}^{k} \overline{x_s} \operatorname{Tr} P_r J P_s J^*. \end{aligned}$$

As $\operatorname{Tr} P_r J F^{-1} J^*$ is real and $\operatorname{Tr} P_r J P_s J^*$ is real and nonnegative, this implies $\operatorname{Im} g_r(\mathbf{x}) \geq 0$. By continuity in F, this must hold also when F is not invertible, establishing (b). $\square$

Lemma 5.19. Let $C, L > 0$ and let $\mathcal{S}$ denote the space of k-tuples $\mathbf{y} = (y_1, \dots, y_k)$ such that each y_r is an analytic function $y_r : \mathbb{C}^+ \to \overline{\mathbb{C}^+}$ and $\sup_{z \in \mathbb{C}^+ : \operatorname{Im} z > L} \|\mathbf{y}(z)\| \leq C$. For sufficiently large C and L (depending on p, n_r, m_r and the matrices H_r and F_{rs} in Theorem 5.13):

(a) $\rho : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ defined by

$$\rho(\mathbf{y}, \tilde{\mathbf{y}}) = \sup_{z \in \mathbb{C}^+ : \operatorname{Im} z > L} \|\mathbf{y}(z) - \tilde{\mathbf{y}}(z)\|$$

is a complete metric on $\mathcal{S}$, and

(b) Letting $g = (g_1, \dots, g_k)$ and $f = (f_1, \dots, f_k)$ where g_r and f_r are as above, $\mathbf{y} \mapsto g(f(z, \mathbf{y}))$ defines a map from $\mathcal{S}$ to itself, and there exists $c \in (0, 1)$ such that for all $\mathbf{y}, \tilde{\mathbf{y}} \in \mathcal{S}$,

$$\rho(g(f(z, \mathbf{y})), g(f(z, \tilde{\mathbf{y}}))) \leq c\rho(\mathbf{y}, \tilde{\mathbf{y}}).$$

Proof. For part (a), ρ is clearly nonnegative, symmetric, and satisfies the triangle inequality. By definition of $\mathcal{S}$, $\rho(\mathbf{y}, \tilde{\mathbf{y}}) < \infty$ for all $\mathbf{y}, \tilde{\mathbf{y}} \in \mathcal{S}$. By uniqueness of analytic extensions, $\rho(\mathbf{y}, \tilde{\mathbf{y}}) = 0 \Leftrightarrow \mathbf{y} = \tilde{\mathbf{y}}$, hence ρ is a metric. If $\{\mathbf{y}^{(l)}\}_{l=1}^{\infty}$ is a Cauchy sequence in $(\mathcal{S}, \rho)$, then for each $z \in \mathbb{C}^+$ with $\operatorname{Im} z > L$, $\{\mathbf{y}^{(l)}(z)\}_{l=1}^{\infty}$ is Cauchy in $(\overline{\mathbb{C}^+})^k$ and hence converges to some $\mathbf{y}(z) = (y_1(z), \dots, y_k(z)) \in (\overline{\mathbb{C}^+})^k$. Then Lemma 5.17 implies each $y_r(z)$ has an analytic extension to all of $\mathbb{C}^+$, and $y_r^{(l)} \to y_r$ uniformly over compact subsets of $\mathbb{C}^+$. This implies $y_r(z) \in \overline{\mathbb{C}^+}$ for all $z \in \mathbb{C}^+$ and $\sup_{z \in \mathbb{C}^+ : \operatorname{Im} z > L} \|\mathbf{y}(z)\| \leq C$, so $\mathbf{y} \in \mathcal{S}$. Furthermore $\rho(\mathbf{y}^{(l)}, \mathbf{y}) \to 0$, hence $(\mathcal{S}, \rho)$ is complete.

For part (b), clearly if $\mathbf{y} = (y_1, \dots, y_k)$ is a k-tuple of analytic functions on $\mathbb{C}^+$, then $g(f(z, \mathbf{y}))$ is as well. Now consider $z \in \mathbb{C}^+$ with $\operatorname{Im} z > L$ and fixed values $\mathbf{y} \in (\overline{\mathbb{C}^+})^k$ with $\|\mathbf{y}\| \leq C$, and define

$$T = (z \operatorname{Id}_p + \mathbf{y} \cdot H^* H)^{-1}, \qquad R = (\operatorname{Id}_M + FD(f(z, \mathbf{y})))^{-1}, \tag{5.50}$$

where invertibility of these quantities follows from Lemma 5.18. Since $H_s^* H_s$ is positive-semidefinite, [CDS11, Lemma 8] implies $\|T\| \leq (\operatorname{Im} z)^{-1}$. Then if $C, D > 0$ (depending on p, m_r, n_r, H_r, F_{rs}) are sufficiently large, we have $|f_r(z, \mathbf{y})| \leq C(\operatorname{Im} z)^{-1}$, $\|FD(f(z, \mathbf{y}))\| < 1/2$, $\|R\| < 2$, and $\|g(f(z, \mathbf{y}))\| \leq C$. This establishes that for sufficiently large $C, L > 0$, if $\mathbf{y} \in \mathcal{S}$, then $g(f(z, \mathbf{y})) \in \mathcal{S}$.

Next, consider also $\tilde{\mathbf{y}} \in (\overline{\mathbb{C}^+})^k$ with $\|\tilde{\mathbf{y}}\| \leq C$, and define $\tilde{T}$ and $\tilde{R}$ by (5.50) with $\tilde{\mathbf{y}}$ in place of $\mathbf{y}$. For each $s = 1, \dots, k$, let P_s be the projection such that $D(\mathbf{x}) = \sum_{s=1}^k x_s P_s$. Then by the matrix identity $A^{-1} - (A + E)^{-1} = A^{-1} E (A + E)^{-1}$,

$$\begin{aligned}
f_r(z, \mathbf{y}) - f_r(z, \tilde{\mathbf{y}}) &= \frac{1}{m_r} \operatorname{Tr}\left(\tilde{T}(T^{-1} - \tilde{T}^{-1}) T H_r^* H_r\right) \\
&= \frac{1}{m_r} \sum_{s=1}^k (y_s - \tilde{y}_s) \operatorname{Tr}\left(\tilde{T} H_s^* H_s T H_r^* H_r\right), \\
g_r(f(z, \mathbf{y})) - g_r(f(z, \tilde{\mathbf{y}})) &= \frac{1}{m_r} \operatorname{Tr} P_r \tilde{R}(R^{-1} - \tilde{R}^{-1}) R F
\end{aligned}$$

$$= \frac{1}{m_r} \sum_{s=1}^{k} (f_s(z, \mathbf{y}) - f_s(z, \tilde{\mathbf{y}})) \operatorname{Tr} P_r \tilde{R} F P_s R F.$$

Then $g(f(z, \mathbf{y})) - g(f(z, \tilde{\mathbf{y}})) = M^{(2)} M^{(1)} (\mathbf{y} - \tilde{\mathbf{y}})$ for the matrices $M^{(1)}, M^{(2)} \in \mathbb{C}^{k \times k}$ having entries

$$M_{rs}^{(1)} = \frac{1}{m_r} \operatorname{Tr} \left(\tilde{T} H_s^* H_s T H_r^* H_r \right), \quad M_{rs}^{(2)} = \frac{1}{m_r} \operatorname{Tr} P_r \tilde{R} F P_s R F.$$

For sufficiently large $C, L > 0$, we have $\|T\| \leq (\operatorname{Im} z)^{-1}$, $\|\tilde{T}\| \leq (\operatorname{Im} z)^{-1}$, $\|M^{(1)}\| \leq C (\operatorname{Im} z)^{-2}$, $\|R\| < 2$, $\|\tilde{R}\| < 2$, and $\|M^{(2)}\| \leq C$, hence $\|M^{(2)} M^{(1)}\| \leq C^2 (\operatorname{Im} z)^{-2} \leq C^2 L^{-2}$. Increasing L if necessary so that $C^2 L^{-2} < 1$, this yields part (b). □

We conclude the proof of Theorem 5.13 using these lemmas, Corollary 5.10, and Lemma 5.16.

Proof of Theorem 5.13. Let $C, L > 0$ be (p, m_r, n_r-dependent values) such that the conclusions of Lemma 5.19 hold. Increasing C if necessary, assume $\|\mathbf{y}^{(0)}\| < C$ where $\mathbf{y}^{(0)} = (y_1^{(0)}, \ldots, y_k^{(0)})$ are the initial values for the iterative procedure of part (c). Lemma 5.19 and the Banach fixed point theorem imply the existence of a unique point $\mathbf{y} \in \mathcal{S}$ such that $g(f(z, \mathbf{y})) = \mathbf{y}$. Defining $\mathbf{x} = f(z, \mathbf{y})$, Lemma 5.18 implies $\mathbf{x} \in (\mathbb{C}^+ \cup \{0\})^k$ for each $z \in \mathbb{C}^+$. Then x_r, y_r satisfy (5.19) and (5.20) for each $z \in \mathbb{C}^+$ by construction, which verifies existence in part (a). For part (c), define the constant functions $\tilde{y}_r^{(0)}(z) \equiv y_r^{(0)}$ over $z \in \mathbb{C}^+$. Then $\tilde{\mathbf{y}}^{(0)} = (\tilde{y}_1^{(0)}, \ldots, \tilde{y}_r^{(0)}) \in \mathcal{S}$. Define iteratively $\tilde{\mathbf{y}}^{(t+1)} = g(f(z, \tilde{\mathbf{y}}^{(t)}))$. Then Lemma 5.19 implies

$$c\rho(\mathbf{y}, \tilde{\mathbf{y}}^{(t)}) \geq \rho(g(f(z, \mathbf{y})), g(f(z, \tilde{\mathbf{y}}^{(t)}))) = \rho(\mathbf{y}, \tilde{\mathbf{y}}^{(t+1)}),$$

for $\mathbf{y}$ the above fixed point and some $c \in (0, 1)$. Hence $\rho(\mathbf{y}, \tilde{\mathbf{y}}^{(t)}) \to 0$ as $t \to \infty$. This implies by Lemma 5.17 that $\tilde{\mathbf{y}}^{(t)}(z) \to \mathbf{y}(z)$ for all $z \in \mathbb{C}^+$, which establishes part (c) upon noting that $\tilde{y}_r^{(t)}(z)$ is exactly the value $y_r^{(t)}$ of the iterative procedure applied at z. Part (c) implies uniqueness in part (a), since $(y_1^{(t)}, \ldots, y_k^{(t)})$ would not converge to $(y_1, \ldots, y_k)$ if this iterative procedure were initialized to a different fixed point. For part (b), Lemma 5.18 verifies that $m_0(z) \in \mathbb{C}^+$ for $z \in \mathbb{C}^+$. As $y_1(z), \ldots, y_k(z)$ are analytic, $m_0(z)$ is also analytic. Furthermore, as $\mathbf{y} \in \mathcal{S}$, $y_1(z), \ldots, y_k(z)$ remain bounded as $\operatorname{Im} z \to \infty$, so $m_0(z) \sim -z^{-1}$ as $\operatorname{Im} z \to \infty$. Then m_0 defines the Stieltjes transform of a probability measure μ_0 by [GH03, Lemma 2].

It remains to verify that μ_0 approximates μ_W. Let $f_{rs}, g_r, h_r \in \mathcal{A}$ be the free deterministic equivalent constructed by Lemma 5.14, and let $N = p + \sum_r m_r + \sum_r n_r$. Uniqueness of the solution x_r, y_r to (5.19) and (5.20) in the stated domains implies that the analytic functions $x_1, \ldots, x_k, y_1, \ldots, y_k$ in Lemma 5.16 must coincide with this solution for $z \in \mathbb{D}$. Then Lemma 5.16 implies, for $z \in \mathbb{D}$,

$$m_w(z) := \tau((w - z)^{-1}) = \frac{p}{N} m_0(z) - \frac{N - p}{Nz}.$$

The conditions of Corollary 5.10 are satisfied by Lemma 5.14, so Corollary 5.10 implies $m_{\tilde{W}}(z) - m_w(z) \to 0$ as $p, n_r, m_r \to \infty$, pointwise a.s. over $\mathbb{D}$, where $\tilde{W} \in \mathbb{C}^{N \times N}$ is the embedding of W and $m_{\tilde{W}}$ is its empirical spectral measure. As

$$m_{\tilde{W}}(z) = \frac{p}{N} m_W(z) - \frac{N-p}{Nz},$$

we have $m_W(z) - m_0(z) \to 0$ pointwise a.s. over $\mathbb{D}$. As $m_W - m_0$ is uniformly bounded over $\{z \in \mathbb{C}^+ : \operatorname{Im} z > \varepsilon\}$ for any $\varepsilon > 0$, Lemma 5.17 implies $m_W(z) - m_0(z) \to 0$ pointwise a.s. for $z \in \mathbb{C}^+$. Hence $\mu_W - \mu_0 \to 0$ vaguely a.s. (see, e.g., [BS10, Theorem B.9]). By the conditions of the theorem, $\|W\|$ is almost surely bounded by a constant for all large p, n_r, m_r. Furthermore, by Lemma 5.14, we have $\tau(w^l) \leq \|w\|^l \leq C^l$ for some constant $C > 0$ and all $l \geq 0$, so m_w and m_0 are Stieltjes transforms of probability measures with bounded support. Then the convergence $\mu_W - \mu_0 \to 0$ holds weakly a.s., concluding the proof of the theorem. □

Appendix A

Marcenko-Pastur model

We collect in this appendix various properties of the Marcenko-Pastur model $\widehat{\Sigma} = X'FX$ and the associated law μ_0 defined in Theorem 2.4. Without loss of generality, we assume $F = T = \operatorname{diag}(t_1, \ldots, t_M)$ is diagonal.

A.1 Density, support, and edges of μ_0

Recall the Stieltjes transform $m_0(z)$ defined by (3.8), and the inverse function $z_0(m)$ from (3.11). Let

$$P = \{0\} \cup \{-t_\alpha^{-1} : t_\alpha \neq 0\}$$

denote the poles of $z_0(m)$. The following characterization of the density and support of μ_0 are from [SC95]:

Proposition A.1. The limit

$$m_0(x) = \lim_{\eta \downarrow 0} m_0(x + i\eta) \tag{A.1}$$

exists for each $x \in \mathbb{R} \setminus \{0\}$. At each such x, the law μ_0 admits a continuous density given by

$$f_0(x) = \frac{1}{\pi} \operatorname{Im} m_0(x).$$

Proof. See [SC95, Theorem 1.1]. □

Proposition A.2. Let $S = \{m \in \mathbb{R} \setminus P : z_0'(m) > 0\}$ and $z_0(S) = \{z_0(m) : m \in S\}$. Then

$$\mathbb{R} \setminus \operatorname{supp}(\mu_0) = z_0(S).$$

Furthermore, $z_0 : S \to \mathbb{R} \setminus \operatorname{supp}(\mu_0)$ is a bijection with inverse $m_0 : \mathbb{R} \setminus \operatorname{supp}(\mu_0) \to S$.

Proof. See [SC95, Theorems 4.1 and 4.2]. ☐

Proposition A.2 implies that μ_0 has bounded support:

Proposition A.3. Under Assumption 3.1, $\operatorname{supp}(\mu_0) \subset [-C, C]$ for a constant $C > 0$.

Proof. Proposition A.2 and the behavior of $z_0(m)$ as $m \to 0$ implies that μ_0 has compact support for each N. Furthermore, each non-zero boundary point of $\operatorname{supp}(\mu_0)$ is given by $z_0(m_*)$ for some $m_* \in \mathbb{R}$ satisfying $z_0'(m_*) = 0$. Rearranging this condition yields

$$1 = \frac{1}{N} \sum_{\alpha=1}^{M} \frac{m_*^2 t_\alpha^2}{(1 + m_* t_\alpha)^2}.$$

Since $\|T\| < C$, this condition implies $|m_*| > c$ for a constant $c > 0$. Furthermore, Cauchy-Schwarz yields

$$\left(\frac{1}{M} \sum_{\alpha=1}^{M} \frac{t_\alpha}{1 + m_* t_\alpha} \right)^2 \leq \frac{1}{M} \sum_{\alpha=1}^{M} \frac{t_\alpha^2}{(1 + m_* t_\alpha)^2} = \frac{N}{M m_*^2}.$$

Combining these yields $|z_0(m_*)| < C$ for a constant $C > 0$, so each non-zero boundary point of $\operatorname{supp}(\mu_0)$ belongs to $[-C, C]$. ☐

We next extend Proposition A.1 to handle the case $x = 0$ (cf. Proposition A.6 below).

Lemma A.4. Denote $m_0(\mathbb{C}^+) = \{m_0(z) : z \in \mathbb{C}^+\}$. For any $m \in \mathbb{R} \setminus P$ such that $z_0'(m) < 0$, m cannot belong to the closure of $m_0(\mathbb{C}^+)$.

Proof. z_0 defines an analytic function on $\mathbb{C} \setminus P$. For any such m, the inverse function theorem implies z_0 has an analytic inverse in a neighborhood B of m in $\mathbb{C} \setminus P$. If m belongs to the closure of $m_0(\mathbb{C}^+)$, then $B \cap m_0(\mathbb{C}^+)$ is non-empty. As $z_0(m_0(z)) = z$ for $z \in \mathbb{C}^+$ by definition of m_0, the inverse of z_0 on B is an analytic extension of m_0 to $z_0(B)$. By the open mapping theorem, $z_0(B)$ is an open set in $\mathbb{C}$ containing m. On the other hand, as m_0 is the Stieltjes transform of μ_0, it permits an analytic extension only to $\mathbb{C} \setminus \operatorname{supp}(\mu_0)$, and this extension is real-valued and increasing on $\mathbb{R} \setminus \operatorname{supp}(\mu_0)$. Then $z_0(B) \cap \mathbb{R}$ must belong to $\mathbb{R} \setminus \operatorname{supp}(\mu_0)$ and z_0 must be increasing on $B \cap \mathbb{R}$, but this contradicts that $z_0'(m) < 0$. ☐

Lemma A.5. Define

$$g(q) = z_0(1/q) = -q + \frac{1}{N} \sum_{\alpha=1}^{M} \left(t_\alpha - \frac{t_\alpha^2}{q + t_\alpha} \right). \tag{A.2}$$

Then for any $c \in \mathbb{R}$, there is at most one value $q \in \mathbb{R}$ for which $g(q) = c$ and $g'(q) \leq 0$.

Proof. Denote by $P' = \{-t_\alpha : t_\alpha \neq 0\}$ the distinct poles of g, and let $I_1, \ldots, I_{|P'|+1}$ be the intervals of $\mathbb{R} \setminus P'$ in increasing order. For any $c \in \mathbb{R}$, boundary conditions of g at P' imply that $g(q) = c$ has at least one root q in each interval $I_2, \ldots, I_{|P'|}$, and hence at least $|P'| - 1$ total roots. In addition, every $q \in \mathbb{R}$ where $g(q) = c$ and $g'(q) \leq 0$ contributes two additional roots to $g(q) = c$, counting multiplicity. As $g(q) = c$ may be written as a polynomial equation in q of degree $|P'|+1$ by clearing denominators, it can have at most $|P'|+1$ total roots counting multiplicity, and hence there is at most one such q. $\square$

Proposition A.6. If $\operatorname{rank}(T) > N$, then the limit (A.1) exists also at $x = 0$, and μ_0 has continuous density $f_0(x) = (1/\pi)\operatorname{Im} m_0(x)$ at $x = 0$.

If $\operatorname{rank}(T) \leq N$, then for any sequence $z_n \to 0$ with $z_n \in \overline{\mathbb{C}^+} \setminus \{0\}$, we have $|m_0(z_n)| \to \infty$.

Proof. Suppose $\operatorname{rank}(T) > N$. Taking imaginary parts of (3.8) yields

$$\operatorname{Im} z = \frac{\operatorname{Im} m_0(z)}{|m_0(z)|^2}\left(1 - \frac{1}{N}\sum_{\alpha=1}^{M} \frac{|t_\alpha m_0(z)|^2}{|1 + t_\alpha m_0(z)|^2}\right). \tag{A.3}$$

Both $\operatorname{Im} z > 0$ and $\operatorname{Im} m_0(z) > 0$ for $z \in \mathbb{C}^+$, whereas if $|m_0(z_n)| \to \infty$ along any sequence $z_n \in \mathbb{C}^+$, then

$$\left(1 - \frac{1}{N}\sum_{\alpha=1}^{M} \frac{|t_\alpha m_0(z_n)|^2}{|1 + t_\alpha m_0(z_n)|^2}\right) \to 1 - \frac{\operatorname{rank}(T)}{N}.$$

When $\operatorname{rank}(T) > N$, this implies $m_0(z)$ is bounded on all of $\mathbb{C}^+$. In particular, it is bounded in a neighborhood of $x = 0$, and the result follows from the same proof as [SC95, Theorem 1.1].

Suppose now $\operatorname{rank}(T) \leq N$. Note (3.8) holds for $z \in \overline{\mathbb{C}^+} \setminus \{0\}$ by continuity of m_0. If $m_0(z_n) \to m$ for some finite m along any sequence $z_n \in \overline{\mathbb{C}^+} \setminus \{0\}$ with $z_n \to 0$, then $z_0(m) = \lim_n z_0(m_0(z_n)) = 0$, and $m \notin P$. Rearranging (3.8) yields

$$z m_0(z) = -1 + \frac{\operatorname{rank}(T)}{N} - \frac{1}{N}\sum_{\alpha : t_\alpha \neq 0} \frac{1}{1 + t_\alpha m_0(z)},$$

and taking real and imaginary parts followed by $z_n \to 0$ yields

$$1 - \frac{\operatorname{rank}(T)}{N} = -\frac{1}{N}\sum_{\alpha : t_\alpha \neq 0} \frac{1 + t_\alpha \operatorname{Re} m}{|1 + t_\alpha m|^2}, \qquad 0 = \frac{1}{N}\sum_{\alpha : t_\alpha \neq 0} \frac{t_\alpha \operatorname{Im} m}{|1 + t_\alpha m|^2}.$$

When $\operatorname{rank}(T) \leq N$, the first equation implies $\operatorname{Re} m \neq 0$ and $\sum_{\alpha : t_\alpha \neq 0} t_\alpha / |1 + t_\alpha m|^2 \neq 0$, and the second equation then implies $\operatorname{Im} m = 0$. Thus $m \in \mathbb{R} \setminus P$. But recalling $g(q)$ from (A.2), we have $g(0) = 0$ and $g'(0) \leq 0$ when $\operatorname{rank}(T) \leq N$, so Lemma A.5 implies $g'(q) > 0$ for every other q where $g(q) = 0$. Thus $z_0'(m) < 0$, but this contradicts Lemma A.4. Hence $|m_0(z_n)| \to \infty$. $\square$

Recall $\mathbb{R}_*$ from (3.10) and the notion of a soft edge from Definition 3.4. We record the following consequence of the above.

Proposition A.7. If E_* is a soft edge of μ_0 with m-value m_*, then $E_* \in \mathbb{R}_*$, m_0 extends continuously to E_*, and $m_0(E_*) = m_*$.

Proof. Recalling $g(q)$ from (A.2), if $E_* = 0$ is a soft edge, then $g(1/m_*) = 0$ and $g'(1/m_*) = 0$. Hence Lemma A.5 implies $g'(0) > 0$, so $\operatorname{rank}(T) > N$. Thus any soft edge E_* belongs to $\mathbb{R}_*$. Propositions A.1 and A.6 then imply continuous extension of m_0 to E_*. Considering $m \in \mathbb{R}$ with $z_0'(m) > 0$ and $m \to m_*$, Proposition A.2 implies $m_0(z_0(m)) = m$, while continuity of z_0 and m_0 yield $z_0(m) \to z_0(m_*) = E_*$ and $m_0(z_0(m)) \to m_0(E_*)$. Hence $m_0(E_*) = m_*$. □

We now establish the characterization of edges of μ_0 given in Proposition 3.3.

Proof of Proposition 3.3. Let $g(q)$ be as in Lemma A.5. If m_j is a local minimum (or maximum) of z_0, then $q_j = 1/m_j$ is a local minimum (resp. maximum) of g, where $q_j = 0$ if $m_j = \infty$. Furthermore these are the only local extrema of g, and they are ordered as $q_1 < \ldots < q_n$. We have $E_j = g(q_j)$ for each $j = 1, \ldots, n$.

Let $P' = \{-t_\alpha : t_\alpha \neq 0\}$ be the poles of g, and let $I_1, \ldots, I_{|P'|+1}$ be the intervals of $\mathbb{R} \setminus P'$ in increasing order. Denoting

$$S' = \{q \in \mathbb{R} \setminus P' : g'(q) < 0\},$$

Proposition A.2 is rephrased in terms of g as

$$\mathbb{R} \setminus \operatorname{supp}(\mu_0) = g(S' \setminus \{0\}). \tag{A.4}$$

(We must remove 0 from S', as $m = \infty$ is not included in S.) As $g'''(q) > 0$ for all $q \in \mathbb{R} \setminus P'$, we have that $g'(q)$ is convex on each I_j. Together with the boundary conditions $g'(q) \to \infty$ as $q \to P'$ and $g'(q) \to -1$ as $q \to \pm\infty$, this implies I_1 contains the single local extremum q_1 (a minimum), $I_{|P'|+1}$ contains the single local extremum q_n (a maximum), and each I_j for $j = 2, \ldots, |P'|$ contains either 0 or 2 local extrema (a maximum followed by a minimum). Hence S' is a union of open intervals, say $J_1, \ldots, J_r$, with at most one such interval contained in each I_j. Lemma A.5 verifies

$$\overline{g(J_j)} \cap \overline{g(J_k)} = \emptyset \tag{A.5}$$

for all $j \neq k$. Together with (A.4), this verifies that the edges of μ_0 are precisely the values $g(q_j)$, with a local maximum q_j corresponding to a left edge and a local minimum q_j corresponding to a right edge. If $0 \in S'$, then it belongs to the interior of some open interval J_j, and $\operatorname{supp}(\mu_0)$ contains an isolated point at 0 which is not considered an edge. This establishes (a) and (b).

The ordering in part (c) follows from a continuity argument as in [KY17, Lemma 2.5]: Define for $\lambda \in (0, 1]$

$$g_\lambda(q) = -q + \frac{\lambda}{N} \sum_{\alpha=1}^{M} \left(t_\alpha - \frac{t_\alpha^2}{q + t_\alpha} \right).$$

Note that $g_\lambda'(q)$ is increasing in λ for each fixed $q \in \mathbb{R} \setminus P'$. Hence for each local minimum (or maximum) q_j of g, we may define a path $q_j(\lambda)$, continuous and increasing (resp. decreasing) in λ, such that $q_j(1) = q_j$ and $q_j(\lambda)$ remains a local minimum (resp. maximum) of g_λ for each $\lambda \in (0, 1]$. As $\lambda \searrow 0$, each $q_j(\lambda)$ converges to a pole $-t_\alpha$ in P', with $g_\lambda(q_j(\lambda)) \searrow t_\alpha$ if $q_j(\lambda) \nearrow -t_\alpha$ and $g_\lambda(q_j(\lambda)) \nearrow t_\alpha$ if $q_j(\lambda) \searrow -t_\alpha$. Hence for sufficiently small $\lambda > 0$,

$$g_\lambda(q_1(\lambda)) > \ldots > g_\lambda(q_n(\lambda)).$$

Lemma A.5 applies to g_λ for each fixed λ, implying in particular that $g_\lambda(q_j(\lambda)) \neq g_\lambda(q_k(\lambda))$ for any $j \neq k$. Hence by continuity in λ, the above ordering is preserved for all $\lambda \in (0, 1]$. In particular it holds at $\lambda = 1$, which establishes (c).

Finally, for part (d), suppose E_j is a soft right edge. Proposition A.7 yields $m_j \in \mathbb{R}_*$ and $m_0(E_j) = m_j$. The previous convexity argument implies $g''(q_j) \neq 0$ for any local extremum q_j, and hence $z_0''(m_j) \neq 0$. Taking $x \nearrow E_j$, continuity of m_0 implies $m_0(x) \to m_j$. As z_0 is analytic at m_j and $z_0'(m_j) = 0$, a Taylor expansion yields, as $x \nearrow E_j$,

$$x - E_j = z_0(m_0(x)) - z_0(m_j) = \frac{z_0''(m_j)}{2}(1 + o(1))(m_0(x) - m_j)^2.$$

Since $\operatorname{Im} m_0(x) > 0$ and $\operatorname{Im} m_j = 0$, this yields

$$m_0(x) - m_j = \sqrt{\frac{2}{z_0''(m_j)}(x - E_j)(1 + o(1))},$$

where we take the square root with branch cut on the positive real axis and having positive imaginary part. Taking imaginary parts and recalling $f_0(x) = (1/\pi) \operatorname{Im} m_0(x)$ yields (d). The case of a left edge is similar. $\square$

A.2 Behavior of $m_0(z)$

First consider $z \in U_\delta = \{z \in \mathbb{C} : \operatorname{dist}(z, \operatorname{supp}(\mu_0)) \geq \delta\}$ for a constant $\delta > 0$. We establish some basic bounds on m_0 and $\operatorname{Im} m_0$.

Proposition A.8. Suppose Assumption 3.1 holds. Fix any constant $\delta > 0$. Then for some constant $c > 0$, all $z \in U_\delta$, and each eigenvalue t_α of T,

$$|1 + t_\alpha m_0(z)| > c.$$

Proof. Note that (2.11) implies $|m_0(z)| \leq 1/\delta$. The result then holds for $|t_\alpha| < \delta/2$. Since $\|T\| < C_0$ for a constant $C_0 > 0$, it also holds when $|m_0(z)| < 1/(2C_0)$. Proposition A.3 shows that $\operatorname{supp}(\mu_0)$ is uniformly bounded, so there is a constant $R > 0$ such that $|m_0(z)| < 1/(2C_0)$ when $|z| > R$. Thus it remains to consider the case

$$|t_\alpha| \geq \delta/2, \qquad |m_0(z)| \geq 1/(2C_0), \qquad |z| \leq R. \tag{A.6}$$

For this case, consider first $z \in U_\delta \cap \mathbb{R}$, so that $m_0(z) \in \mathbb{R}$. The result is immediate if $t_\alpha m_0(z) > 0$. Otherwise, note that $\operatorname{sign}(m_0(z)) = \operatorname{sign}(-1/t_\alpha)$. Since $z \notin \operatorname{supp}(\mu_0)$, Proposition A.2 implies $z_0'(m_0(z)) > 0$. By the behavior of z_0 at its poles, there exists $m_* \in \mathbb{R}$ between $m_0(z)$ and $-1/t_\alpha$ such that $z_0'(m_*) = 0$ and $z_0'(m) > 0$ for each m between m_* and $m_0(z)$. Note that $|1/t_\alpha| > 1/C_0$, so $|m| > 1/(2C_0)$ for each such m. Also, differentiating (3.11) yields $z_0'(m) \leq 1/m^2$. So $0 < z_0'(m) < 4C_0^2$ for each such m. Then, since $z = z_0(m_0(z))$, we have

$$|m_0(z) + 1/t_\alpha| > |m_0(z) - m_*| > |z - z_0(m_*)|/(4C_0^2).$$

Since $z_0(m_*)$ is a boundary of $\operatorname{supp}(\mu_0)$ and $z \in U_\delta$, we have $|z - z_0(m_*)| > \delta$. Multiplying by $|t_\alpha|$ and applying $|t_\alpha| \geq \delta/2$ yields the result when $z \in U_\delta \cap \mathbb{R}$.

To extend to all $z \in U_\delta$ satisfying (A.6), note that for any $z, z' \in U_{\delta/2}$, we have by (2.11)

$$|m_0(z) - m_0(z')| \leq \int \left| \frac{1}{x - z} - \frac{1}{x - z'} \right| \mu_0(dx) \leq C|z - z'|.$$

Thus $|1 + t_\alpha m_0(z)| > c$ for all $z \in U_\delta$ in an ε-neighborhood of $U_{\delta/2} \cap \mathbb{R}$, for a sufficiently small constant $\varepsilon > 0$. For all other $z \in U_\delta$, we have $|\operatorname{Im} z| > \varepsilon$, so the bound $|z| < R$ in (A.6) implies

$$|\operatorname{Im} m_0(z)| = \left| \int \frac{\operatorname{Im} z}{|x - z|^2} \mu_0(dx) \right| > c.$$

Then $|1 + t_\alpha m_0(z)| \geq |t_\alpha| \cdot |\operatorname{Im} m_0(z)| > c$. ☐

Proposition A.9. Suppose Assumption 3.1 holds. Fix $\delta, R > 0$. Then there exist constants $C, c > 0$ such that for all $z \in U_\delta$,

$$|m_0(z)| < C, \qquad |\operatorname{Im} m_0(z)| \leq C|\operatorname{Im} z|,$$

and for all $z \in U_\delta$ with $|z| < R$,

$$|m_0(z)| > c, \qquad |\operatorname{Im} m_0(z)| \geq c|\operatorname{Im} z|.$$

Proof. For each $z \in U_\delta$, we have

$$\operatorname{Im} m_0(z) = \int \frac{\operatorname{Im} z}{|x - z|^2} \mu_0(dx), \qquad |m_0(z)| \leq \int \frac{1}{|x - z|} \mu_0(dx) \leq \frac{1}{\delta}.$$

This yields both bounds on $\operatorname{Im} m_0(z)$ and the upper bound on $|m_0(z)|$. The lower bound on $|m_0(z)|$ follows from (3.8) together with $|z| < R$, $|t_\alpha| < C$, and $|1 + t_\alpha m_0(z)| > c$. ☐

We now turn to the implications of edge regularity, and prove Propositions 3.6, 3.12, and 3.13. The arguments are similar to those of [KY17, Appendix A]. We first quantify continuity of m_0, uniformly in N, near a regular edge E_*. In particular this implies that when $|z - E_*|$ is small, $|m_0(z) - m_*|$ is also small.

Lemma A.10. Suppose Assumption 3.1 holds and E_* is a regular edge with m-value m_*. Then there exist constants $C, \delta > 0$ such that

$$(E_* - \delta, E_* + \delta) \subset \mathbb{R}_*,$$

and for every $z \in \overline{\mathbb{C}^+}$ with $|z - E_*| < \delta$,

$$|m_0(z) - m_*|^2 < C|z - E_*|.$$

Proof. Applying Proposition 3.11, take a constant $\nu > 0$ such that $|m_*| > \nu$. Fix a constant $c < \min(\nu, \tau)$ to be determined later, and define

$$\delta_N = \min\left(c,\ \inf(\delta > 0 : |m_0(z) - m_*| < c \text{ for all } z \in \mathbb{C}^+ \cup \mathbb{R}_* \text{ such that } |z - E_*| \leq \delta)\right).$$

As $m_0(E_*) = m_*$, continuity of m_0 at E_* implies $\delta_N > 0$. Furthermore, if $\operatorname{rank}(T) \leq N$ so that $0 \notin \mathbb{R}_*$, then the divergence of m_0 at 0 from Proposition A.6 implies $(E_* - \delta_N, E_* + \delta_N) \subset \mathbb{R}_*$. A priori, δ_N may depend on N. We will first establish that $|m_0(z) - m_*|^2 < C|z - E_*|$ when $|z - E_*| \leq \delta_N$. This will then imply that δ_N is bounded below by a constant δ.

Consider $z \in \overline{\mathbb{C}^+}$ with $|z - E_*| \leq \delta_N$. Let us write as shorthand $m = m_0(z)$. Then

$$\begin{aligned} |z - E_*| &= |z_0(m) - z_0(m_*)| \\ &= |m - m_*| \left| -\frac{1}{mm_*} + \frac{1}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha^2}{(1 + t_\alpha m)(1 + t_\alpha m_*)} \right| \\ &= |m - m_*|^2 \left| -\frac{1}{mm_*^2} + \frac{1}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha^3}{(1 + t_\alpha m)(1 + t_\alpha m_*)^2} \right|, \end{aligned} \tag{A.7}$$

where the last line adds to the quantity inside the modulus

$$0 = z_0'(m_*) = \frac{1}{m_*^2} - \frac{1}{N} \sum_{\alpha=1}^{M} \frac{t_\alpha^2}{(1 + t_\alpha m_*)^2}.$$

As $|m - m_*| < c$ by definition of δ_N, we have for each non-zero t_α

$$\left| \frac{1}{m} - \frac{1}{m_*} \right| < \frac{c}{\nu(\nu - c)}, \qquad \left| \frac{1}{m + t_\alpha^{-1}} - \frac{1}{m_* + t_\alpha^{-1}} \right| < \frac{c}{\tau(\tau - c)}.$$

Applying this to (A.7) and recalling $\gamma^{-2} = |z_0''(m_*)|/2$ yields

$$|z - E_*| > |m - m_*|^2 \left(\gamma^{-2} - \frac{c}{\nu^3(\nu - c)} - \frac{M}{N} \frac{c}{\tau^3(\tau - c)} \right).$$

As $\gamma^{-2} > \tau^2$, this implies $|m_0(z) - m_*|^2 < C|z - E_*|$ when c is chosen sufficiently small, as desired.

By continuity of m_0 and definition of δ_N, either $\delta_N = c$ or there must exist $z \in \overline{\mathbb{C}^+}$ such that $|z - E_*| = \delta_N$ and $|m_0(z) - m_*| = c$. In the latter case, for this z we have $c^2 = |m_0(z) - m_*|^2 < C|z - E_*| = C\delta_N$, implying $\delta_N > c^2/C$. Thus in both cases δ_N is bounded below by a constant, yielding the lemma. □

Next we bound the third derivative of z_0 near the m-value of a regular edge.

Lemma A.11. Suppose Assumption 3.1 holds and E_* is a regular edge with m-value m_*. Then there exist constants $C, \delta > 0$ such that z_0 is analytic on the disk $\{m \in \mathbb{C} : |m - m_*| < \delta\}$, and for every m in this disk,

$$|z_0'''(m)| < C.$$

Proof. Proposition 3.11 ensures $|m_*| > \nu$ for a constant $\nu > 0$. Taking $\delta < \min(\nu, \tau)$, the disk $D = \{m \in \mathbb{C} : |m - m_*| < \delta\}$ does not contain any pole of z_0, and hence z_0 is analytic on D. We compute

$$z_0'''(m) = \frac{6}{m^4} - \frac{1}{N} \sum_{\alpha : t_\alpha \neq 0} \frac{6}{(t_\alpha^{-1} + m)^4},$$

so $|z_0'''(m)| < C$ for $m \in D$ and sufficiently small δ by the bounds $|m_*| > \nu$ and $|m_* + t_\alpha^{-1}| > \tau$. □

Propositions 3.6, 3.12, and 3.13 now follow:

Proof of Proposition 3.12. This follows from Taylor expansion of z_0'' at m_*, the condition $|z_0''(m_*)| = 2\gamma^{-2} > 2\tau^2$ implied by regularity, and Lemma A.11. □

Proof of Proposition 3.6(a). Let $C, \delta > 0$ be as in Lemma A.10. Reducing δ as necessary and applying Lemma A.11, we may assume z_0 is analytic with $|z_0'''(m)| < C'$ over the disk

$$D = \{m \in \mathbb{C} : |m - m_*| < \sqrt{C\delta}\},$$

for a constant $C' > 0$.

Let E^* be the closest other edge to E_*, and suppose $E^* \in (E_* - \delta, E_* + \delta)$. Let m^* be the m-value for E^*. Then Lemma A.10 implies $m^* \in D$. Applying a Taylor expansion of z_0',

$$z_0'(m^*) = z_0'(m_*) + z_0''(m_*)(m^* - m_*) + \frac{z_0'''(m)}{2}(m^* - m_*)^2$$

for some m between m_* and m^*. Applying $0 = z_0'(m^*) = z_0'(m_*)$, $|z_0''(m_*)| = 2\gamma^{-2} > 2\tau^2$, and $|z_0'''(m)| < C'$, we obtain $|m^* - m_*| > 4\tau^2/C'$. Then Lemma A.10 yields $|E^* - E_*| > c$ for a constant $c > 0$. Reducing δ to c if necessary, we ensure $(E_* - \delta, E_* + \delta)$ contains no other edge E^*. The condition $(E_* - \delta, E_* + \delta) \subset \mathbb{R}_*$ was established in Lemma A.10. $\square$

Proof of Propositions 3.13 and 3.6(b). For any constant $\delta > 0$, if $\eta = \operatorname{Im} z \geq \delta$, then all claims follow from Propositions A.8 and A.9. Hence let us consider $\eta = \operatorname{Im} z < \delta$.

Taking δ sufficiently small, Lemma A.10 implies $|m_0(z) - m_*| < \sqrt{C\delta}$ for all $z \in \mathbf{D}_0$. Then $|m_0(z)| \asymp 1$ and $|1 + t_\alpha m_0(z)| \asymp 1$ by Proposition 3.11. Reducing δ if necessary, by Lemma A.11 we may also ensure z_0 is analytic with $|z_0'''(m)| < C'$ on

$$D = \{m \in \mathbb{C} : |m - m^*| < \sqrt{C\delta}\}.$$

Note $z = z_0(m_0(z))$ by (3.8) while $E_* = z_0(m_*)$. Then taking a Taylor expansion of z_0 and applying the conditions $z_0'(m_*) = 0$, $z_0''(m_*) = 2\gamma^{-2}$, and $|z_0'''(\tilde{m})| < C'$ for all $\tilde{m} \in D$, we have

$$z - E_* = z_0(m_0(z)) - z_0(m_*) = (\gamma^{-2} + r(z))(m_0(z) - m_*)^2 \tag{A.8}$$

where $|r(z)| < C'\sqrt{C\delta}/6$. Taking δ sufficiently small, we ensure

$$|\gamma^{-2} + r(z)| \asymp 1, \qquad \arg(\gamma^{-2} + r(z)) \in (-\varepsilon, \varepsilon) \tag{A.9}$$

for an arbitrarily small constant $\varepsilon > 0$, where $\arg(z)$ denotes the complex argument. Taking the modulus of (A.8) on both sides yields $|m_0(z) - m_*| \asymp \sqrt{|z - E_*|} \asymp \sqrt{\kappa + \eta}$.

For $\operatorname{Im} m_0(z)$, suppose E_* is a right edge. (The case of a left edge is similar.) By Proposition 3.6(a), we may assume $(E_* - \delta, E_*) \subset \operatorname{supp}(\mu_0)$ and $(E_*, E_* + \delta) \subset \mathbb{R} \setminus \operatorname{supp}(\mu_0)$. First suppose $\operatorname{Im} z > 0$ and $E \equiv \operatorname{Re} z \leq E_*$. As $\operatorname{Im} m_0(z) > 0$ by definition, (A.8) yields

$$m_0(z) - m_* = \sqrt{(z - E_*)/(\gamma^{-2} + r(z))}$$

where the square-root has branch cut on the positive real axis and positive imaginary part. Applying $\arg(z - E_*) \in [\pi/2, \pi)$ and (A.9), we have $\operatorname{Im} m_0(z) \asymp \operatorname{Im} \sqrt{z - E_*} \asymp |\sqrt{z - E_*}| \asymp \sqrt{\kappa + \eta}$. By continuity of m_0, this extends to $z \in (E_* - \delta, E_*)$ on the real axis. Hence Proposition 3.6(b) also follows, as $f_0(x) = \pi^{-1} \operatorname{Im} m_0(x)$.

Now, suppose $E \equiv \operatorname{Re} z > E_*$. Let us write

$$\operatorname{Im} m_0(z) = \int_{|\lambda - E_*| < \delta} \frac{\eta}{(\lambda - E)^2 + \eta^2} \mu_0(d\lambda) + \int_{|\lambda - E_*| \geq \delta} \frac{\eta}{(\lambda - E)^2 + \eta^2} \mu_0(d\lambda) \equiv \mathrm{I} + \mathrm{II}.$$

Reducing δ to $\delta/2$, we may assume the closest edge to E is E_*. Then we have $\mathrm{II} \in [0, \eta/\delta^2]$. For I, as μ_0 has density $f_0(x) \asymp \sqrt{E_* - x}$ for $x \in (E_* - \delta, E_*)$ while $(E_*, E_* + \delta) \subset \mathbb{R} \setminus \operatorname{supp}(\mu_0)$,

$$\mathrm{I} \asymp \int_{E_*-\delta}^{E_*} \frac{\eta}{(\lambda - E)^2 + \eta^2} \sqrt{E_* - \lambda}\, d\lambda = \int_0^\delta \frac{\eta}{\eta^2 + (\kappa + x)^2} \sqrt{x}\, dx.$$

Considering separately the integral over $x \in [0, \kappa + \eta]$ and $x \in [\kappa + \eta, \delta]$, we obtain $\mathrm{I} \asymp \eta/\sqrt{\eta + \kappa}$. Then $\mathrm{II} \leq C \cdot \mathrm{I}$, and this yields $\operatorname{Im} m_0(z) \asymp \eta/\sqrt{\eta + \kappa}$. ☐

A.3 Proof of local law

We verify that the proof of the entrywise local law in [KY17] does not require positive definite T. Indeed, Theorem A.13 below, which is a slightly modified version of [KY17, Theorem 3.22], holds in our setting. We deduce from this Theorems 2.5, 3.7, and 3.16.

We use the following notion of stability, analogous to [KY17, Definition 5.4] and [BEK$^+$14, Lemma 4.5].

Definition A.12. Fix a bounded set $S \subset \mathbb{R}$ and a constant $a > 0$, and let

$$\mathbf{D} = \{z \in \mathbb{C}^+ : \operatorname{Re} z \in S, \operatorname{Im} z \in [N^{-1+a}, 1]\}. \tag{A.10}$$

For $z = E + i\eta \in \mathbf{D}$, denote

$$L(z) = \{z\} \cup \{w \in \mathbf{D} : \operatorname{Re} w = E, \operatorname{Im} w \in [\eta, 1] \cap (N^{-5}\mathbb{N})\}.$$

For a function $g : \mathbf{D} \to (0, \infty)$, the Marcenko-Pastur equation (3.8) is ***g*-stable** on $\mathbf{D}$ if the following holds for some constant $C > 0$: Let $u : \mathbb{C}^+ \to \mathbb{C}^+$ be the Stieltjes transform of any probability measure, and let $\Delta : \mathbf{D} \to (0, \infty)$ be any function satisfying

- (Boundedness) $\Delta(z) \in [N^{-2}, (\log N)^{-1}]$ for all $z \in \mathbf{D}$,
- (Lipschitz) $|\Delta(z) - \Delta(w)| \leq N^2 |z - w|$ for all $z, w \in \mathbf{D}$,
- (Monotonicity) $\eta \mapsto \Delta(E + i\eta)$ is non-increasing for each $E \in S$ and $\eta > 0$.

If $z \in \mathbf{D}$ is such that $|z_0(u(w)) - w| \leq \Delta(w)$ for all $w \in L(z)$, then

$$|u(z) - m_0(z)| \leq \frac{C\Delta(z)}{g(z) + \sqrt{\Delta(z)}}. \tag{A.11}$$

Theorem A.13 (Abstract local law)**.** Suppose Assumption 3.1 holds. Fix a bounded set $S \subset \mathbb{R}$ and a constant $a > 0$, and define $\mathbf{D}$ by (A.10). Suppose, for some constants $C, c > 0$ and a bounded function $g : \mathbf{D} \to (0, C)$, that (3.8) is g-stable on $\mathbf{D}$, and furthermore

$$c < |m_0(z)| < C, \qquad c\eta < \operatorname{Im} m_0(z) < Cg(z), \qquad |1 + t_\alpha m_0(z)| > c$$

for all $z = E + i\eta \in \mathbf{D}$ and all $\alpha \in \mathcal{I}_M$. Then, letting $m_N(z), G(z), \Pi(z)$ be as in (3.16), (3.17), and (3.19), and denoting

$$\Psi(z) = \sqrt{\frac{\operatorname{Im} m_0(z)}{N\eta}} + \frac{1}{N\eta},$$

(a) (Entrywise law) For all $z \in \mathbf{D}$ and $A, B \in \mathcal{I}$,

$$\frac{G_{AB}(z) - \Pi_{AB}(z)}{t_A t_B} \prec_a \Psi(z).$$

(b) (Averaged law) For all $z \in \mathbf{D}$,

$$m_N(z) - m_0(z) \prec_a \min\left(\frac{1}{N\eta}, \frac{\Psi(z)^2}{g(z)}\right).$$

Proof. The proof is the same as for [KY17, Theorem 3.22], with only cosmetic differences which we indicate here. The notational identification with [KY17] is $T \leftrightarrow \Sigma$ and $t_\alpha \leftrightarrow \sigma_i$. (We continue to use Greek indices for $\mathcal{I}_M$ and Roman indices for $\mathcal{I}_N$, although this is reversed from the convention in [KY17].) As in [KY17], we may assume T is invertible. The non-invertible case follows by continuity.

We follow [KY17, Section 5], which in turn is based on [BEK+14]. Define

$$Z_i = \sum_{\alpha,\beta \in \mathcal{I}_M} G^{(i)}_{\alpha\beta} X_{\alpha i} X_{\beta i} - N^{-1} \operatorname{Tr} G^{(i)}_M, \qquad Z_\alpha = \sum_{i,j \in \mathcal{I}_N} G^{(\alpha)}_{ij} X_{\alpha i} X_{\alpha j} - N^{-1} \operatorname{Tr} G^{(\alpha)}_N,$$

$$[Z] = \frac{1}{N}\left(\sum_{i \in I_N} Z_i + \sum_{\alpha \in \mathcal{I}_M} \frac{t_\alpha^2}{(1 + t_\alpha m_0)^2} Z_\alpha\right),$$

$$\Theta = N^{-1}\left|\sum_{i \in \mathcal{I}_N} (G - \Pi)_{ii}\right| + M^{-1}\left|\sum_{\alpha \in \mathcal{I}_M} (G - \Pi)_{\alpha\alpha}\right|, \qquad \Psi_\Theta = \sqrt{\frac{\operatorname{Im} m_0 + \Theta}{N\eta}},$$

$$\Lambda_o = \max_{A \neq B \in \mathcal{I}} \frac{|G_{AB}|}{|t_A t_B|}, \qquad \Lambda = \max_{A,B \in \mathcal{I}} \frac{|(G - \Pi)_{AB}|}{|t_A t_B|}, \qquad \Xi = \{\Lambda \leq (\log N)^{-1}\}.$$

These all implicitly depend on an argument $z \in \mathbf{D}$. Then the same steps as in [KY17, Section 5] yield, either for $\eta = 1$ or on the event Ξ, for all $z \in \mathbf{D}$ and $A \in \mathcal{I}$,

$$|Z_A|, \Lambda_o \prec \Psi_\Theta, \tag{A.12}$$

$$z_0(m_N(z)) - z - [Z] \prec \Psi_\Theta^2 \prec (N\eta)^{-1}. \tag{A.13}$$

(In the argument for $\eta = 1$, the use of [KY17, Eq. (4.16)] may be replaced by [KY17, Lemmas 4.8 and 4.9]. Various bounds using σ_i, for example [KY17, Eqs. (5.4), (5.11)], may be replaced by ones using the positive quantity $|t_\alpha|$.) Applying (A.12) and the resolvent identities for G_{ii} and $G_{\alpha\alpha}$, we may also obtain on the event Ξ

$$\Theta \prec |m_N - m_0| + |[Z]| + (N\eta)^{-1}, \qquad \Lambda \prec |m_N - m_0| + \Psi_\Theta. \tag{A.14}$$

The bound (A.12) yields the initial estimate $[Z] \prec \Psi_\Theta \prec (N\eta)^{-1/2}$ on Ξ. The conditions of Definition A.12 hold for $\Delta = (N\eta)^{-1/2}$, so (A.13), the assumed stability of (3.8), and the stochastic continuity argument of [BEK+14, Section 4.1] yield that Ξ holds with high probability (i.e. $1 \prec \mathbb{1}\{\Xi\}$) and $\Lambda \prec (N\eta)^{-1/4}$ on all of $\mathbf{D}$. Next, applying the fluctuation averaging result of [KY17, Lemma 5.6], we obtain for any $c \in (0, 1]$ the implications

$$\Theta \prec (N\eta)^{-c} \Rightarrow \Psi_\Theta \prec \sqrt{\frac{\operatorname{Im} m_0 + (N\eta)^{-c}}{N\eta}} \Rightarrow [Z] \prec \frac{\operatorname{Im} m_0 + (N\eta)^{-c}}{N\eta} \equiv \Delta(z).$$

The conditions of Definition A.12 hold for this $\Delta(z)$, so applying (A.13), stability of (3.8), and $1 \prec \mathbb{1}\{\Xi\}$, we have the implications

$$\Theta \prec (N\eta)^{-c} \Rightarrow |m_N - m_0| \prec \frac{\Delta(z)}{g(z) + \sqrt{\Delta(z)}} \Rightarrow \Theta \prec \frac{\Delta(z)}{g(z) + \sqrt{\Delta(z)}} + \Delta(z) + (N\eta)^{-1}. \tag{A.15}$$

We bound $\Delta(z) \leq C(N\eta)^{-1}$ and

$$\frac{\Delta(z)}{g(z) + \sqrt{\Delta(z)}} \leq \frac{\operatorname{Im} m_0(z)}{N\eta\, g(z)} + (N\eta)^{-(1+c)/2} < C(N\eta)^{-1} + (N\eta)^{-(1+c)/2},$$

where this applies $\operatorname{Im} m_0(z) < Cg(z)$. Hence

$$\Theta \prec (N\eta)^{-c} \Rightarrow \Theta \prec (N\eta)^{-(1+c)/2}.$$

Initializing to $c = 1/4$ and iterating, we obtain $\Theta \prec (N\eta)^{-1+\varepsilon}$ for any $\varepsilon > 0$, so $|m_N - m_0| \leq \Theta \prec (N\eta)^{-1}$. Applying (A.15) once more with $c = 1$, we have for $c = 1$ that $\Delta(z) \leq \Psi(z)^2$ and hence also $|m_N - m_0| \prec \Psi^2/g$. This yields both bounds in the averaged law. The entrywise law $\Lambda \prec \Psi$ follows from (A.14). □

We now verify the stability condition in Definition A.12 near a regular edge and outside the spectrum. The proofs are the same as [KY17, Lemmas A.5 and A.8], which are based on [BEK+14, Lemma 4.5]. For convenience, we reproduce the argument here.

Lemma A.14. Suppose Assumption 3.1 holds.

(a) Fix any constants $\delta, a, C_0 > 0$, and let

$$\mathbf{D} = \{z \in \mathbb{C}^+ : \operatorname{Re} z \in [-C_0, C_0] \setminus \operatorname{supp}(\mu_0)_\delta,\ \operatorname{Im} z \in [N^{-1+a}, 1]\}.$$

Then (3.8) is g-stable on $\mathbf{D}$ for $g(z) \equiv 1$.

(b) Let E_* be a regular edge, and let $\mathbf{D}$ be the domain (3.18), depending on constants $\delta, a > 0$. For $z = E + i\eta \in \mathbf{D}$, denote $\kappa = |E - E_*|$ and let $g(z) = \sqrt{\kappa + \eta}$. Then, for any constant $a > 0$ and any constant $\delta > 0$ sufficiently small, (3.8) is g-stable on $\mathbf{D}$.

Proof. Writing $u = u(z)$, $m = m_0(z)$, and $\Delta_0 = \Delta_0(z) = z_0(u(z)) - z$, we have

$$\begin{aligned}\Delta_0 = z_0(u) - z_0(m) &= \frac{m-u}{um}\left(-1 + \frac{1}{N}\sum_{\alpha=1}^{M} \frac{t_\alpha^2 um}{(1+t_\alpha u)(1+t_\alpha m)}\right)\\ &= \alpha(z)(m-u)^2 + \beta(z)(m-u)\end{aligned}$$

for

$$\alpha(z) = -\frac{1}{u}\cdot\frac{1}{N}\sum_{\alpha=1}^{M}\frac{t_\alpha^2}{(1+t_\alpha u)(1+t_\alpha m)^2},$$

$$\beta(z) = \frac{1}{um}\left(-1 + \frac{1}{N}\sum_{\alpha=1}^{M}\frac{t_\alpha^2 m^2}{(1+t_\alpha m)^2}\right) = -\frac{m}{u} z_0'(m).$$

Viewing this a quadratic equation in $m - u$ and denoting the two roots

$$R_1(z), R_2(z) = \frac{-\beta(z) \pm \sqrt{\beta(z)^2 + 4\alpha(z)\Delta_0(z)}}{2\alpha(z)}, \tag{A.16}$$

we obtain $m_0(z) - u(z) \in \{R_1(z), R_2(z)\}$ for each $z \in \mathbf{D}$. Note that (A.16) implies

$$|R_1(z) - R_2(z)| = \frac{\sqrt{|\beta(z)^2 + 4\alpha(z)\Delta_0(z)|}}{|\alpha(z)|}. \tag{A.17}$$

Also, we have $|R_1 R_2| = |\Delta_0/\alpha|$ and $|R_1 + R_2| = |\beta/\alpha|$. The first statement yields $\min(|R_1|, |R_2|) \leq \sqrt{|\Delta_0/\alpha|} = 2|\Delta_0|/\sqrt{4|\alpha\Delta_0|}$. The second yields $\max(|R_1|, |R_2|) \geq |\beta/(2\alpha)|$, so the first then yields $\min(|R_1|, |R_2|) \leq 2|\Delta_0|/|\beta|$. Combining these,

$$\min(|R_1(z)|, |R_2(z)|) \leq \frac{4|\Delta_0(z)|}{|\beta(z)| + \sqrt{4|\alpha(z)\Delta_0(z)|}}. \tag{A.18}$$

We first show part (a). Let $\Delta(z)$ satisfy the conditions of Definition A.12. We claim that for any constant $\nu > 0$, there exist constants $C_0, c > 0$ such that

1. If $\operatorname{Im} z \geq \nu$ and $|\Delta_0(z)| \leq \Delta(z)$, then

$$|m_0(z) - u(z)| \leq C_0 \Delta(z). \tag{A.19}$$

2. If $|\Delta_0(z)| \leq \Delta(z)$ and $|m_0(z) - u(z)| < (\log N)^{-1/2}$, then

$$\min(|R_1(z)|, |R_2(z)|) \leq C_0 \Delta(z), \qquad |R_1(z) - R_2(z)| \geq c. \tag{A.20}$$

Indeed, if $\operatorname{Im} z \geq \nu$ and $|\Delta_0(z)| \leq \Delta(z) \leq (\log N)^{-1}$, then $\operatorname{Im} z_0(u(z)) \geq \nu/2$. In particular $z_0(u(z)) \in \mathbb{C}^+$, so $m_0(z_0(u(z))) = u(z)$ as Theorem 2.4 guarantees this is the unique root $m \in \mathbb{C}^+$ to the equation $z_0(m) = z_0(u(z))$. Applying $|m_0'(z)| \leq 1/(\operatorname{Im} z)^2$, we obtain

$$|m_0(z) - u(z)| = |m_0(z) - m_0(z_0(u(z)))| \leq (4/\nu^2)|\Delta_0(z)| \leq (4/\nu^2)\Delta(z),$$

and hence (A.19) holds for $C_0 = 4/\nu^2$. On the other hand, if $|m_0(z) - u(z)| < (\log N)^{-1/2}$, then Propositions A.9 and A.8 imply $|\alpha(z)| < C$ and $|\beta(z)| < C$. Taking imaginary parts of (3.8) as in (A.3), we also have $|u(z)m(z)\beta(z)| \geq (\operatorname{Im} z)|m_0(z)|^2/\operatorname{Im} m_0(z) > c$, so $|\beta(z)| > c$. Applying this to (A.17) and (A.18), and increasing C_0 if necessary, we obtain (A.20).

A continuity argument now concludes the proof of part (a): Consider any $z \in \mathbf{D}$ with $|\Delta_0(w)| \leq \Delta(w)$ for all $w \in L(z)$. If $\operatorname{Im} z \geq \nu$, the result follows from (A.19). If $\operatorname{Im} z < \nu$, let $w \in L(z)$ be such that $\operatorname{Im} z < \operatorname{Im} w \leq \operatorname{Im} z + N^{-5}$. Suppose inductively that we have shown (A.19) holds at w. Applying $|u'(z)| \leq 1/(\operatorname{Im} z)^2 \leq N^2$ for any Stieltjes transform $u(z)$ and $z \in \mathbf{D}$, we obtain

$$|m_0(z) - u(z)| \leq C_0 \Delta(w) + 2N^{-3} < (\log N)^{-1/2}.$$

So (A.20) implies $\max(|R_1(z)|, |R_2(z)|) > c/2$. Then $|m_0(z) - u(z)| = \min(|R_1(z)|, |R_2(z)|)$, so (A.20) also shows that (A.19) holds at z. Starting the induction at $\operatorname{Im} z \geq \nu$, we obtain (A.19) for all $w \in L(z)$, and in particular at $w = z$. This establishes part (a).

For part (b), let $g(z) = \sqrt{\kappa + \eta}$. We claim that when $\delta > 0$ is sufficiently small, there exist constants $\nu, C_0, C_1 > 0$ such that

1. If $\operatorname{Im} z \geq \nu$ and $|\Delta_0(z)| \leq \Delta(z)$, then

$$|m_0(z) - u(z)| \leq \frac{C_0 \Delta(z)}{g(z) + \sqrt{\Delta(z)}}. \tag{A.21}$$

2. If $\operatorname{Im} z < \nu$, $|\Delta_0(z)| \leq \Delta(z)$, and $|m_0(z) - u(z)| < (\log N)^{-1/3}$, then

$$\min(|R_1(z)|, |R_2(z)|) \leq \frac{C_0 \Delta(z)}{g(z) + \sqrt{\Delta(z)}}, \tag{A.22}$$

$$C_1^{-1}(g(z) - \sqrt{\Delta(z)}) \leq |R_1(z) - R_2(z)| \leq C_1(g(z) + \sqrt{\Delta(z)}). \tag{A.23}$$

We verify the second claim first: If $\operatorname{Im} z < \nu$ and $|m_0(z) - u(z)| < (\log N)^{-1/3}$, then for ν and δ sufficiently small, Lemma A.10 implies

$$|m_0(z) - m_*| < C\sqrt{\nu + \delta}, \qquad |u(z) - m_*| < C\sqrt{\nu + \delta} \tag{A.24}$$

for a constant $C > 0$ independent of ν, δ. We have

$$\frac{m_* z_0''(m_*)}{2} = -\frac{1}{m_*^2} + \frac{1}{N}\sum_{\alpha=1}^{M} \frac{t_\alpha^3 m_*}{(1 + t_\alpha m_*)^3} = -\frac{1}{N}\sum_{\alpha=1}^{M} \frac{t_\alpha^2}{(1 + t_\alpha m_*)^3},$$

where the second equality applies the identity $0 = z_0'(m_*)$. Comparing the right side with $u(z)\alpha(z)$, and applying (A.24) together with the bounds $|m_*| \asymp 1$, $|z_0''(m_*)| \asymp 1$, and $|1 + t_\alpha m_*| \asymp 1$ from Proposition 3.11, we obtain $c < |\alpha(z)| < C$ for constants $C, c > 0$ and sufficiently small ν, δ. Next, applying again $0 = z_0'(m_*)$, we have

$$z_0'(m) = \int_{m_*}^{m} z_0''(x)dx = (m - m_*)z_0''(m_*) + \int_{m_*}^{m}\int_{m_*}^{x} z_0'''(y)dy\,dx.$$

Applying (A.24), $|z_0''(m_*)| \asymp 1$ from Proposition 3.11, $|m_0(z) - m_*| \asymp \sqrt{\kappa + \eta}$ from Proposition 3.13, and $|z_0'''(y)| < C$ from Lemma A.11, we obtain $cg(z) < |\beta(z)| < Cg(z)$ for ν, δ sufficiently small. Applying these bounds and $|\Delta_0(z)| \leq \Delta(z)$ to (A.18) and (A.17) yields (A.22) and (A.23). Letting ν be small enough such that this holds, for $\operatorname{Im} z \geq \nu$, the same argument as in part (a) implies $|m_0(z) - u(z)| \leq (4/\nu^2)\Delta(z)$. Noting $g(z) \geq \sqrt{\nu}$ and increasing C_0 if necessary, we obtain (A.21).

We again apply a continuity argument to conclude the proof: Consider any $z \in \mathbf{D}$ with $|\Delta_0(w)| \leq \Delta(w)$ for all $w \in L(z)$. If $\operatorname{Im} z \geq \nu$, the result follows from (A.21). If $\operatorname{Im} z < \nu$, suppose first that

$$\frac{C_0\Delta(z)}{g(z) + \sqrt{\Delta(z)}} + 2N^{-3} < (2C_1)^{-1}(g(z) - \sqrt{\Delta(z)}). \tag{A.25}$$

Note that by monotonicity of Δ, the left side is decreasing in $\operatorname{Im} z$ while the right side is increasing in $\operatorname{Im} z$. Thus if (A.25) holds at z, then it holds at all $w \in L(z)$. Let $w \in L(z)$ be such that $\operatorname{Im} z < \operatorname{Im} w \leq \operatorname{Im} z + N^{-5}$, and suppose inductively that we have established (A.21) at w. Then

$$|m_0(z) - u(z)| \leq \frac{C_0\Delta(w)}{g(w) + \sqrt{\Delta(w)}} + 2N^{-3} < (\log N)^{-1/3}.$$

Then (A.23) and (A.25) imply $|m_0(z) - u(z)| = \min(|R_1(z)|, |R_2(z)|)$, so (A.22) implies (A.21) holds at z. Starting the induction at $\operatorname{Im} z \geq \nu$, this establishes (A.21) if z satisfies (A.25).

If z does not satisfy (A.25), then rearranging (A.25) and applying $\Delta(z) > N^{-3}$ yields $g(z)^2 \leq$

$C\Delta(z)$ for a constant $C > 0$. Then

$$\frac{C_0\Delta(z)}{g(z)+\sqrt{\Delta(z)}} + C_1(g(z)+\sqrt{\Delta(z)}) \leq \frac{C_2\Delta(z)}{g(z)+\sqrt{\Delta(z)}}$$

for a constant $C_2 > 0$. We claim

$$|m_0(z) - u(z)| \leq \frac{C_2\Delta(z)}{g(z)+\sqrt{\Delta(z)}}. \tag{A.26}$$

Indeed, let $w \in L(z)$ be such that $\operatorname{Im} z < \operatorname{Im} w \leq \operatorname{Im} z + N^{-5}$, and suppose inductively that we have established (A.26) at w. This implies in particular $|m_0(z) - u(z)| < (\log N)^{-1/3}$ as before, so (A.26) holds at z by (A.22) and (A.23). Starting the induction at the value $w \in L(z)$ satisfying (A.25) which has the smallest imaginary part, this concludes the proof in all cases. □

We now verify Theorems 2.5, 3.7, and 3.16.

Proof of Theorem 2.5. By the bound $\|\widehat{\Sigma}\| \leq \|T\|\|X\|^2$, we may take $C_0 > 0$ sufficiently large such that $\|\widehat{\Sigma}\| \leq C_0$ with probability at least $1 - N^{-D}$. Define

$$\mathbf{D} = \{z \in \mathbb{C}^+ : \operatorname{Re} \in [-C_0, C_0] \setminus \operatorname{supp}(\mu_0)_\delta, \operatorname{Im} z \in [N^{-2/3}, 1]\}.$$

Then Propositions A.8, A.9, and Lemma A.14(a) check the conditions of Theorem A.13 for $g(z) \equiv 1$ over $\mathbf{D}$.

Applying the second bound of Theorem A.13(b), $|m_N(z) - m_0(z)| \prec \Psi(z)^2 \asymp N^{-1} + (N\eta)^{-2}$ for any $z \in \mathbf{D}$. Taking $\eta = N^{-2/3}$ and applying also $\operatorname{Im} m_0(z) \asymp \eta$, we obtain $\operatorname{Im} m_N(z) \prec N^{-2/3} < 1/(2N\eta)$. As the number of eigenvalues of $\widehat{\Sigma}$ in $[E-\eta, E+\eta]$ is at most $2N\eta \cdot \operatorname{Im} m_N(z)$, this implies $\widehat{\Sigma}$ has no eigenvalues in this interval with probability $1 - N^{-D}$ for all $N \geq N_0(D)$. The result follows from a union bound over a grid of values $E \in [-C_0, C_0] \setminus \operatorname{supp}(\mu_0)_\delta$ of cardinality at most $CN^{2/3}$, together with the bound $\|\widehat{\Sigma}\| \leq C_0$. □

Proof of Theorem 3.7. The argument follows [PY14, Eq. (3.4)]. Consider the case of a right edge E_*. (A left edge is analogous.) For each $E \in [E_* + N^{-2/3+\varepsilon}, E_* + \delta]$, denoting $\kappa = E - E_*$, consider $z = E + i\eta$ for

$$\eta = N^{-1/2-\varepsilon/4}\kappa^{1/4} \in [N^{-2/3}, 1],$$

where the inclusion holds for all large N because $\kappa \in [N^{-2/3+\varepsilon}, \delta]$. Proposition 3.13 implies

$$\operatorname{Im} m_0(z) \leq \frac{C\eta}{\sqrt{\kappa+\eta}} \leq \frac{C\eta}{\sqrt{\kappa}} = C(N\eta)^{-1}N^{-\varepsilon/2}.$$

Also by Proposition 3.13 and Lemma A.14(b), we may apply Theorem A.13 with $g(z) = \sqrt{\kappa+\eta}$.

The above bound on $\operatorname{Im} m_0(z)$ yields $\Psi(z)^2 \leq C/(N\eta)^2$, and hence Theorem A.13(b) implies

$$|m_N(z) - m_0(z)| \prec \frac{1}{(N\eta)^2\sqrt{\kappa+\eta}} \leq \frac{1}{(N\eta)^2\sqrt{\kappa}} = \frac{1}{N^{3+\varepsilon/2}\eta^4} \leq (N\eta)^{-1}N^{-\varepsilon/2},$$

where the last bound uses $\eta \geq N^{-2/3}$. Thus we obtain

$$\operatorname{Im} m_N(z) \prec C(N\eta)^{-1}N^{-\varepsilon/2}.$$

Then $\widehat{\Sigma}$ has no eigenvalues in $[E-\eta, E+\eta]$ with probability $1 - N^{-D}$ for all $N \geq N_0(D)$, and the result follows from a union bound over a grid of such values E. $\square$

Proof of Theorem 3.16. This follows from Theorem A.13 applied with $g(z) = \sqrt{\kappa+\eta}$, and Proposition 3.13 and Lemma A.14(b). $\square$

Appendix B

Free deterministic equivalents

In this appendix, we prove the asymptotic freeness results of Chapter 5 and establish the existence of the approximating free deterministic equivalent model.

B.1 Proof of asymptotic freeness

We prove Theorem 5.9 and Corollary 5.10. To ease subscript notation, throughout this section we denote by $M[i, j]$ the (i, j) entry of a matrix M.

Let Q be a $*$-polynomial in $(x_i)_{i\in\mathcal{I}_j, j\in\{1,\ldots,J\}}$ with coefficients in $\langle P_1, \ldots, P_d\rangle$, and let q denote the corresponding $*$-polynomial with coefficients in $\langle p_1, \ldots, p_d\rangle$. For Theorem 5.9, we wish to show for any r, almost surely as $N \to \infty$,

$$\left|N_r^{-1}\operatorname{Tr}_r Q\left(H_i : i \in \mathcal{I}_j, j \in \{1, \ldots, J\}\right) - \tau_r\left(q\left(h_i : i \in \mathcal{I}_j, j \in \{1, \ldots, J\}\right)\right)\right| \to 0. \tag{B.1}$$

The high-level strategy of the proof is the same as [BG09, Theorem 1.6], and follows these steps:

1. By applying linearity of Tr and τ, we may reduce to the case $Q = \prod_{k=1}^K Q_k$, where each Q_k is a simple-valued polynomial of a single family $(H_i : i \in \mathcal{I}_{j_k})$.
2. By "centering" each Q_k and inducting on K, it suffices to consider the case where $j_1 \neq j_2$, $j_2 \neq j_3, \ldots, j_K \neq j_1$ and each Q_k satisfies $\operatorname{Tr} Q_k(H_i : i \in \mathcal{I}_{j_k}) = 0$.
3. The main technical ingredient is Lemma B.2 below, which establishes the result for such Q. We use orthogonal invariance in law of $(H_i : i \in \mathcal{I}_{j_k})$ to introduce independently random block-orthogonal matrices, and then condition on the H_i's to reduce to a statement about Haar-orthogonal and deterministic matrices.

The last step above uses an explicit computation of the trace, together with basic properties of the joint moments of Haar-orthogonal matrices. We follow an approach inspired by [HP00, Theorem

2.1], but which (we believe) fills in an omission in the proof and also extends the combinatorial argument to deal with rectangular matrices and the orthogonal (rather than unitary) case.

Proof of Theorem 5.9. To show (B.1), by linearity of Tr and τ, it suffices to consider the case where Q is a $*$-monomial, which we may always write as a product of $Q_1, \ldots, Q_K$ where each Q_k depends only on the variables of a single family $\mathcal{I}_{j_k}$. Writing $Q_k = (P_1 + \ldots + P_d)Q_k(P_1 + \ldots + P_d)$ and again applying linearity of Tr and τ, it suffices to consider the case where each Q_k is simple-valued, i.e. $P_{r_k} Q_k P_{s_k} = Q_k$ for some $r_k, s_k \in \{1, \ldots, d\}$. If $s_k \neq r_{k+1}$ for any k (with the cyclic identification $r_{K+1} = r_1$), then (B.1) is trivial as both quantities on the left are 0. If $s_k = r_{k+1}$ for all k, then it suffices to consider $r = r_1$ and to replace $N_r^{-1} \operatorname{Tr}_r$ by $N^{-1} \operatorname{Tr}$ and τ_r by τ. The result then follows from Lemma B.1 below. $\square$

Lemma B.1. Under the assumptions of Theorem 5.9, fix $K \geq 1$, $j_1, \ldots, j_K \in \{1, \ldots, J\}$, and $r_1, \ldots, r_K \in \{1, \ldots, d\}$. For each $k = 1, \ldots, K$, let Q_k be a $*$-polynomial with coefficients in $\langle P_1, \ldots, P_d \rangle$ of the variables $(x_i)_{i \in \mathcal{I}_{j_k}}$ of the single family $\mathcal{I}_{j_k}$, such that $P_{r_k} Q_k P_{r_{k+1}} = Q_k$ (with the identification $r_{K+1} := r_1$). Let $q_1, \ldots, q_K$ denote the corresponding $*$-polynomials with coefficients in $\langle p_1, \ldots, p_d \rangle$. Then, almost surely as $N \to \infty$,

$$\left| \frac{1}{N} \operatorname{Tr} \prod_{k=1}^{K} Q_k \left(H_i : i \in \mathcal{I}_{j_k} \right) - \tau \left(\prod_{k=1}^{K} q_k \left(h_i : i \in \mathcal{I}_{j_k} \right) \right) \right| \to 0. \tag{B.2}$$

Proof. We induct on K. For $K = 1$, (B.2) holds by the assumption that $(h_i)_{i \in \mathcal{I}_{j_1}}$ and $(H_i)_{i \in \mathcal{I}_{j_1}}$ are asymptotically equal in $\mathcal{D}$-law a.s.

For $K \geq 2$, assume inductively that (B.2) holds for each value $1, \ldots, K-1$ in place of K. Let

$$t_k = \frac{1}{\tau(p_{r_k})} \tau \left(q_k \left(h_i : i \in \mathcal{I}_{j_k} \right) \right),$$

and define the "centered" $*$-polynomials

$$D_k = Q_k - t_k P_{r_k}, \qquad d_k = q_k - t_k p_{r_k}.$$

We clarify that $t_k \in \mathbb{C}$ is a fixed constant (evaluated at the h_i's, not at the arguments x_i's of these $*$-polynomials), and thus D_k and d_k are still $*$-polynomials of $(x_i)_{i \in \mathcal{I}_{j_k}}$ with coefficients in $\langle P_1, \ldots, P_d \rangle$ and $\langle p_1, \ldots, p_d \rangle$. We have $t_k = 0$ if $r_k \neq r_{k+1}$, because q_k is simple. Denoting by $\mathcal{S}_K$ the collection of all subsets of $\{k : r_k = r_{k+1}\}$ and applying a binomial expansion,

$$\frac{1}{N} \operatorname{Tr} \prod_{k=1}^{K} Q_k \left(H_i : i \in \mathcal{I}_{j_k} \right) = \sum_{S \in \mathcal{S}_K} Q(S)$$

where

$$Q(S) := \prod_{k \in S} t_k \cdot \frac{1}{N} \operatorname{Tr} \prod_{k \in \{1,\ldots,K\} \setminus S} D_k \left(H_i : i \in \mathcal{I}_{j_k}\right).$$

Each D_k still satisfies $P_{r_k} D_k P_{r_{k+1}} = D_k$. Hence, for every $S \neq \emptyset$, applying the induction hypothesis,

$$\left| Q(S) - \prod_{k \in S} t_k \cdot \tau \left(\prod_{k \in \{1,\ldots,K\} \setminus S} d_k \left(h_i : i \in \mathcal{I}_{j_k}\right) \right) \right| \to 0. \tag{B.3}$$

For $S = \emptyset$, if $j_k = j_{k+1}$ for some $k \in \{1, \ldots, K\}$ (or $j_K = j_1$), then combining $D_k D_{k+1}$ into a single polynomial (and applying cyclic invariance of Tr and τ if $j_K = j_1$), the induction hypothesis still yields (B.3).

The remaining case is when $S = \emptyset$ and $j_k \neq j_{k+1}$ for each $k = 1, \ldots, K$. Note, by definition of d_k, that

$$\tau \left(p_r d_k \left(h_i : i \in \mathcal{I}_{j_k}\right) p_r\right) = 0$$

for each r and k, so by freeness of $(h_i)_{i \in \mathcal{I}_1}, \ldots, (h_i)_{i \in \mathcal{I}_k}$ with amalgamation over $\langle p_1, \ldots, p_d \rangle$,

$$\tau \left(\prod_{k=1}^{K} d_k \left(h_i : i \in \mathcal{I}_{j_k}\right) \right) = 0.$$

Thus, it remains to show that $Q(\emptyset) \to 0$. Note first that the definition of the free deterministic equivalent and the condition $N_r/N > c$ imply, almost surely as $N \to \infty$,

$$\left| \frac{N}{N_{r_k}} - \frac{1}{\tau(p_{r_k})} \right| \to 0, \qquad \left| \frac{1}{N} \operatorname{Tr} \left(Q_k \left(H_i : i \in \mathcal{I}_{j_k}\right)\right) - \tau \left(q_k \left(h_i : i \in \mathcal{I}_{j_k}\right)\right) \right| \to 0.$$

Hence $|t_k - T_k| \to 0$ a.s. for

$$T_k = \frac{1}{N_{r_k}} \operatorname{Tr} Q_k \left(H_i : i \in \mathcal{I}_{j_k}\right).$$

Then it suffices to show

$$M(\emptyset) := \frac{1}{N} \operatorname{Tr} \prod_{k=1}^{K} M_k \to 0$$

for the matrices

$$M_k = Q_k \left(H_i : i \in \mathcal{I}_{j_k}\right) - T_k P_{r_k},$$

as we may replace in $Q(\emptyset)$ each t_k by T_k and bound the remainders using the operator norm.

Finally, let us introduce random matrices $(O_{j,r})_{j \in \mathcal{N}, r \in \{1,\ldots,d\}}$ that are independent of each other and of the H_i's, such that each $O_{j,r}$ is orthogonal and Haar-distributed in $\mathbb{R}^{N_r \times N_r}$. For each $j \in \mathcal{N}$, define the block diagonal matrix $O_j = \operatorname{diag}(O_{j,1}, \ldots, O_{j,d})$. By orthogonal invariance in law of

$(H_i)_{i\in\mathcal{I}_{j_k}}$, we have the equality in law

$$M(\emptyset) \stackrel{L}{=} \frac{1}{N}\operatorname{Tr}\prod_{k=1}^{K} O_{j_k} M_k O_{j_k}^{-1}.$$

Write $\check{M}_k \in \mathbb{R}^{N_{r_k}\times N_{r_{k+1}}}$ as the non-zero block of M_k. Then the above may be written as

$$M(\emptyset) \stackrel{L}{=} \frac{1}{N}\operatorname{Tr}\prod_{k=1}^{K} O_{j_k,r_k}\check{M}_k O_{j_k,r_{k+1}}^{-1}\operatorname{Id}_{N_{r_{k+1}}}. \tag{B.4}$$

Conditional on the H_i's, $\check{M}_k$ are deterministic matrices satisfying $\|\check{M}_k\|\leq C$ for some constant $C>0$ and all large N a.s., and if $r_k = r_{k+1}$ then $\operatorname{Tr}\check{M}_k = \operatorname{Tr} M_k = 0$ by definition of T_k. Furthermore, recall that we are in the case $j_k \neq j_{k+1}$ for each k.

The claim $M(\emptyset)\to 0$ follows from the following lemma:

Lemma B.2. Fix $d,K\geq 1$, $l_1,\ldots,l_K\in\mathcal{N}$, $r_1,\ldots,r_K\in\{1,\ldots,d\}$, and $e_1,\ldots,e_K\in\{-1,1\}$. For $N_1,\ldots,N_d\geq 1$, let $\{O_{l,r}\}_{l\in\mathcal{N},r\in\{1,\ldots,d\}}$ be independent random matrices such that each $O_{l,r}$ is a Haar-distributed orthogonal matrix in $\mathbb{R}^{N_r\times N_r}$. Let $D_1\in\mathbb{C}^{N_{r_1}\times N_{r_2}}, D_2\in\mathbb{C}^{N_{r_2}\times N_{r_3}},\ldots,D_K\in\mathbb{C}^{N_{r_K}\times N_{r_1}}$ be deterministic matrices such that, for each $k=1,\ldots,K$ (and cyclically identifying $l_{K+1}:=l_1$, etc.), if $(l_k,r_k,e_k)=(l_{k+1},r_{k+1},-e_{k+1})$, then $\operatorname{Tr} D_k = 0$.

Let $N = N_1+\ldots+N_d$, and suppose there exist constants $C,c>0$ such that, as $N\to\infty$, $N_r/N > c$ for each $r=1,\ldots,d$ and $\|D_k\|< C$ for each $k=1,\ldots,K$. Then, almost surely,

$$N^{-1}\operatorname{Tr}\left(O_{l_1,r_1}^{e_1}D_1O_{l_2,r_2}^{e_2}D_2\ldots O_{l_K,r_K}^{e_K}D_K\right)\to 0.$$

(We emphasize that the matrices $O_{l,r}$ and D_k are N-dependent, while $(l_k,r_k,e_k,k=1,\ldots,K)$ remain fixed as N grows.)

Assuming this lemma for now, write the right side of (B.4) in the form

$$N^{-1}\operatorname{Tr}\left(O_{l_1,r_1}^{e_1}D_1O_{l_2,r_2}^{e_2}D_2\ldots O_{l_{2K},r_{2K}}^{e_{2K}}D_{2K}\right),$$

by making the identifications

$$\begin{aligned}(l_{2k-1},r_{2k-1},e_{2k-1},D_{2k-1}) &\leftarrow (j_k,r_k,1,\check{M}_k)\\ (l_{2k},r_{2k},e_{2k},D_{2k}) &\leftarrow (j_k,r_{k+1},-1,\operatorname{Id}_{N_{r_{k+1}}}).\end{aligned}$$

Then Lemma B.2 implies $M(\emptyset)\to 0$ a.s. conditional on the H_i's, and hence unconditionally as well. Thus (B.3) holds for all $S\in\mathcal{S}_K$.

Finally, reversing the binomial expansion,

$$\sum_{S\in\mathcal{S}_K}\prod_{k\in S} t_k\cdot\tau\left(\prod_{k\in\{1,\ldots,K\}\setminus S} d_k\left(h_i:i\in\mathcal{I}_{j_k}\right)\right)=\tau\left(\prod_{k=1}^{K} q_k\left(h_i:i\in\mathcal{I}_{j_k}\right)\right).$$

This establishes (B.2), completing the induction. □

To conclude the proof of Theorem 5.9, it remains to establish the above Lemma B.2. We require the following fact about joint moments of entries of Haar-orthogonal matrices:

Lemma B.3. Let $O\in\mathbb{R}^{N\times N}$ be a random Haar-distributed real orthogonal matrix, let $K\geq 1$ be any positive integer, and let $i_1,j_1,\ldots,i_K,j_K\in\{1,\ldots,N\}$. Then:

(a) There exists a constant $C:=C_K>0$ such that

$$\mathbb{E}[|O[i_1,j_1]O[i_2,j_2]\ldots O[i_K,j_K]|]\leq CN^{-K/2}.$$

(b) If there exists $i\in\{1,\ldots,N\}$ such that $i_k=i$ for an odd number of indices $k\in\{1,\ldots,K\}$ or $j_k=i$ for an odd number of indices $k\in\{1,\ldots,K\}$, then $\mathbb{E}[O[i_1,j_1]\ldots O[i_K,j_K]]=0$.

Proof. [CŚ06, Eq. (21) and Theorem 3.13] imply $\mathbb{E}[O[i_1,j_1]^2\ldots O[i_K,j_K]^2]\leq CN^{-K}$ for a constant $C:=C_K>0$. Part (a) then follows by Cauchy-Schwarz. Part (b) follows from the fact that the distribution of O is invariant to multiplication of row i or column i by -1, hence if $i_k=i$ or $j_k=i$ for an odd number of indices k, then $\mathbb{E}[O[i_1,j_1]\ldots O[i_K,j_K]]=-\mathbb{E}[O[i_1,j_1]\ldots O[i_K,j_K]]$. □

Proof of Lemma B.2. Define $V_k=O_{l_k,r_k}^{e_k}$ (which is O_{l_k,r_k}' if $e_k=-1$). Expanding the trace,

$$\operatorname{Tr}\left[\prod_{k=1}^{K} V_kD_k\right]=\sum_{\mathbf{i},\mathbf{j}} V(\mathbf{i},\mathbf{j})D(\mathbf{i},\mathbf{j}),\tag{B.5}$$

where the summation is over all tuples $(\mathbf{i},\mathbf{j}):=(i_1,j_1,i_2,j_2,\ldots,i_K,j_K)$ satisfying

$$1\leq i_k,j_k\leq N_{r_k}\tag{B.6}$$

for each $k=1,\ldots,K$, and where we have defined (with the identification $i_{K+1}:=i_1$)

$$V(\mathbf{i},\mathbf{j})=\prod_{k=1}^{K} V_k[i_k,j_k],\quad D(\mathbf{i},\mathbf{j})=\prod_{k=1}^{K} D_k[j_k,i_{k+1}].$$

Denote

$$\mathcal{E}=\mathbb{E}\left[\left|N^{-1}\operatorname{Tr}\left(\prod_{k=1}^{K} V_kD_k\right)\right|^2\right]=N^{-2}\sum_{\mathbf{i},\mathbf{j}}\sum_{\mathbf{i}',\mathbf{j}'} D(\mathbf{i},\mathbf{j})\overline{D(\mathbf{i}',\mathbf{j}')}\mathbb{E}[V(\mathbf{i},\mathbf{j})V(\mathbf{i}',\mathbf{j}')],\tag{B.7}$$

where the second equality uses that each V_k is real and each D_k is deterministic. By the Borel-Cantelli lemma, it suffices to show $\mathcal{E} \leq CN^{-2}$ for some constant $C := C_K > 0$.

Let $\mathcal{R}$ be the set of distinct pairs among (l_k, r_k) for $k = 1, \ldots, K$, corresponding to the set of distinct matrices $O_{l,r}$ that appear in (B.5). By independence of the matrices $O_{l,r}$,

$$\mathbb{E}[V(\mathbf{i},\mathbf{j})V(\mathbf{i}',\mathbf{j}')] = \prod_{(l,r)\in\mathcal{R}} \mathbb{E}\left[\prod_{k:(l_k,r_k)=(l,r)} V_k[i_k, j_k]V_k[i'_k, j'_k]\right]. \tag{B.8}$$

Since $O_{l,r}$ is invariant in law under permutations of rows and columns, each expectation on the right side above depends only on which indices are equal, and not on the actual index values. (For example, denoting $O := O_{l,r}$,

$$O[1,2]O^{-1}[2,3]O[1,4]O^{-1}[3,3] \overset{L}{=} O[8,7]O^{-1}[7,6]O[8,5]O^{-1}[6,6] \tag{B.9}$$

where the equality in law holds by permutation of both the rows and the columns of O.) We therefore analyse $\mathcal{E}$ by decomposing the sum in (B.7) over the different relevant partitions of $(\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}')$ specifying which indices are equal.

More precisely, let

$$\mathcal{I} = (i_k, j_k, i'_k, j'_k : k = 1, \ldots, K)$$

be the collection of all indices, with cardinality $|\mathcal{I}| = 4K$. For each $(l,r) \in \mathcal{R}$, let

$$\mathcal{I}(l,r) = (i_k, j_k, i'_k, j'_k : k \text{ such that } l_k = l, r_k = r).$$

These sets $\mathcal{I}(l,r)$ form a fixed partition of $\mathcal{I}$. For each (l,r), denote by $\mathcal{Q}(l,r)$ any further partition of the indices in $\mathcal{I}(l,r)$, and let

$$\mathcal{Q} = \bigsqcup_{(l,r)\in\mathcal{R}} \mathcal{Q}(l,r) \tag{B.10}$$

be their combined partition of $\mathcal{I}$. Denoting by $Q_{l,r} = |\mathcal{Q}(l,r)|$ the number of elements of $\mathcal{Q}$ that partition $\mathcal{I}(l,r)$, we may identify

$$\mathcal{Q} \equiv \{(l,r,q) : (l,r) \in \mathcal{R},\ q \in \{1, \ldots, Q_{l,r}\}\}.$$

We say that $(\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}')$ *induces* $\mathcal{Q}$ if, for every two indices belonging to the same set $\mathcal{I}(l,r)$, they are equal in value if and only if they belong to the same element of $\mathcal{Q}$.[1] Then $\mathbb{E}[V(\mathbf{i},\mathbf{j})V(\mathbf{i}',\mathbf{j}')]$ is the same for all $(\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}')$ that induce the same partition $\mathcal{Q}$. Thus we may define $E(\mathcal{Q}) = \mathbb{E}[V(\mathbf{i},\mathbf{j})V(\mathbf{i}',\mathbf{j}')]$

[1] For example, if $K = 2$, in display (B.9), both $(i_1, j_1, i_2, j_2, i'_1, j'_1, i'_2, j'_2) = (1,2,2,3,1,4,3,3)$ and $(8,7,7,6,8,5,6,6)$ induce

$$\mathcal{Q}(l,r) = \{\{i_1, i'_1\}, \{j_1, i_2\}, \{j_2, i'_2, j'_2\}, \{j'_1\}\} \quad \text{with} \quad Q_{l,r} = 4.$$

.

for any such $(\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}')$ and write

$$\mathcal{E}=N^{-2}\sum_{\mathcal{Q}}E(\mathcal{Q})\sum_{\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}'|\mathcal{Q}}D(\mathbf{i},\mathbf{j})\overline{D(\mathbf{i}',\mathbf{j}')},$$

where the first sum is over all partitions $\mathcal{Q}$ of the form (B.10), and the second is over all $(\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}')$ satisfying (B.6) and inducing $\mathcal{Q}$.

Applying Lemma B.3(a) and the bound $N_r/N>c$ to (B.8), we have $|E(\mathcal{Q})|\leq CN^{-K}$ for a constant $C:=C_K>0$ and all partitions $\mathcal{Q}$. Thus

$$\mathcal{E}\leq CN^{-2-K}\sum_{\mathcal{Q}:E(\mathcal{Q})\neq 0}|D(\mathcal{Q})| \tag{B.11}$$

where

$$D(\mathcal{Q}):=\sum_{\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}'|\mathcal{Q}}D(\mathbf{i},\mathbf{j})\overline{D(\mathbf{i}',\mathbf{j}')}=\sum_{\mathbf{i},\mathbf{j},\mathbf{i}',\mathbf{j}'|\mathcal{Q}}\prod_{k=1}^{K}D_k[j_k,i_{k+1}]\prod_{k=1}^{K}\overline{D_k}[j'_k,i'_{k+1}].$$

For fixed $\mathcal{Q}$, we may rewrite $D(\mathcal{Q})$ as follows: Denote $L=2K$, $M_k=D_k$, and $M_{K+k}=\overline{D_k}$. Let $\mathfrak{q},\mathfrak{q}':\{1,\ldots,L\}\to\mathcal{Q}$ be the maps such that $\mathfrak{q}(k),\mathfrak{q}'(k),\mathfrak{q}(K+k),\mathfrak{q}'(K+k)$ are the elements of $\mathcal{Q}$ containing $j_k,i_{k+1},j'_k,i'_{k+1}$, respectively. Then

$$D(\mathcal{Q})=\sum_{\alpha}\prod_{\ell=1}^{L}M_\ell[\alpha_{\mathfrak{q}(\ell)},\alpha_{\mathfrak{q}'(\ell)}],$$

where $\sum_\alpha$ denotes the summation over all maps $\alpha:\mathcal{Q}\to\mathcal{N}$ such that $\alpha(l,r,q)\in\{1,\ldots,N_r\}$ for each $(l,r,q)\in\mathcal{Q}$ and $\alpha(l,r,q)\neq\alpha(l,r,q')$ whenever $q\neq q'$. (So α gives the index values, which must be distinct for elements of $\mathcal{Q}$ corresponding to the same $(l,r)\in\mathcal{R}$.)

We may simplify this condition on α by considering the following embedding: Let

$$\tilde{N}=\sum_{(l,r)\in\mathcal{R}}N_r,$$

and consider the corresponding block decomposition of $\mathbb{C}^{\tilde{N}}$ with blocks indexed by $\mathcal{R}$. (So the (l,r) block has size N_r.) For each $\ell=1,\ldots,L$, if $\mathfrak{q}(\ell)=(l,r,q)$ and $\mathfrak{q}'(\ell)=(l',r',q')$, then note that M_ℓ is of size $N_r\times N_{r'}$. Let $\tilde{M}_\ell\in\mathbb{C}^{\tilde{N}\times\tilde{N}}$ be its embedding whose $(l,r)\times(l',r')$ block equals M_ℓ and whose remaining blocks equal 0. Then

$$D(\mathcal{Q})=\sum_{\alpha}\prod_{\ell=1}^{L}\tilde{M}_\ell[\alpha_{\mathfrak{q}(\ell)},\alpha_{\mathfrak{q}'(\ell)}],$$

where $\sum_\alpha$ now denotes the summation over all maps $\alpha:\mathcal{Q}\to\{1,\ldots,\tilde{N}\}$ such that each $\alpha(l,r,q)$

belongs to the (l, r) block of $\{1, \ldots, \tilde{N}\}$, and the values $\alpha(l, r, q)$ are distinct across all $(l, r, q) \in \mathcal{Q}$. Extending the range of summation of each $\alpha(l, r, q)$ to all of $\{1, \ldots, \tilde{N}\}$ simply adds 0 by the definition of $\tilde{M}_\ell$, so we finally obtain

$$D(\mathcal{Q}) = \sum_{\alpha_1, \ldots, \alpha_Q}^{*} \prod_{\ell=1}^{L} \tilde{M}_\ell[\alpha_{\mathfrak{q}(\ell)}, \alpha_{\mathfrak{q}'(\ell)}] \tag{B.12}$$

where $Q = |\mathcal{Q}|$ and the sum is over all tuples of Q distinct indices in $\{1, \ldots, \tilde{N}\}$.

We must bound $|D(\mathcal{Q})|$ for any $\mathcal{Q}$ such that $E(\mathcal{Q}) \neq 0$. By Lemma B.3(b) and the expression (B.8) for $E(\mathcal{Q})$, if $E(\mathcal{Q}) \neq 0$, then for each $(l, r) \in \mathcal{R}$ and each index value $i \in \{1, \ldots, N_r\}$, there must be an even number of indices in $\mathcal{I}(l, r)$ equal in value to i, i.e. each element $S \in \mathcal{Q}$ must have even cardinality. Furthermore, if exactly two indices in $\mathcal{I}(l, r)$ equal i, then they must both be row indices or both be column indices for $O_{l,r}$. In particular, if $S \in \mathcal{Q}$ has cardinality $|S|= 2$, and if $S = \{j_k, i_{k+1}\}$ or $S = \{j'_k, i'_{k+1}\}$, then this implies $(l_k, r_k, e_k) = (l_{k+1}, r_{k+1}, -e_{k+1})$. The condition of the lemma ensures in this case that $\operatorname{Tr} D_k = 0$, so also $\operatorname{Tr} \tilde{M}_k = \operatorname{Tr} \tilde{M}_{K+k} = 0$.

We pause to formulate a lemma which provides the bound for $|D(\mathcal{Q})|$ that we need.

Lemma B.4. Fix integers $L, Q \geq 1$ and a constant $B > 0$. Let $\mathbf{i}, \mathbf{j} : \{1, \ldots, L\} \to \{1, \ldots, Q\}$ be two fixed maps. Let $M_1, \ldots, M_L \in \mathbb{C}^{N \times N}$ be such that $\|M_l\|\leq B$ for all l. Call an index $q \in \{1, \ldots, Q\}$ "good" if both of the following hold:

- Exactly two of $\mathbf{i}(1), \ldots, \mathbf{i}(L), \mathbf{j}(1), \ldots, \mathbf{j}(L)$ are equal to q.
- If $\mathbf{i}(\ell) = \mathbf{j}(\ell) = q$ for some ℓ, then $\operatorname{Tr} M_\ell = 0$.

Let T be the number of good indices $q \in Q$.

Denote by $\sum^{*}_{\alpha_1, \ldots, \alpha_Q}$ the sum over all tuples of Q indices $\alpha_1, \ldots, \alpha_Q \in \{1, \ldots, N\}$ with all values distinct. Then, for some constant $C := C(L, Q, B) > 0$,

$$\left| \sum_{\alpha_1, \ldots, \alpha_Q}^{*} \prod_{\ell=1}^{L} M_\ell[\alpha_{\mathbf{i}(\ell)}, \alpha_{\mathfrak{q}'(\ell)}] \right| \leq C N^{Q-T/2}. \tag{B.13}$$

Assuming this lemma for now, we can complete the proof of Lemma B.2. We saw that any $S \in \mathcal{Q}$ of cardinality $|S|= 2$ is good, for if $S = \{\mathfrak{q}(\ell), \mathfrak{q}'(\ell)\}$, then either $S = \{j_k, i_{k+1}\}$ or $S = \{j'_k, i'_{k+1}\}$ and so $\operatorname{Tr} \tilde{M}_\ell = 0$. Letting T be the number of elements of $\mathcal{Q}$ with cardinality 2, we have $2T + 4(Q-T) \leq 4K$. But T is also the number of good indices q, so Lemma (B.13) implies

$$|D(\mathcal{Q})|\leq C\tilde{N}^{Q-T/2} \leq C\tilde{N}^{K}. \tag{B.14}$$

Noting that $\tilde{N}/N$ and the number of distinct partitions $\mathcal{Q}$ are also both bounded by a K-dependent constant, and combining with (B.11), we obtain $\mathcal{E} \leq CN^{-2}$ as desired, and hence Lemma B.2. $\square$

Proof of Lemma B.4. Denote $[L] = \{1, \ldots, L\}$ and $[Q] = \{1, \ldots, Q\}$. We will show the following claim by induction on t: For any $L, Q \geq 1$ and $B > 0$, if the number of good indices T satisfies $T \geq t$, then there exists a constant $C := C(L, Q, B, t) > 0$ for which

$$\left| \sum_{\alpha_1,\ldots,\alpha_Q}^{*} \prod_{l=1}^{L} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right| \leq CN^{Q-t/2}. \tag{B.15}$$

The desired result follows from this claim applied with $t = T$ and $C = \max_{t=0}^{Q} C(L, Q, B, t)$.

For the base case $t = 0$, the left side of (B.15) is bounded by CN^Q for $C = B^L$, regardless of T, as each entry of M_l is bounded by B.

For the inductive step, let $t \geq 1$, suppose the number T of good indices satisfies $T \geq t$, and suppose the inductive claim holds for $t-1, t-2, \ldots, 0$. We consider two cases corresponding to the two possibilities for goodness of an index q:

Case 1: There exists a good index q and some $l \in [L]$ such that $\mathfrak{q}(l) = \mathfrak{q}'(l) = q$ and $\operatorname{Tr} M_l = 0$. For notational convenience, assume without loss of generality that $q = Q$ and $l = L$. Summing first over $\alpha_1, \ldots, \alpha_{Q-1}$ and then over α_Q, and noting that no other $\mathfrak{q}(l)$ or $\mathfrak{q}'(l)$ equals Q for $l \leq L-1$ because Q is good, the left side of (B.15) may be written as

$$\mathrm{LS} := \left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-1} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) \sum_{\substack{\alpha_Q=1 \\ \alpha_Q \notin \{\alpha_1,\ldots,\alpha_{Q-1}\}}}^{N} M_L[\alpha_Q, \alpha_Q] \right|.$$

Then applying $\operatorname{Tr} M_L = 0$, if $Q = 1$, then LS vanishes and there is nothing further to do. If $Q > 1$, we get

$$\begin{aligned} \mathrm{LS} &= \left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-1} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) \sum_{\alpha_Q \in \{\alpha_1,\ldots,\alpha_{Q-1}\}} M_L[\alpha_Q, \alpha_Q] \right| \\ &\leq \sum_{k=1}^{Q-1} \left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-1} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) M_L[\alpha_k, \alpha_k] \right|. \end{aligned}$$

We may apply the induction hypothesis to each of the $Q-1$ terms of the above sum: Define $\tilde{\mathfrak{q}}, \tilde{\mathfrak{q}}' : [L] \to [Q-1]$ by $\tilde{\mathfrak{q}}(l) = \mathfrak{q}(l)$ and $\tilde{\mathfrak{q}}'(l) = \mathfrak{q}'(l)$ for $l \in [L-1]$ and $\tilde{\mathfrak{q}}(L) = \tilde{\mathfrak{q}}'(L) = k$. Each $q \in [Q-1]$ that was good for i, j remains good for $\tilde{i}, \tilde{j}$, except possibly $q = k$. Thus the number of good indices for $\tilde{\mathfrak{q}}, \tilde{\mathfrak{q}}'$ is at least $\check{t} := \max(t-2, 0)$. The induction hypothesis implies

$$\mathrm{LS} \leq (Q-1) \cdot C(L, Q-1, B, \check{t}) N^{Q-1-\check{t}/2} \leq (Q-1) \cdot C(L, Q-1, B, \check{t}) N^{Q-t/2}.$$

Case 2: There exists a good index q and distinct $l \neq l' \in [L]$ such that one of $\mathfrak{q}(l), \mathfrak{q}'(l)$ and one of $\mathfrak{q}(l'), \mathfrak{q}'(l')$ equal q. For notational convenience, assume without loss of generality that $q = Q$, $l = L-1$, and $l' = L$. By possibly replacing M_{L-1} and/or M_L by M'_{L-1} and/or M'_L, we may further assume $\mathfrak{q}'(L-1) = \mathfrak{q}(L) = Q$.

Summing first over $\alpha_1, \ldots, \alpha_{Q-1}$ and then over α_Q as in Case 1, and noting that no $\mathfrak{q}(l)$ or $\mathfrak{q}'(l)$ equals Q for $l \leq L-2$ because Q is good, the left side of (B.15) may be written as

$$\mathrm{LS} := \left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-2} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) \sum_{\substack{\alpha_Q=1 \\ \alpha_Q \notin \{\alpha_1,\ldots,\alpha_{Q-1}\}}}^{N} M_{L-1}[\alpha_{\mathfrak{q}(L-1)}, \alpha_Q] M_L[\alpha_Q, \alpha_{\mathfrak{q}'(L)}] \right|.$$

Define $M = M_{L-1} M_L$. Then $\|M\| \leq B^2$, and

$$\begin{aligned}
\mathrm{LS} = &\left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-2} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) \left(M[\alpha_{\mathfrak{q}(L-1)}, \alpha_{\mathfrak{q}'(L)}] \right.\right. \\
&\qquad\qquad \left.\left. - \sum_{\alpha_Q \in \{\alpha_1,\ldots,\alpha_{Q-1}\}} M_{L-1}[\alpha_{\mathfrak{q}(L-1)}, \alpha_Q] M_L[\alpha_Q, \alpha_{\mathfrak{q}'(L)}] \right) \right| \\
\leq &\left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-2} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) M[\alpha_{\mathfrak{q}(L-1)}, \alpha_{\mathfrak{q}'(L)}] \right| \\
&\qquad + \sum_{k=1}^{Q-1} \left| \sum_{\alpha_1,\ldots,\alpha_{Q-1}}^{*} \left(\prod_{l=1}^{L-2} M_l[\alpha_{\mathfrak{q}(l)}, \alpha_{\mathfrak{q}'(l)}] \right) M_{L-1}[\alpha_{\mathfrak{q}(L-1)}, \alpha_k] M_L[\alpha_k, \alpha_{\mathfrak{q}'(L)}] \right|.
\end{aligned}$$

We may again apply the induction hypothesis to each term of the above sum: For the first term, each original good index $q \in [Q-1]$ remains good, except possibly $k := \mathfrak{q}(L-1) = \mathfrak{q}'(L)$ if k was originally good but now $\operatorname{Tr} M \neq 0$. Hence for this first term there are still at least $\check{t} := \max(t-2, 0)$ good indices. The other $Q-1$ terms are present only if $Q > 1$. For each of these terms, each original good index $q \in [Q-1]$ remains good, except possibly $q = k$—hence there are also at least $\check{t}$ good indices. Then the induction hypothesis yields, similarly to Case 1,

$$\mathrm{LS} \leq \Big(C(L-1, Q-1, B^2, \check{t}) + (Q-1) \cdot C(L, Q-1, B, \check{t}) \Big) N^{Q-t/2}.$$

This concludes the induction in both cases, upon setting $C(L, Q, B, t) = C(L-1, Q-1, B^2, \check{t}) + (Q-1) \cdot C(L, Q-1, B, \check{t})$. $\square$

This concludes the proof of Theorem 5.9. Finally, we prove Corollary 5.10 which establishes the approximation at the level of Stieltjes transforms.

Proof of Corollary 5.10. Under the given conditions, there exists a constant $C_0 > 0$ such that $|\tau(w^l)| \leq C_0^l$ for all N and $l \geq 0$, and also $|N^{-1} \operatorname{Tr} W^l| \leq \|W\|^l \leq C_0^l$ a.s. for all $l \geq 0$ and all sufficiently large N. Fix $z \in \mathbb{C}^+$ with $|z| > C_0$. Then $m_w(z) = -\sum_{l=0}^{\infty} z^{-(l+1)}\tau(w^l)$ and $m_W(z) = -N^{-1}\operatorname{Tr}(z-W)^{-1} = -\sum_{l=0}^{\infty} z^{-(l+1)}N^{-1}\operatorname{Tr} W^l$ define convergent series for all large N. For any $\varepsilon > 0$, there exists L such that

$$\left|\sum_{l=L+1}^{\infty} z^{-(l+1)}N^{-1}\operatorname{Tr} W^l\right| < \varepsilon, \qquad \left|\sum_{l=L+1}^{\infty} z^{-(l+1)}\tau(w^l)\right| < \varepsilon$$

for all large N, while by Theorem 5.9, as $N \to \infty$

$$\left|\sum_{l=0}^{L} z^{-(l+1)}N^{-1}\operatorname{Tr} W^l - z^{-(l+1)}\tau(w^l)\right| \to 0.$$

Hence $\limsup_{N\to\infty}|m_W(z) - m_w(z)| \leq 2\varepsilon$ a.s., and the result follows by taking $\varepsilon \to 0$. $\square$

B.2 Constructing free approximations

We construct the spaces $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ in Examples 5.5, 5.6, 5.7, and point the reader to the relevant references that establish Lemma 5.14.

Lemma B.5. Rectangular probability spaces $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ satisfying the properties of Examples 5.5, 5.6, and 5.7 exist, such that in each example, $\mathcal{A}$ is a von Neumann algebra and τ is a positive, normal, and faithful trace.

Proof. In Examples 5.5 and 5.6, let $(\Omega, \mathbb{P})$ be a (classical) probability space and let $\mathcal{A}$ be the von Neumann algebra of $d \times d$ random matrices with entries in $L^\infty(\Omega, \mathbb{P})$, the bounded complex-valued random variables on Ω. ($\mathcal{A}$ acts on the Hilbert space H of length-d random vectors with elements in $L^2(\Omega, \mathbb{P})$, endowed with inner-product $v, w \mapsto \mathbb{E}\langle v, w\rangle$.) Defining $\tau(a) = N^{-1}\mathbb{E}[\sum_{r=1}^d N_r a_{rr}]$, τ is a positive and faithful trace. As $a \mapsto \mathbb{E}[a_{rr}]$ is weakly continuous and hence σ-weakly continuous for each $r = 1, \ldots, d$, τ is normal. Letting $p_r \in \mathcal{A}$ be the (deterministic) matrix with (r, r) entry 1 and remaining entries 0, $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ is a rectangular probability space, and $\tau(p_r) = N_r/N$ for each $r = 1, \ldots, d$. For Example 5.5, the element $g \in \mathcal{A}$ may be realized as the random matrix with (r, r) entry equal to X and all other entries 0, where $X \in L^\infty(\Omega, \mathbb{P})$ is a random variable with standard semi-circle distribution on $[-2, 2]$. For Example 5.6, the element $g \in \mathcal{A}$ may be realized as the matrix with (r_1, r_2) entry equal to X and all other entries 0, where $X \in L^\infty(\Omega, \mathbb{P})$ is the square root of a random variable having the Marcenko-Pastur distribution (5.7) with $\lambda = N_{r_2}/N_{r_1}$.

For Example 5.7, we may simply take $(\mathcal{A}, \tau, p_1, \ldots, p_d)$ to be the rectangular probability space of deterministic $N \times N$ matrices from Example 5.1. ($\mathcal{A}$ is the space $B(H)$ for $H = \mathbb{C}^N$, and τ is clearly positive, faithful, and normal as H is finite-dimensional.) We may take the elements $b_1, \ldots, b_k \in \mathcal{A}$ to be the original matrices $B_1, \ldots, B_k$. $\square$

The sub-$*$-algebras $\mathcal{D}$ in the three examples above are isomorphic. They are also finite-dimensional, hence σ-weakly closed, so each is a von Neumann sub-algebra of $\mathcal{A}$.

Proof of Lemma 5.14. For each $r = 1, \ldots, k$, let $(\mathcal{A}^{(r)}, \tau^{(r)}, p_0, \ldots, p_{2k})$ be the space constructed as in Lemma B.5 corresponding to Example 5.6 and containing the element g_r, satisfying conditions 1, 2, and 4. Let $(\mathcal{A}^{(k+1)}, \tau^{(k+1)}, p_0, \ldots, p_{2k})$ and $(\mathcal{A}^{(k+2)}, \tau^{(k+2)}, p_0, \ldots, p_{2k})$ be the spaces constructed as in Lemma B.5 corresponding to Example 5.7 and containing the families $\{h_r\}$ and $\{f_{rs}\}$, respectively, satisfying conditions 1, 2, and 3. $\mathcal{D} = \langle p_0, \ldots, p_{2k}\rangle$ is a common (up to isomorphism) $(2k+1)$-dimensional von Neumann sub-algebra of each $\mathcal{A}^{(r)}$, and each $\tau^{(r)}$ restricts to the same trace on $\mathcal{D}$. Then the construction of the finite von Neumann amalgamated free product of $(\mathcal{A}^{(1)}, \tau^{(1)}), \ldots, (\mathcal{A}^{(k+2)}, \tau^{(k+2)})$ with amalgamation over $\mathcal{D}$ [Voi85, Pop93] yields a von Neumann algebra $\mathcal{A}$ with a positive, faithful, and normal trace τ such that:

- $\mathcal{A}$ contains (as an isomorphically embedded von Neumann sub-algebra) each $\mathcal{A}^{(r)}$, where $\mathcal{A}^{(r)}$ contains the common sub-algebra $\mathcal{D}$.
- Letting $\mathbf{F} : \mathcal{A} \to \mathcal{D}$ and $\mathbf{F}^{(r)} : \mathcal{A}^{(r)} \to \mathcal{D}$ denote the τ-invariant and $\tau^{(r)}$-invariant conditional expectations, $\mathbf{F}|_{\mathcal{A}^{(r)}} \equiv \mathbf{F}^{(r)}$.
- $\tau = \tau^{(r)} \circ \mathbf{F}$ for any r, so in particular, $\tau|_{\mathcal{A}^{(r)}} = \tau^{(r)}$.
- The sub-algebras $\mathcal{A}^{(1)}, \ldots, \mathcal{A}^{(k+2)}$ of $\mathcal{A}$ are free with amalgamation over $\mathcal{D}$ in the $\mathcal{D}$-valued probability space $(\mathcal{A}, \mathcal{D}, \mathbf{F})$.

(For more details about the amalgamated free product construction, see the Introduction of [Dyk95] and also Section 3.8 of [VDN92].) Since τ restricts to $\tau^{(r)}$ on each $\mathcal{A}^{(r)}$, conditions 1–4 continue to hold for the elements p_r, f_{rs}, g_r, h_r in $\mathcal{A}$. The generated von Neumann algebra $\langle D, g_r\rangle_{W^*}$ is contained in $\mathcal{A}^{(r)}$ and similarly for $\langle D, h_1, \ldots, h_k\rangle_{W^*}$ and $\langle D, f_{11}, f_{12}, \ldots, f_{kk}\rangle_{W^*}$, so $\mathcal{D}$-freeness of these algebras is implied by the $\mathcal{D}$-freeness of the sub-algebras $\mathcal{A}^{(r)}$. The elements f_{rs}, g_r, h_r have bounded norms in the original algebras $\mathcal{A}^{(1)}, \ldots, \mathcal{A}^{(k+2)}$ and hence also in the free product. $\square$

Bibliography

[Ame85] Yasuo Amemiya. What should be done when an estimated between-group covariance matrix is not nonnegative definite? *The American Statistician*, 39(2):112–117, 1985.

[BAC+15] Mark W Blows, Scott L Allen, Julie M Collet, Stephen F Chenoweth, and Katrina McGuigan. The phenome-wide distribution of genetic variance. *The American Naturalist*, 186(1):15–30, 2015.

[Bar90] N H Barton. Pleiotropic models of quantitative variation. *Genetics*, 124(3):773–782, 1990.

[BBC+17] Serban T Belinschi, Hari Bercovici, Mireille Capitaine, Maxime Février, et al. Outliers in the spectrum of large deformed unitarily invariant models. *The Annals of Probability*, 45(6A):3571–3625, 2017.

[BBP05] Jinho Baik, Gerard Ben Arous, and Sandrine Péché. Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *The Annals of Probability*, 33(5):1643–1697, 2005.

[BEK+14] Alex Bloemendal, László Erdős, Antti Knowles, Horng-Tzer Yau, and Jun Yin. Isotropic local laws for sample covariance and generalized Wigner matrices. *Electronic Journal of Probability*, 19(33):1–53, 2014.

[BG09] Florent Benaych-Georges. Rectangular random matrices, related convolution. *Probability Theory and Related Fields*, 144(3):471–515, 2009.

[BGGM11] Florent Benaych-Georges, Alice Guionnet, and Mylène Maida. Fluctuations of the extreme eigenvalues of finite rank deformations of random matrices. *Electronic Journal of Probability*, 16:1621–1662, 2011.

[BGN11] Florent Benaych-Georges and Raj Rao Nadakuditi. The eigenvalues and eigenvectors of finite, low rank perturbations of large random matrices. *Advances in Mathematics*, 227(1):494–521, 2011.

[Blo07] Mark W Blows. A tale of two matrices: Multivariate approaches in evolutionary biology. *Journal of Evolutionary Biology*, 20(1):1–8, 2007.

[BM15] Mark W Blows and Katrina McGuigan. The distribution of genetic variance across phenotypic space and the response to selection. *Molecular Ecology*, 24(9):2056–2072, 2015.

[BPZ13] Zhigang Bao, Guangming Pan, and Wang Zhou. Local density of the spectrum on the edge for sample covariance matrices with general population. Technical report, 2013.

[BPZ15] Zhigang Bao, Guangming Pan, and Wang Zhou. Universality for the largest eigenvalue of sample covariance matrices with general population. *The Annals of Statistics*, 43(1):382–421, 2015.

[BS98] Zhidong Bai and Jack W Silverstein. No eigenvalues outside the support of the limiting spectral distribution of large-dimensional sample covariance matrices. *The Annals of Probability*, 26(1):316–345, 1998.

[BS06] Jinho Baik and Jack W Silverstein. Eigenvalues of large sample covariance matrices of spiked population models. *Journal of Multivariate Analysis*, 97(6):1382–1408, 2006.

[BS10] Zhidong Bai and Jack W Silverstein. *Spectral Analysis of Large Dimensional Random Matrices*, volume 20. Springer, 2010.

[BY93] Z D Bai and Y Q Yin. Limit of the smallest eigenvalue of a large dimensional sample covariance matrix. *The Annals of Probability*, 21(3):1275–1294, 1993.

[BY08] Zhidong Bai and Jianfeng Yao. Central limit theorems for eigenvalues in a spiked population model. *Annales de l'Institut Henri Poincaré, Probabilités et Statistiques*, 44(3):447–474, 2008.

[BY12] Zhidong Bai and Jianfeng Yao. On sample eigenvalues in a generalized spiked population model. *Journal of Multivariate Analysis*, 106:167–177, 2012.

[CDS11] Romain Couillet, Mérouane Debbah, and Jack W Silverstein. A deterministic equivalent for the analysis of correlated MIMO multiple access channels. *IEEE Transactions on Information Theory*, 57(6):3493–3514, 2011.

[CL11] C Caratheéodory and E Landau. Beiträge zur konvergenz von funktionenfolgen. *Sitz. Ber. Königl. Preuss. Akad. Wiss., Phys.-math.*, 26:587–613, 1911.

[CMA+18] Julie M Collet, Katrina McGuigan, Scott L Allen, Stephen F Chenoweth, and Mark W Blows. Mutational pleiotropy and the strength of stabilizing selection within and between functional modules of gene expression. *Genetics*, 208(4):1601–1616, 2018.

[Col03] Benoit Collins. Moments and cumulants of polynomial random variables on unitary groups, the Itzykson-Zuber integral, and free probability. *International Mathematics Research Notices*, 2003(17):953–982, 2003.

[CR48] Ralph E Comstock and Harold F Robinson. The components of genetic variance in populations of biparental progenies and their use in estimating the average degree of dominance. *Biometrics*, 4(4):254–266, 1948.

[CŚ06] Benoit Collins and Piotr Śniady. Integration with respect to the Haar measure on unitary, orthogonal and symplectic group. *Communications in Mathematical Physics*, 264(3):773–795, 2006.

[DL11] Florian Dupuy and Philippe Loubaton. On the capacity achieving covariance matrix for frequency selective MIMO channels using the asymptotic approach. *IEEE Transactions on Information Theory*, 57(9):5737–5753, 2011.

[Dyk95] Kenneth J Dykema. Amalgamated free products of multi-matrix algebras and a construction of subfactors of a free group factor. *American Journal of Mathematics*, 117(6):1555–1602, 1995.

[EKY13] László Erdős, Antti Knowles, and Horng-Tzer Yau. Averaging fluctuations in resolvents of random band matrices. *Annales Henri Poincaré*, 8(14):1837–1926, 2013.

[EKYY13a] László Erdős, Antti Knowles, Horng-Tzer Yau, and Jun Yin. The local semicircle law for a general class of random matrices. *Electronic Journal of Probability*, 18(59):1–58, 2013.

[EKYY13b] László Erdős, Antti Knowles, Horng-Tzer Yau, and Jun Yin. Spectral statistics of Erdős–Rényi graphs I: Local semicircle law. *The Annals of Probability*, 41(3B):2279–2375, 2013.

[EYY11] László Erdős, Horng-Tzer Yau, and Jun Yin. Universality for generalized Wigner matrices with Bernoulli distribution. *Journal of Combinatorics*, 2(1):15–81, 2011.

[EYY12] László Erdős, Horng-Tzer Yau, and Jun Yin. Rigidity of eigenvalues of generalized Wigner matrices. *Advances in Mathematics*, 229(3):1435–1515, 2012.

[FBSG$^+$15] Hilary K Finucane, Brendan Bulik-Sullivan, Alexander Gusev, et al. Partitioning heritability by functional annotation using genome-wide association summary statistics. *Nature Genetics*, 47(11):1228, 2015.

[Fis18] Ronald A Fisher. The correlation between relatives on the supposition of Mendelian inheritance. *Transactions of the Royal Society of Edinburgh*, 52(02):399–433, 1918.

[FJ16] Zhou Fan and Iain M Johnstone. Eigenvalue distributions of variance components estimators in high-dimensional random effects models. *arXiv preprint 1607.02201*, 2016.

[FJ17] Zhou Fan and Iain M Johnstone. Tracy-Widom at each edge of real covariance estimators. *arXiv preprint arXiv:1707.02352*, 2017.

[FM96] Douglas S Falconer and Trudy F C Mackay. *Introduction to Quantitative Genetics*. Longman, Harlow, 1996.

[FS10] Ohad N Feldheim and Sasha Sodin. A universality result for the smallest eigenvalues of certain sample covariance matrices. *Geometric and Functional Analysis*, 20(1):88–123, 2010.

[Gem80] Stuart Geman. A limit theorem for the norm of random matrices. *The Annals of Probability*, 8(2):252–261, 1980.

[GH03] Jeffrey S Geronimo and Theodore P Hill. Necessary and sufficient condition that the limit of Stieltjes transforms is a Stieltjes transform. *Journal of Approximation Theory*, 121(1):54–60, 2003.

[HB06] Emma Hine and Mark W Blows. Determining the effective dimensionality of the genetic variance–covariance matrix. *Genetics*, 173(2):1135–1144, 2006.

[HGO10] David Houle, Diddahally R Govindaraju, and Stig Omholt. Phenomics: The next challenge. *Nature Reviews Genetics*, 11(12):855–866, 2010.

[HH81] J F Hayes and W G Hill. Modification of estimates of parameters in the construction of genetic selection indices ('Bending'). *Biometrics*, 37(3):483–493, 1981.

[HHN16] Walid Hachem, Adrien Hardy, and Jamal Najim. Large complex correlated Wishart matrices: Fluctuations and asymptotic independence at the edges. *The Annals of Probability*, 44(3):2264–2348, 2016.

[HLN07] Walid Hachem, Philippe Loubaton, and Jamal Najim. Deterministic equivalents for certain functionals of large random matrices. *The Annals of Applied Probability*, 17(3):875–930, 2007.

[HMB14] Emma Hine, Katrina McGuigan, and Mark W Blows. Evolutionary constraints in high-dimensional trait sets. *The American Naturalist*, 184(1):119–131, 2014.

[Hou10] David Houle. Numbering the hairs on our heads: The shared challenge and promise of phenomics. *Proceedings of the National Academy of Sciences*, 107(suppl 1):1793–1799, 2010.

[HP00] Fumio Hiai and Denes Petz. Asymptotic freeness almost everywhere for random matrices. *Acta Scientiarum Mathematicarum (Szeged)*, 66(3–4):809–834, 2000.

[Joh00] Kurt Johansson. Shape fluctuations and random matrices. *Communications in Mathematical Physics*, 209(2):437–476, 2000.

[Joh01] Iain M Johnstone. On the distribution of the largest eigenvalue in principal components analysis. *The Annals of Statistics*, 29(2):295–327, 2001.

[Kar07] Noureddine El Karoui. Tracy-Widom limit for the largest eigenvalue of a large class of complex sample covariance matrices. *The Annals of Probability*, 35(2):663–714, 2007.

[KM04] Mark Kirkpatrick and Karin Meyer. Direct estimation of genetic principal components. *Genetics*, 168(4):2295–2306, 2004.

[KP69] Jerome Klotz and Joseph Putter. Maximum likelihood estimation of multivariate covariance components for the balanced one-way layout. *The Annals of Mathematical Statistics*, 40(3):1100–1105, 1969.

[KY17] Antti Knowles and Jun Yin. Anisotropic local laws for random matrices. *Probability Theory and Related Fields*, 169(1-2):257–352, 2017.

[LA83] Russell Lande and Stevan J Arnold. The measurement of selection on correlated characters. *Evolution*, 37(6):1210–1226, 1983.

[LaM73] Lynn R LaMotte. Quadratic estimation of variance components. *Biometrics*, 29(2):311–330, 1973.

[Lan79] Russell Lande. Quantitative genetic analysis of multivariate evolution, applied to brain: Body size allometry. *Evolution*, 33(1):402–416, 1979.

[Lix06] Zhang Lixin. *Spectral analysis of large dimensional random matrices*. PhD thesis, National University of Singapore, 2006.

[LS15] Ji Oon Lee and Kevin Schnelli. Edge universality for deformed Wigner matrices. *Reviews in Mathematical Physics*, 27(08):1550018, 2015.

[LS16] Ji Oon Lee and Kevin Schnelli. Tracy-Widom distribution for the largest eigenvalue of real sample covariance matrices with general population. *The Annals of Applied Probability*, 26(6):3786–3839, 2016.

[LTBS$^+$15] Po-Ru Loh, George Tucker, Brendan K Bulik-Sullivan, et al. Efficient Bayesian mixed-model analysis increases association power in large cohorts. *Nature Genetics*, 47(3):284, 2015.

[Lus37] Jay L Lush. *Animal Breeding Plans*. Iowa State Press, 1937.

[LW98] Michael Lynch and Bruce Walsh. *Genetics and Analysis of Quantitative Traits*. Sinauer Sunderland, 1998.

[MAB15] Katrina McGuigan, J David Aguirre, and Mark W Blows. Simultaneous estimation of additive and mutational genetic variance in an outbred population of Drosophila serrata. *Genetics*, 201(3):1239–1251, 2015.

[MCM$^+$14] Katrina McGuigan, Julie M Collet, Elizabeth A McGraw, H Ye Yixin, Scott L Allen, Stephen F Chenoweth, and Mark W Blows. The nature and extent of mutational pleiotropy in gene expression of male Drosophila serrata. *Genetics*, 196(3):911–921, 2014.

[Mey91] Karin Meyer. Estimating variances and covariances for multivariate animal models by restricted maximum likelihood. *Genetics Selection Evolution*, 23(1):67, 1991.

[MH05] Jason G Mezey and David Houle. The dimensionality of genetic variation for wing shape in Drosophila melanogaster. *Evolution*, 59(5):1027–1038, 2005.

[MK05] Karin Meyer and Mark Kirkpatrick. Restricted maximum likelihood estimation of genetic principal components and smoothed covariance matrices. *Genetics Selection Evolution*, 37(1):1, 2005.

[MK08] Karin Meyer and Mark Kirkpatrick. Perils of parsimony: Properties of reduced-rank estimates of genetic covariance matrices. *Genetics*, 180(2):1153–1166, 2008.

[MK10] Karin Meyer and Mark Kirkpatrick. Better estimates of genetic covariance matrices by "bending" using penalized maximum likelihood. *Genetics*, 185(3):1097–1110, 2010.

[MLH$^+$15] Gerhard Moser, Sang Hong Lee, Ben J Hayes, Michael E Goddard, Naomi R Wray, and Peter M Visscher. Simultaneous discovery, estimation and prediction analysis of complex traits using a Bayesian mixture model. *PLoS Genetics*, 11(4):e1004969, 2015.

[MP67] Vladimir A Marcenko and Leonid Andreevich Pastur. Distribution of eigenvalues for some sets of random matrices. *Sbornik: Mathematics*, 1(4):457–483, 1967.

[MS07] Aris L Moustakas and Steven H Simon. On the outage capacity of correlated multiple-path MIMO channels. *IEEE Transactions on Information Theory*, 53(11):3887–3903, 2007.

[Nad08] Boaz Nadler. Finite sample approximation results for principal component analysis: A matrix perturbation approach. *The Annals of Statistics*, 36(6):2791–2817, 2008.

[NS06] Alexandru Nica and Roland Speicher. *Lectures on the Combinatorics of Free Probability*, volume 13. Cambridge University Press, 2006.

[NSS02] Alexandru Nica, Dimitri Shlyakhtenko, and Roland Speicher. Operator-valued distributions. I. Characterizations of freeness. *International Mathematics Research Notices*, 2002(29):1509–1538, 2002.

[Ona08] Alexei Onatski. The Tracy-Widom limit for the largest eigenvalues of singular complex Wishart matrices. *The Annals of Applied Probability*, 18(2):470–490, 2008.

[Pau07] Debashis Paul. Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica*, 17(4):1617–1642, 2007.

[Péc09] Sandrine Péché. Universality results for the largest eigenvalues of some sample covariance matrix ensembles. *Probability Theory and Related Fields*, 143(3-4):481–516, 2009.

[Pop93] Sorin Popa. Markov traces on universal Jones algebras and subfactors of finite index. *Inventiones Mathematicae*, 111(1):375–405, 1993.

[PY14] Natesh S Pillai and Jun Yin. Universality of covariance matrices. *The Annals of Applied Probability*, 24(3):935–1001, 2014.

[Rao72] C Radhakrishna Rao. Estimation of variance and covariance components in linear models. *Journal of the American Statistical Association*, 67(337):112–115, 1972.

[Rob59a] Alan Robertson. Experimental design in the evaluation of genetic parameters. *Biometrics*, 15(2):219–226, 1959.

[Rob59b] Alan Robertson. The sampling variance of the genetic correlation coefficient. *Biometrics*, 15(3):469–485, 1959.

[RV13] Mark Rudelson and Roman Vershynin. Hanson-Wright inequality and sub-gaussian concentration. *Electronic Communications in Probability*, 18, 2013.

[SB95] Jack W Silverstein and Zhidong Bai. On the empirical distribution of eigenvalues of a class of large dimensional random matrices. *Journal of Multivariate Analysis*, 54(2):175–192, 1995.

[SC95] Jack W Silverstein and Sang-Il Choi. Analysis of the limiting spectral distribution of large dimensional random matrices. *Journal of Multivariate Analysis*, 54(2):295–309, 1995.

[Sch13] Joel L Schiff. *Normal Families*. Springer Science & Business Media, 2013.

[SCM09] Shayle R Searle, George Casella, and Charles E McCulloch. *Variance Components*. John Wiley & Sons, 2009.

[Sil95] Jack W Silverstein. Strong convergence of the empirical distribution of eigenvalues of large dimensional random matrices. *Journal of Multivariate Analysis*, 55(2):331–339, 1995.

[Sos02] Alexander Soshnikov. A note on universality of the distribution of the largest eigenvalues in certain sample covariance matrices. *Journal of Statistical Physics*, 108(5):1033–1056, 2002.

[Spe83] T P Speed. Cumulants and partition lattices. *Australian & New Zealand Journal of Statistics*, 25(2):378–388, 1983.

[Spe98] Roland Speicher. *Combinatorial Theory of the Free Product with Amalgamation and Operator-Valued Free Probability Theory*. American Mathematical Society, 1998.

[SR74] S R Searle and T R Rounsaville. A note on estimating covariance components. *The American Statistician*, 28(2):67–68, 1974.

[SS78] William H Swallow and S R Searle. Minimum variance quadratic unbiased estimation (MIVQUE) of variance components. *Technometrics*, 20(3):265–272, 1978.

[SV12] Roland Speicher and Carlos Vargas. Free deterministic equivalents, rectangular random matrix models, and operator-valued free probability theory. *Random Matrices: Theory and Applications*, 1(02):1150008, 2012.

[TW94] Craig A Tracy and Harold Widom. Level-spacing distributions and the Airy kernel. *Communications in Mathematical Physics*, 159(1):151–174, 1994.

[TW96] Craig A Tracy and Harold Widom. On orthogonal and symplectic matrix ensembles. *Communications in Mathematical Physics*, 177(3):727–754, 1996.

[VDN92] D V Voiculescu, K J Dykema, and A Nica. *Free Random Variables*. CRM Monograph Series. American Mathematical Society, 1992.

[VHW08] Peter M Visscher, William G Hill, and Naomi R Wray. Heritability in the genomics era—concepts and misconceptions. *Nature Reviews Genetics*, 9(4):255–266, 2008.

[Voi85] Dan Voiculescu. Symmetries of some reduced free product C^*-algebras. In *Operator algebras and their connections with topology and ergodic theory*, pages 556–588. Springer, 1985.

[Voi91] Dan Voiculescu. Limit laws for random matrices and free products. *Inventiones Mathematicae*, 104(1):201–220, 1991.

[Voi95] Dan Voiculescu. Operations on certain non-commutative operator-valued random variables. *Recent advances in operator algebras (Orléans, 1992)*, Astérisque(232):243–275, 1995.

[Voi98] Dan Voiculescu. A strengthened asymptotic freeness result for random matrices with applications to free entropy. *International Mathematics Research Notices*, 1998(1):41–63, 1998.

[WB09] Bruce Walsh and Mark W Blows. Abundant genetic variation+strong selection=multivariate genetic constraints: A geometric view of adaptation. *Annual Review of Ecology, Evolution, and Systematics*, 40:41–59, 2009.

[Wig55] Eugene P Wigner. Characteristic vectors of bordered matrices with infinite dimensions. *Annals of Mathematics*, 62(3):548–564, 1955.

[Wri35] Sewall Wright. The analysis of variance and the correlations between relatives with respect to deviations from an optimum. *Journal of Genetics*, 30(2):243–256, 1935.

[YBK88] Yong-Quan Yin, Zhidong Bai, and Pathak R Krishnaiah. On the limit of the largest eigenvalue of the large dimensional sample covariance matrix. *Probability Theory and Related Fields*, 78(4):509–521, 1988.

[Yin86] Y Q Yin. Limiting spectral distribution for a class of random matrices. *Journal of multivariate analysis*, 20(1):50–68, 1986.

[YLGV11] Jian Yang, S Hong Lee, Michael E Goddard, and Peter M Visscher. GCTA: a tool for genome-wide complex trait analysis. *The American Journal of Human Genetics*, 88(1):76–82, 2011.

[ZCS13] Xiang Zhou, Peter Carbonetto, and Matthew Stephens. Polygenic modeling with Bayesian sparse linear mixed models. *PLoS Genetics*, 9(2):e1003264, 2013.