Nonlinear spiked covariance matrices and signal propagation in deep neural networks

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Abstract

Many recent works have studied the eigenvalue spectrum of the Conjugate Kernel (CK) defined by the nonlinear feature map of a feedforward neural network. However, existing results only establish weak convergence of the empirical eigenvalue distribution, and fall short of providing precise quantitative characterizations of the "spike" eigenvalues and eigenvectors that often capture the low-dimensional signal structure of the learning problem. In this work, we characterize these signal eigenvalues and eigenvectors for a nonlinear version of the spiked covariance model, including the CK as a special case. Using this general result, we give a quantitative description of how spiked eigenstructure in the input data propagates through the hidden layers of a neural network with random weights. As a second application, we study a simple regime of representation learning where the weight matrix develops a rank-one signal component over training and characterize the alignment of the target function with the spike eigenvector of the CK on test data.

1. Introduction

Kernel matrices associated with the nonlinear feature map of deep neural networks (NNs) provide insight into the optimization dynamics (Jacot et al., 2018; Montanari and Zhong, 2020; Fort et al., 2020) and predictive performance (Lee et al., 2017; Arora et al., 2019; Ortiz-Jiménez et al., 2021); consequently, properties of these kernel matrices can guide the design of network architecture (Xiao et al., 2018; Martens et al., 2021; Li et al., 2022) and learning algorithms (Karakida and Osawa, 2020; Zhou et al., 2022). Particular emphasis has been placed on the *spectral properties* of kernel matrices, due to their connection with the training and test performance of the underlying NN (Bordelon et al., 2020; Loureiro et al., 2021; Wei et al., 2022).

In this paper, we focus on the *conjugate kernel* (CK) (Neal, 1995; Cho and Saul, 2009) defined as the Gram matrix of the features at the penultimate (or more generally, any intermediate) NN layer. In the high-dimensional asymptotic setting where the width of the NN and the number of training samples diverge at the same rate, prior works employed random matrix theory to analyze the limit eigenvalue distribution of the CK matrix at random initialization (Pennington and Worah, 2017; Louart et al., 2018; Péché, 2019; Fan and Wang, 2020). These and related characterizations of the CK resolvent enable precise computations of various errors for NNs with random first-layer weights, known as *random features models* (Mei and Montanari, 2022; Tripuraneni et al., 2021; Hassani and Javanmard, 2022).

It is worth noting that while existing results establish the weak convergence of the empirical spectral measure, the precise behavior of "spike" eigenvalues that are separated from the spectral bulk remains largely unexplored. In learning applications, these spike eigenvalues and corresponding eigenvectors are often the primary spectral features (signal) of interest, because they pertain to low-rank structure of the underlying learning problem (e.g., class labels or the direction of the target function). For the linearly defined *spiked covariance model* $\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{\Sigma}^{1/2} \in \mathbb{R}^{n \times d}$, whose dependence across features is induced by a linear map $\boldsymbol{\Sigma}^{1/2}(\cdot)$ applied to $\boldsymbol{Z}$ having i.i.d. coordinates, classical work in random matrix theory provides a quantitative description of the spike eigenvalue/eigenvector behavior (Johnstone, 2001; Baik and Silverstein, 2006; Benaych-Georges and Nadakuditi, 2012; Bloemendal et al., 2016). In this paper, we establish an analogous characterization of spiked spectral structure for the CK, motivated in part by the following applications:

- **Structured input data.** Real data often contain low-dimensional structure despite the high ambient dimensionality (Lee and Verleysen, 2007; Hastie et al., 2009; Pope et al., 2021), and the leading eigenvectors of the input covariance matrix may be good predictors of the training labels. Common examples where the input features exhibit a low-dimensional spiked structure include Gaussian mixture models (Loureiro et al., 2021; Refinetti et al., 2021; Ben Arous et al., 2023b) and the block-covariance setting of (Ghorbani et al., 2020; Ba et al., 2023; Mousavi-Hosseini et al., 2023). Assuming that the input data $\boldsymbol{X}$ has informative spikes eigenvectors, we ask the natural question:

  How does the low-dimensional signal propagate through nonlinear layers of the NN? When do we observe a similar spiked structure in the CK matrix?

- **Spiked weight matrices in early training.** It is known that NNs can learn useful representations that adapt to the learning problem, and outperform the random features model defined by randomly initialized weights (Ghorbani et al., 2019; Wei et al., 2019; Abbe et al., 2022). Recent works have shown that when the target function is low-dimensional, the gradient update for two-layer NNs around initialization is *low-rank* (Ba et al., 2022; Damian et al., 2022; Wang et al., 2023), and hence the updated weight matrix $\boldsymbol{W}$ is well-approximated by a spiked model. We consider the following question on this pre-trained kernel model in NNs:

  When gradient descent produces a spiked structure in the weight matrix, how does the feature representation of the NN change, in terms of spectral properties of the CK?

1.1. Our Contributions

We analyze the spike eigenstructure in a general nonlinear spiked covariance model, which includes the CK as a special case. Specifically, we characterize the BBP phase transition (Baik et al., 2005) and first-order limits of the eigenvalues and eigenvector alignments in the proportional asymptotics regime, for spike eigenvalues of bounded size. Our work makes the following contributions:

- **Signal propagation in deep random NNs.** Following the setup of Fan and Wang (2020), we consider the CK matrix defined by a multi-layer fully-connected NN at random initialization, where the width of each layer grows linearly with the sample size. Given spiked input data, we compute the magnitude of the leading CK eigenvalues and the alignments between the corresponding CK eigenvectors with those of the input data, across network depth.

- **Feature learning in two-layer NNs.** We consider the early-phase feature learning setting in Ba et al. (2022), where the first-layer weights in a two-layer NN are optimized by gradient descent, and the learned weight matrix exhibits a rank-one spiked structure. We characterize the spiked eigenstructure of the corresponding CK matrix for independent test data, and the alignment of spike eigenvectors with the test labels. This provides a quantitative description of how gradient descent improves the NN representation.

- **Spectral analysis for nonlinear spiked covariance models.** We give a general analysis of the signal eigenvalues/eigenvectors of spiked covariance matrices with arbitrary and possibly nonlinear dependence across features, showing a "Gaussian equivalence" with the quantitative spectral properties of linear spiked covariance models established by Bai and Yao (2012). We prove a deterministic equivalent for the Stieltjes transform and resolvent for any spectral argument separated from the support of the limit spectral measure, extending recent results for spectral arguments bounded away from the positive real line (Chouard, 2022, 2023; Schröder et al., 2023).

1.2. Related Works

Eigenvalues of nonlinear random matrices. Global convergence of the empirical eigenvalue distribution of nonlinear kernel matrices has been studied in both proportional and polynomial scaling regimes (El Karoui, 2010; Cheng and Singer, 2013; Fan and Montanari, 2019; Lu and Yau, 2022; Dubova et al., 2023). Building upon related techniques, recent works characterized the spectrum of the CK matrix (Pennington and Worah, 2017; Louart et al., 2018; Péché, 2019) and the neural tangent kernel (NTK) matrix (Montanari and Zhong, 2020; Adlam and Pennington, 2020), with generalizations to deeper networks studied in Fan and Wang (2020) and Chouard (2023).

Benigni and Péché (2022) gave a precise characterization of the largest eigenvalue in a one-hidden-layer CK matrix when the input data $\boldsymbol{X}$ and weight matrix $\boldsymbol{W}$ both have i.i.d. entries, identifying possible uninformative spike eigenvalues when the nonlinear activation is not an odd function. Guionnet et al. (2023) and Feldman (2023) recently characterized spiked eigenstructure in models where an activation is applied to a spiked Wigner matrix or rectangular information-plus-noise matrix entrywise, for possibly growing spike sizes and activations having degenerate information/Hermite coefficients.

Precise error analysis of NNs. An important application of spectral analyses of the CK matrix is the precise computation of generalization error of random features regression, first performed for two-layer models in proportional scaling regimes (Louart et al., 2018; Mei and Montanari, 2022) and later extended to deep random features models (Schröder et al., 2023; Bosch et al., 2023) and polynomial scaling regimes (Ghorbani et al., 2021; Xiao et al., 2022). These risk analyses reveal a *Gaussian equivalence principle*, where generalization error coincides with that of a Gaussian covariates model, and this equivalence has been extended to other settings of nonlinear (regularized) empirical risk minimization (Hu and Lu, 2020; Goldt et al., 2021; Montanari and Saeed, 2022).

Going beyond random features, Ba et al. (2022) derived the precise asymptotics of representation learning in a two-layer NN when the first-layer weights are trained by one (or finitely many) gradient descent steps; see also Damian et al. (2022); Ba et al. (2023); Dandi et al. (2023). The computation follows from an information-plus-noise characterization of the weight matrix due to a low-rank gradient update. Moniri et al. (2023) derived a corresponding information-plus-noise decomposition of the CK matrix defined by the resulting trained weights, in an asymptotic regime different from ours where the learning rate and spike eigenvalues diverge. Ben Arous et al. (2023a) examined the emerging spike eigenstructure in the NN Hessian that arises during SGD training.

Eigenvalues of sample covariance matrices. Asymptotic spectral analyses of sample covariance matrices have a long history in random matrix theory (Marčenko and Pastur, 1967; Silverstein, 1995; Silverstein and Bai, 1995; Bai and Silverstein, 1998), with the strongest known results in the linearly defined model $\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{\Sigma}^{1/2}$, see e.g. Bloemendal et al. (2014); Knowles and Yin (2017). Outside of this linear setting, Srivastava and Vershynin (2013) and Chafaï and Tikhomirov (2018) develop sharp bounds for the extremal eigenvalues with isotropic population covariance, and Bao and Xu (2022) develop eigenvalue rigidity and Tracy-Widom fluctuation results for isotropic and log-concave distributions.

The spiked covariance model was introduced in Johnstone (2001). Baik et al. (2005); Baik and Silverstein (2006); Paul (2007) initiated the study of spiked eigenstructure and phase transition phenomena for spiked covariance matrices with isotropic bulk covariance. Péché (2006); Benaych-Georges and Nadakuditi (2011, 2012); Capitaine (2013, 2018) studied spiked eigenstructure in related Wigner and information-plus-noise models. Closely related to our work are the results of Bai and Yao (2012) that characterize spike eigenvalues in linearly defined models $\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{\Sigma}^{1/2}$ with general population covariance $\boldsymbol{\Sigma}$, and we extend this characterization to nonlinear settings.

2. Results for neural network models

2.1. Propagation of signal through multi-layer neural networks

Consider input features $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{d \times n}$, where $\boldsymbol{x}_i \in \mathbb{R}^d$ are independent samples. Define a L-hidden-layer feedforward neural network by

$$\boldsymbol{X}_\ell = \frac{1}{\sqrt{d_\ell}}\sigma(\boldsymbol{W}_\ell \boldsymbol{X}_{\ell-1}) \in \mathbb{R}^{d_\ell \times n} \qquad \text{for } \ell = 1 \ldots, L \tag{2.1}$$

with weight matrices $\boldsymbol{W}_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$, $\boldsymbol{X}_0 \equiv \boldsymbol{X}$ and $d_0 \equiv d$, and a nonlinear activation function $\sigma : \mathbb{R} \to \mathbb{R}$ applied entrywise. The Conjugate Kernel (CK) at each layer $\ell = 1, \ldots, L$ is given by the Gram matrix

$$\boldsymbol{K}_\ell = \boldsymbol{X}_\ell^\top \boldsymbol{X}_\ell \in \mathbb{R}^{n \times n}. \tag{2.2}$$

In the limit $n, d_0, \ldots, d_L \to \infty$ with $n/d_\ell \to \gamma_\ell \in (0, \infty)$ for each $\ell = 0, \ldots, L$, under deterministic conditions for the input data $\boldsymbol{X}$ and for random weight matrices $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L$ as specified below, it is shown in Fan and Wang (2020) that the empirical eigenvalue distribution $\widehat{\mu}_\ell$ of $\boldsymbol{K}_\ell$ for each $\ell = 1, \ldots, L$ satisfies the weak convergence

$$\widehat{\mu}_\ell := \frac{1}{n}\sum_{i=1}^n \delta_{\lambda_i(\boldsymbol{K}_\ell)} \to \mu_\ell \text{ a.s.} \tag{2.3}$$

for limit measures $\mu_1, \ldots, \mu_L$ defined as follows: Let μ_0 be the limit eigenvalue distribution of the input gram matrix $\boldsymbol{K}_0 = \boldsymbol{X}^\top \boldsymbol{X}$ (c.f. Assumption 2). Then, for $\ell = 1, \ldots, L$, let

$$\nu_{\ell-1} = b_\sigma^2 \otimes \mu_{\ell-1} \oplus (1 - b_\sigma^2) \tag{2.4}$$

denote the law of $b_\sigma^2 \mathsf{x} + (1 - b_\sigma^2)$ when $\mathsf{x} \sim \mu_{\ell-1}$ and $b_\sigma := \mathbb{E}_{\xi \sim \mathcal{N}(0,1)}[\sigma'(\xi)]$, and define

$$\mu_\ell = \rho_{\gamma_\ell}^{\text{MP}} \boxtimes \nu_{\ell-1}. \tag{2.5}$$

Here, $\rho_\gamma^{\text{MP}} \boxtimes \nu$ denotes the *deformed Marchenko-Pastur law* describing the limit eigenvalue distribution of a sample covariance matrix with limit dimension ratio $\gamma \in (0, \infty)$ and population spectral measure ν, and we review its definition in Appendix A.

In this section, we provide a precise characterization of the spike eigenvalues and eigenvectors of $\boldsymbol{K}_\ell$ for each $\ell = 1, \dots, L$ when the input data $\boldsymbol{X}$ has a fixed number of spike singular values of bounded magnitude. We assume the following conditions on the weights, input data, and activation.

Assumption 1 *The number of layers $L \geq 1$ is fixed, and $n, d_0, \dots, d_L \to \infty$ such that*

$$n/d_\ell \to \gamma_\ell \in (0, \infty) \text{ for each } \ell = 0, \dots, L.$$

The weights $\boldsymbol{W}_1, \dots, \boldsymbol{W}_L$ have entries $[\boldsymbol{W}_\ell]_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1)$, independent of each other and of $\boldsymbol{X}$.

Definition 1 *A feature matrix $\boldsymbol{X} \in \mathbb{R}^{d \times n}$ is τ_n-**orthonormal** if*

$$\big|\|\boldsymbol{x}_\alpha\|_2 - 1\big| \leq \tau_n, \qquad \big|\|\boldsymbol{x}_\beta\|_2 - 1\big| \leq \tau_n, \qquad \big|\boldsymbol{x}_\alpha^\top \boldsymbol{x}_\beta\big| \leq \tau_n$$

for all pairs $\alpha \neq \beta \in [n]$, where $\{\boldsymbol{x}_\alpha\}_{\alpha=1}^n$ are the columns of $\boldsymbol{X}$.

Assumption 2 *For some $\tau_n > 0$ such that $\lim_{n\to\infty} \tau_n \cdot n^{1/3} = 0$, $\boldsymbol{X} \equiv \boldsymbol{X}_0$ is τ_n-orthonormal almost surely for all large n. Furthermore, $\boldsymbol{K}_0 = \boldsymbol{X}^\top \boldsymbol{X}$ has eigenvalues $\lambda_1(\boldsymbol{K}_0), \dots, \lambda_n(\boldsymbol{K}_0)$ (not necessarily ordered by magnitude) such that for some fixed $r \geq 0$, as $n, d \to \infty$,*

(a) There exists a compactly supported probability measure μ_0 on $[0, \infty)$ such that

$$\frac{1}{n - r} \sum_{i=r+1}^n \delta_{\lambda_i(\boldsymbol{K}_0)} \to \mu_0 \text{ weakly a.s.}$$

and for any fixed $\varepsilon > 0$, almost surely for all large n,

$$\lambda_i(\boldsymbol{K}_0) \in \operatorname{supp}(\mu_0) + (-\varepsilon, \varepsilon) \text{ for all } i \geq r + 1.$$

(b) There exist distinct values $\lambda_1, \dots, \lambda_r > 0$ with $\lambda_1, \dots, \lambda_r \notin \operatorname{supp}(\mu_0)$ such that

$$\lambda_i(\boldsymbol{K}_0) \to \lambda_i \quad \text{a.s. for each} \quad i = 1, \dots, r.$$

Assumption 3 *The activation $\sigma : \mathbb{R} \to \mathbb{R}$ is twice differentiable with $\sup_{x\in\mathbb{R}} |\sigma'(x)|, |\sigma''(x)| \leq \lambda_\sigma$ for some $\lambda_\sigma \in (0, \infty)$. Under $\xi \sim \mathcal{N}(0, 1)$, we have $\mathbb{E}[\sigma(\xi)] = 0$ and $\mathbb{E}[\sigma^2(\xi)] = 1$. Furthermore,*

$$b_\sigma := \mathbb{E}[\sigma'(\xi)] \neq 0, \qquad \mathbb{E}[\sigma''(\xi)] = 0. \tag{2.6}$$

Assumption 1 defines the linear-width asymptotic regime. Assumption 2 requires an orthogonality condition for the input features that is similar to (Fan and Wang, 2020, Definition 3.1), and also codifies our spiked eigenstructure assumption for the input data. We briefly comment on (2.6) in Assumption 3: The condition $b_\sigma \neq 0$ ensures that the linear component of $\sigma(\cdot)$ is non-degenerate; if $b_\sigma = 0$, then spiked eigenstructure does not propagate across the NN layers in our studied regime of bounded spike magnitudes. The condition $\mathbb{E}[\sigma''(\xi)] = 0$ ensures that $\boldsymbol{K}_\ell$ does not have uninformative spike eigenvalues; otherwise, as shown in Benigni and Péché (2022), $\boldsymbol{K}_\ell$ may have spike eigenvalues even when the input $\boldsymbol{K}_0$ has no spiked structure. We assume $\mathbb{E}[\sigma''(\xi)] = 0$ for clarity, to avoid characterizing also such uninformative spikes across layers. This condition holds, in particular, for odd activation functions $\sigma(\cdot)$ such as $\tanh$.

The following theorem first extends (Fan and Wang, 2020, Theorem 3.4) by affirming that the weak convergence statement (2.3) holds under the above assumptions, and furthermore, each $\boldsymbol{K}_\ell$ has no outlier eigenvalues outside its limit spectral support when the input $\boldsymbol{K}_0$ has no spike eigenvalues.

Theorem 2 *Suppose Assumptions 1, 2, and 3 hold. Then for each $\ell = 1, \ldots, L$, (2.3) holds weakly a.s. as $n \to \infty$. Furthermore, if the number of spikes is $r = 0$ in Assumption 2, then for any fixed $\varepsilon > 0$, almost surely for all large n,*

$$\boldsymbol{K}_\ell \text{ has no eigenvalues outside } \operatorname{supp}(\mu_\ell) + (-\varepsilon, \varepsilon).$$

Remark 3 *From Theorem 2 and Fan and Wang (2020) we know that for large n and $\gamma_\ell < 1$, the minimum eigenvalue of the CK matrix $\lambda_{\min}(\boldsymbol{K}_\ell)$ is bounded away from 0 almost surely. This implies that the minimum ℓ_2-norm interpolator is well-defined, and provides an affirmative answer to the conjecture in (Mei and Montanari, 2022, Remark 1) regarding the exchangeability of ridgeless limit.*

The main result of this section characterizes the eigenvalues of $\boldsymbol{K}_\ell$ outside $\operatorname{supp}(\mu_\ell)$ when $r \geq 1$. To describe this characterization, define for each $\ell = 1, \ldots, L$ the domain

$$\mathcal{T}_\ell = \{-1/\lambda : \lambda \in \operatorname{supp}(\nu_{\ell-1})\}$$

where $\nu_{\ell-1}$ is defined by (2.4), and define $z_\ell, \varphi_\ell : (0, \infty) \setminus \mathcal{T}_\ell \to \mathbb{R}$ by

$$z_\ell(s) = -\frac{1}{s} + \gamma_\ell \int \frac{\lambda}{1 + \lambda s} \nu_{\ell-1}(d\lambda), \qquad \varphi_\ell(s) = -\frac{s z_\ell'(s)}{z_\ell(s)}. \tag{2.7}$$

It is known from the results of Bai and Yao (2012) and (Yao et al., 2015, Chapter 11) that these are precisely the functions that characterize the spike eigenvalues and eigenvectors in linear spiked covariance models. Set

$$\mathcal{I}_0 = \{1, \ldots, r\}, \qquad s_{i,0} = -\frac{1}{b_\sigma^2 \lambda_i + (1 - b_\sigma^2)} \text{ for } i \in \mathcal{I}_0,$$

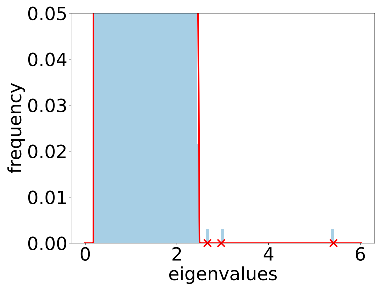
where λ_i and b_σ are defined in Assumptions 2 and 3 respectively. Here, $\mathcal{I}_0$ records the indices of the spike eigenvalues of the input Gram matrix $\boldsymbol{K}_0$. Then define recursively for $\ell = 1, \ldots, L$

$$\mathcal{I}_\ell = \Big\{ i \in \mathcal{I}_{\ell-1} : z_\ell'(s_{i,\ell-1}) > 0 \Big\}, \qquad s_{i,\ell} = -\frac{1}{b_\sigma^2 z_\ell(s_{i,\ell-1}) + (1 - b_\sigma^2)} \text{ for } i \in \mathcal{I}_\ell. \tag{2.8}$$

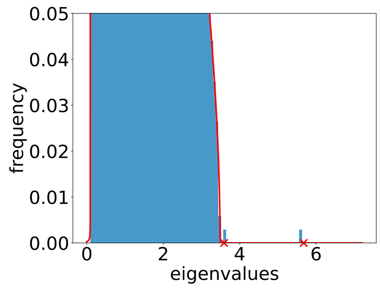
The condition $z_\ell'(s_{i,\ell-1}) > 0$ describes the "phase transition" phenomenon for spike eigenvalues in this model, where spikes $i \in \mathcal{I}_{\ell-1}$ with $z_\ell'(s_{i,\ell-1}) > 0$ induce spike eigenvalues in the CK matrix $\boldsymbol{K}_\ell$ of the next layer, while spikes with $z_\ell'(s_{i,\ell-1}) \leq 0$ are absorbed into the bulk spectrum of $\boldsymbol{K}_\ell$.

Theorem 4 *Suppose Assumptions 1, 2, and 3 hold. Then for each $\ell = 1, \ldots, L$:*

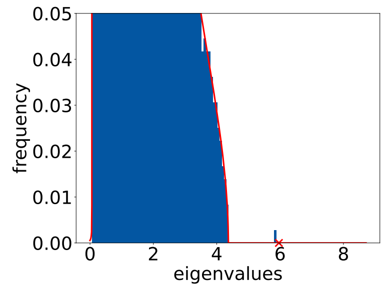
(a) $s_{i,\ell-1} \in (0, \infty) \setminus \mathcal{T}_\ell$ for each $i \in \mathcal{I}_{\ell-1}$, so $z_\ell(s_{i,\ell-1})$ and $\mathcal{I}_\ell$ are well-defined. Furthermore, if $i \in \mathcal{I}_\ell$ (i.e. if $z_\ell'(s_{i,\ell-1}) > 0$) then $z_\ell(s_{i,\ell-1}) > 0$ and $\varphi_\ell(s_{i,\ell-1}) > 0$.



(a) Spectrum of $\boldsymbol{K}_0$



(b) Spectrum of $\boldsymbol{K}_1$



(c) Spectrum of $\boldsymbol{K}_2$

Figure 1: Spectra of three-layer CK matrices defined by (2.2) with $n = 5000$, $d_0 = d_1 = d_2 = 15000$, and $\sigma \propto \arctan$. Input data is a GMM satisfying (2.9) with $r = 3$, $\theta_1 = 2.0$, $\theta_2 = 1.18$, and $\theta_3 = 1.0$. (a)-(c) are theoretically predicted (red) and empirical (blue) bulk distributions and spikes of $\boldsymbol{K}_\ell$ for $\ell = 0, 1, 2$. Observe that the number of informative spikes is non-increasing w.r.t. depth.

(b) For any fixed and sufficiently small $\varepsilon > 0$, almost surely for all large n, there is a 1-to-1 correspondence between the eigenvalues of $\boldsymbol{K}_\ell$ outside $\operatorname{supp}(\mu_\ell) + (-\varepsilon, \varepsilon)$ and $\{i : i \in \mathcal{I}_\ell\}$. Denoting these eigenvalues of $\boldsymbol{K}_\ell$ by $\{\widehat{\lambda}_{i,\ell} : i \in \mathcal{I}_\ell\}$, for each $i \in \mathcal{I}_\ell$ as $n \to \infty$,

$$\widehat{\lambda}_{i,\ell} \to z_\ell(s_{i,\ell-1}) \text{ a.s.}$$

(c) Let $\widehat{\boldsymbol{v}}_{i,\ell}$ be a unit-norm eigenvector of $\boldsymbol{K}_\ell$ corresponding to its eigenvalue $\widehat{\lambda}_{i,\ell}$, and let $\boldsymbol{v}_j$ be a unit-norm eigenvector of $\boldsymbol{K}_0$ corresponding to its spike eigenvalue $\lambda_j(\boldsymbol{K}_0)$. Then for each $i \in \mathcal{I}_\ell$ and $j \in \mathcal{I}_0$, as $n \to \infty$,

$$|\widehat{\boldsymbol{v}}_{i,\ell}^\top \boldsymbol{v}_j|^2 \to \prod_{k=1}^{\ell} \varphi_k(s_{i,k-1}) \cdot \mathbf{1}\{i = j\} \text{ a.s.}$$

Moreover, for each $i \in \mathcal{I}_\ell$ and any unit vector $\boldsymbol{v} \in \mathbb{R}^n$ independent of $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\ell$,

$$|\widehat{\boldsymbol{v}}_{i,\ell}^\top \boldsymbol{v}|^2 - \prod_{k=1}^{\ell} \varphi_k(s_{i,k-1}) \cdot |\boldsymbol{v}_i^\top \boldsymbol{v}|^2 \to 0 \text{ a.s.}$$

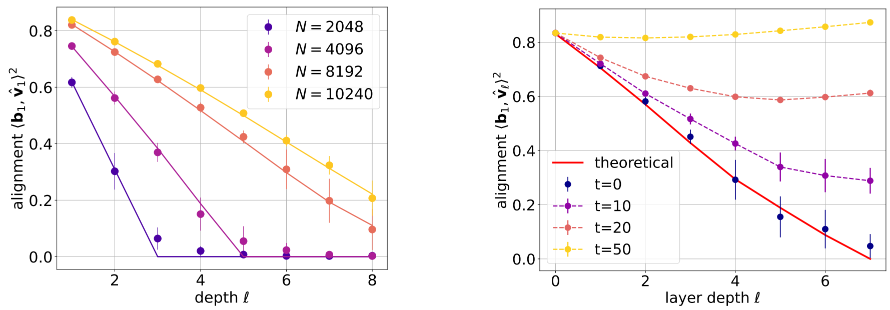
We present the following corollary as a concrete example in which the assumptions of the theorem are satisfied. The corollary encompasses, for instance, Gaussian mixture models with a fixed number r of balanced classes, each class having $\Theta(n)$ samples.

Corollary 5 *Suppose the input data $\boldsymbol{X}$ is itself a low-rank signal-plus-noise matrix*

$$\boldsymbol{X} = \sum_{i=1}^{r} \theta_i \boldsymbol{a}_i \boldsymbol{b}_i^\top + \boldsymbol{Z} \in \mathbb{R}^{d \times n} \tag{2.9}$$

where $\theta_1, \ldots, \theta_r > 0$ are fixed distinct signal strengths, $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_r \in \mathbb{R}^d$ and $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_r \in \mathbb{R}^n$ are orthonormal sets of unit vectors, and $\boldsymbol{Z}$ has i.i.d. $\mathcal{N}(0, 1/d)$ entries. Assume that $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_r$ satisfy the ℓ_∞-delocalization condition: for any sufficiently small $\varepsilon > 0$ and all large n,

$$\max_{i=1}^{r} \|\boldsymbol{b}_i\|_\infty < n^{-1/2+\varepsilon}.$$



(a) Effect of width on alignment.

(b) Effect of GD training.

Figure 2: We consider deep NNs in (2.1) with $\sigma \propto \tanh$ on Gaussian mixture data (2.9) with $r = 1$, and compute the alignment between the largest eigenvector of the CK matrix $\boldsymbol{K}_\ell$ with genuine signal $\boldsymbol{b}_1$ (class labels) for different layer ℓ. (a) NNs at random initialization with varying hidden widths $N = 2048, 4096, 8192, 10240$. (b) NNs trained by gradient descent with learning rate $\eta = 0.1$ for varying steps $T = 0, 10, 20, 50$; we use the μ-parameterization (Yang and Hu, 2020) to encourage feature learning. θ_1 is 2.5 and 1.8 for (a) and (b), respectively. Dots are empirical values (over 10 runs) and solid curves represent theoretical predictions at random initialization from Theorem 4.

Define $\varphi_\ell(\cdot)$ and $s_{i,\ell-1}$ by (2.7) *and* (2.8)*, with the initial measures $\mu_0 = \rho^{\mathrm{MP}}_{\gamma_0}$ and $\nu_0 = b_\sigma^2 \otimes \mu_0 \oplus (1 - b_\sigma^2)$ and initial spike values $\lambda_i = (1 + \theta_i^2)(\gamma_0 + \theta_i^2)/\theta_i^2$ for $i \in \mathcal{I}_0$.*

Then for each $\ell = 1, \ldots, L$, $\boldsymbol{K}_\ell$ has a spike eigenvalue corresponding to the input signal component θ_i if and only if $\theta_i > \gamma_0^{1/4}$ and $i \in \mathcal{I}_\ell$. In this case, its corresponding unit eigenvector $\widehat{\boldsymbol{v}}_{i,\ell}$ satisfies, as $n \to \infty$,

$$|\widehat{\boldsymbol{v}}_{i,\ell}^\top \boldsymbol{b}_i|^2 \to \prod_{k=1}^{\ell} \varphi_k(s_{i,k-1}) \cdot \left(1 - \frac{\gamma_0(1 + \theta_i^2)}{\theta_i^2(\theta_i^2 + \gamma_0)}\right) \text{ a.s.} \tag{2.10}$$

Numerical illustration. A simple illustration of this result for a 3-component Gaussian mixture model is provided in Figure 1. We note that $\mathcal{I}_L \subseteq \cdots \subseteq \mathcal{I}_0$ and $\varphi_\ell(s_{i,\ell-1}) \in (0, 1)$, so the number of spike eigenvalues of $\boldsymbol{K}_\ell$ induced by $\boldsymbol{K}_0$ and the alignment of the spike eigenvectors of $\boldsymbol{K}_\ell$ with the true class label vectors $\{\boldsymbol{b}_i\}_{i=1}^r$ are both non-increasing in the network depth, see also Figure 2. In other words, at random initialization, the input signal diminishes as the depth of the NN increases.

In Figure 2 we highlight two remedies to this "curse of depth" at random initialization.

- In Figure 2(a) we observe that when the width of NN becomes larger, alignment between the leading eigenvector of $\boldsymbol{K}_\ell$ at random initialization and the signal can be preserved across a larger depth. This illustrates the benefit of overparameterization by increasing the network width.
- In Figure 2(b) we observe that gradient descent training on the weight matrices also restores and even amplifies the informative signal in the CK matrix of each layer; specifically, after 50 steps of GD training (yellow curve), the alignment between the class labels and the leading eigenvector of $\boldsymbol{K}_\ell$ may increase through depth. This demonstrates the benefit of gradient-based feature learning. In Section 2.2 we precisely quantify this improved alignment due to gradient descent in a simplified two-layer setting.

2.2. CK matrix after $\mathcal{O}_d(1)$ steps of gradient descent

The preceding section studied the spike eigenstructure of the CK induced by low-rank structure in the input data. Here, focusing on a two-layer model, we study an alternative setting where spiked structure arises instead in the weight matrix $\boldsymbol{W}$ from gradient descent training.

We consider an early training regime studied in Ba et al. (2022), with a width-N two-layer feedforward NN,

$$f_{\text{NN}}(\boldsymbol{x}) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} a_i \sigma(\langle \boldsymbol{x}, \boldsymbol{w}_i \rangle) = \frac{1}{\sqrt{N}} \sigma(\boldsymbol{x}^\top \boldsymbol{W}) \boldsymbol{a}. \tag{2.11}$$

Here $\boldsymbol{x} \in \mathbb{R}^d$ is the input, and $\boldsymbol{W} = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_N] \in \mathbb{R}^{d \times N}$ and $\boldsymbol{a} \in \mathbb{R}^N$ are the network weights. For clarity of the subsequent discussion, we will transpose the notation for $\boldsymbol{X}$ and $\boldsymbol{W}$ from the preceding section, and incorporate a $1/\sqrt{d}$ scaling into $\boldsymbol{W}$ rather than into the input data $\boldsymbol{X}$.

Given are an input feature matrix $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^\top \in \mathbb{R}^{n \times d}$ and labels $\boldsymbol{y} \in \mathbb{R}^n$ for n samples, where $y_i = f_*(\boldsymbol{x}_i) + \text{noise}$. We consider the training of first-layer weights $\boldsymbol{W}$ to minimize the mean squared error

$$\mathcal{L}(\boldsymbol{W}) = \frac{1}{2n} \sum_{i=1}^{n} (f_{\text{NN}}(\boldsymbol{x}_i) - y_i)^2,$$

fixing the second-layer weight vector $\boldsymbol{a}$. From a random initialization $\boldsymbol{W}_0 \in \mathbb{R}^{d \times N}$, and over T steps with learning rates $\eta_1, \ldots, \eta_T$ scaled by $\sqrt{N}$, the gradient descent (GD) updates take the form

$$\boldsymbol{W}_{t+1} = \boldsymbol{W}_t + \eta_{t+1} \sqrt{N} \cdot \boldsymbol{G}_t, \qquad \boldsymbol{G}_t = -\nabla \mathcal{L}(\boldsymbol{W}_t). \tag{2.12}$$

Of interest is the information about the label function f_* that is learned by $\boldsymbol{W}_{\text{trained}} \equiv \boldsymbol{W}_T$, which may be characterized by the spectral alignment of the CK matrix with the class label vector on independent test data $(\tilde{\boldsymbol{X}}, \tilde{\boldsymbol{y}})$. This use of independent test data may be understood as a pre-training setup, also considered previously in Ba et al. (2022); Moniri et al. (2023) and studied for real-world data in Wei et al. (2022).

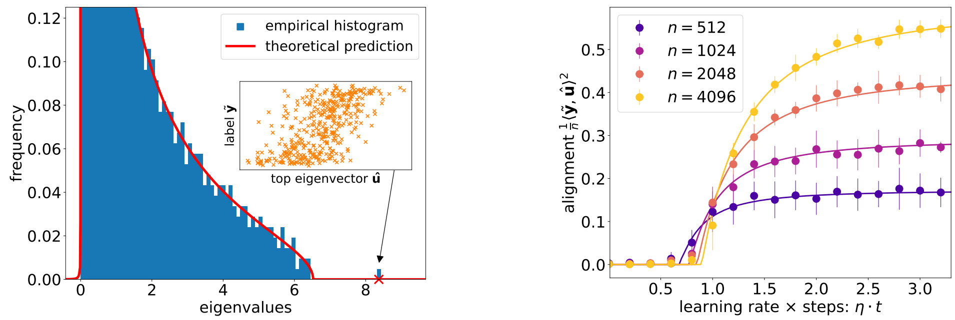
It was shown in Ba et al. (2022) that in a training regime with initialization $\|\boldsymbol{W}_0\| \asymp 1$ such that $|f_{\text{NN}}(\boldsymbol{x}_i)| \ll 1$ for each $i = 1, \ldots, N$, and with learning rates $\eta_1, \ldots, \eta_T \asymp 1$ for a fixed number T of GD steps, the weight matrix $\boldsymbol{W}$ undergoes a change during training that is $O(1)$ in operator norm and approximately rank-1,

$$\boldsymbol{W}_{\text{trained}} \approx \boldsymbol{W}_0 + \frac{\eta b_\sigma}{n} \boldsymbol{X}^\top \boldsymbol{y} \boldsymbol{a}^\top \qquad \text{where} \qquad \eta = \sum_{t=1}^{T} \eta_t.$$

(Ba et al., 2022, Conjecture 4) conjectured that for the CK matrix

$$\boldsymbol{K} = \frac{1}{N} \sigma(\tilde{\boldsymbol{X}} \boldsymbol{W}_{\text{trained}}) \sigma(\tilde{\boldsymbol{X}} \boldsymbol{W}_{\text{trained}})^\top \in \mathbb{R}^{n \times n} \tag{2.13}$$

defined by the pre-trained weights and test data $\tilde{\boldsymbol{X}}$, the resulting spike eigenvalue and the alignment of its spike eigenvector with the test labels $\tilde{\boldsymbol{y}} \in \mathbb{R}^n$ are accurately predicted by a Gaussian equivalent model. Our main result of this section is an affirmative verification of this conjecture and precise characterization of the spike eigenstructure of $\boldsymbol{K}$, in the following representative setting.



(a) Spectrum of the updated CK.

(b) Eigenvector alignment of the updated CK.

Figure 3: (a) We set $n = 2000, d = 1600, N = 2400, \eta \cdot t = 2$, and $\sigma = \sigma_* = \text{erf}$. (b) We set $d = 2048, N = 1024, \eta = 0.2, \sigma = \tanh, \sigma_* = \text{SoftPlus}$, and vary the sample size n and number of GD steps t; dots represent empirical simulations (over 10 runs) and solid curves are theoretical predictions from Theorem 6.

Assumption 4 *For a two-layer NN in (2.11) with GD training defined by (2.12), we assume that*

(a) $n, d, N \to \infty$ *such that* $N/d \to \gamma_0 \in (0, \infty)$ *and* $N/n \to \gamma_1 \in (0, \infty)$.

(b) Training features $\boldsymbol{X} = [\boldsymbol{x}_1, \dots, \boldsymbol{x}_n]^\top \in \mathbb{R}^{n \times d}$ *have entries* $[\boldsymbol{X}]_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1)$, *training labels* $\boldsymbol{y} \in \mathbb{R}^n$ *have entries* $y_i = \sigma_*(\boldsymbol{\beta}_*^\top \boldsymbol{x}_i) + \varepsilon_i$ *where* $\boldsymbol{\beta}_* \in \mathbb{R}^d$ *is a deterministic unit vector and* $\varepsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2)$, *and test data* $(\tilde{\boldsymbol{X}}, \tilde{\boldsymbol{y}})$ *is an independent copy of* $(\boldsymbol{X}, \boldsymbol{y})$.

(c) The NN activation $\sigma : \mathbb{R} \to \mathbb{R}$ *and label function* $\sigma_* : \mathbb{R} \to \mathbb{R}$ *both satisfy Assumption 3, with* $b_\sigma := \mathbb{E}[\sigma'(\xi)] \neq 0$ *and* $b_{\sigma_*} := \mathbb{E}[\sigma_*'(\xi)] \neq 0$.

(d) The weight initializations satisfy $[\boldsymbol{W}_0]_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1/d)$ *and* $a_j \overset{iid}{\sim} \mathcal{N}(0, 1/N)$.

(e) The number of iterations T *and learning rates* $\eta_1, \dots, \eta_T$ *are fixed independently of* n, d, N.

Under these assumptions, the following theorem characterizes the spike eigenvalue of the CK matrix and the alignment between the corresponding eigenvector and the test labels, as a function of the learning rate η_t and the number of gradient descent steps T.

Theorem 6 *Suppose that Assumption 4 holds, and set* $\eta = \sum_{t=1}^T \eta_t$. *Define*

$$\theta_1 = b_\sigma \eta \cdot \sqrt{(\gamma_1/\gamma_0)(1 + \sigma_\varepsilon^2) + b_{\sigma_*}^2}, \qquad \theta_2 = b_\sigma b_{\sigma_*} \eta. \tag{2.14}$$

Let $z(\cdot)$ *and* $\varphi(\cdot)$ *be defined by (2.7) for* $\ell = 1$ *with* γ_1 *and* $\nu_0 = b_\sigma^2 \otimes \rho_{\gamma_0}^{\text{MP}} \oplus (1 - b_\sigma^2)$, *and set*

$$\lambda_1 = b_\sigma^2 \frac{(1 + \theta_1^2)(\gamma_0 + \theta_1^2)}{\theta_1^2} + 1 - b_\sigma^2.$$

Then $\boldsymbol{K}$ *defined by (2.13) has a spike eigenvalue if and only if* $\theta_1 > \gamma_0^{1/4}$ *and* $z'(-1/\lambda_1) > 0$. *In this case,* $\lambda_{\max}(\boldsymbol{K}) \to \gamma_1^{-1} z(-1/\lambda_1)$ *a.s., and the leading unit eigenvector* $\widehat{\boldsymbol{u}} \in \mathbb{R}^n$ *of* $\boldsymbol{K}$ *satisfies*

$$\frac{1}{\sqrt{n}} |\tilde{\boldsymbol{y}}^\top \widehat{\boldsymbol{u}}| \to b_\sigma b_{\sigma_*} \frac{\sqrt{z(-1/\lambda_1)\varphi(-1/\lambda_1)}}{\lambda_1} \cdot \frac{\theta_2 \sqrt{(\theta_1^4 - \gamma_0)(\gamma_0 + \theta_1^2)}}{\theta_1^3} > 0 \text{ a.s.} \tag{2.15}$$

Numerical illustration. Figure 3 empirically validates the predictions of Theorem 6, for a two-layer NN trained with a small number of GD steps. Figure 3(a) shows that one spike eigenvalue emerges over training in the test-data CK, the location of which is accurately predicted by Theorem 6; moreover, the leading eigenvector $\widehat{\boldsymbol{u}}$ aligns with the labels $\tilde{\boldsymbol{y}}$. This is quantified in Figure 3(b), where above a phase transition threshold, the alignment $\langle \widehat{\boldsymbol{u}}, \tilde{\boldsymbol{y}} \rangle^2$ (predicted by (2.15)) increases with the learning rate or number of GD steps; in addition, alignment also increases with the training set size n. Compared with random initialization ($\eta = 0$), this illustrates that training improves the NN representation, and the test-data CK contains information on the label function f_*.

3. Analysis of a nonlinear spiked covariance model

The results of Sections 2.1 and 2.2 rest on an analysis of spiked eigenstructure in a general nonlinear spiked covariance model. We describe the assumptions and statement of this general result informally here, deferring formal and more quantitative statements to Appendix B.

Let $\boldsymbol{G} = \frac{1}{\sqrt{N}}[\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N]^\top \in \mathbb{R}^{N \times n}$ have independent rows $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N \in \mathbb{R}^n$ with mean 0 and common covariance $\boldsymbol{\Sigma} \in \mathbb{R}^{n \times n}$. We assume that the law of $\boldsymbol{g}_i$ satisfies concentration of quadratic forms $\boldsymbol{g}_i^\top \boldsymbol{A} \boldsymbol{g}_j$, but has otherwise arbitrary dependence across coordinates. As $n, N \to \infty$ with $n/N \to \gamma \in (0, \infty)$, the eigenvalues of $\boldsymbol{\Sigma}$ satisfy

$$\lambda_i(\boldsymbol{\Sigma}) \to \lambda_i \text{ for } i = 1, \ldots, r, \qquad \frac{1}{n-r} \sum_{i=r+1}^{n} \delta_{\lambda_i(\boldsymbol{\Sigma})} \to \nu \text{ weakly},$$

for fixed spike values $\lambda_1, \ldots, \lambda_r > 0$ and a deterministic limit spectral law ν. Then the empirical spectral law of the sample covariance matrix $\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G}$ satisfies

$$\frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\boldsymbol{K})} \to \mu = \rho_\gamma^{\mathrm{MP}} \boxtimes \nu \text{ weakly a.s.}$$

Under these assumptions, let us define

$$z(s) = -\frac{1}{s} + \gamma \int \frac{\lambda}{1 + \lambda s} d\nu(\lambda), \qquad \varphi(s) = \frac{z'(s)}{(-1/s) z(s)}.$$

Theorem 7 (informal)

(a) If $r = 0$, then all eigenvalues of $\boldsymbol{K}$ converge to $\operatorname{supp}(\mu) \cup \{0\}$. More generally for $r \geq 0$, the eigenvalues of $\boldsymbol{K}$ asymptotically separated from $\operatorname{supp}(\mu) \cup \{0\}$ are in 1-to-1 correspondence with $\mathcal{I} = \{i : z'(-1/\lambda_i) > 0\}$, and $\widehat{\lambda}_i(\boldsymbol{K}) \to z(-1/\lambda_i)$.

(b) For each $i \in \mathcal{I}$ and any deterministic unit vector $\boldsymbol{v} \in \mathbb{R}^n$, $(\boldsymbol{v}^\top \widehat{\boldsymbol{v}}_i)^2 - \varphi(-1/\lambda_i)(\boldsymbol{v}^\top \boldsymbol{v}_i)^2 \to 0$, where $\boldsymbol{v}_i, \widehat{\boldsymbol{v}}_i$ are the unit eigenvectors of $\boldsymbol{\Sigma}, \boldsymbol{K}$ for eigenvalues $\lambda_i(\boldsymbol{\Sigma}), \widehat{\lambda}_i(\boldsymbol{K})$.

(c) Let $\boldsymbol{u} = \frac{1}{\sqrt{N}}(u_1, \ldots, u_N)^\top \in \mathbb{R}^N$ be such that $[\boldsymbol{u}, \boldsymbol{G}] \in \mathbb{R}^{N \times (n+1)}$ has i.i.d. rows $\{[u_j, \boldsymbol{g}_j]\}_{j=1}^N$, and denote $\mathbb{E}[u\boldsymbol{g}] = \mathbb{E}[u_j \boldsymbol{g}_j]$ for all $j \in [N]$. Then for each $i \in \mathcal{I}$,

$$(\boldsymbol{u}^\top \widehat{\boldsymbol{u}}_i)^2 - \frac{z(-1/\lambda_i)\varphi(-1/\lambda_i)}{\lambda_i^2} (\mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{v}_i)^2 \to 0$$

where $\widehat{\boldsymbol{u}}_i$ is the unit eigenvector of $\boldsymbol{G}\boldsymbol{G}^\top$ for its eigenvalue $\widehat{\lambda}_i(\boldsymbol{G}\boldsymbol{G}^\top) = \widehat{\lambda}_i(\boldsymbol{K})$.

Statements (a–b) are known in a linear setting $\boldsymbol{g}_i = \boldsymbol{\Sigma}^{1/2}\boldsymbol{z}_i$ when $\boldsymbol{z}_i$ has i.i.d. entries, see e.g. (Bai and Yao, 2012) and (Yao et al., 2015, Theorems 11.3 and 11.5). The above theorem thus verifies an exact asymptotic equivalence between spiked spectral phenomena in a nonlinear spiked covariance model with those of a linearly defined (possibly Gaussian) model.

In Section 2.1, each CK matrix $\boldsymbol{K}_\ell$ has (approximately) the structure of the above matrix $\boldsymbol{K}$ over the randomness of $\boldsymbol{W}_\ell$, conditional on the features $\boldsymbol{X}_{\ell-1}$ of the preceding layer, and Theorem 4 follows from Theorem 7(a,b). In Section 2.2, the CK matrix $\boldsymbol{K}$ defined by trained weights has (approximately) this structure over the randomness of $\tilde{\boldsymbol{X}}$, conditional on $\boldsymbol{W}_{\text{trained}}$, and Theorem 6 follows from Theorem 7(a,c).

Proof ideas. Analyses in the linearly defined model $\boldsymbol{g}_i = \boldsymbol{\Sigma}^{1/2}\boldsymbol{z}_i$ commonly stem from block matrix inversion identities with respect to the block decompositions

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Sigma}_0 \end{pmatrix}, \qquad \boldsymbol{G} = \begin{pmatrix} \boldsymbol{G}_r & \boldsymbol{G}_0 \end{pmatrix}$$

where $\boldsymbol{\Sigma}_r$ contains the spike eigenvalues of $\boldsymbol{\Sigma}$, and $\boldsymbol{G}_r$ is independent of $\boldsymbol{G}_0$. This independence does not hold in our setting, and we develop a different "master equation" approach.

Let $\widehat{\lambda}^{1/2}$ be a spike singular value of $\boldsymbol{G}$ with corresponding unit singular vectors $(\widehat{\boldsymbol{u}}, \widehat{\boldsymbol{v}})$. We consider the linearized equation

$$0 = \begin{pmatrix} -\widehat{\lambda}\boldsymbol{I} & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I} \end{pmatrix} \begin{pmatrix} \widehat{\boldsymbol{v}} \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}} \end{pmatrix}. \tag{3.1}$$

Writing $\boldsymbol{V}_r \in \mathbb{R}^{n \times r}$ for the r spike eigenvectors of $\boldsymbol{\Sigma}$, we define a generalized resolvent

$$\boldsymbol{\mathcal{R}}(z, \alpha) = \begin{pmatrix} -z\boldsymbol{I} - \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I} \end{pmatrix}^{-1},$$

add to (3.1) the quantity $-\alpha \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}$ on both sides for some large $\alpha > 0$, and rewrite this as

$$\begin{pmatrix} \widehat{\boldsymbol{v}} \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}} \end{pmatrix} = -\alpha\, \boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}. \tag{3.2}$$

We will show that $\boldsymbol{\mathcal{R}}(z, \alpha)$ exists and is bounded in operator norm for any z separated from the limit bulk spectral support of $\boldsymbol{K}$ and any large enough $\alpha > 0$. Then, multiplying (3.2) by $(\boldsymbol{V}_r^\top \; \boldsymbol{0})$ and applying a block matrix inversion identity,

$$\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}} = -\alpha \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix}^\top \boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}} = -\alpha \boldsymbol{V}_r^\top \left(\boldsymbol{G}^\top \boldsymbol{G} - \widehat{\lambda}\boldsymbol{I} - \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top \right)^{-1} \boldsymbol{V}_r \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}.$$

As a result, spike eigenvalues $\widehat{\lambda}$ are roots $z = \widehat{\lambda}$ of the master equation

$$\det\left(\boldsymbol{I}_r + \alpha \boldsymbol{V}_r^\top \left(\boldsymbol{G}^\top \boldsymbol{G} - z\boldsymbol{I} - \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top \right)^{-1} \boldsymbol{V}_r \right) = 0,$$

for any fixed and large $\alpha > 0$. Singular vector alignments may be characterized likewise from (3.2).

The core of the proof is an asymptotic analysis of this master equation via a deterministic equivalent approximation

$$\boldsymbol{v}_1^\top \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{v}_2 := \boldsymbol{v}_1^\top (\boldsymbol{G}^\top \boldsymbol{G} - \boldsymbol{\Gamma})^{-1}\boldsymbol{v}_2 \approx -\boldsymbol{v}_1^\top (\boldsymbol{\Gamma} + z\tilde{m}(z)\boldsymbol{\Sigma})^{-1}\boldsymbol{v}_2 \tag{3.3}$$

for any deterministic unit vectors $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^n$ and low-rank perturbations $\boldsymbol{\Gamma}$ of $z\boldsymbol{I}$, where $\tilde{m}(z)$ is the Stieltjes transform of the "companion" limit measure $\tilde{\mu}$ for the eigenvalue distribution of $\boldsymbol{G}\boldsymbol{G}^\top \in \mathbb{R}^{N\times N}$. We extend results of Chouard (2022); Schröder et al. (2023) by establishing this approximation not only for $\boldsymbol{\Gamma} = z\boldsymbol{I}$ but also perturbations thereof, and for spectral arguments $z \in \mathbb{C}\setminus\operatorname{supp}(\mu)$ that may belong to the positive real line. The latter extension requires showing, a priori, that all eigenvalues of $\boldsymbol{K} = \boldsymbol{G}^\top\boldsymbol{G}$ fall close to $\operatorname{supp}(\mu)$ in the absence of spiked structure. We show this by adapting an argument of Bai and Silverstein (1998) and using a fluctuation averaging lemma described below.

Let us conclude with a brief discussion of our proof of (3.3): From manipulations of the identity

$$\operatorname{Tr}\boldsymbol{B} = \operatorname{Tr}(\boldsymbol{G}^\top\boldsymbol{G} - \boldsymbol{\Gamma})\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B} = -\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Gamma} + \frac{1}{N}\sum_{i=1}^N \boldsymbol{g}_i^\top \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{g}_i$$

for appropriately chosen matrices $\boldsymbol{B} \in \mathbb{C}^{n\times n}$, the Sherman-Morrison (leave-one-out) formula for matrix inversion applied to $\boldsymbol{R}(\boldsymbol{\Gamma})$, and the concentration of bilinear forms in $\boldsymbol{g}_i$, one may show

$$\boldsymbol{v}_1^\top(\boldsymbol{\Gamma} + z\tilde{m}(z)\boldsymbol{\Sigma})^{-1}\boldsymbol{v}_2 \approx -\boldsymbol{v}_1^\top\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{v}_2 + \frac{1}{1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})} \cdot \frac{1}{N}\sum_{i=1}^N (1 - \mathbb{E}_{\boldsymbol{g}_i})T_i \tag{3.4}$$

where $T_i = \boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{v}_2 \cdot \boldsymbol{v}_1^\top(\boldsymbol{\Gamma} + zm_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i$. Here, $\boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})$ and $m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})$ are generalized leave-one-out resolvents and empirical Stieltjes transforms defined by $\{\boldsymbol{g}_j\}_{j\neq i}$, and $\mathbb{E}_{\boldsymbol{g}_i}$ is the partial expectation over only $\boldsymbol{g}_i$. Under our assumptions for $\boldsymbol{g}_i$, each error term $(1 - \mathbb{E}_{\boldsymbol{g}_i})T_i$ has mean 0 and $O(1)$ fluctuations. We develop a fluctuation averaging lemma using recursive applications of the Sherman-Morrison identity to further resolve the dependence of $\boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})$ and $m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})$ on fixed subsets of rows $\{\boldsymbol{g}_j\}_{j\neq i}$, to show that the errors $(1 - \mathbb{E}_{\boldsymbol{g}_i})T_i$ are weakly correlated across $i \in [N]$. Hence their average has a mean 0 and fluctuates on the asymptotically negligible scale of $O(N^{-1/2})$, and applying this to (3.4) shows (3.3).

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Organization of the Appendices

- Appendix A introduces relevant notation and background.
- Appendix B states our main results for the general nonlinear spiked covariance model

$$\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G},$$

formalizing the discussion in Section 3. These results are divided into two subsections: Appendix B.1 gives a "no outliers" statement for $\boldsymbol{K}$ and a deterministic equivalent approximation for its resolvent, under minimal asymptotic assumptions. Appendix B.2 then states the main characterizations of spike eigenvalues/eigenvectors in an asymptotic setting with a spiked eigenstructure.

- Appendix C develops a general fluctuation averaging lemma for the sample covariance model, and proves the results of Appendix B.1.
- Appendix D proves the results of Appendix B.2.
- Finally, Appendix E proves the results of Section 2.1 on propagation of spiked eigenstructure through the layers of a neural network, and Appendix F proves the results of Section 2.2 on the eigenstructure of the CK after gradient descent training.

Appendix A. Notations and background

A.1. Stochastic domination

We use the following standard notation for stochastic domination of random variables, see e.g. (Erdős et al., 2013, Definition 2.4): For random variables $X \equiv X(u)$ and $Y \equiv Y(u) \geq 0$ depending implicitly on N and a parameter $u \in U_N$, as $N \to \infty$, we write

$$X \prec Y \text{ or } X = O_\prec(Y) \text{ uniformly over } u \in U_N$$

if, for any fixed $\varepsilon, D > 0$ and all large N,

$$\sup_{u \in U_N} \mathbb{P}\Big[|X(u)| > N^\varepsilon Y(u)\Big] < N^{-D}.$$

Throughout, "for all large N" means for all $N \geq N_0$ where N_0 may depend on ε, D, any quantities that are constant in the context of the statement, and convergence rates of the spike eigenvalues and empirical spectral measures in the given assumptions.

If $X = \mathbf{1}\{\mathcal{E}\}$ is the indicator of an event $\mathcal{E} \equiv \mathcal{E}_N$, then $\mathbf{1}\{\mathcal{E}\} \prec 0$ means $\mathbb{P}[\mathcal{E}] < N^{-D}$ for any fixed $D > 0$ and all large N. If X and Y are both deterministic, then $X \prec Y$ means $|X| \leq N^\varepsilon Y$ (deterministically) for any $\varepsilon > 0$ and all large N. For an event $\mathcal{E} \equiv \mathcal{E}_N$, we will write

$$X = O_\prec^{\mathcal{E}}(Y)$$

as shorthand for $X \cdot \mathbf{1}\{\mathcal{E}\} \prec Y$.

We will use the following basic properties often implicitly.

Proposition 8 *Suppose $X \prec Y$ uniformly over $u \in U_N$.*

(a) If $|U_N| \le N^C$ for a constant $C > 0$, then for any fixed $\varepsilon, D > 0$ and all large N,

$$\mathbb{P}\Big[\text{there exists } u \in U_N \text{ with } |X(u)| \ge N^{\varepsilon} Y(u)\Big] \le N^{-D}.$$

(b) If $|U_N| \le N^C$ for a constant $C > 0$, then $\sum_{u \in U_N} X(u) \prec \sum_{u \in U_N} Y(u)$.

(c) If $|U_N| \le C$ for a constant $C > 0$, then $\prod_{u \in U_N} X(u) \prec \prod_{u \in U_N} Y(u)$.

(d) If Y is deterministic, and $\mathbb{E}[X^2] \le N^C$ and $Y \ge N^{-C}$ for a constant $C > 0$, then also $\mathbb{E}[|X|] \prec Y$ uniformly over $u \in U_N$.

Proof. The first three statements follow from a union bound over U_N. For the last statement, for any fixed $\varepsilon > 0$, observe that

$$\mathbb{E}|X| \le N^{\varepsilon/2} Y + \mathbb{E}\Big[|X| \mathbf{1}\{|X| > N^{\varepsilon/2} Y\}\Big] \le N^{\varepsilon/2} Y + \mathbb{E}[X^2]^{1/2} \mathbb{P}[|X| > N^{\varepsilon/2} Y]^{1/2}.$$

Applying $\mathbb{E}[X^2] \le N^C$, $Y \ge N^{-C}$, and $\mathbb{P}[|X| > N^{\varepsilon/2} Y] < N^{-D}$ for sufficiently large $D > 0$ shows that the second term is less than $N^{\varepsilon/2} Y$ for all large N, hence $\mathbb{E}|X| < N^{\varepsilon} Y$. ■

A.2. Deformed Marcenko-Pastur law

For a probability measure ν supported on $[0, \infty)$ and an aspect ratio parameter $\gamma > 0$, consider the deformed Marcenko–Pastur measure

$$\mu = \rho_{\gamma}^{\text{MP}} \boxtimes \nu$$

and its "companion" probability measure

$$\tilde{\mu} = \gamma \mu + (1 - \gamma) \delta_0.$$

Here, μ and $\tilde{\mu}$ represent the limit eigenvalue distributions of $\boldsymbol{G}^\top \boldsymbol{G} \in \mathbb{R}^{n \times n}$ and $\boldsymbol{G}\boldsymbol{G}^\top \in \mathbb{R}^{N \times N}$ respectively, when $\boldsymbol{G} = \frac{1}{\sqrt{N}}[\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N] \in \mathbb{R}^{N \times n}$ has i.i.d. rows with mean 0 and covariance $\boldsymbol{\Sigma}$, and $n, N \to \infty$ with $n/N \to \gamma$ and $\frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\boldsymbol{\Sigma})} \to \nu$ weakly.

These measures $\mu, \tilde{\mu}$ may be defined by their Stieltjes transform

$$m(z) = \int \frac{1}{x - z} d\mu(x), \qquad \tilde{m}(z) = \int \frac{1}{x - z} d\tilde{\mu}(x) \tag{A.1}$$

where $\tilde{m}(z) = \gamma m(z) + (1 - \gamma)(-1/z)$. By the results of (Marčenko and Pastur, 1967; Silverstein and Bai, 1995), for any $z \in \mathbb{C}^+$, $m(z)$ and $\tilde{m}(z)$ are the unique roots in $\{m \in \mathbb{C} : \gamma m + (1 - \gamma)(-1/z) \in \mathbb{C}^+\}$ and $\mathbb{C}^+$, respectively, to the *Marcenko-Pastur equations*

$$m(z) = \int \frac{1}{\lambda(1 - \gamma - \gamma z m(z)) - z} d\nu(\lambda), \quad z = -\frac{1}{\tilde{m}(z)} + \gamma \int \frac{\lambda}{1 + \lambda \tilde{m}(z)} d\nu(\lambda). \tag{A.2}$$

We define $m(z), \tilde{m}(z)$ via (A.1) also on the full domains $\mathbb{C} \setminus \operatorname{supp}(\mu)$ and $\mathbb{C} \setminus \operatorname{supp}(\tilde{\mu})$ respectively, where the support sets $\operatorname{supp}(\mu)$ and $\operatorname{supp}(\tilde{\mu})$ may differ only at the single point $\{0\}$.

In the setting $\boldsymbol{\Sigma} = \boldsymbol{I}$ (and $\nu = \delta_1$), the law $\mu = \rho_\gamma^{\mathrm{MP}}$ is the standard Marcenko-Pastur law, with explicit density function with respect to Lebesgue measure

$$d\rho_\gamma^{\mathrm{MP}}(\lambda) = \frac{1}{2\pi}\frac{\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}}{\gamma\lambda} \cdot \mathbf{1}_{\lambda\in[\lambda_-,\lambda_+]}\, d\lambda, \qquad \lambda_\pm := (1 \pm \sqrt{\gamma})^2$$

for $\gamma \leq 1$, and an additional point mass $(1 - 1/\gamma)$ at 0 when $\gamma > 1$.

In general, μ and $\tilde{\mu}$ do not have analytically explicit densities. However, $\mathrm{supp}(\tilde{\mu})$ is explicitly characterized in Silverstein and Choi (1995), and we review this characterization here: Define

$$\mathcal{T} = \{0\} \cup \{-1/\lambda : \lambda \in \mathrm{supp}(\nu)\}. \tag{A.3}$$

For $\tilde{m} \in \mathbb{C} \setminus \mathcal{T}$, define

$$z(\tilde{m}) = -\frac{1}{\tilde{m}} + \gamma \int \frac{\lambda}{1 + \lambda\tilde{m}} d\nu(\lambda). \tag{A.4}$$

In light of the second equation of (A.2), this may be understood as a formal inverse of $\tilde{m}(z)$. From (Silverstein and Choi, 1995, Theorems 4.1 and 4.2), we have the following properties.

Proposition 9 *$\tilde{m}(\cdot)$ defines a bijection from $\{z \in \mathbb{R} \setminus \mathrm{supp}(\tilde{\mu})\}$ to $\{\tilde{m} \in \mathbb{R} \setminus \mathcal{T} : z'(\tilde{m}) > 0\}$, whose inverse function is $z(\cdot)$. In particular, $x \in \mathbb{R}$ does not belong to $\mathrm{supp}(\tilde{\mu})$ if and only if there exists $\tilde{m} \in \mathbb{R} \setminus \mathcal{T}$ such that $z'(\tilde{m}) > 0$ and $z(\tilde{m}) = x$.*

A.3. Additional notation

For a probability measure μ, its support is the closed set

$$\mathrm{supp}(\mu) = \{x \in \mathbb{R} : \mu(O) > 0 \text{ for any open neighborhood } O \ni x\}.$$

We write $\mathrm{dist}(x, A) = \inf\{|x - y| : y \in A\}$ and define the ε-neighborhood

$$\mathrm{supp}(\mu) + (-\varepsilon, \varepsilon) = \{x \in \mathbb{R} : \mathrm{dist}(x, \mathrm{supp}(\mu)) < \varepsilon\}.$$

We write δ_x for the probability measure given by a point mass at $x \in \mathbb{R}$, $a\mu_0 + (1 - a)\mu_1$ for the convex combination of μ_0, μ_1, and $a \otimes \mu \oplus b$ for the law of $a\mathsf{x} + b$ when $\mathsf{x} \sim \mu$.

For vectors, $\|\boldsymbol{v}\| \equiv \|\boldsymbol{v}\|_2$ is the Euclidean norm. For matrices, $\|\boldsymbol{M}\|$ is the operator norm $\sup_{\boldsymbol{v}:\|\boldsymbol{v}\|=1} \|\boldsymbol{M}\boldsymbol{v}\|$, $\|\boldsymbol{M}\|_F$ is the Frobenius norm $(\mathrm{Tr}\, \boldsymbol{M}^\top \boldsymbol{M})^{1/2}$, Tr is the (unnormalized) matrix trace, and $\boldsymbol{A} \odot \boldsymbol{B}$ is the entrywise (Hadamard) product. We write $\mathrm{diag}(\boldsymbol{v})$ for the diagonal matrix with vector $\boldsymbol{v}$ along the main diagonal, and $\boldsymbol{I}_n$ for the $n \times n$ identity matrix.

Appendix B. Results for the nonlinear spiked covariance model

B.1. Deterministic equivalent for the resolvent

We consider the sample covariance and Gram matrix

$$\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G} \in \mathbb{R}^{n\times n}, \quad \widetilde{\boldsymbol{K}} = \boldsymbol{G}\boldsymbol{G}^\top \in \mathbb{R}^{N\times N}, \quad \text{where} \quad \boldsymbol{G} = \frac{1}{\sqrt{N}}[\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N]^\top \in \mathbb{R}^{N\times n}.$$

The following are our basic assumptions, where we recall that $\mathbf{1}\{\mathcal{E}\} \prec 0$ means $\mathbb{P}[\mathcal{E}] \leq N^{-D}$ for any fixed $D > 0$ and all large N.

Assumption 5 *The rows of $\boldsymbol{G}$ are independent and satisfy $\mathbb{E}[\boldsymbol{g}_i] = \boldsymbol{0}$ and $\mathbb{E}[\boldsymbol{g}_i \boldsymbol{g}_i^\top] = \boldsymbol{\Sigma}$ for all $i \in [N]$, such that:*

(a) There exist constants $C, c > 0$ such that $c < n/N < C$ and $\|\boldsymbol{\Sigma}\| < C$.

(b) There exists a constant $B > 0$ such that $\mathbf{1}\{\|\boldsymbol{K}\| > B\} \prec 0$.

(c) Uniformly over deterministic matrices $\boldsymbol{A} \in \mathbb{C}^{n \times n}$ and over $i \neq j \in [N]$,

$$\boldsymbol{g}_i^\top \boldsymbol{A} \boldsymbol{g}_i - \mathbb{E}[\boldsymbol{g}_i^\top \boldsymbol{A} \boldsymbol{g}_i] \prec \|\boldsymbol{A}\|_F, \qquad \boldsymbol{g}_i^\top \boldsymbol{A} \boldsymbol{g}_j \prec \|\boldsymbol{A}\|_F.$$

(d) For any integer $\alpha > 0$, there exists a constant $C = C(\alpha) > 0$ such that $\mathbb{E}[\|\boldsymbol{g}_i\|^\alpha] \leq N^C$.

Denote the finite-N dimension ratio and empirical eigenvalue distribution of $\boldsymbol{\Sigma}$ by

$$\gamma_N = \frac{n}{N}, \qquad \nu_N = \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\boldsymbol{\Sigma})}. \tag{B.1}$$

Let

$$\mu_N = \rho_{\gamma_N}^{\text{MP}} \boxtimes \nu_N, \qquad \tilde{\mu}_N = \gamma_N \mu_N + (1 - \gamma_N) \delta_0.$$

Denote the Stieltjes transforms of $\mu_N, \tilde{\mu}_N$ by $m_N(z), \tilde{m}_N(z)$. These are characterized exactly as in (A.2) with (γ_N, ν_N) in place of (γ, ν).

We first establish that with high probability, $\boldsymbol{K}$ and $\widetilde{\boldsymbol{K}}$ have no outlier eigenvalues far from the support set

$$\mathcal{S}_N = \operatorname{supp}(\mu_N) \cup \{0\} = \operatorname{supp}(\tilde{\mu}_N) \cup \{0\}. \tag{B.2}$$

Theorem 10 *Suppose Assumption 5 holds. Then for any fixed $\varepsilon > 0$,*

$$\mathbf{1}\Big\{\boldsymbol{K} \textit{ has an eigenvalue outside } \mathcal{S}_N + (-\varepsilon, \varepsilon)\Big\} \prec 0.$$

In asymptotic settings where $\nu_N \to \nu$ and $\mu_N \to \mu$ weakly and $\boldsymbol{\Sigma}$ has no spike eigenvalues, this set $\mathcal{S}_N$ will converge to $\mathcal{S} := \operatorname{supp}(\mu) \cup \{0\}$. In general, $\mathcal{S}_N$ may contain intervals around spike eigenvalues of $\boldsymbol{K}$ that are separated from $\operatorname{supp}(\mu) \cup \{0\}$ if $\boldsymbol{\Sigma}$ has a spiked structure, and this will be clarified in the subsequent section.

Next, we establish a deterministic equivalent approximation for the resolvent of $\boldsymbol{K}$, for spectral arguments separated from this support set $\mathcal{S}_N$. Let us denote by

$$\boldsymbol{R}(z) = (\boldsymbol{K} - z\boldsymbol{I})^{-1}, \qquad m_{\boldsymbol{K}}(z) = \frac{1}{n} \operatorname{Tr} \boldsymbol{R}(z)$$

the resolvent and Stieltjes transform of $\boldsymbol{K}$ for $z \notin \operatorname{supp}(\mu_N)$. For any $\varepsilon > 0$, define the domain

$$U_N(\varepsilon) = \Big\{z \in \mathbb{C} : \, |z| \leq \varepsilon^{-1}, \operatorname{dist}(z, \mathcal{S}_N) \geq \varepsilon\Big\}. \tag{B.3}$$

Theorem 11 *Suppose Assumption 5 holds. Then for any fixed $\varepsilon > 0$, uniformly over $z \in U_N(\varepsilon)$ and over deterministic matrices $\boldsymbol{A} \in \mathbb{C}^{n \times n}$, we have*

$$m_{\boldsymbol{K}}(z) - m_N(z) \prec \frac{1}{N}, \qquad \operatorname{Tr}\Big[\boldsymbol{R}(z)\boldsymbol{A} - (-z\tilde{m}_N(z)\boldsymbol{\Sigma} - z\boldsymbol{I})^{-1}\boldsymbol{A}\Big] \prec \frac{1}{\sqrt{N}} \|\boldsymbol{A}\|_F.$$

For spectral arguments $z \in \mathbb{C} \setminus \mathbb{R}_+$ separated from the positive real line, such a result has been shown recently in Chouard (2022); Schröder et al. (2023) (using different proof techniques). We use Theorem 10 as an input to establish this approximation also for spectral arguments in $\mathbb{R}_+ \setminus \mathcal{S}_N$, as such a result (and its extension to a generalized resolvent) is needed for our analysis of spiked eigenstructure to follow.

B.2. Spike eigenvalues and eigenvectors

Now we consider an asymptotic setting with a specific spiked structure for the population covariance matrix $\mathbf{\Sigma}$, having a fixed number of spikes outside the support of the weak limit of its spectral law. This assumption is summarized as follows.

Assumption 6 *$\mathbf{\Sigma}$ has eigenvalues $\lambda_1(\mathbf{\Sigma}), \ldots, \lambda_n(\mathbf{\Sigma})$ (not necessarily ordered by magnitude) where, for a fixed integer $r \geq 0$, as $N \to \infty$:*

(a) $n/N \to \gamma \in (0, \infty)$.

(b) There exists a probability measure ν with compact support in $(0, \infty)$, such that

$$\frac{1}{n-r} \sum_{i=r+1}^{n} \delta_{\lambda_i(\mathbf{\Sigma})} \to \nu \text{ weakly.}$$

Furthermore, for any fixed $\varepsilon > 0$ and all large N,

$$\lambda_i(\mathbf{\Sigma}) \in \operatorname{supp}(\nu) + (-\varepsilon, \varepsilon) \text{ for all } i \geq r+1.$$

(c) There exist distinct values $\lambda_1, \ldots, \lambda_r > 0$ with $\lambda_1, \ldots, \lambda_r \notin \operatorname{supp}(\nu)$ such that

$$\lambda_i(\mathbf{\Sigma}) \to \lambda_i \text{ for all } i = 1, \ldots, r.$$

Under this assumption, we analyze the outlier singular values of $\boldsymbol{G}$ and their corresponding singular vectors. Let

$$\gamma_{N,0} = \frac{n-r}{N}, \qquad \nu_{N,0} = \frac{1}{n-r} \sum_{i=r+1}^{n} \delta_{\lambda_i(\mathbf{\Sigma})}$$

be the finite-N aspect ratio and population spectral measure corresponding to the bulk component of $\mathbf{\Sigma}$. Define the laws

$$\mu_{N,0} = \rho^{\text{MP}}_{\gamma_{N,0}} \boxtimes \nu_{N,0}, \qquad \tilde{\mu}_{N,0} = \gamma_{N,0}\mu_{N,0} + (1-\gamma_{N,0})\delta_0$$

and let $m_{N,0}(z), \tilde{m}_{N,0}(z)$ be their Stieltjes transforms. In the setting of Assumption 6, we note that $\mu_{N,0} \to \mu = \rho^{\text{MP}}_{\gamma} \boxtimes \nu$ and $\tilde{\mu}_{N,0} \to \tilde{\mu} = \gamma\mu + (1-\gamma)\delta_0$ weakly as $N \to \infty$, where the Stieltjes transforms $m(z), \tilde{m}(z)$ of these limits $\mu, \tilde{\mu}$ are characterized by (A.2).

Denote the limit support set

$$\mathcal{S} = \operatorname{supp}(\mu) \cup \{0\} = \operatorname{supp}(\tilde{\mu}) \cup \{0\}. \tag{B.4}$$

Under Assumption 6 when $r = 0$, i.e. $\mathbf{\Sigma}$ does not have spike eigenvalues, the following is a corollary of Theorem 10. A similar "no outlier" statement has been shown for linearly defined sample covariance models in (Bai and Silverstein, 1998).

Corollary 12 *Suppose Assumptions 5 and 6 hold, where $r = 0$. Then for any fixed $\varepsilon > 0$,*

$$\mathbf{1}\Big\{\boldsymbol{K} \text{ has an eigenvalue outside } \mathcal{S} + (-\varepsilon, \varepsilon)\Big\} \prec 0.$$

We now give a more quantitative version of Theorem 7 stated informally in Section 3, which describes the spike eigenvalues of $\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G}$ and corresponding singular vectors of $\boldsymbol{G}$ when there are possibly spike eigenvalues in $\boldsymbol{\Sigma}$. Define the domain

$$\mathcal{T}_{N,0} = \{0\} \cup \{-1/\lambda : \lambda \in \operatorname{supp}(\nu_{N,0})\}.$$

For $\tilde{m} \in \mathbb{C} \setminus \mathcal{T}_{N,0}$, define the functions

$$z_{N,0}(\tilde{m}) = -\frac{1}{\tilde{m}} + \gamma_{N,0} \int \frac{\lambda}{1 + \lambda \tilde{m}} d\nu_{N,0}(\lambda), \qquad \varphi_{N,0}(\tilde{m}) = -\frac{\tilde{m} z'_{N,0}(\tilde{m})}{z_{N,0}(\tilde{m})}. \tag{B.5}$$

We note that under Assumption 6, the domain $\mathcal{T}_{N,0}$ converges in Hausdorff distance to $\mathcal{T}$ as defined in (A.3). We will verify in the proof (c.f. Lemma 24) that $z_{N,0}(\tilde{m}) \to z(\tilde{m})$ and $z'_{N,0}(\tilde{m}) \to z'(\tilde{m})$ for each fixed $\tilde{m} \in \mathbb{C} \setminus \mathcal{T}$, where $z(\cdot)$ is as defined in (A.4). Then also $\varphi_{N,0}(\tilde{m}) \to \varphi(\tilde{m})$ for the limiting function

$$\varphi(\tilde{m}) = -\frac{\tilde{m} z'(\tilde{m})}{z(\tilde{m})}. \tag{B.6}$$

Theorem 13 *Suppose Assumptions 5 and 6 hold. Let*

$$\mathcal{I} = \big\{i \in \{1, \ldots, r\} : z'(-1/\lambda_i) > 0\big\}.$$

(a) For any sufficiently small constant $\varepsilon > 0$ and all large N, on an event $\mathcal{E} \equiv \mathcal{E}_N$ satisfying $\mathbf{1}\{\mathcal{E}^c\} \prec 0$, there is a 1-to-1 correspondence between the eigenvalues of $\boldsymbol{K}$ outside $\mathcal{S} + (-\varepsilon, \varepsilon)$ and $\{\lambda_i : i \in \mathcal{I}\}$. Denoting these eigenvalues of $\boldsymbol{K}$ by $\{\widehat{\lambda}_i : i \in \mathcal{I}\}$, we have

$$\widehat{\lambda}_i - z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) = O_\prec^{\mathcal{E}}\Big(\frac{1}{\sqrt{N}}\Big)$$

for each $i \in \mathcal{I}$, where $z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) \to z(-1/\lambda_i) > 0$ as $N \to \infty$.

(b) On this event $\mathcal{E}$, for each $i \in \mathcal{I}$, let $\widehat{\boldsymbol{v}}_i \in \mathbb{R}^n$ be a unit-norm eigenvector of $\boldsymbol{K}$ (i.e. right singular vector of $\boldsymbol{G}$) corresponding to its eigenvalue $\widehat{\lambda}_i$, and let $\boldsymbol{v}_i$ be a unit-norm eigenvector of $\boldsymbol{\Sigma}$ corresponding to $\lambda_i(\boldsymbol{\Sigma})$. Then, uniformly over (deterministic) unit vectors $\boldsymbol{v} \in \mathbb{R}^n$,

$$|\boldsymbol{v}^\top \widehat{\boldsymbol{v}}_i| - \sqrt{\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))} \cdot |\boldsymbol{v}^\top \boldsymbol{v}_i| = O_\prec^{\mathcal{E}}\Big(\frac{1}{\sqrt{N}}\Big) \tag{B.7}$$

where $\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) \to \varphi(-1/\lambda_i) > 0$ as $N \to \infty$. In particular, for each $i \in \mathcal{I}$, $|\boldsymbol{v}_i^\top \widehat{\boldsymbol{v}}_i|^2 \to \varphi(-1/\lambda_i)$ and $\sup_{j \in [n]: j \neq i} |\boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i|^2 \to 0$ almost surely as $N \to \infty$.

(c) Let $\boldsymbol{u} = \frac{1}{\sqrt{N}}(u_1, \ldots, u_N)^\top \in \mathbb{R}^N$ be a random vector such that $[\boldsymbol{u}, \boldsymbol{G}] \in \mathbb{R}^{N \times (n+1)}$ has independent rows also satisfying Assumption 5. Denote by $\mathbb{E}[u\boldsymbol{g}] \in \mathbb{R}^n$ the common value of $\mathbb{E}[u_j \boldsymbol{g}_j]$ for all $j \in [N]$.

On this event $\mathcal{E}$, for each $i \in \mathcal{I}$, let $\widehat{\boldsymbol{u}}_i \in \mathbb{R}^N$ be a unit-norm eigenvector of $\widetilde{\boldsymbol{K}}$ (i.e. left singular vector of $\boldsymbol{G}$) corresponding to its eigenvalue $\widehat{\lambda}_i$, and let $\boldsymbol{v}_i$ be the eigenvector of $\boldsymbol{\Sigma}$ as in part (b). Then

$$|\boldsymbol{u}^\top \widehat{\boldsymbol{u}}_i| - \frac{\sqrt{z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))}}{\lambda_i(\boldsymbol{\Sigma})} \cdot \Big|\mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{v}_i\Big| = O_\prec^{\mathcal{E}}\Big(\frac{1}{\sqrt{N}}\Big). \tag{B.8}$$

Appendix C. Analysis of the resolvent

We prove the results of Appendix B.1. Appendix C.1 first develops a fluctuation averaging lemma for the sample covariance model. Appendix C.2 applies this lemma within the arguments of Bai and Silverstein (1998), to prove the "no outliers" result of Theorem 10. Appendix C.3 uses Theorem 10 and a second application of the fluctuation averaging lemma to prove the deterministic equivalent approximation of Theorem 11.

C.1. Fluctuation averaging lemma

Recall the definitions

$$\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G}, \qquad \widetilde{\boldsymbol{K}} = \boldsymbol{G}\boldsymbol{G}^\top.$$

For $S \subset [N]$, let $\boldsymbol{G}^{(S)} \in \mathbb{R}^{(N-|S|)\times n}$ be the matrix obtained by removing the rows of $\boldsymbol{G}$ corresponding to $i \in S$, and define

$$\boldsymbol{K}^{(S)} = \boldsymbol{G}^{(S)\top}\boldsymbol{G}^{(S)} = \frac{1}{N}\sum_{i\in[N]\setminus S} \boldsymbol{g}_i\boldsymbol{g}_i^\top \in \mathbb{R}^{n\times n}.$$

Then, for $\boldsymbol{\Gamma} \in \mathbb{C}^{n\times n}$, define

$$\begin{aligned} \boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) = (\boldsymbol{K}^{(S)} - \boldsymbol{\Gamma})^{-1}, \qquad m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) = \frac{1}{n}\operatorname{Tr}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}), \\ \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) = \gamma_N m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) + (1-\gamma_N)\left(-\frac{1}{z}\right) = \frac{1}{N}\operatorname{Tr}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) + \left(1-\frac{n}{N}\right)\left(-\frac{1}{z}\right). \end{aligned} \tag{C.1}$$

Importantly, these quantities are independent of $\{\boldsymbol{g}_i : i \in S\}$. We say that $\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})$ exists (and hence also $m_{\boldsymbol{K}}^{(S)}, \tilde{m}_{\boldsymbol{K}}^{(S)}$ exist) when $\boldsymbol{K}^{(S)} - \boldsymbol{\Gamma}$ is invertible. For simplicity, we write $\boldsymbol{R} = \boldsymbol{R}^{\emptyset}$, $\boldsymbol{R}^{(i)} = \boldsymbol{R}^{(\{i\})}$, $\boldsymbol{R}^{(Si)} = \boldsymbol{R}^{(S\cup\{i\})}$, and similarly for $m_{\boldsymbol{K}}$ and $\tilde{m}_{\boldsymbol{K}}$.

Lemma 14 *Suppose Assumption 5 holds. Suppose also that there are constants $C_0, c_0, \delta, \upsilon > 0$, N-dependent domains $U \subset \mathbb{C}\setminus\{0\}$ and $\mathcal{D}_\Gamma, \mathcal{D}_A \subseteq \mathbb{C}^{n\times n}$, and N-dependent maps $\Phi_N : \mathcal{D}_\Gamma \times \mathcal{D}_A \to (N^{-\upsilon}, N^{\upsilon})$ and $\Psi_N : \mathcal{D}_\Gamma \to (N^{-\upsilon}, N^{1-\delta})$, such that for any fixed $L \geq 1$, the events*

$$\begin{aligned} \mathcal{E}(z,\boldsymbol{\Gamma},\boldsymbol{A},S) = \Big\{ &\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) \text{ exists, } \|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{A}\|_F \leq \Phi_N(\boldsymbol{\Gamma},\boldsymbol{A}),\ \|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\|_F \leq \Psi_N(\boldsymbol{\Gamma}), \\ &\|(z^{-1}\boldsymbol{\Gamma} + \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\| \leq C_0, \text{ and } |1 + N^{-1}\boldsymbol{g}_j^\top \boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{g}_j| \geq c_0 \text{ for all } j \in S \Big\} \end{aligned} \tag{C.2}$$

satisfy $\mathbf{1}\{\mathcal{E}(z,\boldsymbol{\Gamma},\boldsymbol{A},S)^c\} \prec 0$ uniformly over $z \in U$, $\boldsymbol{\Gamma} \in \mathcal{D}_\Gamma$, $\boldsymbol{A} \in \mathcal{D}_A$, and $S \subset [N]$ with $|S| \leq L$.

Then, denoting by $\mathbb{E}_{\boldsymbol{g}_i}$ the partial expectation over only $\boldsymbol{g}_i$ (i.e. conditional on $\{\boldsymbol{g}_j\}_{j\neq i}$), also uniformly over $z \in U$, $\boldsymbol{\Gamma} \in \mathcal{D}_\Gamma$, and $\boldsymbol{A} \in \mathcal{D}_A$,

$$\frac{1}{N}\sum_{i=1}^N (1-\mathbb{E}_{\boldsymbol{g}_i})\big[\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + \tilde{m}_{\boldsymbol{K}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i\big] \prec \max\left(\frac{\Psi_N(\boldsymbol{\Gamma})}{N}, \frac{1}{\sqrt{N}}\right)\cdot \Phi_N(\boldsymbol{\Gamma},\boldsymbol{A}). \tag{C.3}$$

We remark that applying Assumption 5(c) and the conditions of $\mathcal{E}(z, \mathbf{\Gamma}, \boldsymbol{A}, i)$ separately to each summand of the left side of (C.3) gives the naive bound

$$\frac{1}{N}\sum_{i=1}^{N}(1-\mathbb{E}_{\boldsymbol{g}_i})[\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\mathbf{\Gamma})\boldsymbol{A}(z^{-1}\mathbf{\Gamma}+\tilde{m}_{\boldsymbol{K}}^{(i)}(\mathbf{\Gamma})\mathbf{\Sigma})^{-1}\boldsymbol{g}_i]$$
$$\prec \max_{i=1}^{N}\|\boldsymbol{R}^{(i)}(\mathbf{\Gamma})\boldsymbol{A}\|_F \cdot \|(z^{-1}\mathbf{\Gamma}+\tilde{m}_{\boldsymbol{K}}^{(i)}(\mathbf{\Gamma})\mathbf{\Sigma})^{-1}\| \prec \Phi_N(\mathbf{\Gamma}, \boldsymbol{A}).$$

The content of the lemma is to improve this by the additional factor of $\max(\frac{\Psi_N(\mathbf{\Gamma})}{N}, \frac{1}{\sqrt{N}}) \ll 1$.

In this work, we will apply Lemma 14 only to spectral arguments z with $O(1)$-separation from $\operatorname{supp}(\mu_N)$ (and matrices $\mathbf{\Gamma} = z\boldsymbol{I}$ or a finite-rank perturbation thereof), in which case we will take $\Psi_N(\mathbf{\Gamma}) = C/\sqrt{N}$ for a constant $C > 0$. For full-rank matrices $\boldsymbol{A}$ having bounded operator norm, we will also take $\Phi_N(\mathbf{\Gamma}, \boldsymbol{A}) = C/\sqrt{N}$, whereas for finite-rank matrices $\boldsymbol{A}$ we will take $\Phi_N(\mathbf{\Gamma}, \boldsymbol{A}) = C$. We state the result here more abstractly, as it may be of independent interest to prove local laws in this nonlinear sample covariance model for spectral arguments z that approach $\operatorname{supp}(\mu_N)$.

In the remainder of this section, we prove Lemma 14. Fix $z \in U$, $\mathbf{\Gamma} \in \mathcal{D}_\Gamma$, and $\boldsymbol{A} \in \mathcal{D}_A$, and write as shorthand

$$\boldsymbol{R}^{(S)} = \boldsymbol{R}^{(S)}(\mathbf{\Gamma}), \qquad \tilde{m}^{(S)} = \tilde{m}_{\boldsymbol{K}}^{(S)}(\mathbf{\Gamma}), \qquad \mathbf{\Omega}^{(S)} = (z^{-1}\mathbf{\Gamma} + \tilde{m}_{\boldsymbol{K}}^{(S)}(\mathbf{\Gamma})\mathbf{\Sigma})^{-1},$$
$$\Phi_N = \Phi_N(\mathbf{\Gamma}, \boldsymbol{A}), \qquad \Psi_N = \Psi_N(\mathbf{\Gamma}), \qquad \mathcal{E}(S) = \mathcal{E}(z, \mathbf{\Gamma}, \boldsymbol{A}, S).$$

All subsequent instances of $\prec$ will be implicitly uniform over $z \in U$, $\mathbf{\Gamma} \in \mathcal{D}_\Gamma$, and $\boldsymbol{A} \in \mathcal{D}_A$. Define the quantities, for $i \in S$, $j, k \in S \setminus \{i\}$, and $d \geq 0$,

$$\begin{aligned}
Y_i^{(S)}[d] &= \operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \mathbf{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{A}\mathbf{\Omega}^{(S)}[\mathbf{\Sigma}\mathbf{\Omega}^{(S)}]^d,\\
Z_{ijk}^{(S)}[d] &= N^{-1}\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \mathbf{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{g}_j\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\mathbf{\Omega}^{(S)}[\mathbf{\Sigma}\mathbf{\Omega}^{(S)}]^d,\\
B_{jk}^{(S)} &= N^{-1}\boldsymbol{g}_j^\top\boldsymbol{R}^{(S)}\boldsymbol{g}_k,\\
C_{jk}^{(S)} &= N^{-2}\boldsymbol{g}_j^\top(\boldsymbol{R}^{(S)})^2\boldsymbol{g}_k,\\
Q_j^{(S)} &= (1 + N^{-1}\boldsymbol{g}_j^\top\boldsymbol{R}^{(S)}\boldsymbol{g}_j)^{-1}.
\end{aligned}$$

For each $L \geq 1$, define also the event

$$\mathcal{E}_L = \bigcap_{S \subset [N]: |S| \leq L} \mathcal{E}(S). \tag{C.4}$$

Lemma 15 *For any fixed $L, D \geq 1$, uniformly over $S \subset [N]$ with $|S| \leq L$, and over $i \in S$ and $j, k \in S \setminus \{i\}$ and $d \leq D$,*

$$\begin{gathered}
Y_i^{(S)}[d] = O_\prec^{\mathcal{E}(S)}(\Phi_N), \quad Z_{ijk}^{(S)}[d] = O_\prec^{\mathcal{E}(S)}\big(N^{-1}\Psi_N\Phi_N\big),\\
B_{jk}^{(S)} = O_\prec^{\mathcal{E}(S)}\big(N^{-1}\Psi_N\big) \text{ for } j \neq k, \quad C_{jk}^{(S)} = O_\prec^{\mathcal{E}(S)}\big(N^{-2}\Psi_N^2\big), \quad Q_j^{(S)} = O_\prec^{\mathcal{E}(S)}(1).
\end{gathered} \tag{C.5}$$

Furthermore, for any $\alpha > 0$, there exists a constant $C = C(\alpha, L, D) > 0$ such that

$$\begin{gathered}
\mathbb{E}\big[|Y_i^{(S)}[d]|^\alpha \mathbf{1}\{\mathcal{E}(S)\}\big] < N^C, \quad \mathbb{E}\big[|Z_{ijk}^{(S)}[d]|^\alpha \mathbf{1}\{\mathcal{E}(S)\}\big] < N^C,\\
\mathbb{E}\big[|B_{jk}^{(S)}|^\alpha \mathbf{1}\{\mathcal{E}(S)\}\big] < N^C, \quad \mathbb{E}\big[|C_{jk}^{(S)}|^\alpha \mathbf{1}\{\mathcal{E}(S)\}\big] < N^C, \quad \mathbb{E}\big[|Q_j^{(S)}|^\alpha \mathbf{1}\{\mathcal{E}(S)\}\big] < N^C.
\end{gathered} \tag{C.6}$$

Proof. On the event $\mathcal{E}(S)$, we have by definition $Q_j^{(S)} \leq 1/c_0$, so the two statements for $Q_j^{(S)}$ hold immediately. The remaining statements of (C.6) follow easily from Holder's inequality, the moment bounds for $\|\boldsymbol{g}_i\|$ in Assumption 5(d), the bound $\|\boldsymbol{\Sigma}\| < C$ in Assumption 5(a), and the conditions $\|\boldsymbol{R}^{(S)}\boldsymbol{A}\| \leq \Phi_N \leq N^v$, $\|\boldsymbol{R}^{(S)}\|_F \leq \Psi_N \leq N$, and $\|\boldsymbol{\Omega}^{(S)}\| \leq C_0$ defining $\mathcal{E}(S)$.

For the bounds for $B_{jk}^{(S)}$ and $C_{jk}^{(S)}$ in (C.5), note that when $j \neq k$, Assumption 5(c) implies $B_{jk}^{(S)} \prec N^{-1}\|\boldsymbol{R}^{(S)}\|_F$ and $C_{jk}^{(S)} \prec N^{-2}\|(\boldsymbol{R}^{(S)})^2\|_F \leq N^{-2}\|\boldsymbol{R}^{(S)}\|_F^2$. When $j = k$, Assumption 5(c) implies also

$$
\begin{aligned}
C_{jj}^{(S)} &\prec N^{-2}|\operatorname{Tr}\boldsymbol{\Sigma}(\boldsymbol{R}^{(S)})^2| + N^{-2}\|(\boldsymbol{R}^{(S)})^2\|_F \\
&\leq N^{-2}\|\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}\|_F\|\boldsymbol{R}^{(S)}\|_F + N^{-2}\|\boldsymbol{R}^{(S)}\|_F^2 \leq N^{-2}(\|\boldsymbol{\Sigma}\|+1)\|\boldsymbol{R}^{(S)}\|_F^2.
\end{aligned}
$$

Then these bounds in (C.5) follow from the condition $\|\boldsymbol{R}^{(S)}\|_F \leq \Psi_N$ defining $\mathcal{E}(S)$.

Finally, for the bounds for $Y_i^{(S)}[d]$ and $Z_{ijk}^{(S)}[d]$ in (C.5), observe that for any matrix $\boldsymbol{A} \in \mathbb{C}^{n\times n}$ independent of $\boldsymbol{g}_i$, we have $\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{A} \prec \|\boldsymbol{A}\|_F$ by Assumption 5(c). Then $Y_i^{(S)}[d] \prec \|\boldsymbol{R}^{(S)}\boldsymbol{A}\boldsymbol{\Omega}^{(S)}[\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(S)}]^d\|_F \leq \|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F \cdot \|\boldsymbol{\Omega}^{(S)}\|^{d+1}\|\boldsymbol{\Sigma}\|^d$, so the bound for $Y_i^{(S)}[d]$ in (C.5) follows from the conditions $\|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F \leq \Phi_N$ and $\|\boldsymbol{\Omega}^{(S)}\| \leq C_0$ defining $\mathcal{E}(S)$. For $Z_{ijk}^{(S)}[d]$, similarly by Assumption 5(c),

$$
Z_{ijk}^{(S)} \prec N^{-1}\|\boldsymbol{R}^{(S)}\boldsymbol{g}_j\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\boldsymbol{\Omega}^{(S)}[\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(S)}]^d\|_F \leq N^{-1}\|\boldsymbol{R}^{(S)}\boldsymbol{g}_j\|\cdot\|\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\|\cdot\|\boldsymbol{\Omega}^{(S)}\|^{d+1}\|\boldsymbol{\Sigma}\|^d.
$$

Applying again Assumption 5(c), we have

$$
\|\boldsymbol{R}^{(S)}\boldsymbol{g}_j\|_2^2 = \boldsymbol{g}_j^\top(\boldsymbol{R}^{(S)})^*\boldsymbol{R}^{(S)}\boldsymbol{g}_j \prec |\operatorname{Tr}\boldsymbol{\Sigma}(\boldsymbol{R}^{(S)})^*\boldsymbol{R}^{(S)}| + \|(\boldsymbol{R}^{(S)})^*\boldsymbol{R}^{(S)}\|_F \prec \|\boldsymbol{R}^{(S)}\|_F^2
$$

and similarly $\|\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\|_2^2 \prec \|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F^2$. Then the bound for $Z_{ijk}^{(S)}[d]$ in (C.5) follows from the conditions $\|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F \leq \Phi_N$, $\|\boldsymbol{R}^{(S)}\|_F \leq \Psi_N$, and $\|\boldsymbol{\Omega}^{(S)}\| \leq C_0$ defining $\mathcal{E}(S)$. ■

Lemma 16 *Fix any $L, D \geq 1$. Then there exist coefficients $\alpha(d, d', D) \in \mathbb{R}$ such that the following holds: Uniformly over $S \subset [N]$ with $|S| \leq L-1$, and over $i \in S$, $j,k \in S \setminus \{i\}$, $l \in [N]\setminus S$, and $d \leq D$,*

$$
Y_i^{(S)}[d] = \sum_{d'=d}^{d+\lceil D/2\rceil} \alpha(d,d',D)\Big[C_{ll}^{(Sl)}Q_l^{(Sl)}\Big]^{d'-d}\Big(Y_i^{(Sl)}[d'] - Z_{ill}^{(Sl)}[d']Q_l^{(Sl)}\Big) + O_\prec^{\mathcal{E}_L}\big(N^{-D}\Psi_N^D\Phi_N\big) \tag{C.7}
$$

$$
\begin{aligned}
Z_{ijk}^{(S)}[d] = \sum_{d'=d}^{d+\lceil D/2\rceil} &\alpha(d,d',D)\Big[C_{ll}^{(Sl)}Q_l^{(Sl)}\Big]^{d'-d}\Big(Z_{ijk}^{(Sl)}[d'] - Z_{ilk}^{(Sl)}[d']B_{lj}^{(Sl)}Q_l^{(Sl)} \\
&- Z_{ijl}^{(Sl)}[d']B_{kl}^{(Sl)}Q_l^{(Sl)} + Z_{ill}^{(Sl)}[d']B_{lj}^{(Sl)}B_{kl}^{(Sl)}(Q_l^{(Sl)})^2\Big) + O_\prec^{\mathcal{E}_L}\big(N^{-D}\Psi_N^D\Phi_N\big), \qquad \text{(C.8)}
\end{aligned}
$$

$$
B_{jk}^{(S)} = B_{jk}^{(Sl)} - B_{jl}^{(Sl)}B_{lk}^{(Sl)}Q_l^{(Sl)}, \tag{C.9}
$$

$$
C_{jk}^{(S)} = C_{jk}^{(Sl)} - B_{jl}^{(Sl)}C_{lk}^{(Sl)}Q_l^{(Sl)} - C_{jl}^{(Sl)}B_{lk}^{(Sl)}Q_l^{(Sl)} + B_{jl}^{(Sl)}C_{ll}^{(Sl)}B_{lk}^{(Sl)}(Q_l^{(Sl)})^2, \tag{C.10}
$$

$$
Q_j^{(S)} = \sum_{d=1}^{\lceil D/2\rceil}\Big(Q_j^{(Sl)}\Big)^d\Big[(B_{jl}^{(Sl)})^2Q_l^{(Sl)}\Big]^{d-1} + O_\prec^{\mathcal{E}_L}\big(N^{-D}\Psi_N^D\big). \tag{C.11}
$$

Proof. By the Sherman-Morrison formula, on the event $\mathcal{E}_L$ where $\boldsymbol{R}^{(S)}$ and $\boldsymbol{R}^{(Sl)}$ both exist, we have

$$\boldsymbol{R}^{(S)} = \boldsymbol{R}^{(Sl)} - N^{-1}\boldsymbol{R}^{(Sl)}\boldsymbol{g}_l\boldsymbol{g}_l^\top \boldsymbol{R}^{(Sl)} \cdot Q_l^{(Sl)}. \tag{C.12}$$

Applying this to each copy of $\boldsymbol{R}^{(S)}$ defining $B_{jk}^{(S)}$ and $C_{jk}^{(S)}$ yields immediately (C.9) and (C.10), as well as the identities

$$\begin{aligned} z^{-1}\boldsymbol{\Gamma} + \tilde{m}^{(S)}\boldsymbol{\Sigma} &= z^{-1}\boldsymbol{\Gamma} + \Big(N^{-1}\operatorname{Tr}\boldsymbol{R}^{(S)} + (1-\gamma_N)(-1/z)\Big)\boldsymbol{\Sigma} \\ &= (z^{-1}\boldsymbol{\Gamma} + \tilde{m}^{(Sl)}\boldsymbol{\Sigma}) - C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}, \\ 1 + B_{jj}^{(S)} &= 1 + B_{jj}^{(Sl)} - (B_{jl}^{(Sl)})^2 Q_l^{(Sl)}. \end{aligned}$$

Taking inverses and applying the expansion

$$(\boldsymbol{A}-\boldsymbol{\Delta})^{-1} = \sum_{d=1}^{\lceil D/2\rceil} \boldsymbol{A}^{-1}(\boldsymbol{\Delta}\boldsymbol{A}^{-1})^{d-1} + (\boldsymbol{A}-\boldsymbol{\Delta})^{-1}(\boldsymbol{\Delta}\boldsymbol{A}^{-1})^{\lceil D/2\rceil},$$

we obtain

$$\boldsymbol{\Omega}^{(S)} = \sum_{d=1}^{\lceil D/2\rceil} \boldsymbol{\Omega}^{(Sl)}[C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d-1} + \boldsymbol{E}, \tag{C.13}$$

$$Q_j^{(S)} = \sum_{d=1}^{\lceil D/2\rceil} Q_j^{(Sl)}[(B_{jl}^{(Sl)})^2 Q_l^{(Sl)}Q_j^{(Sl)}]^{d-1} + e, \tag{C.14}$$

for remainder terms $\boldsymbol{E} \in \mathbb{C}^{n\times n}$ and $e \in \mathbb{C}$ satisfying, by the bounds of Lemma 15,

$$\|\boldsymbol{E}\| = O_\prec^{\mathcal{E}_L}\Big(|C_{ll}^{(Sl)}|^{D/2}\Big) = O_\prec^{\mathcal{E}_L}\big((N^{-1}\Psi)^D\big), \quad |e| = O_\prec^{\mathcal{E}_L}\Big(|(B_{jl}^{(Sl)})^2|^{D/2}\Big) = O_\prec^{\mathcal{E}_L}\big((N^{-1}\Psi)^D\big).$$

In particular, (C.14) shows (C.11). Applying (C.13) to the definitions of $Y_i^{(S)}[d]$ and $Z_{ijk}^{(S)}[d]$, we get

$$\begin{aligned} Y_i^{(S)}[d] = \operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{A}\left(\sum_{d'=1}^{\lceil D/2\rceil} \boldsymbol{\Omega}^{(Sl)}[C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d'-1} + \boldsymbol{E}\right) \\ \cdot\left(\boldsymbol{\Sigma}\left[\sum_{d'=1}^{\lceil D/2\rceil} \boldsymbol{\Omega}^{(Sl)}[C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d'-1} + \boldsymbol{E}\right]\right)^d, \\ Z_{ijk}^{(S)}[d] = \frac{1}{N}\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{g}_j\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\left(\sum_{d'=1}^{\lceil D/2\rceil} \boldsymbol{\Omega}^{(Sl)}[C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d'-1} + \boldsymbol{E}\right) \\ \cdot\left(\boldsymbol{\Sigma}\left[\sum_{d'=1}^{\lceil D/2\rceil} \boldsymbol{\Omega}^{(Sl)}[C_{ll}^{(Sl)}Q_l^{(Sl)}\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d'-1} + \boldsymbol{E}\right]\right)^d. \end{aligned}$$

For any matrix $\boldsymbol{B} \in \mathbb{C}^{n\times n}$ independent of $\boldsymbol{g}_i$, observe that $\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{A}\boldsymbol{B} = O_\prec^{\mathcal{E}(S)}(\Phi_N\|\boldsymbol{B}\|)$ and $\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{g}_j\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\boldsymbol{B} = O_\prec^{\mathcal{E}(S)}(\Psi_N\Phi_N\|\boldsymbol{B}\|)$ by the same arguments as those bounding $Y_i^{(S)}[d]$ and $Z_{ijk}^{(S)}[d]$ in the proof of Lemma 15. Then, expanding the above and absorbing all terms containing $\boldsymbol{E}$ and all terms with combined power of $C_{ll}^{(Sl)}$ larger than $D/2$ into $O_\prec^{\mathcal{E}(S)}\big(N^{-D}\Psi_N^D\Phi_N\big)$ remainders, we obtain for some coefficients $\alpha(d,d',D) \in \mathbb{R}$ that

$$\begin{aligned} Y_i^{(S)}[d] &= \operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{A}\sum_{d'=0}^{\lceil D/2\rceil}\alpha(d,d',D)[C_{ll}^{(Sl)}Q_l^{(Sl)}]^{d'}\boldsymbol{\Omega}^{(Sl)}[\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d+d'} \\ &\qquad + O_\prec^{\mathcal{E}(S)}\big(N^{-D}\Psi_N^D\Phi_N\big), \\ Z_{ijk}^{(S)}[d] &= \frac{1}{N}\operatorname{Tr}(\boldsymbol{g}_i\boldsymbol{g}_i^\top - \boldsymbol{\Sigma})\boldsymbol{R}^{(S)}\boldsymbol{g}_j\boldsymbol{g}_k^\top\boldsymbol{R}^{(S)}\boldsymbol{A}\sum_{d'=0}^{\lceil D/2\rceil}\alpha(d,d',D)[C_{ll}^{(Sl)}Q_l^{(Sl)}]^{d'}\boldsymbol{\Omega}^{(Sl)}[\boldsymbol{\Sigma}\boldsymbol{\Omega}^{(Sl)}]^{d+d'} \\ &\qquad + O_\prec^{\mathcal{E}(S)}\big(N^{-D}\Psi_N^D\Phi_N\big). \end{aligned}$$

Finally, applying the Sherman-Morrison formula (C.12) to expand each copy of $\boldsymbol{R}^{(S)}$, and re-indexing the summations by $d + d' \mapsto d'$, we get (C.7) and (C.8). ■

Lemma 17 *Fix any $L, D \geq 1$. Uniformly over $S \subset [N]$ with $|S| \leq L$ and over $i \in S$, the following holds: Denote $\bar{S} = S \setminus \{i\}$. Then there exists a collection of monomials $\mathcal{M}_{i,S}$ such that $Y_i^{(i)}[0]$ can be approximated as*

$$Y_i^{(i)}[0] = \sum_{q\in\mathcal{M}_{i,S}} q\bigg(\{Y_i^{(S)}[d]\}_{d\leq\lfloor D/2\rfloor}, \{Z_{ijk}^{(S)}[d]\}_{j,k\in\bar{S},d\leq\lfloor D/2\rfloor}, \{B_{jk}^{(S)}\}_{j\neq k\in\bar{S}}, \{C_{jk}^{(S)}\}_{j,k\in\bar{S}}, \{Q_j^{(S)}\}_{j\in\bar{S}}\bigg) + O_\prec^{\mathcal{E}_L}\big(N^{-D}\Psi_N^D\Phi_N\big). \quad \text{(C.15)}$$

Each monomial $q \in \mathcal{M}_{i,S}$ is a product of a real-valued scalar coefficient and one or more factors of the form $Y_i^{(S)}[d]$, $Z_{ijk}^{(S)}[d]$, $B_{jk}^{(S)}$ with $j \neq k$, $C_{jk}^{(S)}$, $Q_j^{(S)}$ for $j,k \in \bar{S}$ and $d \leq \lfloor D/2\rfloor$. We have $q = O_\prec^{\mathcal{E}_L}(\Phi_N)$ uniformly over $q \in \mathcal{M}_{i,S}$, and the number of monomials $|\mathcal{M}_{i,S}|$ is most a constant depending on L, D. Furthermore:

(a) There is exactly one factor of the form $Y_i^{(S)}[d]$ or $Z_{ijk}^{(S)}[d]$ appearing in q.

(b) The number of factors $Z_{ijk}^{(S)}[d]$, $B_{jk}^{(S)}$, and $C_{jk}^{(S)}$ appearing in q is no less than the number of distinct indices of $\bar{S}$ (not including i) that appear as lower indices across all factors of q.

Proof. We arbitrarily order the indices of $\bar{S} = S \setminus \{i\}$ as $l_1, l_2, \ldots, l_{|S|-1}$. Beginning with the monomial $Y_i^{(i)}[0]$, iteratively for $j = 1, 2, \ldots, |S| - 1$, we replace all factors with superscript $(il_1 \ldots l_{j-1})$ by a sum of terms with superscript $(il_1 \ldots l_j)$, using the recursions (C.7)–(C.11). It is then direct to check that this gives a representation of the form (C.15), where:

- Each application of (C.7)–(C.8) replaces a factor $Y_i^{(\ldots)}[d]$ or $Z_{ijk}^{(\ldots)}[d]$ by terms having exactly one such factor. Thus, each monomial $q \in \mathcal{M}_{i,S}$ has exactly one factor $Y_i^{(S)}[d]$ or $Z_{ijk}^{(S)}[d]$.

- The number of total applications of (C.7)–(C.11) is bounded by a constant depending on L, D, so $|\mathcal{M}_{i,S}|$ and the scalar coefficient of each $q \in \mathcal{M}_{i,S}$ are both bounded by constants depending on L, D. Then, by the bounds of (C.5), each $q \in \mathcal{M}_{i,S}$ satisfies $q = O_{\prec}^{\mathcal{E}_L}(\Phi_N)$, and the remainder in (C.15) is at most $O_{\prec}^{\mathcal{E}_L}\big(N^{-D}\Psi_N^D\Phi_N\big)$. If q has the term $Y_i^{(S)}[d]$ or $Z_i^{(S)}[d]$, then it also has combined power of $\{C_{jk}^{(S)}\}_{j,k\in\bar{S}}$ equal to d, and hence may be absorbed into the remainder of (C.15) if $d > D/2$.
- Each term on the right side of (C.7)–(C.11) that contains the new lower index l has at least one more factor of the form $Z_{ijk}^{(\dots)}[d]$, $B_{jk}^{(\dots)}$, or $C_{jk}^{(\dots)}$ than the left side. Thus, each monomial $q \in \mathcal{M}_{i,S}$ is such that the number of distinct lower indices of $\bar{S}$ across all of its factors is no greater than the number of its factors of the form $Z_{ijk}^{(\dots)}[d]$, $B_{jk}^{(\dots)}$, or $C_{jk}^{(\dots)}$.

Combining these observations yields the lemma. ■

Proof of Lemma 14. For each $\varepsilon, D > 0$, let us fix an even integer $L = L(\varepsilon, D) > D/\varepsilon$. The assumption of this lemma guarantees $\mathbf{1}\{\mathcal{E}(S)^c\} \prec 0$ uniformly over $S \subset [N]$ with $|S| \le L$. Since the number of such subsets is at most N^L, we may take a union bound (c.f. Proposition 8(a)) to obtain $\mathbf{1}\{\mathcal{E}_L^c\} \prec 0$ for the intersection event $\mathcal{E}_L$ of (C.4). Noting that $(1 - \mathbb{E}_{\boldsymbol{g}_i})[\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)} \boldsymbol{A}\boldsymbol{\Omega}\boldsymbol{g}_i] = Y_i^{(i)}[0]$, to prove the lemma, it suffices to show for any $\varepsilon, D > 0$ and all sufficiently large N that

$$\mathbb{P}\left[\left(\frac{1}{N}\sum_{i=1}^N Y_i^{(i)}[0]\right)\mathbf{1}\{\mathcal{E}_L\} > \max\left(\frac{\Psi_N}{N}, \frac{1}{\sqrt{N}}\right)\Phi_N \cdot N^\varepsilon\right] < N^{-D}. \tag{C.16}$$

In anticipation of applying Markov's inequality, we analyze

$$\mathbb{E}\left[\left(\sum_{i=1}^N Y_i^{(i)}[0]\right)^L \mathbf{1}\{\mathcal{E}_L\}\right] = \sum_{i_1,\dots,i_L=1}^N \underbrace{\mathbb{E}\left[\prod_{l=1}^L Y_{i_l}^{(i_l)}[0]\mathbf{1}\{\mathcal{E}_L\}\right]}_{:=\mathbb{E}[m(i_1,\dots,i_L)]}. \tag{C.17}$$

Fix any index tuple $(i_1, \dots, i_L)$. Letting $S = \{i_1, \dots, i_L\}$ be the set of distinct indices in this tuple, we apply Lemma 17 to each term $Y_{i_l}^{(i_l)}[0]$, with this set S and with $D = L$. This gives

$$m(i_1, \dots, i_L) = \sum_{q^{(1)}\in\mathcal{M}(i_1,S)} \cdots \sum_{q^{(l)}\in\mathcal{M}(i_l,S)} \prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\} + O_\prec\big((N^{-1}\Psi_N)^L \Phi_N^L\big), \tag{C.18}$$

where each $\mathcal{M}(i_l, S)$ is the collection of monomials arising in the approximation of $Y_{i_l}^{(i_l)}[0]$, and we have applied $q^{(l)} = O_\prec^{\mathcal{E}_L}(\Phi_N)$ to bound the remainder. Observe that by (C.6) and Holder's inequality, we have $\mathbb{E}[|m(i_1, \dots, i_L)|^2] \le N^C$ and $\mathbb{E}[|\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}|^2] \le N^C$ for all $q^{(1)}, \dots, q^{(L)}$ and a constant $C > 0$. By this and the given condition $\Psi_N, \Phi_N \ge N^{-\upsilon}$, we may take expectations in (C.18) using Proposition 8(d) to get

$$\mathbb{E}[m(i_1, \dots, i_L)] = \sum_{q^{(1)}\in\mathcal{M}(i_1,S)} \cdots \sum_{q^{(l)}\in\mathcal{M}(i_l,S)} \mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}\right] + O_\prec\big((N^{-1}\Psi_N)^L \Phi_N^L\big). \tag{C.19}$$

Now to bound $\mathbb{E}[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}]$, we consider separately two cases, focusing on those indices i_l which appear exactly once in $(i_1, \ldots, i_L)$. In the first case, suppose there is some such index i_l that does not appear as a lower index of $q^{(l')}$ for any $l' \neq l$. Fixing this set $S = \{i_1, \ldots, i_L\}$ and index $i_l \in S$, let us introduce

$$\mathcal{E}' = \Bigg\{ \boldsymbol{R}^{(S)} \text{ exists, } \|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F \leq \Phi_N,\ \|\boldsymbol{R}^{(S)}\|_F \leq \Psi_N,\ \|(z^{-1}\boldsymbol{\Gamma} + \tilde{m}^{(S)}\boldsymbol{\Sigma})^{-1}\| \leq C_0, \\ \text{and } |1 + N^{-1}\boldsymbol{g}_j^\top \boldsymbol{R}^{(S)}\boldsymbol{g}_j| \geq c_0 \text{ for all } j \in S \setminus \{i_l\} \Bigg\}.$$

Comparing with the definition of $\mathcal{E}(S)$ from (C.2), observe that only the last condition defining $\mathcal{E}'$ is different (where we do not require the bound for $j = i_l$), so that this event $\mathcal{E}'$ is independent of $\boldsymbol{g}_{i_l}$. Then $\mathcal{E}_L \subseteq \mathcal{E}(S) \subseteq \mathcal{E}'$, and

$$\mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}\right] = \mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}'\}\right] - \mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}'\}\mathbf{1}\{\mathcal{E}_L^c\}\right]. \tag{C.20}$$

For the first term of (C.20), observe that both $\{q^{(l')} : l' \neq l\}$ and $\mathcal{E}'$ are independent of $\boldsymbol{g}_{i_l}$, and only the one factor $Y_{i_l}^{(S)}[d]$ or $Z_{i_l jk}^{(S)}[d]$ in $q^{(l)}$ depends on $\boldsymbol{g}_{i_l}$. Then, noting that $\mathbb{E}_{\boldsymbol{g}_i}[Y_i^{(S)}[d]] = 0$ and $\mathbb{E}_{\boldsymbol{g}_i}[Z_{ijk}^{(S)}[d]] = 0$, the first term of (C.20) is 0. For the second term of (C.20), observe that all statements of (C.6) continue to hold with $\mathcal{E}(S)$ replaced by $\mathcal{E}'$, except for the bound on $Q_{i_l}^{(S)}$. But $Q_{i_l}^{(S)}$ appears neither in $\{q^{(l')} : l' \neq l\}$ nor in $q^{(l)}$, so we may apply Holder's inequality to get $\mathbb{E}[|\prod_{l=1}^L q^{(l)}|^2 \mathbf{1}\{\mathcal{E}'\}] \leq N^C$ for a constant $C > 0$. Then, applying Cauchy-Schwarz and $\mathbf{1}\{\mathcal{E}_L^c\} \prec 0$, the second term of (C.20) is bounded by $N^{-D'}$ for any fixed constant $D' > 0$ and all large N. Thus,

$$\mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}\right] \leq N^{-D'}. \tag{C.21}$$

In the second case, every index i_l that appears exactly once in $(i_1, \ldots, i_L)$ appears as a lower index of $q^{(l')}$ for some $l' \neq l$. Call the number of such indices K. Then condition (b) of Lemma 17 implies that the total number of factors of the forms $Z_{ijk}^{(S)}[d]$, $B_{jk}^{(S)}$ for $j \neq k$, and $C_{jk}^{(S)}$ across all monomials $q^{(1)}, \ldots, q^{(L)}$ is at least K. Then, by the bounds of Lemma 15 and Proposition 8(d), we have

$$\mathbb{E}\left[\prod_{l=1}^L q^{(l)} \cdot \mathbf{1}\{\mathcal{E}_L\}\right] \prec (N^{-1}\Psi_N)^K \Phi_N^L. \tag{C.22}$$

Under the given condition $\Phi_N, \Psi_N \geq N^{-\upsilon}$, we have $N^{-D'} \leq (N^{-1}\Psi_N)^K \Phi_N^L$ for large enough D'. Then, combining the two cases (C.21) and (C.22) and applying this back to (C.19), we get

$$\mathbb{E}[m(i_1, \ldots, i_L)] \prec (N^{-1}\Psi_N)^K \Phi_N^L \tag{C.23}$$

where K is the number of indices in $S = \{i_1, \ldots, i_L\}$ that appear exactly once in $(i_1, \ldots, i_L)$. Let J be the number of distinct indices in $S = \{i_1, \ldots, i_L\}$ that appear at least twice in $(i_1, \ldots, i_L)$.

Then $2J + K \leq L$, and the number of index tuples $(i_1, \ldots, i_L) \in [N]^L$ with these values of (J, K) is at most CN^{J+K}, for a constant $C = C(J, K) > 0$. Then, applying (C.23) back to (C.17) yields

$$\mathbb{E}\left[\left(\sum_{i=1}^{N} Y_i^{(i)}[0]\right)^L \mathbf{1}\{\mathcal{E}_L\}\right] \prec \max_{J,K \geq 0:\, 2J+K \leq L} N^{J+K} \cdot (N^{-1}\Psi_N)^K \Phi_N^L$$

$$= \max_{J,K \geq 0:\, 2J+K \leq L} (\sqrt{N})^{2J} \Psi_N^K \Phi_N^L \leq \max(\Psi_N, \sqrt{N})^L \Phi_N^L.$$

Finally, by Markov's inequality, the probability in (C.16) is at most

$$\max(\Psi_N, \sqrt{N})^{-L} \Phi_N^{-L} N^{-\varepsilon L} \cdot \mathbb{E}\left[\left(\sum_{i=1}^{N} Y_i^{(i)}[0]\right)^L \mathbf{1}\{\mathcal{E}_L\}\right] \prec N^{-\varepsilon L},$$

and (C.16) follows as desired under our initial choice $L = L(\varepsilon, D) > D/\varepsilon$. ■

C.2. No eigenvalues outside the support

We now prove Theorem 10. Let $m_N(z), \tilde{m}_N(z)$ be the Stieltjes transform of the N-dependent deterministic measures $\mu_N, \tilde{\mu}_N$. For each $z \in \mathbb{C}^+$, $\tilde{m}_N(z)$ is the unique root in $\mathbb{C}^+$ to the equation

$$z = -\frac{1}{\tilde{m}_N(z)} + \gamma_N \int \frac{\lambda}{1 + \lambda \tilde{m}_N(z)} d\nu_N(\lambda), \tag{C.24}$$

and $m_N(z), \tilde{m}_N(z)$ are related by $\tilde{m}_N(z) = \gamma_N m_N(z) + (1 - \gamma_N)(-1/z)$. Define the discrete set

$$\mathcal{T}_N = \{0\} \cup \{-1/\lambda : \lambda \in \operatorname{supp}(\nu_N)\}. \tag{C.25}$$

On the domain $\mathbb{C} \setminus \mathcal{T}_N$, we may define the formal inverse of (C.24),

$$z_N(\tilde{m}) = -\frac{1}{\tilde{m}} + \gamma_N \int \frac{\lambda}{1 + \lambda \tilde{m}} d\nu_N(\lambda), \tag{C.26}$$

which is a finite-N analogue of (A.4). Let $\mathcal{S}_N$ be the deterministic support defined in (B.2), and let $U_N(\varepsilon)$ be the spectral domain (B.3). The following basic properties of $\mathcal{S}_N$ and $\tilde{m}_N(z)$ are known.

Proposition 18 *Suppose Assumption 5(a) holds, and fix any $\varepsilon > 0$. Then there exist constants $C_0, c_0 > 0$, depending only on ε and the constants C, c of Assumption 5(a), such that for all $x \in \mathcal{S}_N$ we have $|x| \leq C$, and for all $z = x + i\eta \in U_N(\varepsilon)$ we have*

$$c < |\tilde{m}_N(z)| < C, \qquad c\eta \leq |\operatorname{Im} \tilde{m}_N(z)| \leq C\eta, \qquad \min_{\lambda \in \operatorname{supp}(\nu_N)} |1 + \lambda\, \tilde{m}_N(z)| \geq c$$

Proof. See (Fan and Johnstone, 2022, Propositions A.3, B.1, B.2). ■

Let $m_{\widetilde{\boldsymbol{K}}}(z) = N^{-1} \operatorname{Tr}(\widetilde{\boldsymbol{K}} - z\boldsymbol{I})^{-1}$ be the Stieltjes transform of the empirical eigenvalue distribution of $\widetilde{\boldsymbol{K}} = \boldsymbol{G}\boldsymbol{G}^\top$. Since $\widetilde{\boldsymbol{K}}$ and $\boldsymbol{K} = \boldsymbol{G}^\top \boldsymbol{G}$ have the same eigenvalues up to $|N - n|$ 0's, we have

$$m_{\widetilde{\boldsymbol{K}}}(z) = \gamma_N m_{\boldsymbol{K}}(z) + (1 - \gamma_N)(-1/z), \tag{C.27}$$

so in particular $m_{\tilde{\boldsymbol{K}}}$ coincides with $\tilde{m}_{\boldsymbol{K}}^{(\emptyset)}$ from (C.1). We begin with a preliminary estimate for the Stieltjes transform $m_{\tilde{\boldsymbol{K}}}(z)$ when $\operatorname{Im} z \geq N^{-1/11}$. Similar statements have been shown in (Silverstein, 1995; Bai and Silverstein, 1998), and we provide an argument here following ideas of (Bai and Silverstein, 1998, Section 3) for later reference.

Lemma 19 *Fix any $\varepsilon > 0$, and suppose Assumption 5 holds. Then, uniformly over $z = x + i\eta \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1/11}$,*

$$m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z) \prec \frac{1}{\sqrt{N}\eta^4}.$$

Proof. Let $\boldsymbol{R}^{(i)}$ and $\tilde{m}_{\boldsymbol{K}}^{(i)}$ be as defined in (C.1) with $\boldsymbol{\Gamma} = z\boldsymbol{I}$. Applying the Sherman-Morrison formula

$$\boldsymbol{R} = \boldsymbol{R}^{(i)} - \frac{N^{-1}\boldsymbol{R}^{(i)}\boldsymbol{g}_i\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}}{1 + N^{-1}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{g}_i}, \tag{C.28}$$

for any matrix $\boldsymbol{B} \in \mathbb{C}^{n\times n}$ we have

$$\begin{aligned}\operatorname{Tr}\boldsymbol{B} = \operatorname{Tr}(\boldsymbol{K} - z\boldsymbol{I})\boldsymbol{R}\boldsymbol{B} &= -z\operatorname{Tr}\boldsymbol{R}\boldsymbol{B} + \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{g}_i^\top\boldsymbol{R}\boldsymbol{B}\boldsymbol{g}_i \\ &= -z\operatorname{Tr}\boldsymbol{R}\boldsymbol{B} + \frac{1}{N}\sum_{i=1}^{N}\frac{\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{B}\boldsymbol{g}_i}{1 + N^{-1}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{g}_i}.\end{aligned} \tag{C.29}$$

Choosing $\boldsymbol{B} = \boldsymbol{I}$ in (C.29), applying $\operatorname{Tr}\boldsymbol{R} = n\, m_{\boldsymbol{K}} = N\, m_{\tilde{\boldsymbol{K}}} + (n - N)(-1/z)$, and rearranging, we obtain the identity

$$m_{\tilde{\boldsymbol{K}}} = -\frac{1}{Nz}\sum_{i=1}^{N}\frac{1}{1 + N^{-1}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{g}_i}. \tag{C.30}$$

Now fix any deterministic matrix $\boldsymbol{A} \in \mathbb{C}^{n\times n}$, define

$$d_i = \frac{1}{N}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i - \frac{1}{N}\operatorname{Tr}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{\Sigma},$$

and choose $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}$ in (C.29). Then, applying also the identity (C.30), we get

$$\begin{aligned}&\operatorname{Tr}\boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1} \\ &= -z\operatorname{Tr}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1} - zm_{\tilde{\boldsymbol{K}}}\operatorname{Tr}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{\Sigma} + \sum_{i=1}^{N}\frac{d_i}{1 + N^{-1}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{g}_i} \\ &= -z\operatorname{Tr}\boldsymbol{R}\boldsymbol{A} + \sum_{i=1}^{N}\frac{d_i}{1 + N^{-1}\boldsymbol{g}_i^\top\boldsymbol{R}^{(i)}\boldsymbol{g}_i}.\end{aligned} \tag{C.31}$$

We proceed to bound d_i, where (for later purposes) we derive estimates in terms of the Frobenius norms of $\boldsymbol{R}, \boldsymbol{R}\boldsymbol{A}, \boldsymbol{R}^{(i)}, \boldsymbol{R}^{(i)}\boldsymbol{A}$ rather than their operator norms. Note that Assumption 5(c) implies, for any matrix $\boldsymbol{B} \in \mathbb{C}^{n\times n}$ independent of $\boldsymbol{g}_i$,

$$\|\boldsymbol{B}\boldsymbol{g}_i\|^2 = \boldsymbol{g}_i^\top\boldsymbol{B}^*\boldsymbol{B}\boldsymbol{g}_i \prec \operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{B}^*\boldsymbol{B} + \|\boldsymbol{B}^*\boldsymbol{B}\|_F \prec \|\boldsymbol{B}\|_F^2. \tag{C.32}$$

We have also, by Assumption 5(c) and the Sherman-Morrison formula (C.28),

$$\begin{aligned} N^{-1}|\operatorname{Tr} \boldsymbol{R}\boldsymbol{B} - \operatorname{Tr} \boldsymbol{R}^{(i)}\boldsymbol{B}| &= N^{-2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}|\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{B}\boldsymbol{R}^{(i)}\boldsymbol{g}_i| \\ &\prec N^{-2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\Big(|\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}^{(i)}\boldsymbol{B}\boldsymbol{R}^{(i)}| + \|\boldsymbol{R}^{(i)}\boldsymbol{B}\boldsymbol{R}^{(i)}\|_F\Big) \\ &\prec N^{-2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}^{(i)}\boldsymbol{B}\|_F\|\boldsymbol{R}^{(i)}\|_F. \end{aligned} \tag{C.33}$$

Define $d_i = d_{i,1} + d_{i,2} + d_{i,3} + d_{i,4}$ where

$$\begin{aligned} d_{i,1} &= N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i - N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i, \\ d_{i,2} &= N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i - N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}, \\ d_{i,3} &= N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1} - N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}, \\ d_{i,4} &= N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1} - N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}. \end{aligned} \tag{C.34}$$

Applying the identity $\boldsymbol{A}^{-1} - \boldsymbol{B}^{-1} = \boldsymbol{A}^{-1}(\boldsymbol{B}-\boldsymbol{A})\boldsymbol{B}^{-1}$, the definition of $\tilde{m}_{\boldsymbol{K}}^{(i)}$ in (C.1), and the bounds (C.32) and (C.33) (the latter with $\boldsymbol{B} = \boldsymbol{I}$),

$$\begin{aligned} |d_{i,1}| &\le N^{-1}\|\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{A}\|\|(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\|\|(\tilde{m}_{\boldsymbol{K}}^{(i)} - m_{\tilde{\boldsymbol{K}}})\boldsymbol{\Sigma}\|\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|\|\boldsymbol{g}_i\| \\ &\prec N^{-5/2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}^{(i)}\boldsymbol{A}\|_F\|\boldsymbol{R}^{(i)}\|_F^2\|(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\|\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|. \end{aligned} \tag{C.35}$$

Applying Assumption 5(c),

$$|d_{i,2}| \prec N^{-1}\|\boldsymbol{R}^{(i)}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|_F \le N^{-1}\|\boldsymbol{R}^{(i)}\boldsymbol{A}\|_F\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|. \tag{C.36}$$

Applying the Sherman-Morrison identity (C.28), $|\operatorname{Tr} \boldsymbol{u}\boldsymbol{v}^\top| \le \|\boldsymbol{u}\|\|\boldsymbol{v}\|$, and (C.32),

$$\begin{aligned} |d_{i,3}| &\le N^{-2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{\Sigma}\boldsymbol{R}^{(i)}\boldsymbol{g}_i\|\|\boldsymbol{g}_i^\top \boldsymbol{A}\boldsymbol{R}^{(i)}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\| \\ &\prec N^{-2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}^{(i)}\boldsymbol{A}\|_F\|\boldsymbol{R}^{(i)}\|_F\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|. \end{aligned} \tag{C.37}$$

Finally, applying $\boldsymbol{A}^{-1} - \boldsymbol{B}^{-1} = \boldsymbol{A}^{-1}(\boldsymbol{B}-\boldsymbol{A})\boldsymbol{B}^{-1}$, (C.33) (with $\boldsymbol{B} = \boldsymbol{I}$), and $|\operatorname{Tr} \boldsymbol{A}\boldsymbol{B}| \le \|\boldsymbol{A}\|_F\|\boldsymbol{B}\|_F \le \sqrt{N}\|\boldsymbol{A}\|_F\|\boldsymbol{B}\|$,

$$\begin{aligned} |d_{i,4}| &= N^{-1}\Big|\operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}\boldsymbol{A}(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}(\tilde{m}_{\boldsymbol{K}}^{(i)} - m_{\tilde{\boldsymbol{K}}})\boldsymbol{\Sigma}(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\Big| \\ &\prec N^{-5/2}|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}\boldsymbol{A}\|_F\|\boldsymbol{R}\|_F^2\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|\|(\boldsymbol{I}+m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\|. \end{aligned} \tag{C.38}$$

For the current proof, we apply (C.31) and the definitions (C.34) with $\boldsymbol{A} = \boldsymbol{I}$. Recalling $\operatorname{Tr} \boldsymbol{R} = n\, m_{\boldsymbol{K}} = N\, m_{\tilde{\boldsymbol{K}}} + (n-N)(-1/z)$ and rearranging (C.31) with $\boldsymbol{A} = \boldsymbol{I}$, we get the identity

$$z_N(m_{\tilde{\boldsymbol{K}}}) - z = -\frac{1}{m_{\tilde{\boldsymbol{K}}}} \cdot \frac{1}{N}\sum_{i=1}^N \frac{d_i}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i} \tag{C.39}$$

where $z_N(m) = -(1/m) + N^{-1}\operatorname{Tr} \boldsymbol{\Sigma}(\boldsymbol{I}+m\boldsymbol{\Sigma})^{-1}$ is the function defined in (C.26). For any $z = x + i\eta$ with $\eta > 0$, we have

$$|z(1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i)| \ge \operatorname{Im}[z(1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i)] \ge \operatorname{Im} z = \eta, \tag{C.40}$$

$$\max(\|\boldsymbol{R}\|_F, \|\boldsymbol{R}^{(i)}\|_F) \le N^{1/2} \max(\|\boldsymbol{R}\|, \|\boldsymbol{R}^{(i)}\|) \le N^{1/2}\eta^{-1}. \tag{C.41}$$

Here, the second inequalities of both (C.40) and (C.41) follow from the spectral representations of $\boldsymbol{R}, \boldsymbol{R}^{(i)}$, i.e. writing $(\lambda_j, \boldsymbol{v}_j)_{j=1}^n$ for the eigenvalues and unit eigenvectors of $\boldsymbol{K}^{(i)}$, we have

$$\begin{aligned}
\operatorname{Im}[z\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)} \boldsymbol{g}_i] &= \operatorname{Im}\left[z\boldsymbol{g}_i^\top\left(\sum_{j=1}^n \frac{1}{\lambda_j - z}\boldsymbol{v}_j\boldsymbol{v}_j^\top\right)\boldsymbol{g}_i\right] = \sum_{j=1}^n \operatorname{Im}\frac{z}{\lambda_j - z}\cdot(\boldsymbol{g}_i^\top \boldsymbol{v}_j)^2 \\
&= \sum_{j=1}^n \frac{\lambda_j \operatorname{Im} z}{|\lambda_j - z|^2}\cdot(\boldsymbol{g}_i^\top \boldsymbol{v}_j)^2 \ge 0, \\
\|\boldsymbol{R}^{(i)}\| &= \left\|\sum_{j=1}^n \frac{1}{\lambda_j - z}\boldsymbol{v}_j\boldsymbol{v}_j^\top\right\| = \max_{j=1}^n |\lambda_j - z|^{-1} \le \eta^{-1},
\end{aligned}$$

and similarly for $\|\boldsymbol{R}\|$. In particular, (C.40) and (C.41) imply

$$(1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i)^{-1} \prec \eta^{-1}, \qquad \|\boldsymbol{R}\|_F, \|\boldsymbol{R}^{(i)}\|_F \prec N^{1/2}\eta^{-1}. \tag{C.42}$$

Next, observe that if $m(z) = \int \frac{1}{\lambda - z} d\mu(\lambda)$ is the Stieltjes transform of any probability measure μ supported on $[-B, B]$, then for $z = x + i\eta$ with $\eta > 0$ and $|z| \le \varepsilon^{-1}$, we have

$$\operatorname{Im} m(z) = \int \frac{\eta}{|\lambda - z|^2} d\mu(\lambda) \ge c\eta, \quad |\operatorname{Re} m(z)| \le \int \frac{|\lambda - x|}{|\lambda - z|^2} d\mu(\lambda) \le (C/\eta) \operatorname{Im} m(z)$$

for some constants $C, c > 0$ depending on ε, B. Consequently, for any $\lambda \ge 0$, either $\lambda \cdot |\operatorname{Re} m(z)| < 1/2$ or $\lambda \cdot \operatorname{Im} m(z) \ge 2\eta/C$, so $|1 + \lambda m(z)| \ge \max(2, 2\eta/C)$. By Assumption 5(b) and Weyl's inequality, we have $\mathbf{1}\{\|\boldsymbol{K}\| > B\} \prec 0$ and $\mathbf{1}\{\|\boldsymbol{K}^{(i)}\| > B\} \prec 0$, and on the event where $\|\boldsymbol{K}\|, \|\boldsymbol{K}^{(i)}\| \le B$, we have that $m_{\tilde{\boldsymbol{K}}}, \tilde{m}_{\boldsymbol{K}}^{(i)}$ are Stieltjes transforms of probability measures supported on $[-B, B]$. Thus, this implies

$$|m_{\tilde{\boldsymbol{K}}}|^{-1} \le |\operatorname{Im} m_{\tilde{\boldsymbol{K}}}|^{-1} \prec \eta^{-1}, \quad \max(\|(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\|, \|(\boldsymbol{I} + \tilde{m}_{\boldsymbol{K}}^{(i)}\boldsymbol{\Sigma})^{-1}\|) \prec \eta^{-1}. \tag{C.43}$$

Applying these bounds (C.42) and (C.43) to (C.35)–(C.38), we get $d_i \prec N^{-1}\eta^{-6} + N^{-1/2}\eta^{-2} \le 2N^{-1/2}\eta^{-2}$ for $\eta \ge N^{-1/11}$. Then, applying these bounds (C.42) and (C.43) also to (C.39), we get

$$z_N(m_{\tilde{\boldsymbol{K}}}) - z \prec \frac{1}{\sqrt{N}\eta^4}. \tag{C.44}$$

The proof is completed by the following stability argument: When $\eta \ge N^{-1/11}$, we have $1/(\sqrt{N}\eta^4) \ll \eta = \operatorname{Im} z$, so (C.44) implies in particular that

$$\mathbf{1}\{z_N(m_{\tilde{\boldsymbol{K}}}) \notin \mathbb{C}^+\} \prec 0. \tag{C.45}$$

On the event $z_N(m_{\tilde{\boldsymbol{K}}}) \in \mathbb{C}^+$, recalling the implicit definition of $\tilde{m}_N : \mathbb{C}^+ \to \mathbb{C}^+$ by (C.24), the value $\tilde{m}_N(z_N(m_{\tilde{\boldsymbol{K}}}))$ must be the unique root $u \in \mathbb{C}^+$ to the equation

$$z_N(m_{\tilde{\boldsymbol{K}}}) = -\frac{1}{u} + \gamma_N \int \frac{\lambda}{1 + \lambda u} d\nu_N(\lambda),$$

i.e. to the equation $z_N(m_{\tilde{\boldsymbol{K}}}) = z_N(u)$. This equation is satisfied by $u = m_{\tilde{\boldsymbol{K}}} \in \mathbb{C}^+$, so we deduce that $\tilde{m}_N(z_N(m_{\tilde{\boldsymbol{K}}})) = m_{\tilde{\boldsymbol{K}}}$. Then, applying that $z \in U_N(\varepsilon)$ and that $\tilde{m}_N : \mathbb{C}^+ \to \mathbb{C}^+$ is $(4/\varepsilon^2)$-Lipschitz over the domain $U_N(\varepsilon/2)$, we obtain from (C.44) that

$$\mathbf{1}\{z_N(m_{\tilde{\boldsymbol{K}}}) \in \mathbb{C}^+\}\Big(m_{\tilde{\boldsymbol{K}}} - \tilde{m}_N(z)\Big) = \mathbf{1}\{z_N(m_{\tilde{\boldsymbol{K}}}) \in \mathbb{C}^+\}\Big(\tilde{m}_N(z_N(m_{\tilde{\boldsymbol{K}}})) - \tilde{m}_N(z)\Big) \prec \frac{1}{\sqrt{N}\eta^4}.$$

Together with (C.45), this yields the lemma. ■

Corollary 20 *Fix any $\varepsilon > 0$, and suppose Assumption 5 holds. Then there is a constant $C > 0$ such that uniformly over $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1/11}$,*

$$\mathbf{1}\{\|\boldsymbol{R}(z)\|_F > C\sqrt{N}\} \prec 0.$$

Proof. Since $m_{\tilde{\boldsymbol{K}}}(z) = \gamma_N m_{\boldsymbol{K}}(z) + (1-\gamma_N)(-1/z)$ and $\tilde{m}_N(z) = \gamma_N m_N(z) + (1-\gamma_N)(-1/z)$, Lemma 19 implies also

$$m_{\boldsymbol{K}}(z) - m_N(z) \prec \frac{1}{\sqrt{N}\eta^4} \ll \eta.$$

Observe that $\operatorname{Im} m_N(z) = \int \eta/|\lambda - z|^2 d\mu_N(\lambda) \leq \eta\varepsilon^{-2}$ for $z \in U_N(\varepsilon)$, so $\mathbf{1}\{\operatorname{Im} m_{\boldsymbol{K}}(z) > (1+\varepsilon^{-2})\eta\} \prec 0$. Then by the identity $\|\boldsymbol{R}(z)\|_F^2 = \sum_i 1/|z - \lambda_i(\boldsymbol{K})|^2 = (n/\eta) \operatorname{Im} m_{\boldsymbol{K}}(z)$, we get $\mathbf{1}\{\|\boldsymbol{R}(z)\|_F > C\sqrt{N}\} \prec 0$ for a constant $C = C(\varepsilon) > 0$, as desired. ■

We may now apply Corollary 20 and the fluctuation averaging result of Lemma 14 to improve the estimate of Lemma 19 to the following result.

Lemma 21 *Fix any $\varepsilon > 0$, and suppose Assumption 5 holds. Then, uniformly over $z = x + i\eta \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1/11}$,*

$$m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z) \prec \frac{1}{N}.$$

Proof. We derive an improved estimate for (C.39). First, combining Lemma 19 with the bounds for $\tilde{m}_N(z)$ in Proposition 18, there are constants $C_0, c_0 > 0$ for which

$$\mathbf{1}\{|m_{\tilde{\boldsymbol{K}}}| > C_0\} \prec 0, \qquad \mathbf{1}\{|m_{\tilde{\boldsymbol{K}}}| < c_0\} \prec 0, \qquad \mathbf{1}\{\|(\boldsymbol{I} + m_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\| > C_0\} \prec 0 \tag{C.46}$$

uniformly over $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1/11}$. Next, applying Assumption 5(c), we have also uniformly over $i \in [N]$,

$$\begin{aligned} N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)} \boldsymbol{g}_i &= N^{-1} \operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R}^{(i)} + O_\prec\Big(N^{-1}\|\boldsymbol{R}^{(i)}\|_F\Big) \\ &= N^{-1} \operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R} + O_\prec\Big(N^{-2}|1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}^{(i)}\|_F^2\Big) + O_\prec\Big(N^{-1}\|\boldsymbol{R}^{(i)}\|_F\Big) \end{aligned}$$

where the second line follows from (C.33) applied with $\boldsymbol{B} = \boldsymbol{\Sigma}$. Applying $\|\boldsymbol{R}^{(i)}\|_F \prec N^{1/2}$ by Corollary 20 and the estimate $|1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1} \prec \eta^{-1}$ from (C.42), this gives

$$1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i = 1 + N^{-1} \operatorname{Tr} \boldsymbol{\Sigma}\boldsymbol{R} + O_\prec\Big(N^{-1/2}\Big). \tag{C.47}$$

Then, applying this and $|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1} \prec \eta^{-1}$ to (C.30),

$$m_{\tilde{\boldsymbol{K}}} = -\frac{1}{z}\cdot\frac{1}{1+N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}} + O_\prec\Big(N^{-1/2}\eta^{-2}\Big).$$

Together with the first bound of (C.46) and the bound $|z| \le \varepsilon^{-1}$ for $z \in U_N(\varepsilon)$, this implies for a constant $c_0 > 0$ that $\mathbf{1}\{|1+N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}| < c_0\} \prec 0$, and thus $\mathbf{1}\{|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i| < c_0\} \prec 0$.

Applying Corollary 20 and the above arguments now for $\boldsymbol{K}^{(S)}$ and $\boldsymbol{R}^{(S)}$ in place of $\boldsymbol{K}$ and $\boldsymbol{R}$, we obtain for any fixed $L \ge 1$ and some constants $C_0, c_0 > 0$, uniformly over $S \subset [N]$ with $|S| \le L$, over $i \in S$, and over $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \ge N^{-1/11}$,

$$\begin{gathered}\mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}| > C_0\} \prec 0, \quad \mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}| < c_0\} \prec 0, \quad \mathbf{1}\{\|(\boldsymbol{I}+\tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma})^{-1}\| > C_0\} \prec 0,\\ \mathbf{1}\{\|\boldsymbol{R}^{(S)}\|_F > C\sqrt{N}\} \prec 0, \quad \mathbf{1}\{|1+N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}| < c_0\} \prec 0,\\ \mathbf{1}\{|1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(S)}\boldsymbol{g}_i| < c_0\} \prec 0.\end{gathered} \tag{C.48}$$

(We remark that a direct application of the above arguments for $\boldsymbol{K}^{(S)}$ yields the first three estimates of (C.48) for the quantity $\frac{N}{N-|S|}\tilde{m}_{\boldsymbol{K}}^{(S)} = \frac{1}{N-|S|}\operatorname{Tr}\boldsymbol{R}^{(S)} + \frac{n}{N-|S|}(-1/z)$ in place of $\tilde{m}_{\boldsymbol{K}}^{(S)}$, and the estimates for $\tilde{m}_{\boldsymbol{K}}^{(S)}$ then follow for slightly modified constants $C_0, c_0 > 0$ because $|S| \le L$.)

Finally, applying (C.47) and (C.48) back to (C.39) and (C.35)–(C.38) with $\boldsymbol{A} = \boldsymbol{I}$, we get $|d_{i,1}|, |d_{i,3}|, |d_{i,4}| \prec N^{-1}$, $|d_{i,2}| \prec N^{-1/2}$, and

$$\begin{aligned}|z_N(m_{\tilde{\boldsymbol{K}}}) - z| &\prec \left|\frac{1}{N}\sum_{i=1}^N \frac{d_{i,2}}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i}\right| + O_\prec(N^{-1})\\ &= \frac{1}{N}\cdot\frac{1}{1+N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}}\cdot\left|\sum_{i=1}^N d_{i,2}\right| + O_\prec(N^{-1}).\end{aligned}$$

The statements of (C.48) verify the needed assumptions of Lemma 14 with $\boldsymbol{A} = \boldsymbol{I}$, $\boldsymbol{\Gamma} = z\boldsymbol{I}$, and $\Phi_N = \Psi_N = C\sqrt{N}$. Then Lemma 14 gives $\sum_{i=1}^N d_{i,2} \prec 1$, and hence

$$|z_N(m_{\tilde{\boldsymbol{K}}}) - z| \prec N^{-1}.$$

The proof is then completed by the same stability argument as in the conclusion of the proof of Lemma 19. ■

Proof of Theorem 10. We apply the idea of (Bai and Silverstein, 1998, Section 6). Let $z = x + i\eta$, where $\operatorname{dist}(x, \mathcal{S}_N) \ge \varepsilon$ and $\eta = N^{-1/11}$. Taking imaginary part in the estimate $m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z) \prec N^{-1}$ of Lemma 21 and multiplying by η gives

$$\frac{1}{N}\sum_{j=1}^N \frac{\eta^2}{(\lambda_j(\widetilde{\boldsymbol{K}}) - x)^2 + \eta^2} - \int \frac{\eta^2}{(\lambda - x)^2 + \eta^2} d\tilde{\mu}_N(\lambda) \prec \frac{\eta}{N}.$$

Fix any integer $P \ge 1$, and apply this instead at the point $z = x + i\sqrt{p}\,\eta$ for each $p = 1, \ldots, P$. Then

$$\frac{1}{N}\sum_{j=1}^N \frac{\eta^2}{(\lambda_j(\widetilde{\boldsymbol{K}}) - x)^2 + p\eta^2} - \int \frac{\eta^2}{(\lambda - x)^2 + p\eta^2} d\tilde{\mu}_N(\lambda) \prec \frac{\eta}{N} \text{ for all } p = 1, \ldots, P.$$

Taking successive finite differences using

$$\frac{1}{r-q+1}\left(\frac{1}{\prod_{p=q}^{r}(\lambda-x)^2+p\eta^2}-\frac{1}{\prod_{p=q+1}^{r+1}(\lambda-x)^2+p\eta^2}\right)=\frac{\eta^2}{\prod_{p=q}^{r+1}(\lambda-x)^2+p\eta^2},$$

we then obtain

$$\frac{1}{N}\sum_{j=1}^{N}\frac{\eta^{2P}}{\prod_{p=1}^{P}[(\lambda_j(\widetilde{\boldsymbol{K}})-x)^2+p\eta^2]}-\int\frac{\eta^{2P}}{\prod_{p=1}^{P}[(\lambda-x)^2+p\eta^2]}d\tilde{\mu}_N(\lambda)\prec\frac{\eta}{N}. \tag{C.49}$$

Since $\operatorname{dist}(x,\mathcal{S}_N)\geq\varepsilon$, the second integral term of (C.49) is bounded by $C\eta^{2P}$ for a constant $C:=C(\varepsilon,P)>0$. Thus, we get

$$\frac{1}{N}\sum_{j=1}^{N}\mathbf{1}\{\lambda_j(\widetilde{\boldsymbol{K}})\in(x-\eta,x+\eta)\}\leq\frac{C}{N}\sum_{j=1}^{N}\frac{\eta^{2P}}{\prod_{p=1}^{P}[(\lambda_j(\widetilde{\boldsymbol{K}})-x)^2+p\eta^2]}\prec\frac{\eta}{N}+\eta^{2P}$$

where the first inequality holds for a constant $C:=C(P)>0$. Finally, recalling $\eta=N^{-1/11}$ and taking any $P\geq 6$, we get $\eta/N+\eta^{2P}\ll 1/N$, hence

$$\mathbf{1}\big\{\text{there exists an eigenvalue of }\widetilde{\boldsymbol{K}}\text{ in }(x-\eta,x+\eta)\big\}\prec 0.$$

Recalling Assumption 5(b) and taking a union bound over x belonging to a η-net of $[-B,B]\setminus(\mathcal{S}_N+(-\varepsilon,\varepsilon))$ (with cardinality at most $CN^{1/11}$), we obtain

$$\mathbf{1}\big\{\text{there exists an eigenvalue of }\widetilde{\boldsymbol{K}}\text{ in }\mathcal{S}_N+(-\varepsilon,\varepsilon)\big\}\prec 0.$$

The theorem follows from the observation that $\boldsymbol{K}$ has the same non-zero eigenvalues as $\widetilde{\boldsymbol{K}}$, and all 0 eigenvalues belong by definition to $\mathcal{S}_N$. ■

C.3. Deterministic equivalent for the resolvent

In this section, we prove Theorem 11.

Lemma 22 *Suppose Assumption 5 holds. Let*

$$\gamma_N^{(S)}=\frac{n}{N-|S|},\qquad \mu_N^{(S)}=\rho^{\mathrm{MP}}_{\gamma_N^{(S)}}\boxtimes\nu_N,\qquad \tilde{\mu}_N^{(S)}=\gamma_N^{(S)}\mu_N^{(S)}+(1-\gamma_N^{(S)})\delta_0$$

be the analogues of $\gamma_N,\mu_N,\tilde{\mu}_N$ defined with the dimension $N-|S|$ in place of N. Then for any fixed $\varepsilon>0$ and $L\geq 1$, all large N, and all $S\subset[N]$ with $|S|\leq L$,

$$\operatorname{supp}(\tilde{\mu}_N^{(S)})\subseteq\operatorname{supp}(\tilde{\mu}_N)+(-\varepsilon,\varepsilon)$$

Proof. Let $\mathcal{T}_N$ and $z_N:\mathbb{C}\setminus\mathcal{T}_N\to\mathbb{C}$ be as defined by (C.25) and (C.26). Define similarly

$$z_N^{(S)}(\tilde{m})=-\frac{1}{\tilde{m}}+\gamma_N^{(S)}\int\frac{\lambda}{1+\lambda\tilde{m}}d\nu_N(\lambda),\qquad z_N^{(S)}:\mathbb{C}\setminus\mathcal{T}_N\to\mathbb{C}.$$

We recall from Proposition 9 that $x \in \mathbb{R} \setminus \operatorname{supp}(\tilde{\mu}_N)$ if and only if there exists $\tilde{m} \in \mathbb{R} \setminus \mathcal{T}_N$ where $z_N(\tilde{m}) = x$ and $z_N'(\tilde{m}) > 0$; the analogous characterization holds for $\mathbb{R} \setminus \operatorname{supp}(\tilde{\mu}_N^{(S)})$ and $z_N^{(S)}(\tilde{m})$.

Now fix any $\varepsilon, L > 0$. By Proposition 18, there is a constant $C_0 > 0$ such that $\operatorname{supp}(\tilde{\mu}_N^{(S)}) \subseteq [-C_0, C_0]$ for all $|S| \le L$ and all large N. Consider any $x \in [-C_0, C_0] \setminus (\operatorname{supp}(\tilde{\mu}_N) + (-\varepsilon, \varepsilon))$. Then $[x-\varepsilon/2, x+\varepsilon/2] \subset \mathbb{R} \setminus \operatorname{supp}(\tilde{\mu}_N)$, so $\tilde{m}_N$ is well-defined and increasing on $[x-\varepsilon/2, x+\varepsilon/2]$. Define $[\tilde{m}_-, \tilde{m}_+] = [\tilde{m}_N(x-\varepsilon/2), \tilde{m}_N(x+\varepsilon/2)]$. Then Proposition 9 implies that z_N is increasing on $[\tilde{m}_-, \tilde{m}_+]$, and $z_N([\tilde{m}_-, \tilde{m}_+]) = [x-\varepsilon/2, x+\varepsilon/2]$. Again by Proposition 18, there is a constant $c > 0$ such that, for any such $x \in [-C_0, C_0] \setminus (\operatorname{supp}(\tilde{\mu}_N) + (-\varepsilon, \varepsilon))$, we have

$$\min_{y \in [x-\varepsilon/2, x+\varepsilon/2]} \min_{\lambda \in \operatorname{supp}(\nu_N)} |1 + \lambda \tilde{m}_N(y)| > c.$$

This then implies that there is a constant $C > 0$ for which

$$|z_N^{(S)}(\tilde{m}) - z_N(\tilde{m})| = |\gamma_N^{(S)} - \gamma_N| \cdot \left| \int \frac{\lambda}{1 + \lambda \tilde{m}} d\nu_N(\lambda) \right| \le \frac{C}{N} < \varepsilon/2$$

for all $\tilde{m} \in [\tilde{m}_-, \tilde{m}_+]$, $|S| \le L$, and large N. Then $z_N^{(S)}(\tilde{m}_-) < z_N(\tilde{m}_-) + \varepsilon/2 = x$ and $z_N^{(S)}(\tilde{m}_+) > z_N(\tilde{m}_+) - \varepsilon/2 = x$. (Silverstein and Choi, 1995, Theorem 4.3) shows that if $m_1, m_2 \in [\tilde{m}_-, \tilde{m}_+]$ satisfy ${z_N^{(S)}}'(m_1) \ge 0$ and ${z_N^{(S)}}'(m_2) \ge 0$, then ${z_N^{(S)}}'(m) > 0$ strictly for all $m \in [m_1, m_2]$. By this and the continuity and differentiability of $z_N^{(S)}$ on $[\tilde{m}_-, \tilde{m}_+]$, there must be a point $\tilde{m} \in (\tilde{m}_-, \tilde{m}_+)$ where $z_N^{(S)}(\tilde{m}) = x$ and ${z_N^{(S)}}'(\tilde{m}) > 0$ strictly. Then Proposition 9 implies that $x \notin \operatorname{supp}(\tilde{\mu}_N^{(S)})$. This holds for all $x \in [-C_0, C_0] \setminus (\operatorname{supp}(\tilde{\mu}_N) + (-\varepsilon, \varepsilon))$, implying $\operatorname{supp}(\tilde{\mu}_N^{(S)}) \subseteq \operatorname{supp}(\tilde{\mu}_N) + (-\varepsilon, \varepsilon)$ as desired. ■

The following now applies Lemma 22 and Theorem 10 to extend the estimates (C.48) previously obtained over $\{z \in U_N(\varepsilon) : \operatorname{Im} z \ge N^{-1/11}\}$ to all of $U_N(\varepsilon)$.

Lemma 23 *Fix any $\varepsilon > 0$ and $L \ge 1$. Then for some constants $C_0, c_0 > 0$, uniformly over $z \in U_N(\varepsilon)$, $S \subset [N]$ with $|S| \le L$, and $i \in S$, we have*

$$\mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(z)| > C_0\} \prec 0, \quad \mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(z)| < c_0\} \prec 0, \quad \mathbf{1}\{\|(\boldsymbol{I} + \tilde{m}_{\boldsymbol{K}}^{(S)}(z)\boldsymbol{\Sigma})^{-1}\| > C_0\} \prec 0,$$
$$\mathbf{1}\{\|\boldsymbol{R}^{(S)}(z)\| > C_0\} \prec 0, \quad \mathbf{1}\{|1 + N^{-1} \operatorname{Tr} \boldsymbol{\Sigma} \boldsymbol{R}^{(S)}(z)| < c_0\} \prec 0,$$
$$\mathbf{1}\{|1 + N^{-1} \boldsymbol{g}_i^\top \boldsymbol{R}^{(S)}(z) \boldsymbol{g}_i| < c_0\} \prec 0.$$

Proof. By conjugation symmetry, it suffices to show the statements for $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \ge 0$. Denote for simplicity $\boldsymbol{R}^{(S)} = \boldsymbol{R}^{(S)}(z)$ and $\tilde{m}_{\boldsymbol{K}}^{(S)} = \tilde{m}_{\boldsymbol{K}}^{(S)}(z)$. Let $\mathcal{S}_N^{(S)} = \operatorname{supp}(\mu_N^{(S)}) \cup \{0\} = \operatorname{supp}(\tilde{\mu}_N^{(S)}) \cup \{0\}$ where $\mu_N^{(S)}, \tilde{\mu}_N^{(S)}$ are as defined in Lemma 22. Then Theorem 10 applied to $\boldsymbol{K}^{(S)}$ guarantees that

$$\mathbf{1}\{\boldsymbol{K}^{(S)} \text{ has an eigenvalue outside } \mathcal{S}_N^{(S)} + (-\varepsilon/4, \varepsilon/4)\} \prec 0,$$

uniformly over all $S \subset [N]$ with $|S| \le L$. Note that $\mathcal{S}_N^{(S)} + (-\varepsilon/4, \varepsilon/4) \subseteq \mathcal{S}_N + (-\varepsilon/2, \varepsilon/2)$ by Lemma 22. Then, applying the bound $\|\boldsymbol{R}^{(S)}\| \le 1/\operatorname{dist}(z, \mathcal{S}_N^{(S)})$ and the condition $z \in U_N(\varepsilon)$, we get

$$\mathbf{1}\{\|\boldsymbol{R}^{(S)}\| > 2/\varepsilon\} \prec 0. \tag{C.50}$$

The remaining statements have already been shown for $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1/11}$ in (C.48). For $z = x + i\eta$ where $\eta \in [0, N^{-1/11}]$, define $z' = x + iN^{-1/11}$. On the event that $\boldsymbol{K}^{(S)}$ has no eigenvalues outside $\mathcal{S}_N + (-\varepsilon/2, \varepsilon/2)$, both $N^{-1} \operatorname{Tr} \boldsymbol{\Sigma} \boldsymbol{R}^{(S)}(z)$ and $\tilde{m}_{\boldsymbol{K}}^{(S)}(z) = N^{-1} \operatorname{Tr} \boldsymbol{R}^{(S)}(z) + \gamma_N(-1/z)$ are C-Lipschitz over $z \in U_N(\varepsilon)$ for a constant $C = C(\varepsilon) > 0$, and $N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(S)}(z)\boldsymbol{g}_i$ is $CN^{-1}\|\boldsymbol{g}_i\|^2$-Lipschitz where $N^{-1}\|\boldsymbol{g}_i\|^2 \prec 1$ by Assumption 5. Then

$$N^{-1} \operatorname{Tr} \boldsymbol{\Sigma} \boldsymbol{R}^{(S)}(z) - N^{-1} \operatorname{Tr} \boldsymbol{\Sigma} \boldsymbol{R}^{(S)}(z') \prec N^{-1/11}, \quad \tilde{m}_{\boldsymbol{K}}^{(S)}(z) - \tilde{m}_{\boldsymbol{K}}^{(S)}(z') \prec N^{-1/11},$$

$$N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(S)}(z)\boldsymbol{g}_i - N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(S)}(z')\boldsymbol{g}_i \prec N^{-1/11},$$

so the remaining statements of the lemma hold also for $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \in [0, N^{-1/11}]$. ■

Proof of Theorem 11. Again by conjugation symmetry, it suffices to show the result for $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq 0$. Denote for simplicity $\boldsymbol{R}^{(S)} = \boldsymbol{R}^{(S)}(z)$ and $\tilde{m}_{\boldsymbol{K}}^{(S)} = \tilde{m}_{\boldsymbol{K}}^{(S)}(z)$. The first estimate of Lemma 23 implies

$$\mathbf{1}\{\|\boldsymbol{R}^{(S)}\|_F > C\sqrt{N}\} \prec 0, \qquad \mathbf{1}\{\|\boldsymbol{R}^{(S)}\boldsymbol{A}\|_F > C\|\boldsymbol{A}\|_F\} \prec 0 \tag{C.51}$$

uniformly over $z \in U_N(\varepsilon)$ and $\boldsymbol{A} \in \mathbb{C}^{n\times n}$. Then also, by Assumption 5(c) and (C.33) applied with $\boldsymbol{B} = \boldsymbol{\Sigma}$,

$$\begin{aligned} 1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i &= 1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R} + O_\prec\Big(N^{-2}|1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i|^{-1}\|\boldsymbol{R}^{(i)}\|_F^2 + \|\boldsymbol{R}^{(i)}\|_F\Big) \\ &= 1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R} + O_\prec\Big(N^{-1/2}\Big). \end{aligned} \tag{C.52}$$

Let $d_i = d_{i,1} + d_{i,2} + d_{i,3} + d_{i,4}$ be as defined in (C.34) with $\boldsymbol{A} = \boldsymbol{I}$. Then, applying (C.51), (C.52), and the bounds of Lemma 23, we obtain exactly as in the proof of Lemma 21 (using again the fluctuation averaging result of Lemma 14) that, uniformly over $z \in U_N(\varepsilon)$, we have $|d_{i,1}|, |d_{i,3}|, |d_{i,4}| \prec N^{-1}$, $|d_{i,2}| \prec N^{-1/2}$, and

$$|z_N(m_{\tilde{\boldsymbol{K}}}) - z| \prec \frac{1}{N} \cdot \frac{1}{1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}} \cdot \left|\sum_{i=1}^N d_{i,2}\right| + O_\prec(N^{-1}) = O_\prec(N^{-1}).$$

Fix any $\iota > 0$. If $\operatorname{Im} z \geq N^{-1+\iota}$, then this implies $\mathbf{1}\{z_N(m_{\tilde{\boldsymbol{K}}}) \notin \mathbb{C}^+\} \prec 0$. By the same stability argument as in Lemma 19, we get $m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z) \prec N^{-1}$ uniformly over $z \in U_N(\varepsilon)$ with $\operatorname{Im} z \geq N^{-1+\iota}$. For $\operatorname{Im} z \in [0, N^{-1+\iota}]$, on the event that all eigenvalues of $\boldsymbol{K}$ belong to $\mathcal{S}_N + (-\varepsilon/2, \varepsilon/2)$, we may apply that both $m_{\tilde{\boldsymbol{K}}}(z)$ and $\tilde{m}_N(z)$ are $C(\varepsilon)$-Lipschitz over $z \in U_N(\varepsilon)$ to compare values at $z = x + i\eta$ and $z' = x + iN^{-1+\iota}$. Applying $m_{\tilde{\boldsymbol{K}}}(z') - \tilde{m}_N(z') \prec N^{-1}$, we then get for any $D > 0$, all $z \in U_N(\varepsilon)$, some constant $C > 0$, and all large N,

$$\mathbb{P}[|m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z)| > CN^{-1+\iota}] \leq N^{-D}.$$

Since $\iota > 0$ is arbitrary, this shows $m_{\tilde{\boldsymbol{K}}}(z) - \tilde{m}_N(z) \prec N^{-1}$ uniformly over $z \in U_N(\varepsilon)$. The bound $m_{\boldsymbol{K}}(z) - m_N(z) \prec N^{-1}$ then follows from $m_{\tilde{\boldsymbol{K}}}(z) = \gamma_N m_{\boldsymbol{K}}(z) + (1 - \gamma_N)(-1/z)$ and $\tilde{m}_N(z) = \gamma_N m_N(z) + (1 - \gamma_N)(-1/z)$.

For the estimate of $\operatorname{Tr} \boldsymbol{R}\boldsymbol{A}$, we apply the definition of $d_i = d_{i,1} + d_{i,2} + d_{i,3} + d_{i,4}$ from (C.34) and the identity (C.31) now with this matrix $\boldsymbol{A}$. Then (C.31) gives

$$\operatorname{Tr}\left[\boldsymbol{R}\boldsymbol{A} - (-z\boldsymbol{I} - zm_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{A}\right] = \frac{1}{z}\sum_{i=1}^{N} \frac{d_i}{1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i}.$$

Applying (C.51), (C.52), and the bounds of Lemma 23 to (C.35)–(C.38), uniformly over $z \in U_N(\varepsilon)$ and $\boldsymbol{A} \in \mathbb{C}^{n\times n}$, we have $|d_{i,1}|, |d_{i,3}|, |d_{i,4}| \prec N^{-3/2}\|\boldsymbol{A}\|_F$, $|d_{i,2}| \prec N^{-1}\|\boldsymbol{A}\|_F$, and hence

$$\left|\sum_{i=1}^{N} \frac{d_i}{1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}\boldsymbol{g}_i}\right| \prec \frac{1}{1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}}\left|\sum_{i=1}^{N} d_{i,2}\right| + O_\prec\left(N^{-1/2}\|\boldsymbol{A}\|_F\right).$$

Finally, applying Lemma 14 with $\boldsymbol{\Gamma} = z\boldsymbol{I}$, $\Psi_N(\boldsymbol{\Gamma}) = C\sqrt{N}$, and $\Phi_N(\boldsymbol{\Gamma}, \boldsymbol{A}) = C\|\boldsymbol{A}\|_F$ (where we may assume without loss of generality $\|\boldsymbol{A}\|_F \in (N^{-\upsilon}, N^{\upsilon})$ by scale invariance of the desired estimate with respect to $\boldsymbol{A}$), we get $|\sum_i d_{i,2}| \prec N^{-1/2}\|\boldsymbol{A}\|_F$. Thus,

$$\operatorname{Tr}\left[\boldsymbol{R}\boldsymbol{A} - (-z\boldsymbol{I} - zm_{\tilde{\boldsymbol{K}}}\boldsymbol{\Sigma})^{-1}\boldsymbol{A}\right] \prec \frac{1}{\sqrt{N}}\|\boldsymbol{A}\|_F.$$

■

Appendix D. Analysis of spiked eigenstructure

We now consider the asymptotic setup of Appendix B.2 and prove Corollary 12 and Theorem 13. As all the desired statements are invariant under conjugation of $\boldsymbol{\Sigma}$ by an orthogonal matrix, we may assume without loss of generality that $\boldsymbol{\Sigma}$ is diagonal and of the form

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_r & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Sigma}_0 \end{pmatrix}, \qquad \boldsymbol{\Sigma}_r = \operatorname{diag}(\lambda_1(\boldsymbol{\Sigma}), \ldots, \lambda_r(\boldsymbol{\Sigma})), \qquad \boldsymbol{\Sigma}_0 = \operatorname{diag}(\lambda_{r+1}(\boldsymbol{\Sigma}), \ldots, \lambda_n(\boldsymbol{\Sigma})).$$

Denote the block decomposition of $\boldsymbol{G}$ corresponding to $\boldsymbol{\Sigma}_r, \boldsymbol{\Sigma}_0$ as

$$\boldsymbol{G} = [\boldsymbol{G}_r, \boldsymbol{G}_0], \qquad \boldsymbol{G}_r \in \mathbb{R}^{N\times r}, \qquad \boldsymbol{G}_0 \in \mathbb{R}^{N\times(n-r)}.$$

We remind the reader that $\boldsymbol{G}_r$ and $\boldsymbol{G}_0$ need not be independent.

D.1. No outliers outside the limit support

We consider first the setting of $r = 0$, and prove Corollary 12 together with some uniform convergence properties of $\tilde{m}_N$ and z_N that will be used in the later analysis.

Recall the domain $\mathcal{T}_N$ and function $z_N : \mathbb{C} \setminus \mathcal{T}_N \to \mathbb{C}$ from (C.25) and (C.26), and their asymptotic analogues $\mathcal{T}$ and $z : \mathbb{C} \setminus \mathcal{T} \to \mathbb{C}$ from (A.3) and (A.4).

Lemma 24 *Suppose Assumption 5 holds, and Assumption 6 holds with $r = 0$. Then, as $N \to \infty$,*

(a) $z_N(\tilde{m})$ and its derivative $z_N'(\tilde{m})$ converge uniformly over compact subsets of $\mathbb{C} \setminus \mathcal{T}$ to $z(\tilde{m})$ and $z'(\tilde{m})$.

(b) For any $\varepsilon > 0$ and all large N,

$$\operatorname{supp}(\tilde{\mu}_N) \subseteq \operatorname{supp}(\tilde{\mu}) + (-\varepsilon, \varepsilon).$$

(c) $\tilde{m}_N(z)$ and its derivative $\tilde{m}'_N(z)$ converge uniformly over compact subsets of $\mathbb{C} \setminus \operatorname{supp}(\tilde{\mu})$ to $\tilde{m}(z)$ and $\tilde{m}'(z)$.

Proof. For part (a), let $K \subset \mathbb{C} \setminus \mathcal{T}$ be any fixed compact set. Then K does not intersect some sufficiently small open neighborhood of the compact domain $\mathcal{T}$. If Assumption 6 holds with $r = 0$, then $\mathcal{T}_N$ is contained in this open neighborhood of $\mathcal{T}$ for all large N, so $K \subset \mathbb{C} \setminus \mathcal{T}_N$, and both z_N and z are well-defined on K. The pointwise convergences $z_N(\tilde{m}) \to z(\tilde{m})$ and $z'_N(\tilde{m}) \to z'(\tilde{m})$ on K then follow from $\gamma_N \to \gamma$, the weak convergence $\nu_N \to \nu$, and the uniform boundedness of the functions $\lambda \mapsto \lambda/(1 + \lambda\tilde{m})$ and $\lambda \mapsto \lambda^2/(1 + \lambda\tilde{m})^2$ on an open neighborhood of $\operatorname{supp}(\nu)$, for $\tilde{m} \in K$. This convergence is furthermore uniform because $\{z_N\}$ and $\{z'_N\}$ are both equicontinuous over K.

For part (b), consider any $x \notin \operatorname{supp}(\tilde{\mu}) + (-\varepsilon, \varepsilon)$. Then $[x - \varepsilon/2, x + \varepsilon/2] \subset \mathbb{R} \setminus \operatorname{supp}(\tilde{\mu})$, so $\tilde{m}$ is well-defined and increasing on $[x - \varepsilon/2, x + \varepsilon/2]$. Let $[\tilde{m}_-, \tilde{m}_+] = [\tilde{m}(x - \varepsilon/2), \tilde{m}(x + \varepsilon/2)]$. Then by Proposition 9, $z'(\tilde{m}) > 0$ for all $\tilde{m} \in [\tilde{m}_-, \tilde{m}_+]$, and $z([\tilde{m}_-, \tilde{m}_+]) = [x - \varepsilon/2, x + \varepsilon/2]$. The uniform convergence in part (a) implies for all large N that $z_N(\tilde{m}_-) < x$, $z_N(\tilde{m}_+) > x$, and $z'_N(\tilde{m}) > 0$ for all $\tilde{m} \in [\tilde{m}_-, \tilde{m}_+]$. Then there exists $\tilde{m} \in [\tilde{m}_-, \tilde{m}_+]$ where $z_N(\tilde{m}) = x$ and $z'_N(\tilde{m}) > 0$, implying by Proposition 9 that $x \notin \operatorname{supp}(\tilde{\mu}_N)$. So $\operatorname{supp}(\tilde{\mu}_N) \subseteq \operatorname{supp}(\tilde{\mu}) + (-\varepsilon, \varepsilon)$ as desired.

For part (c), let $K \subset \mathbb{C} \setminus \operatorname{supp}(\tilde{\mu})$ be any fixed compact set. Then K does not intersect some sufficiently small open neighborhood of the compact set $\operatorname{supp}(\tilde{\mu})$, so the inclusion of part (b) implies $K \subset \mathbb{C} \setminus \operatorname{supp}(\tilde{\mu}_N)$ for all large N, and both $\tilde{m}_N$ and $\tilde{m}$ are well-defined on K. The uniform convergence $\tilde{m}_N(z) \to \tilde{m}(z)$ and $\tilde{m}'_N(z) \to \tilde{m}'(z)$ on K then follow from the weak convergence $\tilde{\mu}_N \to \tilde{\mu}$, the uniform boundedness of the functions $\lambda \mapsto 1/(\lambda - z)$ and $\lambda \mapsto 1/(\lambda - z)^2$ on an open neighborhood of $\operatorname{supp}(\tilde{\mu})$ for $z \in K$, and the equicontinuity of $\{\tilde{m}_N\}$ and $\{\tilde{m}'_N\}$ on K. ■

Proof of Corollary 12. By Lemma 24(b), for any fixed $\varepsilon > 0$, we have $\mathcal{S}_N + (-\varepsilon/2, \varepsilon/2) \subseteq \mathcal{S} + (-\varepsilon, \varepsilon)$ for all large N. Then by Theorem 10,

$$\begin{aligned}&\mathbf{1}\{\boldsymbol{K} \text{ has an eigenvalue in } \mathbb{R} \setminus (\mathcal{S} + (-\varepsilon, \varepsilon))\\&\leq \mathbf{1}\{\boldsymbol{K} \text{ has an eigenvalue in } \mathbb{R} \setminus (\mathcal{S}_N + (-\varepsilon/2, \varepsilon/2))\} \prec 0.\end{aligned}$$

■

D.2. Deterministic equivalents for generalized resolvents

We next introduce two generalized resolvents for the matrix $\boldsymbol{K}$, and extend Theorem 11 to establish deterministic equivalents for these generalized resolvents.

Define the spectral domain

$$U(\varepsilon) = \left\{z \in \mathbb{C} : |z| \leq \varepsilon^{-1},\ \operatorname{dist}(z, \mathcal{S}) \geq \varepsilon\right\}$$

where $\mathcal{S}$ is the limit support set defined in (B.4). Given $z \in U(\varepsilon)$ and $\alpha \in \mathbb{C}$, define a diagonal matrix

$$\boldsymbol{\Gamma} := \boldsymbol{\Gamma}(z,\alpha) = z\boldsymbol{I}_n + \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top = \begin{pmatrix} (z+\alpha)\boldsymbol{I}_r & \boldsymbol{0} \\ \boldsymbol{0} & z\boldsymbol{I}_{n-r} \end{pmatrix} \in \mathbb{C}^{n\times n}, \quad \boldsymbol{V}_r = \begin{pmatrix} \boldsymbol{I}_r \\ \boldsymbol{0} \end{pmatrix} \in \mathbb{R}^{n\times r}. \tag{D.1}$$

Define the first generalized resolvent

$$\boldsymbol{\mathcal{R}}(z,\alpha) = \begin{pmatrix} -\boldsymbol{\Gamma} & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I}_N \end{pmatrix}^{-1} \in \mathbb{C}^{(n+N)\times(n+N)}. \tag{D.2}$$

This matrix inverse exists if and only if the Schur complement $\boldsymbol{G}^\top \boldsymbol{G} - \boldsymbol{\Gamma} = \boldsymbol{K} - \boldsymbol{\Gamma}$ for its lower right block is invertible, in which case the upper-left block of $\boldsymbol{\mathcal{R}}(z,\alpha)$ is $\boldsymbol{R}(\boldsymbol{\Gamma}) = (\boldsymbol{K} - \boldsymbol{\Gamma})^{-1}$. The following provides a deterministic equivalent for this block of $\boldsymbol{\mathcal{R}}(z,\alpha)$.

Lemma 25 *Under the assumptions of Theorem 13, for any fixed $\varepsilon > 0$, there exist $C_0, \alpha_0 > 0$ (depending on ε) such that fixing any $\alpha \in \mathbb{C}$ with $|\alpha| > \alpha_0$, the following hold:*

(a) The event

$$\mathcal{E} = \Big\{ \boldsymbol{\mathcal{R}}(z,\alpha) \text{ exists and } \|\boldsymbol{\mathcal{R}}(z,\alpha)\| \le C_0 \text{ for all } z \in U(\varepsilon) \Big\}$$

satisfies $\mathbf{1}\{\mathcal{E}^c\} \prec 0$.

(b) Uniformly over $z \in U(\varepsilon)$ and deterministic unit vectors $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^n$,

$$\left\| \begin{pmatrix} \boldsymbol{v}_1^\top & \boldsymbol{0} \end{pmatrix} \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{v}_2 \\ \boldsymbol{0} \end{pmatrix} + \boldsymbol{v}_1^\top (\boldsymbol{\Gamma} + z \cdot \tilde{m}_{N,0}(z)\boldsymbol{\Sigma})^{-1} \boldsymbol{v}_2 \right\| \prec \frac{1}{\sqrt{N}}. \tag{D.3}$$

In the setting of Theorem 13(c), let $\boldsymbol{u} = \frac{1}{\sqrt{N}}(u_1, \ldots, u_N) \in \mathbb{R}^N$ be the additional given vector for which $\{(u_j, \boldsymbol{g}_j^\top)\}_{j=1}^N$ are independent vectors in $\mathbb{R}^{n+1}$. For $z \in U(\varepsilon)$ and $\alpha \in \mathbb{C}$, define

$$\widetilde{\boldsymbol{\Sigma}} = \begin{pmatrix} \mathbb{E}[u^2] & \mathbb{E}[u\boldsymbol{g}]^\top \\ \mathbb{E}[u\boldsymbol{g}] & \boldsymbol{\Sigma} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}, \tag{D.4}$$

$$\widetilde{\boldsymbol{\Gamma}} = \widetilde{\boldsymbol{\Gamma}}(z,\alpha) = \begin{pmatrix} z+\alpha & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Gamma} \end{pmatrix} \in \mathbb{C}^{(n+1)\times(n+1)}$$

where $\mathbb{E}[u^2]$ and $\mathbb{E}[u\boldsymbol{g}]$ denote the common values of $\mathbb{E}[u_j^2]$ and $\mathbb{E}[u_j \boldsymbol{g}_j]$ for $j = 1, \ldots, N$. Define the second generalized resolvent

$$\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha) = \begin{pmatrix} -\widetilde{\boldsymbol{\Gamma}} & [\boldsymbol{u}, \boldsymbol{G}]^\top \\ [\boldsymbol{u}, \boldsymbol{G}] & -\boldsymbol{I} \end{pmatrix}^{-1} = \begin{pmatrix} -(z+\alpha) & \boldsymbol{0} & \boldsymbol{u}^\top \\ \boldsymbol{0} & -\boldsymbol{\Gamma} & \boldsymbol{G}^\top \\ \boldsymbol{u} & \boldsymbol{G} & -\boldsymbol{I}_N \end{pmatrix}^{-1} \in \mathbb{C}^{(n+1+N)\times(n+1+N)}. \tag{D.5}$$

We have the following deterministic equivalent for the upper-left block of $\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)$, which is analogous to Lemma 25.

Lemma 26 *Under the assumptions of Theorem 13(c), for any fixed $\varepsilon > 0$, there exist $C_0, \alpha_0 > 0$ (depending on ε) such that fixing any $\alpha \in \mathbb{C}$ with $|\alpha| > \alpha_0$, the following hold:*

(a) The event

$$\widetilde{\mathcal{E}} = \Big\{ \widetilde{\mathcal{R}}(z,\alpha) \text{ exists and } \|\widetilde{\mathcal{R}}(z,\alpha)\| \le C_0 \text{ for all } z \in U(\varepsilon) \Big\}$$

satisfies $\mathbf{1}\{\widetilde{\mathcal{E}}^c\} \prec 0$.

(b) Uniformly over $z \in U(\varepsilon)$ *and deterministic unit vectors* $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^{n+1}$,

$$\left\| \begin{pmatrix} \boldsymbol{v}_1^\top & \mathbf{0} \end{pmatrix} \widetilde{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{v}_2 \\ \mathbf{0} \end{pmatrix} + \boldsymbol{v}_1^\top \Big(\widetilde{\boldsymbol{\Gamma}} + z \cdot \tilde{m}_{N,0}(z) \widetilde{\boldsymbol{\Sigma}} \Big)^{-1} \boldsymbol{v}_2 \right\| \prec \frac{1}{\sqrt{N}}. \tag{D.6}$$

In the remainder of this section, we prove Lemmas 25 and 26. Recall

$$\mu_{N,0} = \rho^{\text{MP}}_{\gamma_{N,0}} \boxtimes \nu_{N,0}, \qquad \tilde{\mu}_{N,0} = \gamma_{N,0}\mu_{N,0} + (1-\gamma_{N,0})\delta_0.$$

Define the bulk components of the sample covariance and Gram matrices

$$\boldsymbol{K}_0 = \boldsymbol{G}_0^\top \boldsymbol{G}_0 \in \mathbb{R}^{(n-r)\times(n-r)}, \qquad \widetilde{\boldsymbol{K}}_0 = \boldsymbol{G}_0 \boldsymbol{G}_0^\top \in \mathbb{R}^{N\times N}. \tag{D.7}$$

Define also the N-dependent bulk spectral support and spectral domain

$$\begin{aligned} \mathcal{S}_{N,0} &= \operatorname{supp}(\mu_{N,0}) \cup \{0\} = \operatorname{supp}(\tilde{\mu}_{N,0}) \cup \{0\}, \\ U_{N,0}(\varepsilon) &= \{ z \in \mathbb{C} : |z| \le \varepsilon^{-1}, \operatorname{dist}(z, \mathcal{S}_{N,0}) \ge \varepsilon \}. \end{aligned} \tag{D.8}$$

Lemma 24(b) shows $\mathcal{S}_{N,0} \subseteq \mathcal{S} + (-\varepsilon/2, \varepsilon/2)$ for any fixed $\varepsilon > 0$ and all large N, so also $U(\varepsilon) \subseteq U_{N,0}(\varepsilon/2)$ for all large N. Thus, the results of Appendix C applied to $\boldsymbol{K}_0$, which hold uniformly over $z \in U_{N,0}(\varepsilon/2)$ for any fixed $\varepsilon > 0$, also hold uniformly over $z \in U(\varepsilon)$. In particular, the following is an immediate consequence of Corollary 12 and Theorem 11, which we record here for future reference.

Lemma 27 *Suppose Assumptions 5 and 6 hold. Then for any fixed* $\varepsilon > 0$,

$$\mathbf{1}\{\boldsymbol{K}_0 \text{ has an eigenvalue outside } \mathcal{S} + (-\varepsilon, \varepsilon)\} \prec 0.$$

Furthermore, uniformly over $z \in U(\varepsilon)$,

$$m_{\boldsymbol{K}_0} - m_{N,0}(z) \prec 1/N, \quad m_{\tilde{\boldsymbol{K}}_0} - \tilde{m}_{N,0}(z) \prec 1/N.$$

We now check that for sufficiently large $|\alpha|$, the generalized resolvent $\mathcal{R}(z,\alpha)$ exists and has bounded operator norm with high probability.

Proof of Lemma 25(a). Let

$$\mathcal{E}' = \Big\{ \text{all eigenvalues of } \boldsymbol{K}_0 \text{ belong to } \mathcal{S} + (-\varepsilon/2, \varepsilon/2), \text{ and } \|\boldsymbol{G}\| < \sqrt{B} \Big\}.$$

By Assumption 5(b) and Lemma 27, $\mathbf{1}\{\mathcal{E}'^c\} \prec 0$, so it suffices to show $\mathcal{E}' \subseteq \mathcal{E}$. On this event $\mathcal{E}'$, for any $z \in U(\varepsilon)$, we have that each eigenvalue of $\boldsymbol{K}_0$ is separated by at least $\varepsilon/2$ from z. Then

$$\mathcal{R}_0(z) := \begin{pmatrix} -z\boldsymbol{I}_{n-r} & \boldsymbol{G}_0^\top \\ \boldsymbol{G}_0 & -\boldsymbol{I}_N \end{pmatrix}^{-1} \in \mathbb{C}^{(n-r+N)\times(n-r+N)} \tag{D.9}$$

exists for all $z \in U(\varepsilon)$ because the Schur complement $\boldsymbol{K}_0 - z\boldsymbol{I}_{n-r}$ of its lower-right block is invertible. Furthermore, denoting $\boldsymbol{R}_0 = (\boldsymbol{K}_0 - z\boldsymbol{I}_{n-r})^{-1}$, we have $\|\boldsymbol{R}_0\| \le 2/\varepsilon$ and $\|\boldsymbol{G}_0\| \le \|\boldsymbol{G}\| < \sqrt{B}$, so

$$\|\boldsymbol{\mathcal{R}}_0(z)\| = \left\| \begin{pmatrix} \boldsymbol{R}_0 & \boldsymbol{R}_0\boldsymbol{G}_0^\top \\ \boldsymbol{G}_0\boldsymbol{R}_0 & \boldsymbol{G}_0\boldsymbol{R}_0\boldsymbol{G}_0^\top - \boldsymbol{I}_N \end{pmatrix} \right\| \le C_1 \tag{D.10}$$

for some constant C_1 depending only on ε, B.

Now write $\boldsymbol{\mathcal{R}}(z,\alpha)$ as defined in (D.2) in its block decomposition with blocks of sizes r and $n-r+N$. Then the Schur complement of the upper left block of size $r \times r$ is given by

$$\boldsymbol{S} = -\begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix} \boldsymbol{\mathcal{R}}_0(z) \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix} - (\alpha+z)\boldsymbol{I}_r. \tag{D.11}$$

Notice that

$$\boldsymbol{S}\boldsymbol{S}^* = |\alpha+z|^2\boldsymbol{I}_r + \begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix} \boldsymbol{\mathcal{R}}_0(z) \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix} \begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix} \overline{\boldsymbol{\mathcal{R}}_0(z)} \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix} \tag{D.12}$$

$$+ (\bar{\alpha}+\bar{z}) \begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix} \boldsymbol{\mathcal{R}}_0(z) \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix} + (\alpha+z) \begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix} \overline{\boldsymbol{\mathcal{R}}_0(z)} \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix} \tag{D.13}$$

where the first two terms are positive semi-definite. Therefore, applying (D.10) and $\|\boldsymbol{G}_r\| \le \|\boldsymbol{G}\| < \sqrt{B}$ on the event $\mathcal{E}'$, there exist $\alpha_0, c_0 > 0$ depending only on ε, B, such that

$$\lambda_{\min}(\boldsymbol{S}\boldsymbol{S}^*) \ge |\alpha+z|^2 - 2(|\alpha|+|z|)\|\boldsymbol{G}_r\|^2\|\boldsymbol{\mathcal{R}}_0(z)\| > c_0 \tag{D.14}$$

for any $z \in U(\varepsilon)$ and $|\alpha| > \alpha_0$. Consequently, under the event $\mathcal{E}'$, the Schur complement $\boldsymbol{S}$ in (D.11) is invertible with $\|\boldsymbol{S}^{-1}\| < c_0^{-1/2}$. Then $\boldsymbol{\mathcal{R}}(z,\alpha)$ exists, and

$$\|\boldsymbol{\mathcal{R}}(z,\alpha)\| = \left\| \begin{pmatrix} \boldsymbol{S}^{-1} & -\boldsymbol{S}^{-1}\begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix}\boldsymbol{\mathcal{R}}_0(z) \\ -\boldsymbol{\mathcal{R}}_0(z)\begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix}\boldsymbol{S}^{-1} & \boldsymbol{\mathcal{R}}_0(z) + \boldsymbol{\mathcal{R}}_0(z)\begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{G}_r \end{pmatrix}\boldsymbol{S}^{-1}\begin{pmatrix} \boldsymbol{0} & \boldsymbol{G}_r^\top \end{pmatrix}\boldsymbol{\mathcal{R}}_0(z) \end{pmatrix} \right\| \le C_0 \tag{D.15}$$

for a constant $C_0 > 0$ depending only on ε, B. This shows $\mathcal{E}' \subseteq \mathcal{E}$ as desired. ■

For the matrix $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}(z,\alpha)$ in (D.1), recall the definitions of $\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})$ and $\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})$ from (C.1). The following provides an analogue of Lemma 23 for these quantities.

Lemma 28 *Fix any $\varepsilon > 0$ and $L \ge 1$. Then there exist $C_0, c_0, \alpha_0 > 0$ such that for any fixed $\alpha \in \mathbb{C}$ with $|\alpha| > \alpha_0$, uniformly over $S \subset [N]$ with $|S| \le L$, over $j \in S$, and over $z \in U(\varepsilon)$,*

$$\boldsymbol{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| > C_0\} \prec 0, \quad \boldsymbol{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| < c_0\} \prec 0, \quad \boldsymbol{1}\{\|(z^{-1}\boldsymbol{\Gamma} + \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\| > C_0\} \prec 0,$$
$$\boldsymbol{1}\{\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| > C_0\} \prec 0, \quad \boldsymbol{1}\{|1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})| < c_0\} \prec 0,$$
$$\boldsymbol{1}\{|1 + N^{-1}\boldsymbol{g}_j^\top\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{g}_j| < c_0\} \prec 0.$$

Proof. Suppose $|\alpha|$ is large enough so that Lemma 25(a) holds. Since $\boldsymbol{R}(\boldsymbol{\Gamma})$ is the upper-left block of $\boldsymbol{\mathcal{R}}(z,\alpha)$, Lemma 25(a) applied with $\boldsymbol{G}^{(S)}$ in place of $\boldsymbol{G}$ shows that $\mathbf{1}\{\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| > C_0\} \prec 0$ for a constant $C_0 > 0$, uniformly over $S \subset [N]$ with $|S| \leq L$ and over $z \in U(\varepsilon)$. For the remaining statements, let $\boldsymbol{G}_0^{(S)} \in \mathbb{R}^{(N-|S|)\times(n-r)}$ be the submatrix of $\boldsymbol{G}_0$ with the rows of S removed, and define

$$\boldsymbol{K}_0^{(S)} = \boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_0^{(S)}, \quad \widetilde{\boldsymbol{K}}_0^{(S)} = \boldsymbol{G}_0^{(S)}\boldsymbol{G}_0^{(S)\top},$$

$$\boldsymbol{R}_0^{(S)} = (\boldsymbol{K}_0^{(S)} - z\boldsymbol{I}_{n-r})^{-1}, \quad m_{\boldsymbol{K}_0}^{(S)} = \frac{1}{n-r}\operatorname{Tr}\boldsymbol{R}_0^{(S)}, \quad \tilde{m}_{\boldsymbol{K}_0}^{(S)} = \gamma_{N,0}m_{\boldsymbol{K}_0}^{(S)} + (1-\gamma_{N,0})\Big(-\frac{1}{z}\Big).$$

Then by Lemma 27 applied to $\boldsymbol{K}_0^{(S)}$, also $\mathbf{1}\{\|\boldsymbol{R}_0^{(S)}\| > C_0\} \prec 0$ for a constant $C_0 > 0$.

Using these bounds, we first show the comparisons

$$|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) - \tilde{m}_{\boldsymbol{K}_0}^{(S)}| \prec 1/N, \quad \Big|N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) - N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}_0\boldsymbol{R}_0^{(S)}\Big| \prec 1/N. \tag{D.16}$$

For the first comparison, notice that in the decompositions into blocks of sizes r and $n-r$,

$$\frac{n-r}{n}m_{\boldsymbol{K}_0}^{(S)} = \frac{1}{n}\operatorname{Tr}\begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{R}_0^{(S)}\end{pmatrix}$$

and

$$\begin{aligned} m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) &= \frac{1}{n}\operatorname{Tr}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\\ &= \frac{1}{n}\operatorname{Tr}\begin{pmatrix}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_r^{(S)} - (\alpha+z)\boldsymbol{I}_r & \boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\\ \boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)} & \boldsymbol{K}_0^{(S)} - z\boldsymbol{I}_{N-|S|}\end{pmatrix}^{-1}\\ &= \frac{1}{n}\operatorname{Tr}\begin{pmatrix}(\boldsymbol{S}_r^{(S)})^{-1} & -(\boldsymbol{S}_r^{(S)})^{-1}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}\\ -\boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)}(\boldsymbol{S}_r^{(S)})^{-1} & \boldsymbol{R}_0^{(S)} + \boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)}(\boldsymbol{S}_r^{(S)})^{-1}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}\end{pmatrix}, \end{aligned}$$

where

$$\boldsymbol{S}_r^{(S)} := \boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_r^{(S)} - (\alpha+z)\boldsymbol{I}_r - \boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)} \tag{D.17}$$

is the Schur complement of the lower-right block. We have $\|(\boldsymbol{S}_r^{(S)})^{-1}\| \leq \|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| \prec 1$, $\|\boldsymbol{R}_0^{(S)}\| \prec 1$, and by Assumption 5, $\|\boldsymbol{G}_0^{(S)}\| \prec 1$ and $\|\boldsymbol{G}_r^{(S)}\| \prec 1$. Combining these bounds and using $|\operatorname{Tr}\boldsymbol{A}| \leq r\|\boldsymbol{A}\|$ when $\boldsymbol{A}$ has rank r (as follows from the von Neumann trace inequality),

$$\begin{aligned} &\Big|m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) - \frac{n-r}{n}m_{\boldsymbol{K}_0}^{(S)}\Big|\\ &= \left|\frac{1}{n}\operatorname{Tr}\begin{pmatrix}(\boldsymbol{S}_r^{(S)})^{-1} & -(\boldsymbol{S}_r^{(S)})^{-1}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}\\ -\boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)}(\boldsymbol{S}_r^{(S)})^{-1} & \boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)}(\boldsymbol{S}_r^{(S)})^{-1}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}\end{pmatrix}\right|\\ &\leq \frac{1}{n}|\operatorname{Tr}(\boldsymbol{S}_r^{(S)})^{-1}| + \frac{1}{n}|\operatorname{Tr}\boldsymbol{R}_0^{(S)}\boldsymbol{G}_0^{(S)\top}\boldsymbol{G}_r^{(S)}(\boldsymbol{S}_r^{(S)})^{-1}\boldsymbol{G}_r^{(S)\top}\boldsymbol{G}_0^{(S)}\boldsymbol{R}_0^{(S)}|\\ &\leq \frac{r}{n}\|(\boldsymbol{S}_r^{(S)})^{-1}\| + \frac{r}{n}\|\boldsymbol{G}_r^{(S)}\|^2\|\boldsymbol{G}_0^{(S)}\|^2\|\boldsymbol{R}_0^{(S)}\|^2\|(\boldsymbol{S}_r^{(S)})^{-1}\| \prec 1/N. \end{aligned}$$

Then also $|m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) - m_{\boldsymbol{K}_0}^{(S)}| \prec 1/N$ since $|m_{\boldsymbol{K}_0}^{(S)}| \leq \|\boldsymbol{R}_0^{(S)}\| \prec 1$ and $(n-r)/n = 1 + O_\prec(1/N)$. Hence $|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) - \tilde{m}_{\boldsymbol{K}_0}^{(S)}| \prec 1/N$ from the definitions $\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) = \gamma_N m_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma}) + (1-\gamma_N)(-1/z)$

and $\tilde{m}_{\boldsymbol{K}_0}^{(S)} = \gamma_{N,0} m_{\boldsymbol{K}_0}^{(S)} + (1-\gamma_{N,0})(-1/z)$, as $|1/z| \le \varepsilon$ for $z \in U(\varepsilon)$ and $\gamma_{N,0} = \gamma_N + O_{\prec}(1/N)$. The proof of the second comparison of (D.16) is analogous, considering in addition

$$\frac{1}{n}\operatorname{Tr}\left(\boldsymbol{\Sigma} - \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_0 \end{pmatrix}\right)\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) = \frac{1}{n}\operatorname{Tr}\begin{pmatrix} \boldsymbol{\Sigma}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) \le \frac{r}{n}\|\boldsymbol{\Sigma}_r\|\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| \prec \frac{1}{N}. \tag{D.18}$$

Now, Lemma 23 applied with $\boldsymbol{K}_0$ shows, uniformly over $S \subset [N]$ with $|S| \le L$ and over $z \in U(\varepsilon)$,

$$\mathbf{1}\{|\tilde{m}_{\boldsymbol{K}_0}^{(S)}| > C_0\} \prec 0, \quad \mathbf{1}\{|\tilde{m}_{\boldsymbol{K}_0}^{(S)}| < c_0\} \prec 0, \quad \mathbf{1}\{|1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}_0\boldsymbol{R}_0^{(S)}| < c_0\} \prec 0,$$

which together with (D.16) implies

$$\mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| > C_0\} \prec 0, \quad \mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| < c_0\} \prec 0, \quad \mathbf{1}\{|1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})| < c_0\} \prec 0$$

for adjusted constants $C_0, c_0 > 0$. Also by Assumption 5, uniformly over $j \in S$,

$$N^{-1}\boldsymbol{g}_j^\top \boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{g}_j - N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma}) \prec N^{-1}\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\|_F \le N^{-1/2}\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| \prec N^{-1/2}, \tag{D.19}$$

so $\mathbf{1}\{|1 + N^{-1}\boldsymbol{g}_j^\top \boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{g}_j| < c\} \prec 0$ for a constant $c > 0$. Lastly, from the definition of $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}(z,\alpha)$ in (D.1), we have

$$z^{-1}\boldsymbol{\Gamma} + \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma} = \begin{pmatrix} \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}_r + (\frac{\alpha}{z}+1)\boldsymbol{I}_r & \mathbf{0} \\ \mathbf{0} & \tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}_0 + \boldsymbol{I}_{n-r} \end{pmatrix}. \tag{D.20}$$

By (D.16) and Lemma 23, we have

$$\mathbf{1}\left\{\left\|\left(\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}_0 + \boldsymbol{I}_{n-r}\right)^{-1}\right\| > C\right\} \prec 0 \tag{D.21}$$

for some constant $C > 0$. We have already proved $\mathbf{1}\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| > C_0\} \prec 0$, and applying $\|\boldsymbol{\Sigma}_r\| \le C$ under Assumption 5, we can deduce for the smallest singular value that

$$\sigma_{\min}\left(\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}_r + (\alpha/z+1)\boldsymbol{I}_r\right) \ge \frac{|\alpha|}{|z|} - 1 - |\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})|\|\boldsymbol{\Sigma}_r\| \ge c \tag{D.22}$$

on the event $\{|\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})| \le C_0\}$, for any $z \in U(\varepsilon)$, $|\alpha| \ge \alpha_0$, and some $\alpha_0, c > 0$ depending on ε, C_0. Thus also

$$\mathbf{1}\{\|(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\| > C\} \prec 0 \tag{D.23}$$

for a constant $C > 0$, showing all statements of the lemma. ■

Proof of Lemma 25(b). Recalling the form of $\boldsymbol{\mathcal{R}}(z,\alpha)$ in (D.2), the quantity we wish to approximate is

$$\begin{pmatrix} \boldsymbol{v}_1^\top & \mathbf{0} \end{pmatrix}\boldsymbol{\mathcal{R}}(z,\alpha)\begin{pmatrix} \boldsymbol{v}_2 \\ \mathbf{0} \end{pmatrix} = \boldsymbol{v}_1^\top \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{v}_2 = \boldsymbol{v}_1^\top(\boldsymbol{K} - \boldsymbol{\Gamma})^{-1}\boldsymbol{v}_2.$$

Analogous to (C.29) in the proof of Lemma 19, for any matrix $\boldsymbol{B} \in \mathbb{C}^{n\times n}$, we have

$$\operatorname{Tr} \boldsymbol{B} = \operatorname{Tr}(\boldsymbol{K} - \boldsymbol{\Gamma})\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B} = -\operatorname{Tr} \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Gamma} + \frac{1}{N}\sum_{i=1}^{N} \frac{\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{g}_i}{1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i}. \tag{D.24}$$

Applying the definition $m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) = N^{-1}\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma}) + (1-\gamma_N)(-1/z)$ and the identity (D.24) with $\boldsymbol{B} = \boldsymbol{I}$, we obtain analogously to (C.30) that

$$\begin{aligned} m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) &= (1-\gamma_N)(-1/z) + \frac{1}{Nz}\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{\Gamma} - \frac{1}{N}\operatorname{Tr}(z^{-1}\boldsymbol{\Gamma} - \boldsymbol{I})\boldsymbol{R}(\boldsymbol{\Gamma}) \\ &= -\frac{1}{Nz}\sum_{i=1}^{N}\frac{1}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i} - \frac{1}{N}\operatorname{Tr}(z^{-1}\boldsymbol{\Gamma} - \boldsymbol{I})\boldsymbol{R}(\boldsymbol{\Gamma}). \end{aligned}$$

Then, noting that $z^{-1}\boldsymbol{\Gamma} - \boldsymbol{I}$ has rank r and hence $|N^{-1}\operatorname{Tr}(z^{-1}\boldsymbol{\Gamma} - \boldsymbol{I})\boldsymbol{R}(\boldsymbol{\Gamma})| \leq \frac{r}{N}\frac{|\alpha|}{|z|}\|\boldsymbol{R}(\boldsymbol{\Gamma})\| \prec N^{-1}$, this gives

$$m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) = -\frac{1}{Nz}\sum_{i=1}^{N}\frac{1}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i} + O_\prec\big(N^{-1}\big). \tag{D.25}$$

Fixing the unit vectors $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^n$, let us now choose $\boldsymbol{A} = \boldsymbol{v}_2\boldsymbol{v}_1^\top$ and $\boldsymbol{B} = \boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\cdot\boldsymbol{\Sigma})^{-1}$ in (D.24), and define

$$\begin{aligned} d_i &= \frac{1}{N}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{g}_i - \frac{1}{N}\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Sigma} \\ &= \frac{1}{N}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}\big(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}\big)^{-1}\boldsymbol{g}_i - \frac{1}{N}\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{A}\big(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma}\big)^{-1}\boldsymbol{\Sigma}. \end{aligned}$$

Then, combining (D.24) and (D.25), we get

$$\begin{aligned} &\boldsymbol{v}_1^\top(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{v}_2 = \operatorname{Tr}\boldsymbol{B} \\ &= -\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Gamma} + \operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Sigma}\cdot\big(-zm_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) + O_\prec\big(N^{-1}\big)\big) + \sum_{i=1}^{N}\frac{d_i}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i} \\ &= -z\cdot\boldsymbol{v}_1^\top \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{v}_2 + \sum_{i=1}^{N}\frac{d_i}{1+N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i} + O_\prec\big(N^{-1}\big), \end{aligned} \tag{D.26}$$

where the last equality applies the definition of $\boldsymbol{B}$ to combine the first two terms, and applies also $|\operatorname{Tr}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{B}\boldsymbol{\Sigma}| \leq \|(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})\| \prec 1$ by Lemma 28 to obtain the $O_\prec\big(N^{-1}\big)$ remainder.

Considering a similar decomposition as in Lemma 19, we define $d_i = d_{i,1} + d_{i,2} + d_{i,3} + d_{i,4}$ where

$$\begin{aligned} d_{i,1} &= \frac{1}{N}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i - \frac{1}{N}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i, \\ d_{i,2} &= \frac{1}{N}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}\boldsymbol{g}_i - \frac{1}{N}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}, \\ d_{i,3} &= \frac{1}{N}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1} - \frac{1}{N}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}, \\ d_{i,4} &= \frac{1}{N}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1} - \frac{1}{N}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{A}(z^{-1}\boldsymbol{\Gamma} + m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma})\boldsymbol{\Sigma})^{-1}. \end{aligned} \tag{D.27}$$

For $\boldsymbol{A} = \boldsymbol{v}_2\boldsymbol{v}_1^\top$, by the bound $\mathbf{1}\{\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\| > C_0\} \prec 0$ from Lemma 28, we have for a constant $C > 0$ that

$$\mathbf{1}\Big\{\Big\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\Big\|_F > C\sqrt{N}\Big\} \prec 0, \quad \mathbf{1}\Big\{\Big\|\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})\boldsymbol{A}\Big\|_F > C\Big\} \prec 0 \tag{D.28}$$

uniformly over $z \in U(\varepsilon)$. Then, employing Lemma 28 and the same bounds as (C.35)–(C.38) from the proof of Lemma 23 (where here, the bounds for $\|\boldsymbol{R}^{(i)}\boldsymbol{A}\|_F, \|\boldsymbol{R}\boldsymbol{A}\|_F$ are improved by a factor of $N^{-1/2}$ because $\boldsymbol{A}$ is low-rank), we conclude that $|d_{i,1}|, |d_{i,3}|, |d_{i,4}| \prec N^{-3/2}$ and $|d_{i,2}| \prec N^{-1}$. Hence, applying also $1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i = 1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma}) + O_\prec\big(N^{-1/2}\big)$ as follows from (D.19) and the bound (C.33),

$$\sum_{i=1}^N \frac{d_i}{1 + N^{-1}\boldsymbol{g}_i^\top \boldsymbol{R}^{(i)}(\boldsymbol{\Gamma})\boldsymbol{g}_i} = \frac{1}{1 + N^{-1}\operatorname{Tr}\boldsymbol{\Sigma}\boldsymbol{R}(\boldsymbol{\Gamma})} \cdot \sum_{i=1}^N d_{i,2} + O_\prec\Big(N^{-1/2}\Big).$$

By Lemma 14 applied with $\Psi_N(\boldsymbol{\Gamma}) = C\sqrt{N}$ and $\Phi_N(\boldsymbol{\Gamma}, \boldsymbol{A}) = C$ for a constant $C > 0$, we have $|\sum_i d_{i,2}| \prec N^{-1/2}$. Thus the above quantity is of size $O_\prec\big(N^{-1/2}\big)$, so applying this back to (D.26),

$$\boldsymbol{v}_1^\top(\boldsymbol{\Gamma} + z m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) \cdot \boldsymbol{\Sigma})^{-1}\boldsymbol{v}_2 + \boldsymbol{v}_1^\top \boldsymbol{R}(\boldsymbol{\Gamma})\boldsymbol{v}_2 \prec N^{-1/2}.$$

Finally, from (D.16) and Lemma 27 we have $m_{\tilde{\boldsymbol{K}}}(\boldsymbol{\Gamma}) = \tilde{m}_{N,0}(z) + O_\prec\big(N^{-1}\big)$, and applying this above completes the proof. ∎

Proof of Lemma 26. The proof is similar to Lemma 25, replacing r and n throughout by $r+1$ and $n+1$, $\boldsymbol{G}_r^{(S)}$ by $[\boldsymbol{u}^{(S)}, \boldsymbol{G}_r^{(S)}]$, $\boldsymbol{\Sigma}$ by $\widetilde{\boldsymbol{\Sigma}}$, and $\boldsymbol{R}^{(S)}(\boldsymbol{\Gamma})$ and $\tilde{m}_{\boldsymbol{K}}^{(S)}(\boldsymbol{\Gamma})$ by

$$\boldsymbol{R}^{(S)}(\widetilde{\boldsymbol{\Gamma}}) = \big([\boldsymbol{u}^{(S)}, \boldsymbol{G}^{(S)}]^\top[\boldsymbol{u}^{(S)}, \boldsymbol{G}^{(S)}] - \widetilde{\boldsymbol{\Gamma}}\big)^{-1}, \quad \tilde{m}_{\boldsymbol{K}}^{(S)}(\widetilde{\boldsymbol{\Gamma}}) = \frac{1}{N}\operatorname{Tr}\boldsymbol{R}^{(S)}(\widetilde{\boldsymbol{\Gamma}}) + \Big(1 - \frac{n+1}{N}\Big)\Big(-\frac{1}{z}\Big).$$

The only difference here is that $\widetilde{\boldsymbol{\Sigma}}$ is no longer diagonal, leading to the following minor modifications of the preceding proof: The bound

$$\frac{1}{n+1}\operatorname{Tr}\left(\widetilde{\boldsymbol{\Sigma}} - \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\Sigma}_0 \end{pmatrix}\right)\boldsymbol{R}^{(S)}(\widetilde{\boldsymbol{\Gamma}}) \prec \frac{1}{N}$$

analogous to (D.18) follows upon noting that (with $\mathbb{E}[u\boldsymbol{g}]^\top = \big(\mathbb{E}[u\boldsymbol{g}_r]^\top \quad \mathbb{E}[u\boldsymbol{g}_0]^\top\big)$)

$$\widetilde{\boldsymbol{\Sigma}} - \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\Sigma}_0 \end{pmatrix} = \begin{pmatrix} \mathbb{E}[u^2] & \mathbb{E}[u\boldsymbol{g}_r]^\top & \mathbb{E}[u\boldsymbol{g}_0]^\top \\ \mathbb{E}[u\boldsymbol{g}_r] & \boldsymbol{\Sigma}_r & \mathbf{0} \\ \mathbb{E}[u\boldsymbol{g}_0] & \mathbf{0} & \mathbf{0} \end{pmatrix}$$

still is of low rank, with rank at most $r+2$. Writing as shorthand $\tilde{m}_{\boldsymbol{K}}^{(S)} = \tilde{m}_{\boldsymbol{K}}^{(S)}(\widetilde{\boldsymbol{\Gamma}})$, the bound

$$\mathbf{1}\{\|(z^{-1}\widetilde{\boldsymbol{\Gamma}} + \tilde{m}_{\boldsymbol{K}}^{(S)}\widetilde{\boldsymbol{\Sigma}})^{-1}\| > C_0\} \prec 0$$

analogous to (D.23) follows from

$$(z^{-1}\widetilde{\boldsymbol{\Gamma}} + \tilde{m}_{\boldsymbol{K}}^{(S)}\widetilde{\boldsymbol{\Sigma}})^{-1} = \begin{pmatrix} \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u^2] + \frac{\alpha}{z} + 1 & \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_r]^\top & \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_0]^\top \\ \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_r] & \tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma}_r + (\frac{\alpha}{z} + 1)\boldsymbol{I}_r & \mathbf{0} \\ \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_0] & \mathbf{0} & \tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma}_0 + \boldsymbol{I} \end{pmatrix}^{-1},$$

the bound $\mathbf{1}\{\|\tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma}_0+\boldsymbol{I}\|^{-1}>C\}\prec 0$ for the lower-right block as follows from (D.21), and the bound for the inverse of its Schur-complement

$$\mathbf{1}\Bigg\{\Bigg\|\Bigg[\begin{pmatrix}\tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u^2]+\frac{\alpha}{z}+1 & \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_r]^\top \\ \tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_r] & \tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma}_r+(\frac{\alpha}{z}+1)\boldsymbol{I}_r\end{pmatrix}$$
$$-\begin{pmatrix}\tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_0]^\top \\ \mathbf{0}\end{pmatrix}(\tilde{m}_{\boldsymbol{K}}^{(S)}\boldsymbol{\Sigma}_0+\boldsymbol{I})^{-1}\Big(\tilde{m}_{\boldsymbol{K}}^{(S)}\mathbb{E}[u\boldsymbol{g}_0]\quad \mathbf{0}\Big)\Bigg]^{-1}\Bigg\|>C\Bigg\}\prec 0$$

which holds uniformly over $z\in U(\varepsilon)$ for any $|\alpha|>\alpha_0$ sufficiently large, by an argument analogous to (D.22). The remainder of the proof is identical to that of Lemma 25, and we omit the details. ■

D.3. Analysis of outliers

Let $\boldsymbol{V}_r,\boldsymbol{\Gamma}(z,\alpha),\boldsymbol{\mathcal{R}}(z,\alpha),\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)$ be as defined in the preceding section. Consider the decomposition of $\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)$ as in (D.5) into its blocks of dimensions 1, n, and N, and define

$$\widetilde{\mathcal{R}}_{11}(z,\alpha):=\begin{pmatrix}1\\0\\0\end{pmatrix}^\top\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)\begin{pmatrix}1\\0\\0\end{pmatrix}=\frac{1}{-z-\alpha+\boldsymbol{u}^\top\boldsymbol{u}-\boldsymbol{u}^\top\boldsymbol{G}(\boldsymbol{G}^\top\boldsymbol{G}-\boldsymbol{\Gamma}(z,\alpha))^{-1}\boldsymbol{G}^\top\boldsymbol{u}},\tag{D.29}$$

$$\widetilde{\boldsymbol{\mathcal{R}}}_{1V}(z,\alpha):=\begin{pmatrix}1\\0\\0\end{pmatrix}^\top\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)\begin{pmatrix}0\\\boldsymbol{V}_r\\0\end{pmatrix}=-\widetilde{\mathcal{R}}_{11}(z,\alpha)\cdot\boldsymbol{u}^\top\boldsymbol{G}\Big(\boldsymbol{G}^\top\boldsymbol{G}-\boldsymbol{\Gamma}(z,\alpha)\Big)^{-1}\boldsymbol{V}_r,\tag{D.30}$$

where the second equalities follow from block matrix inversion of the lower 2×2 blocks of $\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)$, followed by block matrix inversion of the full matrix $\widetilde{\boldsymbol{\mathcal{R}}}(z,\alpha)$. Set

$$\boldsymbol{M}_{\boldsymbol{K}}(z,\alpha)=\boldsymbol{I}_r+\alpha\big(\boldsymbol{V}_r^\top\quad\mathbf{0}\big)\boldsymbol{\mathcal{R}}(z,\alpha)\begin{pmatrix}\boldsymbol{V}_r\\\mathbf{0}\end{pmatrix}.\tag{D.31}$$

Proposition 29 *Fix any $\varepsilon>0$ and any $\alpha\in\mathbb{R}$ sufficiently large that satisfies Lemmas 25 and 26. Then on the event $\mathcal{E}\cap\widetilde{\mathcal{E}}$ of Lemmas 25 and 26, for all sufficiently large N,*

(a) $\widehat{\lambda}\in U(\varepsilon)\cap\mathbb{R}$ is an eigenvalue of $\boldsymbol{G}^\top\boldsymbol{G}$ if and only if $\det\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda},\alpha)=0$, and its multiplicity as an eigenvalue of $\boldsymbol{G}^\top\boldsymbol{G}$ equals the dimension of $\ker\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda},\alpha)$.

(b) Let $\widehat{\boldsymbol{v}}\in\mathbb{R}^n$ be a unit eigenvector of $\boldsymbol{G}^\top\boldsymbol{G}$ (i.e. right singular vector of $\boldsymbol{G}$) corresponding to an eigenvalue $\widehat{\lambda}\in U(\varepsilon)\cap\mathbb{R}$. Then $\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}$ is a non-zero vector in $\ker\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda},\alpha)$, and

$$\frac{1}{\alpha^2}=\widehat{\boldsymbol{v}}^\top\boldsymbol{V}_r\begin{pmatrix}\boldsymbol{V}_r\\\mathbf{0}\end{pmatrix}^\top\boldsymbol{\mathcal{R}}(\widehat{\lambda},\alpha)\begin{pmatrix}\boldsymbol{I}_n&\mathbf{0}\\\mathbf{0}&\mathbf{0}\end{pmatrix}\boldsymbol{\mathcal{R}}(\widehat{\lambda},\alpha)\begin{pmatrix}\boldsymbol{V}_r\\\mathbf{0}\end{pmatrix}\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}\tag{D.32}$$

For any vector $\boldsymbol{v}\in\mathbb{R}^n$, we have

$$\boldsymbol{v}^\top\widehat{\boldsymbol{v}}+\alpha\big(\boldsymbol{v}^\top\quad\mathbf{0}\big)\boldsymbol{\mathcal{R}}(\widehat{\lambda},\alpha)\begin{pmatrix}\boldsymbol{V}_r\\\mathbf{0}\end{pmatrix}\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}=0.\tag{D.33}$$

(c) *Let* $\boldsymbol{u}$ *be as in Theorem 13(c), and let* $\hat{\mathbf{u}} \in \mathbb{R}^N$ *be a unit eigenvector of* $\boldsymbol{G}\boldsymbol{G}^\top$ *(i.e. left singular vector of* $\boldsymbol{G}$*) corresponding to the eigenvalue* $\widehat{\lambda} \in U(\varepsilon) \cap \mathbb{R}$*. Then*

$$\boldsymbol{u}^\top \widehat{\boldsymbol{u}} = \frac{\alpha}{\widehat{\lambda}^{1/2}\, \widetilde{\mathcal{R}}_{11}(\widehat{\lambda}, \alpha)} \widetilde{\boldsymbol{\mathcal{R}}}_{1V}(\widehat{\lambda}, \alpha) \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}. \tag{D.34}$$

Proof. For part (a), note that if $\widehat{\lambda}$ is an eigenvalue of $\boldsymbol{G}^\top \boldsymbol{G}$, i.e. $\widehat{\lambda}^{1/2}$ is a singular value of $\boldsymbol{G}$ with left and right unit singular vectors $\widehat{\boldsymbol{u}}$ and $\widehat{\boldsymbol{v}}$, then

$$0 = \begin{pmatrix} -\widehat{\lambda}\boldsymbol{I}_n & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I}_N \end{pmatrix} \begin{pmatrix} \widehat{\boldsymbol{v}} \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}} \end{pmatrix}$$

which implies, for any $\alpha \in \mathbb{R}$,

$$-\alpha \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}} = \begin{pmatrix} -\widehat{\lambda}\boldsymbol{I}_n - \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I}_N \end{pmatrix} \begin{pmatrix} \widehat{\boldsymbol{v}} \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}} \end{pmatrix}.$$

Fixing $\alpha \in \mathbb{R}$ large enough, on the event $\mathcal{E}$ of Lemma 25, the generalized resolvent

$$\boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha) = \begin{pmatrix} -\widehat{\lambda}\boldsymbol{I}_n - \alpha \boldsymbol{V}_r \boldsymbol{V}_r^\top & \boldsymbol{G}^\top \\ \boldsymbol{G} & -\boldsymbol{I}_N \end{pmatrix}^{-1}$$

exists, and multiplying both sides by $\boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha)$ gives

$$\begin{pmatrix} \widehat{\boldsymbol{v}} \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}} \end{pmatrix} = -\alpha \boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}. \tag{D.35}$$

Then, multiplying by $(\boldsymbol{V}_r^\top \ \boldsymbol{0})$ on both sides and re-arranging, we get $\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}, \alpha) \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}} = 0$.

We remark that if $\widehat{\lambda}$ is an eigenvalue of multiplicity k, and $\boldsymbol{G}$ has corresponding linearly independent left singular vectors $\widehat{\boldsymbol{u}}_1, \ldots, \widehat{\boldsymbol{u}}_k$ and right singular vectors $\widehat{\boldsymbol{v}}_1, \ldots, \widehat{\boldsymbol{v}}_k$, then the vectors $\{(\widehat{\boldsymbol{v}}_j, \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}}_j)\}_{j=1}^k$ on the left side of (D.35) are linearly independent, implying that the vectors $\{\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_j\}_{j=1}^k$ on the right side must also be (non-zero and) linearly independent vectors in $\ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}, \alpha)$. Conversely, if $\{\boldsymbol{y}_j\}_{j=1}^k$ are linearly independent vectors in $\ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}, \alpha)$, then defining

$$\begin{pmatrix} \widehat{\boldsymbol{v}}_j \\ \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}}_j \end{pmatrix} = -\alpha \boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \boldsymbol{0} \end{pmatrix} \cdot \boldsymbol{y}_j$$

and multiplying by $(\boldsymbol{V}_r^\top \ \boldsymbol{0})$, we must have $\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_j = (-\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}, \alpha) + \boldsymbol{I})\boldsymbol{y}_j = \boldsymbol{y}_j$. Thus the pairs $(\widehat{\boldsymbol{v}}_j, \widehat{\lambda}^{1/2}\widehat{\boldsymbol{u}}_j)$ are linearly independent vectors satisfying (D.35), and multiplying by $\boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha)^{-1}$ and rearranging shows that $\widehat{\lambda}^{1/2}$ must be a singular value of $\boldsymbol{G}$ with multiplicity at least k, with corresponding singular vectors $\{(\widehat{\boldsymbol{v}}_j, \widehat{\boldsymbol{u}}_j)\}_{j=1}^k$. This establishes part (a).

For part (b), the above argument has shown $\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}} \in \ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}, \alpha)$. Multiplying (D.35) on the left by

$$\begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}$$

and taking the squared norm (noting that $\widehat{\lambda}, \alpha$ and $\boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha)$ here are real) shows (D.32). Multiplying (D.35) on the left by $(\boldsymbol{v}^\top\ \boldsymbol{0})$ shows (D.33). For part (c), multiplying (D.35) by $(\boldsymbol{0}\ \boldsymbol{u}^\top)$, we have

$$\widehat{\lambda}^{1/2}\boldsymbol{u}^\top\widehat{\boldsymbol{u}} = -\alpha\begin{pmatrix}\boldsymbol{0}\\ \boldsymbol{u}\end{pmatrix}^\top \boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha)\begin{pmatrix}\boldsymbol{V}_r\\ \boldsymbol{0}\end{pmatrix}\cdot \boldsymbol{V}_r^\top\widehat{\boldsymbol{v}} = -\alpha\boldsymbol{u}^\top\boldsymbol{G}\Big(\boldsymbol{G}^\top\boldsymbol{G} - \boldsymbol{\Gamma}(\widehat{\lambda}, \alpha)\Big)^{-1}\boldsymbol{V}_r\cdot\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}$$

where the second equality follows from the block matrix inversion of $\boldsymbol{\mathcal{R}}(\widehat{\lambda}, \alpha)$. Then, recalling the forms of $\widetilde{\mathcal{R}}_{11}$ and $\widetilde{\boldsymbol{\mathcal{R}}}_{1V}$ from (D.29) and (D.30), this gives

$$\boldsymbol{u}^\top\widehat{\boldsymbol{u}} = \frac{\alpha\widetilde{\boldsymbol{\mathcal{R}}}_{1V}(\widehat{\lambda}, \alpha)}{\widehat{\lambda}^{1/2}\,\widetilde{\mathcal{R}}_{11}(\widehat{\lambda}, \alpha)}\cdot\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}$$

which is (D.34). ■

For notational convenience, let us now introduce the shorthand

$$\psi_{N,0}(z) = z\tilde{m}_{N,0}(z), \qquad \psi(z) = z\tilde{m}(z).$$

By Lemma 25(b) applied with $(\boldsymbol{v}_1, \boldsymbol{v}_2)$ being the columns of $\boldsymbol{V}_r$, we see that $\boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)$ is well-approximated by the (deterministic, N-dependent) matrix

$$\boldsymbol{M}_N(z, \alpha) := \boldsymbol{I}_r - \alpha\Big((\alpha+z)\boldsymbol{I}_r + \psi_{N,0}(z)\operatorname{diag}(\lambda_1(\boldsymbol{\Sigma}), \ldots, \lambda_r(\boldsymbol{\Sigma}))\Big)^{-1}. \tag{D.36}$$

To show Theorem 13(a), we translate this approximation into a comparison of the roots of $0 = \det\boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)$ and $0 = \det\boldsymbol{M}_N(z, \alpha)$, where the latter are explicitly given by $z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))$ for the function $z_{N,0}(\cdot)$ defined in (B.5).

Proof of Theorem 13(a). Let us fix any $\varepsilon > 0$ and $\alpha \in \mathbb{R}$ satisfying Lemmas 25 and 26, and denote

$$f_{N,i}(z, \alpha) = 1 - \frac{\alpha}{\alpha + z + \psi_{N,0}(z)\lambda_i(\boldsymbol{\Sigma})}$$

for each $i \in [r]$. Then $\det\boldsymbol{M}_N(z, \alpha) = \prod_{i=1}^r f_{N,i}(z, \alpha)$. Define also the limiting functions

$$f_i(z, \alpha) = 1 - \frac{\alpha}{\alpha + z + \psi(z)\lambda_i}, \qquad \boldsymbol{M}(z, \alpha) = \boldsymbol{I}_r - \alpha\Big((\alpha+z)\boldsymbol{I}_r + \psi(z)\operatorname{diag}(\lambda_1, \ldots, \lambda_r)\Big)^{-1}$$

so $\det\boldsymbol{M}(z, \alpha) = \prod_{i=1}^r f_i(z, \alpha)$. We first analyze the roots of $0 = \det\boldsymbol{M}(z, \alpha)$: By the definition $\psi(z) = z\tilde{m}(z)$, observe that $z \in \mathbb{R}\setminus\operatorname{supp}(\tilde{\mu})$ satisfies $0 = \det\boldsymbol{M}(z, \alpha)$ if and only if either $z = 0$ or

$$\tilde{m}(z) = -1/\lambda_i \text{ for some } i \in [r].$$

(This condition is the same for any non-zero $\alpha \in \mathbb{R}$.) Let $\mathcal{T} = \{0\} \cup \{-1/\lambda : \lambda \in \operatorname{supp}(\nu)\}$ be as in (A.3) where ν is the limit spectral law of $\boldsymbol{\Sigma}_0$. Then $-1/\lambda_i \in \mathbb{R}\setminus\mathcal{T}$ for all $i \in [r]$ under Assumption 6, so Proposition 9 implies that $\tilde{m}(z) = -1/\lambda_i$ holds for some $z \in \mathbb{R}\setminus\operatorname{supp}(\tilde{\mu})$ if and only if $z'(-1/\lambda_i) > 0$, i.e. $i \in \mathcal{I}$. If $i \in \mathcal{I}$, then $\tilde{m}(z) = -1/\lambda_i$ holds for $z = z(-1/\lambda_i)$, and we must have $z(-1/\lambda_i) > 0$ strictly because for any $z \le 0$, we have $\tilde{m}(z) > 0$ (and hence $\tilde{m}(z) \neq -1/\lambda_i$) by the definition $\tilde{m}(z) = \int \frac{1}{x-z}d\tilde{\mu}(x)$. Thus the roots of $0 = \det\boldsymbol{M}(z, \alpha)$ in

$\mathbb{R} \setminus \mathcal{S} = \mathbb{R} \setminus (\text{supp}(\tilde{\mu}) \cup \{0\})$ — and hence in $U(\varepsilon) \cap \mathbb{R}$ for any sufficiently small $\varepsilon > 0$ — are given precisely by

$$z_i := z(-1/\lambda_i) \text{ for } i \in \mathcal{I}.$$

Since $\tilde{m}'(z) = \int \frac{1}{(x-z)^2} d\tilde{\mu}(x) > 0$ for all $z \in \mathbb{R} \setminus \mathcal{S}$, and $\{\lambda_i : i \in \mathcal{I}\}$ are distinct by assumption, these values $\{z_i : i \in \mathcal{I}\}$ are simple roots of $0 = \det \boldsymbol{M}(z_i, \alpha)$. Then $(\det \boldsymbol{M})'(z_i, \alpha) \neq 0$ where $(\det \boldsymbol{M})'$ denotes the derivative in z.

Lemma 24(c) implies $\tilde{m}_{N,0}(z) \to \tilde{m}(z)$ and $\tilde{m}'_{N,0}(z) \to \tilde{m}'(z)$ uniformly over $z \in U(\varepsilon)$. Since also $\lambda_i(\boldsymbol{\Sigma}) \to \lambda_i$, we have $\det \boldsymbol{M}_N(z, \alpha) \to \det \boldsymbol{M}(z, \alpha)$ and $(\det \boldsymbol{M}_N)'(z, \alpha) \to (\det \boldsymbol{M})'(z, \alpha)$ uniformly over $z \in U(\varepsilon)$. This, together with the above condition $(\det \boldsymbol{M})'(z_i, \alpha) \neq 0$, imply that for all large N, the roots $z_{N,i} \in U(\varepsilon) \cap \mathbb{R}$ of $0 = \det \boldsymbol{M}_N(z, \alpha)$ are in 1-to-1 correspondence with, and converge to, the above roots $z_i \in U(\varepsilon) \cap \mathbb{R}$ of $0 = \det \boldsymbol{M}(z, \alpha)$. We note that $0 = \det \boldsymbol{M}_N(z, \alpha)$ if and only if either $z = 0$ or

$$\tilde{m}_{N,0}(z) = -1/\lambda_i(\boldsymbol{\Sigma}) \text{ for some } i \in [r]. \tag{D.37}$$

For each $i \in \mathcal{I}$, we have $\lambda_i(\boldsymbol{\Sigma}) \to \lambda_i$ where $z'(-1/\lambda_i) > 0$. Recall from Lemma 24(a) that $z_{N,0}(\tilde{m}) \to z(\tilde{m})$ and $z'_{N,0}(\tilde{m}) \to z'(\tilde{m})$ uniformly over compact subsets of $\mathbb{R} \setminus \mathcal{T}$. Then $z'_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) \to z'(-1/\lambda_i)$, so also $z'_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) > 0$ for all large N. Then Proposition 9 implies that (D.37) holds for $z_{N,i} := z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))$. We have $z_{N,i} \to z_i = z(-1/\lambda_i)$, so these must be the roots of $\det \boldsymbol{M}_N(z, \alpha)$ in $U(\varepsilon) \cap \mathbb{R}$. Thus we have shown that for any sufficiently small $\varepsilon > 0$ and all large N, the roots $z \in U(\varepsilon) \cap \mathbb{R}$ of $0 = \det \boldsymbol{M}_N(z, \alpha)$ are precisely the values

$$z_{N,i} := z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) \text{ for } i \in \mathcal{I},$$

and $z_{N,i} \to z_i > 0$ for each $i \in \mathcal{I}$.

Finally, we apply Lemma 25(b) with $(\boldsymbol{v}_1, \boldsymbol{v}_2)$ being the columns of $\boldsymbol{V}_r$. On the event $\mathcal{E}$ of Lemma 25(a), we have

$$\|\boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)\| \leq C, \qquad \big\|\boldsymbol{M}_{\boldsymbol{K}}(z, \alpha) - \boldsymbol{M}_{\boldsymbol{K}}(z', \alpha)\big\| \leq C|z - z'| \tag{D.38}$$

for some $C > 0$ and all $z, z' \in U(\varepsilon/2)$. Also $|\tilde{m}_{N,0}(z)|, |\tilde{m}'_{N,0}(z)| < C$ for a constant $C > 0$, all $z \in U(\varepsilon)$, and all large N, and thus

$$\|\boldsymbol{M}_N(z, \alpha)\| \leq C, \qquad \big\|\boldsymbol{M}_N(z, \alpha) - \boldsymbol{M}_N(z', \alpha)\big\| \leq C|z - z'| \tag{D.39}$$

for some $C > 0$ and all $z, z' \in U(\varepsilon/2)$. Then, applying Lemma 25(b) and the Lipschitz bounds of (D.38) and (D.39) to take a union bound over a sufficiently fine covering net of $U(\varepsilon/2)$, we get

$$\sup_{z \in U(\varepsilon/2)} \|\boldsymbol{M}_N(z, \alpha) - \boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)\| \prec 1/\sqrt{N}. \tag{D.40}$$

Applying also the first bounds of (D.38) and (D.39), this gives

$$\sup_{z \in U(\varepsilon/2)} |\det \boldsymbol{M}_N(z, \alpha) - \det \boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)| \prec 1/\sqrt{N}. \tag{D.41}$$

Since $\det \boldsymbol{M}_N(z, \alpha)$ and $\det \boldsymbol{M}_{\boldsymbol{K}}(z, \alpha)$ are both holomorphic over $z \in U(\varepsilon/2)$ on this event $\mathcal{E}$, the Cauchy integral formula then implies

$$\sup_{z \in U(\varepsilon)} |(\det \boldsymbol{M}_N)'(z, \alpha) - (\det \boldsymbol{M}_{\boldsymbol{K}})'(z, \alpha)| \prec 1/\sqrt{N}.$$

In particular, combining with the uniform convergence statements $\det \boldsymbol{M}_N(z,\alpha) \to \det \boldsymbol{M}(z,\alpha)$ and $(\det \boldsymbol{M}_N)'(z,\alpha) \to (\det \boldsymbol{M})'(z,\alpha)$ over $z \in U(\varepsilon)$ as argued above, this shows that on an event $\mathcal{E}$ satisfying $\mathbf{1}\{\mathcal{E}^c\} \prec 0$ and for some $\delta_N \to 0$, we have

$$\sup_{z\in U(\varepsilon)\cap\mathbb{R}} |\det \boldsymbol{M}(z,\alpha) - \det \boldsymbol{M}_{\boldsymbol{K}}(z,\alpha)|, |(\det \boldsymbol{M})'(z,\alpha) - (\det \boldsymbol{M}_{\boldsymbol{K}})'(z,\alpha)| < \delta_N.$$

Thus, on this event $\mathcal{E}$ and as $N \to \infty$, the roots $\widehat{\lambda}_i \in U(\varepsilon)\cap\mathbb{R}$ of $0 = \det \boldsymbol{M}_{\boldsymbol{K}}(z,\alpha)$ are also in 1-to-1 correspondence with, and converge to, the roots $z_i \in U(\varepsilon)\cap\mathbb{R}$ of $0 = \det \boldsymbol{M}(z,\alpha)$. Furthermore, the condition $(\det \boldsymbol{M})'(z_i,\alpha) \neq 0$ implies that $|(\det \boldsymbol{M}_N)'(z,\alpha)|$ and $|(\det \boldsymbol{M}_{\boldsymbol{K}})'(z,\alpha)|$ are bounded away from 0 in a neighborhood of each such root z_i, so (D.41) then implies that the corresponding roots $\widehat{\lambda}_i$ and $z_{N,i}$ of $0 = \det \boldsymbol{M}_{\boldsymbol{K}}(z,\alpha)$ and $0 = \det \boldsymbol{M}_N(z,\alpha)$ satisfy

$$|\widehat{\lambda}_i - z_{N,i}| \prec 1/\sqrt{N}.$$

Proposition 29 shows that on this event $\mathcal{E}$, these roots $\{\widehat{\lambda}_i : i \in \mathcal{I}\}$ are precisely the eigenvalues of $\boldsymbol{G}^\top\boldsymbol{G}$ in $U(\varepsilon)\cap\mathbb{R}$. By the definition of $\boldsymbol{M}(z_i,\alpha)$, each root z_i of $\det \boldsymbol{M}(z_i,\alpha)$ is such that $\ker \boldsymbol{M}(z_i,\alpha)$ has dimension 1. Since $\mathbf{1}\{\mathcal{E}\}(\widehat{\lambda}_i - z_i) \to 0$, we have $\mathbf{1}\{\mathcal{E}\}\|\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha) - \boldsymbol{M}(z_i,\alpha)\| \to 0$, so $\ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha)$ also has dimension 1 on this event $\mathcal{E}$ for all large N. Then Proposition 29 implies that the eigenvalues $\{\widehat{\lambda}_i : i \in \mathcal{I}\}$ of $\boldsymbol{G}^\top\boldsymbol{G}$ are simple, and thus in 1-to-1 correspondence with $\{\lambda_i : i \in \mathcal{I}\}$. This proves part (a) of the theorem. ■

Lemma 30 *Under the assumptions of Theorem 13, for any fixed $\varepsilon > 0$, there exists $\alpha_0 > 0$ such that fixing any $\alpha \in \mathbb{C}$ with $|\alpha| > \alpha_0$, uniformly over $z \in U(\varepsilon)$,*

$$\left\| \begin{pmatrix} \boldsymbol{V}_r \\ \mathbf{0} \end{pmatrix}^\top \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{I}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \mathbf{0} \end{pmatrix} - ((\alpha+z)\boldsymbol{I}_r + \psi_{N,0}(z)\boldsymbol{\Sigma}_r)^{-2}\big(\boldsymbol{I}_r + \psi'_{N,0}(z)\boldsymbol{\Sigma}_r\big) \right\| \prec \frac{1}{\sqrt{N}}.$$

Proof. Fix any $\alpha \in \mathbb{C}$ satisfying Lemma 25, and denote

$$f_N(z,\alpha) := \begin{pmatrix} \boldsymbol{V}_r^\top & \mathbf{0} \end{pmatrix} \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \mathbf{0} \end{pmatrix}, \qquad g_N(z,\alpha) := -((\alpha+z)\boldsymbol{I}_r + \psi_{N,0}(z)\boldsymbol{\Sigma}_r)^{-1}.$$

Applying Lemma 25(b) and the Lipschitz continuity statements of (D.38) and (D.39) to take a union bound over a sufficiently fine covering net of $U(\varepsilon/2)$, we have

$$\sup_{z\in U(\varepsilon/2)} \|f_N(z,\alpha) - g_N(z,\alpha)\| \prec 1/\sqrt{N}.$$

Then by the Cauchy integral formula, $\sup_{z\in U(\varepsilon)} \|f'_N(z,\alpha) - g'_N(z,\alpha)\| \prec 1/\sqrt{N}$ where f'_N and g'_N denote the entrywise derivatives in z. The lemma follows, since differentiating $\boldsymbol{\mathcal{R}}(z,\alpha)$ in (D.2) shows

$$f'_N(z,\alpha) = \begin{pmatrix} \boldsymbol{V}_r^\top & \mathbf{0} \end{pmatrix} \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \boldsymbol{\mathcal{R}}(z,\alpha) \begin{pmatrix} \boldsymbol{V}_r \\ \mathbf{0}, \end{pmatrix}$$

while $g'_N(z,\alpha) = ((\alpha+z)\boldsymbol{I}_r + \psi_{N,0}(z)\boldsymbol{\Sigma}_r)^{-2}(\boldsymbol{I}_r + \psi'_{N,0}(z)\boldsymbol{\Sigma}_r)$. ■

Proof of Theorem 13(b). Let $\widehat{\boldsymbol{v}}_i$ be the given unit-norm eigenvector of $\boldsymbol{K}$ with eigenvalue $\widehat{\lambda}_i$. Let $z_{N,i} = z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))$ and $z_i = z(-1/\lambda_i)$. Then, fixing any $\alpha \in \mathbb{R}$ large enough to satisfy Lemmas 25 and 26, Proposition 29(b) shows that $\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_i \in \ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha)$. By (D.40), (D.39), and the bound $|\widehat{\lambda}_i - z_{N,i}| \prec N^{-1/2}$ of part (a) of the theorem already proven, we have

$$\left\|\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha) - \boldsymbol{M}_N(z_{N,i},\alpha)\right\| \leq \left\|\boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha) - \boldsymbol{M}_N(\widehat{\lambda}_i,\alpha)\right\| + \left\|\boldsymbol{M}_N(\widehat{\lambda}_i,\alpha) - \boldsymbol{M}_N(z_{N,i},\alpha)\right\| \prec N^{-1/2}. \tag{D.42}$$

Let $\boldsymbol{v}_1,\ldots,\boldsymbol{v}_r$ denote the columns of $\boldsymbol{V}_r$, which are the unit eigenvectors of $\boldsymbol{\Sigma}$. Then, applying $\boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_i \in \ker \boldsymbol{M}_{\boldsymbol{K}}(\widehat{\lambda}_i,\alpha)$, (D.42), and the definition of $\boldsymbol{M}_N(z,\alpha)$, and noting that $\psi_{N,0}(z_{N,i}) = z_{N,i}\tilde{m}_{N,0}(z_{N,i}) = -z_{N,i}/\lambda_i(\boldsymbol{\Sigma})$, we have

$$\left\|\boldsymbol{M}_N(z_{N,i},\alpha)\cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_i\right\|^2 = \sum_{j=1}^r \left(1 - \frac{\alpha}{\alpha + z_{N,i}(1-\lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma}))}\right)^2 (\boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i)^2 \prec 1/N.$$

For each $j \in [r]\setminus\{i\}$, we have that $z_{N,i}(1-\lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma}))$ is bounded away from 0 as $N\to\infty$ because $z_{N,i}\to z_i>0$ and $\lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma}) \to \lambda_j/\lambda_i \neq 1$. So this implies

$$|\boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i|^2 \prec 1/N \quad \text{for all} \quad j\in[r]\setminus\{i\}. \tag{D.43}$$

At the same time, applying Lemma 30 and $|\widehat{\lambda}_i - z_{N,i}| \prec N^{-1/2}$ to bound (D.32) in Proposition 29(b), we have

$$\begin{aligned}
\frac{1}{\alpha^2} &= \widehat{\boldsymbol{v}}_i^\top \boldsymbol{V}_r \begin{pmatrix}\boldsymbol{V}_r\\ \boldsymbol{0}\end{pmatrix}^\top \boldsymbol{\mathcal{R}}(z_{N,i},\alpha)\begin{pmatrix}\boldsymbol{I}_n & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{0}\end{pmatrix}\boldsymbol{\mathcal{R}}(z_{N,i},\alpha)\begin{pmatrix}\boldsymbol{V}_r\\ \boldsymbol{0}\end{pmatrix}\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}_i + O_\prec\left(N^{-1/2}\right)\\
&= \widehat{\boldsymbol{v}}_i^\top \boldsymbol{V}_r\Big((\alpha+z_{N,i})\boldsymbol{I}_r + \psi_{N,0}(z_{N,i})\boldsymbol{\Sigma}_r\Big)^{-2}\Big(\boldsymbol{I}_r + \psi'_{N,0}(z_{N,i})\boldsymbol{\Sigma}_r\Big)\boldsymbol{V}_r^\top\widehat{\boldsymbol{v}}_i + O_\prec\left(N^{-1/2}\right)\\
&= |\boldsymbol{v}_i^\top\widehat{\boldsymbol{v}}_i|^2\cdot\frac{1+\psi'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma})}{\alpha^2}\\
&\qquad + \sum_{j\neq i}|\boldsymbol{v}_j^\top\widehat{\boldsymbol{v}}_i|^2\cdot\frac{1+\psi'_{N,0}(z_{N,i})\lambda_j(\boldsymbol{\Sigma})}{(\alpha+z_{N,i}(1-\lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma})))^2} + O_\prec\left(N^{-1/2}\right)\\
&= |\boldsymbol{v}_i^\top\widehat{\boldsymbol{v}}_i|^2\cdot\frac{1+\psi'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma})}{\alpha^2} + O_\prec\left(N^{-1/2}\right),
\end{aligned} \tag{D.44}$$

the last equality applying (D.43). Observe that

$$\begin{aligned}
1+\psi'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma}) &= 1 + z_{N,i}\tilde{m}'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma}) + \tilde{m}_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma})\\
&= z_{N,i}\tilde{m}'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma}) = z_{N,i}\lambda_i(\boldsymbol{\Sigma})/z'_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})),
\end{aligned}$$

where the last two equalities use $z_{N,i} = z_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))$ and $\tilde{m}_{N,0}(\cdot)$ is the inverse function of $z_{N,0}(\cdot)$. Then, multiplying by $\alpha^2/(1+\psi'_{N,0}(z_{N,i})\lambda_i(\boldsymbol{\Sigma}))$ we obtain

$$|\boldsymbol{v}_i^\top\widehat{\boldsymbol{v}}_i|^2 = \frac{z'_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))}{z_{N,i}\lambda_i(\boldsymbol{\Sigma})} + O_\prec\left(N^{-1/2}\right) = \varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) + O_\prec\left(N^{-1/2}\right),$$

where we recall $\varphi_{N,0}$ from (B.5). We have $\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma})) \to \varphi(-1/\lambda_i) = z'(-1/\lambda_i)/(\lambda_i z_i) > 0$, so taking a square root gives

$$|\boldsymbol{v}_i^\top \widehat{\boldsymbol{v}}_i| = \sqrt{\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))} + O_\prec\Big(N^{-1/2}\Big). \tag{D.45}$$

Finally, for any unit vector $\boldsymbol{v} \in \mathbb{R}^n$, by (D.33) in Proposition 29(b), Lemma 25(b), and the bound $|\widehat{\lambda}_i - z_{N,i}| \prec N^{-1/2}$ in part (a) of the theorem already shown, we know that

$$\begin{aligned}
\boldsymbol{v}^\top \widehat{\boldsymbol{v}}_i &= -\alpha \cdot \begin{pmatrix}\boldsymbol{v}^\top & \mathbf{0}\end{pmatrix} \boldsymbol{\mathcal{R}}(z_{N,i}, \alpha) \begin{pmatrix}\boldsymbol{V}_r \\ \mathbf{0}\end{pmatrix} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_i + O_\prec\Big(N^{-1/2}\Big) \\
&= -\alpha \sum_{j=1}^r \frac{\boldsymbol{v}^\top \boldsymbol{v}_j \cdot \boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i}{\alpha + z_{N,i} + \psi_{N,0}(z_{N,i})\lambda_j(\boldsymbol{\Sigma})} + O_\prec\Big(N^{-1/2}\Big) \\
&= -\alpha \sum_{j=1}^r \frac{\boldsymbol{v}^\top \boldsymbol{v}_j \cdot \boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i}{\alpha + z_{N,i} \cdot (1 - \lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma}))} + O_\prec\Big(N^{-1/2}\Big).
\end{aligned}$$

Applying (D.43) and (D.45), only the summand with $j = i$ contributes, and we obtain as desired

$$|\boldsymbol{v}^\top \widehat{\boldsymbol{v}}_i| = \sqrt{\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))} \cdot |\boldsymbol{v}^\top \boldsymbol{v}_i| + O_\prec\Big(N^{-1/2}\Big).$$

■

Proof of Theorem 13(c). Applying Lemma 26(b) and block matrix inversion of $\widetilde{\boldsymbol{\Gamma}} + \psi_{N,0}(z)\widetilde{\boldsymbol{\Sigma}}$ to the definitions of $\widetilde{\mathcal{R}}_{11}$ and $\widetilde{\boldsymbol{\mathcal{R}}}_{1V}$ in (D.29) and (D.30), we have

$$\left|\widetilde{\mathcal{R}}_{11}(z,\alpha) + \Big(z + \alpha + \psi_{N,0}(z) \cdot \mathbb{E}[u^2] - \psi_{N,0}(z)^2 \cdot \mathbb{E}[u\boldsymbol{g}]^\top (\boldsymbol{\Gamma} + \psi_{N,0}(z)\boldsymbol{\Sigma})^{-1}\mathbb{E}[u\boldsymbol{g}]\Big)^{-1}\right| \prec \frac{1}{\sqrt{N}},$$

$$\left\|\widetilde{\boldsymbol{\mathcal{R}}}_{1V}(z,\alpha) - \frac{\psi_{N,0}(z) \cdot \mathbb{E}[u\boldsymbol{g}]^\top (\boldsymbol{\Gamma} + \psi_{N,0}(z)\boldsymbol{\Sigma})^{-1}\boldsymbol{V}_r}{z + \alpha + \psi_{N,0}(z) \cdot \mathbb{E}[u^2] - \psi_{N,0}(z)^2 \cdot \mathbb{E}[u\boldsymbol{g}]^\top (\boldsymbol{\Gamma} + \psi_{N,0}(z)\boldsymbol{\Sigma})^{-1}\mathbb{E}[u\boldsymbol{g}]}\right\| \prec \frac{1}{\sqrt{N}}.$$

Hence,

$$\left\|\frac{\widetilde{\boldsymbol{\mathcal{R}}}_{1V}(z,\alpha)}{\widetilde{\mathcal{R}}_{11}(z,\alpha)} + \psi_{N,0}(z) \cdot \mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{V}_r \cdot ((\alpha + z)\boldsymbol{I}_r + \psi_{N,0}(z)\boldsymbol{\Sigma}_r)^{-1}\right\| \prec \frac{1}{\sqrt{N}}.$$

Applying this and the bound $|\widehat{\lambda}_i - z_{N,i}| \prec N^{-1/2}$ to Proposition 29(c),

$$\begin{aligned}
\boldsymbol{u}^\top \widehat{\boldsymbol{u}}_i = \frac{\alpha}{\widehat{\lambda}_i^{1/2}} \frac{\widetilde{\boldsymbol{\mathcal{R}}}_{1V}(\widehat{\lambda}_i, \alpha)}{\widetilde{\mathcal{R}}_{11}(\widehat{\lambda}_i, \alpha)} \cdot \boldsymbol{V}_r^\top \widehat{\boldsymbol{v}}_i &= -\frac{\alpha}{\sqrt{z_{N,i}}} \sum_{j=1}^r \frac{\psi_{N,0}(z_{N,i}) \cdot \mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{v}_j \cdot \boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i}{\alpha + z_{N,i} + \psi_{N,0}(z_{N,i})\lambda_j(\boldsymbol{\Sigma})} + O_\prec\Big(N^{-1/2}\Big) \\
&= -\frac{\alpha}{\sqrt{z_{N,i}}} \sum_{j=1}^r \frac{\psi_{N,0}(z_{N,i}) \cdot \mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{v}_j \cdot \boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i}{\alpha + z_{N,i}(1 - \lambda_j(\boldsymbol{\Sigma})/\lambda_i(\boldsymbol{\Sigma}))} + O_\prec\Big(N^{-1/2}\Big).
\end{aligned}$$

Then, applying again (D.43) and (D.45), only the summand with $j = i$ contributes, and this gives

$$|\boldsymbol{u}^\top \widehat{\boldsymbol{u}}_i| = \frac{|\mathbb{E}[u\boldsymbol{g}]^\top \boldsymbol{v}_i| \cdot |\psi_{N,0}(z_{N,i})| \sqrt{\varphi_{N,0}(-1/\lambda_i(\boldsymbol{\Sigma}))}}{\sqrt{z_{N,i}}} + O_\prec\Big(N^{-1/2}\Big).$$

Recalling $\psi_{N,0}(z_{N,i}) = -z_{N,i}/\lambda_i(\boldsymbol{\Sigma})$, this yields part (c) of the theorem. ■

Appendix E. Proofs for propagation of spiked eigenstructure in deep NNs

We next prove Theorems 2 and 4. Appendix E.1 first establishes these results for a one-hidden-layer NN, $L = 1$. We then apply this result for $L = 1$ inductively in Appendix E.2 to obtain these results for general L. Appendix E.3 proves Corollary 5.

E.1. Spike analysis for one-hidden-layer CK

Consider the setup in Section 2.1 with a single hidden layer $L = 1$. In this setting, let us simplify notation and denote

$$\boldsymbol{X} = \boldsymbol{X}_0, \qquad \boldsymbol{W} = \boldsymbol{W}_0, \qquad d = d_0, \qquad N = d_1,$$

$$\boldsymbol{Y} = \boldsymbol{X}_1 = \frac{1}{\sqrt{N}}\sigma(\boldsymbol{W}\boldsymbol{X}), \qquad \boldsymbol{K} = \boldsymbol{K}_1 = \boldsymbol{Y}^\top \boldsymbol{Y}.$$

We denote the rows of $\boldsymbol{W}$ and columns of $\boldsymbol{X}$ respectively by

$$\boldsymbol{w}_i^\top \in \mathbb{R}^d \text{ for } i \in [N], \qquad \boldsymbol{x}_\alpha \in \mathbb{R}^d \text{ for } \alpha \in [n].$$

We write $\mathbb{E}_{\boldsymbol{w}}$ for the expectation over a standard Gaussian vector $\boldsymbol{w} \sim \mathcal{N}(0, \boldsymbol{I})$ in $\mathbb{R}^d$.

Note that for a sufficiently large constant $B > 0$ (depending on $\operatorname{supp}(\nu)$ and $\lambda_1, \ldots, \lambda_r$), Assumption 2 implies that the event

$$\mathcal{E}(\boldsymbol{X}) = \Big\{ \|\boldsymbol{X}\| < B,\ |\boldsymbol{x}_\alpha^\top \boldsymbol{x}_\beta| < \tau_n \text{ and } |\|\boldsymbol{x}_\alpha\|_2 - 1| < \tau_n \text{ for all } \alpha \neq \beta \in [n] \Big\} \tag{E.1}$$

holds almost surely for all large n. We will use throughout this section the following argument: Since $\boldsymbol{W} \equiv \boldsymbol{W}^{(n)}$ is independent of $\boldsymbol{X} \equiv \boldsymbol{X}^{(n)}$, and $\mathcal{E}(\boldsymbol{X}^{(n)})$ holds for all large n with probability 1 over $\{\boldsymbol{X}^{(n)}\}_{n=1}^\infty$, to prove any almost-sure statement, it suffices to show that the statement holds with probability 1 over $\{\boldsymbol{W}^{(n)}\}_{n=1}^\infty$, for any deterministic matrices $\{\boldsymbol{X}^{(n)}\}_{n=1}^\infty$ satisfying $\mathcal{E}(\boldsymbol{X}^{(n)})$. Thus, we assume in the remainder of this section that $\boldsymbol{X}$ is deterministic and satisfies $\mathcal{E}(\boldsymbol{X})$ for all large n, and write $\mathbb{E}, \mathbb{P}$ for the expectation and probability over only the random weight matrix $\boldsymbol{W}$.

We will apply Theorem 13 to a centered version of $\boldsymbol{Y}$,

$$\boldsymbol{G} := \boldsymbol{Y} - \mathbb{E}\boldsymbol{Y} = \frac{1}{\sqrt{N}}[\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N]^\top, \qquad \boldsymbol{g}_i^\top := \sigma(\boldsymbol{w}_i^\top \boldsymbol{X}) - \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})].$$

Note that these rows $\boldsymbol{g}_i^\top$ are i.i.d. with mean $\mathbf{0}$ and covariance

$$\boldsymbol{\Sigma} := \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})^\top \sigma(\boldsymbol{w}^\top \boldsymbol{X})] - \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})]^\top \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})] \in \mathbb{R}^{n \times n}. \tag{E.2}$$

Lemma 31 *Suppose Assumptions 1, 2, and 3 hold, with $L = 1$ and deterministic $\boldsymbol{X}$. Then*

$$\|\mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})]\|_2 \to 0, \qquad \|\mathbb{E}\boldsymbol{Y}\| \to 0.$$

Proof. Denote $\xi \sim \mathcal{N}(0,1)$. Applying $\mathbb{E}[\sigma(\xi)] = 0$, $\mathbb{E}[\sigma'(\xi)\xi] = \mathbb{E}[\sigma''(\xi)] = 0$, and a Taylor approximation of σ, for any $\alpha \in [n]$,

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{x}_\alpha)] &= \mathbb{E}[\sigma(\|\boldsymbol{x}_\alpha\|\xi)] - \mathbb{E}[\sigma(\xi)] \\
&= \mathbb{E}[\sigma'(\xi)\xi(\|\boldsymbol{x}_\alpha\| - 1)] + \mathbb{E}[\sigma''(\eta)\xi^2(\|\boldsymbol{x}_\alpha\| - 1)^2] = \mathbb{E}[\sigma''(\eta)\xi^2(\|\boldsymbol{x}_\alpha\| - 1)^2]
\end{aligned}$$

for some η between ξ and $\|\boldsymbol{x}_i\|\xi$. Then, applying $|\sigma''(x)| \leq \lambda_\sigma$ and the τ_n-orthonormality of $\boldsymbol{X}$ under $\mathcal{E}(\boldsymbol{X})$,

$$|\mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{x}_\alpha)]| \leq \lambda_\sigma \tau_n^2.$$

This gives $\|\mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})]\|_2 \leq \lambda_\sigma \tau_n^2 \sqrt{n} \to 0$, so also $\|\mathbb{E}\boldsymbol{Y}\| = \left\| \frac{1}{\sqrt{N}} \mathbf{1}_N \cdot \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})] \right\| \to 0$. ■

Next, we recall from Wang and Zhu (2021) an approximation of $\boldsymbol{\Sigma}$ by the linearized matrix

$$\boldsymbol{\Sigma}_{\text{lin}} := b_\sigma^2 \boldsymbol{X}^\top \boldsymbol{X} + (1 - b_\sigma^2)\boldsymbol{I}_n \tag{E.3}$$

in the operator norm.

Lemma 32 *Suppose Assumptions 1, 2, and 3 hold, with $L = 1$ and deterministic $\boldsymbol{X}$.*

$$\|\boldsymbol{\Sigma} - \boldsymbol{\Sigma}_{\text{lin}}\| \to 0.$$

Consequently, ordering $\lambda_1(\boldsymbol{\Sigma}), \ldots, \lambda_n(\boldsymbol{\Sigma})$ in the same order as $\lambda_1(\boldsymbol{X}^\top \boldsymbol{X}), \ldots, \lambda_n(\boldsymbol{X}^\top \boldsymbol{X})$,

$$\sup_{i \in [n]} \left| b_\sigma^2 \lambda_i(\boldsymbol{X}^\top \boldsymbol{X}) + (1 - b_\sigma^2) - \lambda_i(\boldsymbol{\Sigma}) \right| \to 0. \tag{E.4}$$

Proof. Denote $\xi \sim \mathcal{N}(0, 1)$. Let $\zeta_k(\sigma) = \mathbb{E}[\sigma(\xi) h_k(\xi)]$ be the k-th Hermite coefficient of σ, where $h_k(x)$ is the k-th Hermite polynomial normalized so that $\mathbb{E}[h_k(\xi)^2] = 1$. Note that by Gaussian integration by parts and the assumption $\mathbb{E}[\sigma''(\xi)] = 0$,

$$\zeta_1(\sigma) = \mathbb{E}[\xi\sigma(\xi)] = \mathbb{E}[\sigma'(\xi)] = b_\sigma, \qquad \sqrt{2}\,\zeta_2(\sigma) = \mathbb{E}[(\xi^2 - 1)\sigma(\xi)] = \mathbb{E}[\xi\sigma'(\xi)] = \mathbb{E}[\sigma''(\xi)] = 0.$$

Then by (Wang and Zhu, 2021, Lemma 5.2) and the first statement of Lemma 31, we have

$$\|\boldsymbol{\Sigma}_0 - \boldsymbol{\Sigma}\| \leq \|\boldsymbol{\Sigma}_0 - \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})^\top \sigma(\boldsymbol{w}^\top \boldsymbol{X})]\| + \|\mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^\top \boldsymbol{X})^\top \sigma(\boldsymbol{w}^\top \boldsymbol{X})] - \boldsymbol{\Sigma}\| \to 0$$

where

$$\boldsymbol{\Sigma}_0 = \zeta_1(\sigma)^2 \boldsymbol{X}^\top \boldsymbol{X} + \zeta_3(\sigma)^2 (\boldsymbol{X}^\top \boldsymbol{X})^{\odot 3} + (1 - \zeta_1(\sigma)^2 - \zeta_3(\sigma)^2)\boldsymbol{I}_n.$$

(Here, examination of the proof of (Wang and Zhu, 2021, Lemma 5.2) shows that the condition $\sum_\alpha (\|\boldsymbol{x}_\alpha\|_2 - 1)^2 \leq B^2$ for (ε, B)-orthonormality is not used when $\zeta_2(\sigma) = 0$, and the remaining conditions of (ε, B)-orthonormality hold under $\mathcal{E}(\boldsymbol{X})$.) The lemma then follows upon observing that under $\mathcal{E}(\boldsymbol{X})$,

$$\begin{aligned}
\left\| (\boldsymbol{X}^\top \boldsymbol{X})^{\odot 3} - \boldsymbol{I}_n \right\| &\leq \left\| \operatorname{diag}((\boldsymbol{X}^\top \boldsymbol{X})^{\odot 3} - \boldsymbol{I}_n) \right\| + \left\| \operatorname{offdiag}(\boldsymbol{X}^\top \boldsymbol{X})^{\odot 3} \right\|_F \\
&\leq \max_{\alpha \in [n]} \left| \|\boldsymbol{x}_\alpha\|^6 - 1 \right| + n \cdot \max_{\alpha \neq \beta \in [n]} |\boldsymbol{x}_\alpha^\top \boldsymbol{x}_\beta|^3 \leq C(\tau_n + n\tau_n^3),
\end{aligned}$$

so that $\|\boldsymbol{\Sigma}_{\text{lin}} - \boldsymbol{\Sigma}_0\| = \zeta_3(\sigma)^2 \left\| (\boldsymbol{X}^\top \boldsymbol{X})^{\odot 3} - \boldsymbol{I}_n \right\| \to 0$ when $\lim_{n\to\infty} \tau_n \cdot n^{1/3} = 0$. ■

Theorem 13 will provide a characterization of outlier eigenvalues of $\boldsymbol{K}$ that are separated from $\mathcal{S}_1 = \operatorname{supp}(\mu_1) \cup \{0\}$, which is different from $\operatorname{supp}(\mu_1)$ when $\gamma_1 < 1$. For $\gamma_1 < 1$, we augment this statement with a small-ball argument to bound the smallest eigenvalue of $\boldsymbol{K}$, using the following result of (Yaskov, 2016, Theorem 2.1).

Lemma 33 (Yaskov (2016)) *Let $G = \frac{1}{\sqrt{N}}[g_1, \ldots, g_N]^\top \in \mathbb{R}^{N\times n}$ where the rows $g_i \in \mathbb{R}^n$ are i.i.d. and equal in law to $g \in \mathbb{R}^n$. Define*

$$\Sigma = \mathbb{E}gg^\top, \qquad c_g = \inf_{v\in\mathbb{R}^n:\|v\|_2=1} \mathbb{E}|g^\top v|, \qquad L_g(\delta,\iota) = \sup_{\Pi:\mathrm{rank}(\Pi)\geq \iota n} \mathbb{P}\Big[|\Pi g|^2 \leq \delta\,\mathrm{rank}(\Pi)\Big]$$

where the latter supremum is taken over all orthogonal projections $\Pi \in \mathbb{R}^{n\times n}$ with rank at least $\iota \cdot n$.

Suppose $\lambda_{\max}(\Sigma) \leq 1$, $c(g) \geq c$, and $n/N \leq y$ for some constants $c > 0$ and $y \in (0,1)$. Then there exist constants $s_0, \iota > 0$ depending only on (c, y) such that for any $\delta \in (0,1)$ and $s > 0$,

$$\mathbb{P}[\lambda_{\min}(G^\top G) \geq (s_0 - L(\delta,\iota; g) - s)\delta] \geq 1 - 2e^{-yns^2/2}.$$

Lemma 34 *Suppose Assumptions 1, 2, and 3 hold, with $L = 1$ and deterministic X. Let $G = Y - \mathbb{E}Y$.*

(a) If $\gamma_1 \geq 1$, then $0 \in \mathrm{supp}(\mu_1)$.

(b) If $\gamma_1 < 1$, then there is a constant $c > 0$ such that $\lambda_{\min}(G^\top G) > c$ almost surely for all large n.

Proof. If $\gamma_1 > 1$ strictly, then by definition

$$\mu_1 = \frac{1}{\gamma_1}\,\tilde{\mu}_1 + \frac{\gamma_1 - 1}{\gamma_1}\,\delta_0$$

is a mixture of $\tilde{\mu}_1$ and a point mass at 0, so $0 \in \mathrm{supp}(\mu_1)$. If $\gamma = 1$, then $\mu_1 = \tilde{\mu}_1$. In this case, recall from Proposition 9 that $\mathrm{supp}(\tilde{\mu}_1)$ is characterized by the function

$$z(\tilde{m}) = -\frac{1}{\tilde{m}} + \gamma_1 \int \frac{\lambda}{1+\lambda\tilde{m}} d\nu_0(\lambda).$$

When $\gamma_1 = 1$, we have for all $\tilde{m} \in (0,\infty)$ that

$$z(\tilde{m}) < 0, \qquad z'(\tilde{m}) = \frac{1}{\tilde{m}^2} - \int \frac{\lambda^2}{(1+\lambda\tilde{m})^2} d\nu(\lambda) > 0,$$

so $z(\tilde{m})$ increases from $-\infty$ to 0 over the positive line $\tilde{m} \in (0,\infty)$. Suppose by contradiction that $0 \notin \mathrm{supp}(\tilde{\mu})$. Then by Proposition 9, there must be a point $\tilde{m} \in \mathbb{R} \setminus \mathcal{T}$ where $z(\tilde{m}) = 0$ and $z'(\tilde{m}) > 0$ strictly, implying that there is an open interval $(\tilde{m}_-, \tilde{m}_+) \ni \tilde{m}$ on which $z(\cdot)$ increases from $z(\tilde{m}_-) < 0$ to $z(\tilde{m}_+) > 0$. We must have $\tilde{m} < 0$ by the above behavior of $z(\cdot)$ on $(0,\infty)$, and the range $[z(\tilde{m}_-), z(\tilde{m}_+)]$ must overlap with $[z(a), z(b)]$ for some sufficiently large $a, b \in (0,\infty)$. But this contradicts the non-intersecting property shown in (Silverstein and Choi, 1995, Theorem 4.4). So also in this case $0 \in \mathrm{supp}(\tilde{\mu}_1) = \mathrm{supp}(\mu_1)$, showing part (a).

For part (b), we apply Lemma 33. Under $\mathcal{E}(X)$, the condition $b_\sigma \neq 0$ implies $c_0 < \lambda_{\min}(\Sigma_{\mathrm{lin}}) \leq \lambda_{\max}(\Sigma_{\mathrm{lin}}) < C_0$ for some constants $C_0, c_0 > 0$. Hence also

$$c_0 < \lambda_{\min}(\Sigma) \leq \lambda_{\max}(\Sigma) < C_0 \tag{E.5}$$

for all large n, by Lemma 32. We may assume without loss of generality that $\lambda_{\max}(\mathbf{\Sigma}) \leq 1$ as needed in Lemma 33; otherwise, the following argument may be applied to a rescaling of $\mathbf{\Sigma}$ and $\boldsymbol{G}$.

To lower bound $c_{\boldsymbol{g}}$ in Lemma 33, observe that for any unit vector $\boldsymbol{v} \in \mathbb{R}^n$ we have

$$\mathbb{E}[(\boldsymbol{g}^\top \boldsymbol{v})^2] = \boldsymbol{v}^\top \mathbf{\Sigma} \boldsymbol{v} > c_0.$$

Viewing $F(\boldsymbol{w}) = \boldsymbol{g}^\top \boldsymbol{v} = \sigma(\boldsymbol{w}^\top \boldsymbol{X})\boldsymbol{v} = \sum_{\alpha=1}^n v_\alpha \sigma(\boldsymbol{w}^\top \boldsymbol{x}_\alpha)$ as a function of $\boldsymbol{w} \sim \mathcal{N}(0, \boldsymbol{I})$, we have $\nabla F(\boldsymbol{w}) = \sum_{\alpha=1}^n v_\alpha \sigma'(\boldsymbol{w}^\top \boldsymbol{x}_\alpha)\boldsymbol{x}_\alpha = \boldsymbol{X}(\boldsymbol{v} \odot \sigma'(\boldsymbol{w}^\top \boldsymbol{X}))$ where $\sigma'(\cdot)$ is applied coordinatewise and $\odot$ is the coordinatewise product. Then, applying $|\sigma'(x)| \leq \lambda_\sigma$, observe that $\|\nabla F(\boldsymbol{w})\|_2 \leq \|\boldsymbol{X}\| \cdot \|\boldsymbol{v} \odot \sigma'(\boldsymbol{w}^\top \boldsymbol{X})\|_2 \leq \lambda_\sigma \|\boldsymbol{X}\|$, so $F(\boldsymbol{w})$ is C-Lipschitz in $\boldsymbol{w}$ for a constant $C > 0$ (not depending on $\boldsymbol{v}$) on the event $\mathcal{E}(\boldsymbol{X})$. This implies by Gaussian concentration-of-measure that $\boldsymbol{g}^\top \boldsymbol{v}$ is sub-gaussian, i.e. for some constants $C, c > 0$ and any $t > 0$, $\mathbb{P}[|\boldsymbol{g}^\top \boldsymbol{v}| \geq t] \leq Ce^{-ct^2}$. Integrating this tail bound, for some constant $t > 0$ sufficiently large, we have $\mathbb{E}[(\boldsymbol{g}^\top \boldsymbol{v})^2 \mathbf{1}_{\{|\boldsymbol{g}^\top \boldsymbol{v}| > t\}}] \leq c_0/2$, and hence

$$c_0 < \mathbb{E}[(\boldsymbol{g}^\top \boldsymbol{v})^2] \leq \mathbb{E}[(\boldsymbol{g}^\top \boldsymbol{v})^2 \mathbf{1}_{\{|\boldsymbol{g}^\top \boldsymbol{v}| \leq t\}}] + \frac{c_0}{2} \leq t \cdot \mathbb{E}|\boldsymbol{g}^\top \boldsymbol{v}| + \frac{c_0}{2}.$$

So $\mathbb{E}|\boldsymbol{g}^\top \boldsymbol{v}| \geq c_0/(2t)$, and hence $c_{\boldsymbol{g}} \geq c_0/(2t) > c$ for a constant $c > 0$.

Now let $s_0, \iota > 0$ be the constants depending on (c, γ_1) in the statement of Lemma 33. By the nonlinear Hanson-Wright inequality of (Wang and Zhu, 2021, Eq. (3.3)), for any orthogonal projection $\mathbf{\Pi} \in \mathbb{R}^{n \times n}$, any $t > 0$, and some constant $c > 0$, we have

$$\mathbb{P}\big[|\boldsymbol{g}^\top \mathbf{\Pi} \boldsymbol{g} - \mathbb{E}\boldsymbol{g}^\top \mathbf{\Pi} \boldsymbol{g}| > t\big] \leq 2e^{-c\min(t^2/\|\mathbf{\Pi}\|_F^2, t/\|\mathbf{\Pi}\|)}.$$

Here $\mathbb{E}\boldsymbol{g}^\top \mathbf{\Pi} \boldsymbol{g} = \operatorname{Tr} \mathbf{\Pi} \mathbf{\Sigma} > c_0 \operatorname{rank}(\mathbf{\Pi})$, $\|\mathbf{\Pi}\|_F^2 = \operatorname{rank}(\mathbf{\Pi})$, and $\|\mathbf{\Pi}\| = 1$, so applying this with $t = (c_0/2)\operatorname{rank}(\mathbf{\Pi})$ yields

$$\mathbb{P}[|\mathbf{\Pi} \boldsymbol{g}|^2 \leq (c_0/2)\operatorname{rank}(\mathbf{\Pi})] \leq 2e^{-c' \operatorname{rank}(\mathbf{\Pi})}.$$

Then, choosing $\delta = c_0/2$, we get $L_{\boldsymbol{g}}(\delta, \iota) \to 0$ as $n \to \infty$. Then Lemma 33 implies $\lambda_{\min}(\boldsymbol{G}^\top \boldsymbol{G}) > s_0\delta/2$ almost surely for all large n, as desired. ■

The following is the main result of this section, showing that Theorems 2 and 4 hold in this setting of $L = 1$.

Lemma 35 *Theorems 2 and 4 hold for a single layer $L = 1$. Furthermore, $\boldsymbol{Y}$ is $C\tau_n$-orthonormal for some constant $C > 0$, almost surely for all large n.*

Proof. We condition on $\boldsymbol{X}$ as discussed at the start of this section, and apply Theorem 13 to the centered matrix $\boldsymbol{G} = \boldsymbol{Y} - \mathbb{E}\boldsymbol{Y} = \frac{1}{\sqrt{N}}[\boldsymbol{g}_1, \ldots, \boldsymbol{g}_N]^\top$. Let us verify Assumption 5 for $\boldsymbol{G}$: We have shown Assumption 5(a) in (E.5). The rows $\boldsymbol{g}_i$ are sub-gaussian as shown in the above proof of Lemma 34(b), so Assumption 5(b) holds by (Vershynin, 2010, Eq. (5.26)), and Assumption 5(d) holds by (Jin et al., 2019, Lemma 2). The nonlinear Hanson-Wright inequality of (Wang and Zhu, 2021, Eq. (3.3)) implies

$$|\boldsymbol{g}_i^\top \boldsymbol{A} \boldsymbol{g}_i - \operatorname{Tr} \boldsymbol{A}\mathbf{\Sigma}| \prec \|\boldsymbol{A}\|_F$$

uniformly over $i \in [N]$ and deterministic matrices $\boldsymbol{A} \in \mathbb{C}^{n \times n}$. Furthermore, it is clear from the argument preceding (Wang and Zhu, 2021, Eq. (3.3)) that for any $i \neq j \in [N]$, the joint vector $(\boldsymbol{g}_i, \boldsymbol{g}_j) \in \mathbb{R}^{2n}$ also satisfies Lipschitz concentration, hence

$$\left| \begin{pmatrix} \boldsymbol{g}_i^\top & \boldsymbol{g}_j^\top \end{pmatrix} \boldsymbol{B} \begin{pmatrix} \boldsymbol{g}_i \\ \boldsymbol{g}_j \end{pmatrix} - \operatorname{Tr} \boldsymbol{B} \begin{pmatrix} \mathbf{\Sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Sigma} \end{pmatrix} \right| \prec \|\boldsymbol{B}\|_F$$

uniformly over $i \neq j \in [N]$ and deterministic matrices $\boldsymbol{B} \in \mathbb{C}^{2n \times 2n}$. Applying this with

$$\boldsymbol{B} = \begin{pmatrix} \mathbf{0} & \boldsymbol{A} \\ \boldsymbol{A} & \mathbf{0} \end{pmatrix}$$

verifies both statements of Assumption 5(c).

Next, we check Assumption 6 for the population covariance matrix $\boldsymbol{\Sigma}$. Combining Assumption 2 and (E.4) from Lemma 32, we have

$$\frac{1}{n-r} \sum_{i=r+1}^{n} \delta_{\lambda_i(\boldsymbol{\Sigma})} \to \nu_0 := b_\sigma^2 \otimes \mu_0 \oplus (1 - b_\sigma^2) \text{ weakly,} \tag{E.6}$$

$$\lambda_i(\boldsymbol{\Sigma}) \to -\frac{1}{s_{i,0}} := b_\sigma^2 \lambda_i + (1 - b_\sigma^2) \notin \operatorname{supp}(\nu_0) \text{ for } i = 1, \ldots, r. \tag{E.7}$$

Here, the statement $-1/s_{i,0} \notin \operatorname{supp}(\nu_0)$ in (E.7) follows from the assumptions $\lambda_i \notin \operatorname{supp}(\mu_0)$ and $b_\sigma \neq 0$. This then implies by the definition of $\mathcal{T}_1$ that $s_{i,0} \in \mathbb{R} \setminus \mathcal{T}_1$, as claimed in Theorem 4(a). Furthermore, for any fixed $\varepsilon > 0$ and all large n, Assumption 2 and (E.4) imply also that

$$\lambda_i(\boldsymbol{\Sigma}) \in \operatorname{supp}(\nu_0) + (-\varepsilon, \varepsilon) \text{ for all } i \geq r + 1.$$

Thus Assumption 6 holds for $\boldsymbol{\Sigma}$ as $n \to \infty$.

Then we can apply Theorems 11 and 13 for $\bar{\boldsymbol{K}} := \boldsymbol{G}^\top \boldsymbol{G}$. The Stieltjes transform approximation in Theorem 11 and Lemma 24(c) together imply $m_{\bar{\boldsymbol{K}}}(z) \to m_1(z)$ almost surely for each fixed $z \in \mathbb{C}^+$, where $m_1(z)$ is the Stieltjes transform of the measure $\mu_1 = \rho_{\gamma_1}^{\text{MP}} \boxtimes \nu_0$. This implies the weak convergence

$$\frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\bar{\boldsymbol{K}})} \to \mu_1 \text{ a.s.} \tag{E.8}$$

Theorem 13(a,b) further justifies:

- Let $z_1(\cdot)$ and $\mathcal{I}_1$ be defined by (2.7) and (2.8) with $\ell = 1$. Then for any sufficiently small constant $\varepsilon > 0$, almost surely for all large n, there is a 1-to-1 correspondence between the eigenvalues of $\bar{\boldsymbol{K}}$ outside $\mathcal{S}_1 + (-\varepsilon, \varepsilon)$ and $\{i : i \in \mathcal{I}_1\}$. Furthermore, for each $i \in \mathcal{I}_1$,

$$\lambda_i(\bar{\boldsymbol{K}}) \to z_1(s_{i,0}) > 0. \tag{E.9}$$

  almost surely as $n \to \infty$.

- Let $\varphi_1(\cdot)$ be defined by (2.7) with $\ell = 1$. For each $i \in \mathcal{I}_1$, let $\boldsymbol{v}_i(\bar{\boldsymbol{K}}) \in \mathbb{R}^n$ be a unit-norm eigenvector of $\bar{\boldsymbol{K}}$ corresponding to $\lambda_i(\bar{\boldsymbol{K}})$, and for each $j \in [r]$, let $\boldsymbol{v}_j(\boldsymbol{\Sigma})$ be a unit-norm eigenvector of $\boldsymbol{\Sigma}$ corresponding to $\lambda_j(\boldsymbol{\Sigma})$. Then almost surely as $n \to \infty$, for each $i \in \mathcal{I}_1$ and $j \in [r]$,

$$|\boldsymbol{v}_j(\boldsymbol{\Sigma})^\top \boldsymbol{v}_i(\bar{\boldsymbol{K}})| \to \sqrt{\varphi_1(s_{i,0})} \cdot \mathbf{1}\{i = j\} \tag{E.10}$$

  where $\varphi_1(s_{i,0}) > 0$. Moreover, letting $\boldsymbol{v} \in \mathbb{R}^n$ be any unit vector independent of $\boldsymbol{W}$, almost surely

$$|\boldsymbol{v}^\top \boldsymbol{v}_i(\bar{\boldsymbol{K}})| - \sqrt{\varphi_1(s_{i,0})} \cdot |\boldsymbol{v}^\top \boldsymbol{v}_i(\boldsymbol{\Sigma})| \to 0. \tag{E.11}$$

If $\gamma_1 \geq 1$, then Lemma 34(a) shows that $\operatorname{supp}(\mu_1) = \operatorname{supp}(\mu_1) \cup \{0\} = \mathcal{S}_1$. If $\gamma_1 < 1$, then Lemma 34(b) shows that for any sufficiently small constant $\varepsilon > 0$, $\bar{\boldsymbol{K}}$ has no eigenvalues in $[0, \varepsilon)$ almost surely for all large n. Thus, in both cases, the first statement above in fact establishes a 1-to-1 correspondence between $\{i : i \in \mathcal{I}_1\}$ and all eigenvalues of $\bar{\boldsymbol{K}}$ outside $\operatorname{supp}(\mu_1) + (-\varepsilon, \varepsilon)$, almost surely for all large n.

To translate these statements to the non-centered matrix $\boldsymbol{K} = \boldsymbol{Y}^\top \boldsymbol{Y}$, recall from Lemma 31 that $\|\boldsymbol{Y} - \boldsymbol{G}\| \to 0$ almost surely, and from Assumption 5(b) verified above that $\mathbf{1}\{\|\boldsymbol{G}^\top \boldsymbol{G}\| > B'\} \prec 0$ for a constant $B' > 0$. Then, almost surely as $n \to \infty$,

$$\left\|\boldsymbol{K} - \bar{\boldsymbol{K}}\right\| \to 0.$$

Therefore, by Weyl's inequality and (E.8), the empirical eigenvalue distribution $\widehat{\mu}_1$ of $\boldsymbol{K}$ converges also to μ_1 weakly a.s., as claimed in Theorem 2. Furthermore, by (E.9), almost surely for all large n, the eigenvalues $\widehat{\lambda}_{i,1}$ of $\boldsymbol{K}$ outside $\operatorname{supp}(\mu_1) + (-\varepsilon, \varepsilon)$ are also in 1-to-1 correspondence with $\{i : i \in \mathcal{I}_1\}$, where $\widehat{\lambda}_{i,1} \to z_1(s_{i,0})$ for each $i \in \mathcal{I}_1$. In particular, if $r = 0$, then also $|\mathcal{I}_1| = 0$, so $\boldsymbol{K}$ has no eigenvalues outside $\operatorname{supp}(\mu_1) + (-\varepsilon, \varepsilon)$. This proves Theorem 2.

For each $i \in \mathcal{I}_1$, let $\widehat{\boldsymbol{v}}_{i,1} \in \mathbb{R}^n$ be a unit-norm eigenvector of $\boldsymbol{K}$ corresponding to $\widehat{\lambda}_{i,1}$. Then by the Davis-Kahan Theorem Davis and Kahan (1970), we may choose a sign for $\widehat{\boldsymbol{v}}_{i,1}$ such that

$$\left\|\widehat{\boldsymbol{v}}_{i,1} - \boldsymbol{v}_i(\bar{\boldsymbol{K}})\right\| \leq \frac{\sqrt{2}\|\boldsymbol{K} - \bar{\boldsymbol{K}}\|}{\operatorname{dist}(\widehat{\lambda}_{i,1}, \operatorname{spec}(\bar{\boldsymbol{K}}) \setminus \{\lambda_i(\bar{\boldsymbol{K}})\})}.$$

We note that $\widehat{\lambda}_{i,1} \to z_1(s_{i,0})$ a.s., which is distinct from the limit values $\{z_1(s_{j,0}) : j \in \mathcal{I}_1 \setminus \{i\}\}$ of $\{\lambda_j(\bar{\boldsymbol{K}}) : \mathcal{I}_1 \setminus \{i\}\}$ by bijectivity of the map $z_1(\cdot)$ in Proposition 9. Furthermore $z_1(s_{i,0})$ falls outside $\operatorname{supp}(\mu_1) + (-\varepsilon, \varepsilon)$ for sufficiently small $\varepsilon > 0$, which contains all other eigenvalues of $\bar{\boldsymbol{K}}$. Thus $\operatorname{dist}(\widehat{\lambda}_{i,1}, \operatorname{spec}(\bar{\boldsymbol{K}}) \setminus \{\lambda_i(\bar{\boldsymbol{K}})\}) \geq c$ for a constant $c > 0$ almost surely for all large n, so

$$\left\|\widehat{\boldsymbol{v}}_{i,1} - \boldsymbol{v}_i(\bar{\boldsymbol{K}})\right\| \to 0 \text{ a.s.}$$

Similarly, by the convergence $\|\boldsymbol{\Sigma} - \boldsymbol{\Sigma}_{\text{lin}}\| \to 0$ and the assumption $b_\sigma \neq 0$, we have $\|\boldsymbol{v}_j(\boldsymbol{\Sigma}) - \boldsymbol{v}_j\| \to 0$ for each $j \in [r]$, where $\boldsymbol{v}_j$ is the unit-norm eigenvector of $\boldsymbol{\Sigma}_{\text{lin}}$ corresponding to its eigenvalue $b_\sigma^2 \lambda_j(\boldsymbol{X}^\top \boldsymbol{X}) + (1 - b_\sigma^2)$, i.e. the eigenvector of $\boldsymbol{X}^\top \boldsymbol{X}$ corresponding to $\lambda_j(\boldsymbol{X}^\top \boldsymbol{X})$. Then (E.10) and (E.11) imply also

$$|\boldsymbol{v}_j^\top \widehat{\boldsymbol{v}}_i|^2 \to \varphi_1(s_{i,0}) \cdot \mathbf{1}\{i = j\}, \qquad |\boldsymbol{v}^\top \widehat{\boldsymbol{v}}_i|^2 - \varphi_1(s_{i,0}) \cdot |\boldsymbol{v}^\top \boldsymbol{v}_i|^2 \to 0.$$

This shows all claims of Theorem 4 for $L = 1$.

Finally, on $\mathcal{E}(\boldsymbol{X})$, the matrix $\boldsymbol{Y}$ is $C\tau_n$-orthonormal for a constant $C > 0$ by (Fan and Wang, 2020, Lemma D.3(b)). (The proof of (Fan and Wang, 2020, Lemma D.3(b)) again does not use the condition $\sum_\alpha (\|\boldsymbol{x}_\alpha\|_2^2 - 1)^2 \leq B^2$ of (ε, B)-orthonormality therein, and the remaining conditions of (ε, B)-orthonormality hold under $\mathcal{E}(\boldsymbol{X})$.) This shows the last claim of the lemma. ■

E.2. Spike analysis for multiple layers

We now prove Theorem 4 by inductively applying the result for $L = 1$ through multiple layers. We follow the notations of Section 2.1.

Proof of Theorem 4. Suppose inductively that Assumption 2 holds with $\boldsymbol{X}_{\ell-1}$ in place of $\boldsymbol{X}_0$, and all conclusions of Theorem 4 hold for $\boldsymbol{K}_\ell$. The base case of $\ell = 1$ follows from Lemma 35.

Then the last statement of Lemma 35 implies that $\boldsymbol{X}_\ell$ is τ_n'-orthonormal almost surely for all large n, for some τ_n' satisfying $\tau_n' \cdot n^{1/3} \to 0$. Furthermore, the conclusions of Theorem 4(b,c) for $\boldsymbol{K}_\ell$ imply that statements (a) and (b) of Assumption 2 also hold for $\boldsymbol{X}_\ell$, in the following sense: Let $r_\ell = |\mathcal{I}_\ell|$. Then

$$\frac{1}{n - |r_\ell|} \sum_{i \notin \mathcal{I}_\ell} \delta_{\lambda_i(\boldsymbol{X}_\ell^\top \boldsymbol{X}_\ell)} \to \mu_\ell \text{ weakly a.s.}$$

For any fixed $\varepsilon > 0$, almost surely for all large n, $\widehat{\lambda}_{i,\ell} := \lambda_i(\boldsymbol{X}_\ell^\top \boldsymbol{X}_\ell) \in \operatorname{supp}(\mu_\ell) + (-\varepsilon, \varepsilon)$ for all $i \notin \mathcal{I}_\ell$. Furthermore, for each $i \in \mathcal{I}_\ell$, $\widehat{\lambda}_{i,\ell} \to z_\ell(s_{i,\ell-1}) \notin \operatorname{supp}(\mu_\ell)$.

Then we may apply Lemma 35 with input data $\boldsymbol{X} = \boldsymbol{X}_\ell$ in place of $\boldsymbol{X}_0$. This shows that for any fixed $\varepsilon > 0$ and all large n, there is a 1-to-1 correspondence between the eigenvalues $\widehat{\lambda}_{i,\ell+1}$ of $\boldsymbol{K}_{\ell+1}$ outside $\operatorname{supp}(\mu_{\ell+1}) + (-\varepsilon, \varepsilon)$ and $\{i : i \in \mathcal{I}_{\ell+1}\}$, where $\widehat{\lambda}_{i,\ell+1} \to z_{\ell+1}(s_{i,\ell}) > 0$ a.s., and $s_{i,\ell} \in \mathbb{R} \setminus \mathcal{T}_{\ell+1}$. Moreover, for any unit vector $\boldsymbol{v} \in \mathbb{R}^n$ independent of $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\ell+1}$,

$$|\widehat{\boldsymbol{v}}_{i,\ell+1}^\top \boldsymbol{v}|^2 - \varphi_{\ell+1}(s_{i,\ell}) \cdot |\widehat{\boldsymbol{v}}_{i,\ell}^\top \boldsymbol{v}|^2 \to 0,$$

where also $\varphi_{\ell+1}(s_{i,\ell}) > 0$. Then by the induction hypothesis for $|\widehat{\boldsymbol{v}}_{i,\ell}^\top \boldsymbol{v}|^2$,

$$|\widehat{\boldsymbol{v}}_{i,\ell+1}^\top \boldsymbol{v}|^2 \to \prod_{k=1}^{\ell+1} \varphi_k(s_{i,k-1}) \cdot |\boldsymbol{v}_i^\top \boldsymbol{v}|^2,$$

and specializing to $\boldsymbol{v} = \boldsymbol{v}_j$ for $j \in [r]$ gives

$$|\widehat{\boldsymbol{v}}_{i,\ell+1}^\top \boldsymbol{v}_j|^2 \to \prod_{k=1}^{\ell+1} \varphi_k(s_{i,k-1}) \cdot \mathbf{1}\{i = j\}.$$

This verifies all conclusions of Theorem 4 for $\boldsymbol{K}_{\ell+1}$, completing the induction. ■

E.3. Corollary for signal-plus-noise input data

Proof of Corollary 5. It is shown in (Benaych-Georges and Nadakuditi, 2012, Section 3.1) that asymptotically as $d, n \to \infty$ with $n/d \to \gamma_0$, the data matrix $\boldsymbol{X}$ has a spike singular value corresponding to θ_i if and only if $\theta_i > \gamma_0^{1/4}$, in which case

$$\lambda_i(\boldsymbol{K}_0) \to \lambda_i := \frac{(1 + \theta_i^2)(\gamma_0 + \theta_i^2)}{\theta_i^2}, \qquad |\boldsymbol{b}_i^\top \boldsymbol{v}_i|^2 \to 1 - \frac{\gamma_0(1 + \theta_i^2)}{\theta_i^2(\theta_i^2 + \gamma_0)}$$

where $\boldsymbol{v}_i$ is the unit eigenvector of the input Gram matrix $\boldsymbol{K}_0 = \boldsymbol{X}^\top \boldsymbol{X}$. Thus claims (a) and (b) of Assumption 2 hold with $r = |\{i : \theta_i > \gamma_0^{1/4}\}|$, $\mu_0 = \rho_{\gamma_0}^{\text{MP}}$ being the standard Marcenko-Pastur law, and $\lambda_i = (1 + \theta_i^2)(\gamma_0 + \theta_i^2)/\theta_i^2$ being the above values.

We note that $\boldsymbol{X}$ is $n^{-1/2+\varepsilon}$-orthonormal for any $\varepsilon > 0$ almost surely for all large n, by the given condition $\max_{i=1}^r \|\boldsymbol{b}_i\|_\infty < n^{-1/2+\varepsilon}$ and the bounds, for any $\alpha, \beta \in [n]$,

$$\|\boldsymbol{x}_\alpha\|_2 = \|\boldsymbol{z}_\alpha\|_2 + \sum_{i=1}^r O_\prec(\|\boldsymbol{a}_i\|_2 |\theta_i| |b_{i,\alpha}|) = \|\boldsymbol{z}_\alpha\|_2 + O_\prec\Big(n^{-1/2+\varepsilon}\Big) = 1 + O_\prec\Big(n^{-1/2+\varepsilon}\Big),$$

$$\boldsymbol{x}_\alpha^\top \boldsymbol{x}_\beta = \boldsymbol{z}_\alpha^\top \boldsymbol{z}_\beta + \sum_{i=1}^r O_\prec\Big(|\theta_i|\Big(|\boldsymbol{a}_i^\top \boldsymbol{z}_\alpha||b_{i,\alpha}| + |\boldsymbol{a}_i^\top \boldsymbol{z}_\beta||b_{i,\beta}|\Big) + \theta_i^2\|\boldsymbol{a}_i\|_2^2|b_{i,\alpha}b_{i,\beta}|\Big) = O_\prec\Big(n^{-1/2+\varepsilon}\Big).$$

Hence Theorem 4 applies, showing that $\boldsymbol{K}_\ell$ has an outlier eigenvalue corresponding to each input signal θ_i if and only if $\theta_i > \gamma_0^{1/4}$ and $i \in \mathcal{I}_\ell$. The statement (2.10) follows from Theorem 4(c) applied with $\boldsymbol{v} = \boldsymbol{b}_i$. ■

Appendix F. Proofs for spiked eigenstructure of the trained CK

In this section, we prove Theorem 6. The proof is an application of Theorem 13 as in the one-layer setting of the preceding section, but now reversing the roles of $\boldsymbol{X}$ and $\boldsymbol{W}$. We abbreviate

$$\boldsymbol{W} = \boldsymbol{W}_{\text{trained}}, \qquad \boldsymbol{Y} = \frac{1}{\sqrt{N}}\sigma(\tilde{\boldsymbol{X}}\boldsymbol{W}), \qquad \boldsymbol{K} = \boldsymbol{Y}\boldsymbol{Y}^\top$$

where $\boldsymbol{K}$ is the CK matrix of interest. In contrast to the preceding section, the theorem requires characterizing the *left* spike singular vector of $\boldsymbol{Y}$, and we will do so using Theorem 13(c).

We first recall the following approximation of $\boldsymbol{W}$ from Ba et al. (2022).

Proposition 36 *Under Assumption 4, set $\eta = \sum_{t=1}^T \eta_t$, and let θ_1, θ_2 be as defined in (2.14). Then*

$$\|\boldsymbol{W} - \widetilde{\boldsymbol{W}}\| \prec N^{-1/2} \quad \textit{where} \quad \widetilde{\boldsymbol{W}} = \boldsymbol{W}_0 + \frac{b_\sigma \eta}{n}\boldsymbol{X}^\top \boldsymbol{y}\boldsymbol{a}^\top. \tag{F.1}$$

The largest singular value $s_{\max}(\boldsymbol{W})$ falls outside the limit of its empirical singular value distribution if and only if $\theta_1 > \gamma_0^{1/4}$, in which case $s_{\max}(\boldsymbol{W})$ and its unit-norm left singular vector $\boldsymbol{u}(\boldsymbol{W})$ satisfy

$$s_{\max}(\boldsymbol{W}) \to s_1 := \sqrt{\frac{(1+\theta_1^2)(\gamma_0+\theta_1^2)}{\theta_1^2}}, \quad |\boldsymbol{u}(\boldsymbol{W})^\top \boldsymbol{\beta}_*|^2 \to \frac{\theta_2^2}{\theta_1^2}\left(1 - \frac{\gamma_0+\theta_1^2}{\theta_1^2(\theta_1^2+1)}\right) \quad \textit{a.s.} \tag{F.2}$$

Proof. Notice that each gradient update matrix $\boldsymbol{G}_t$ of (2.12) takes the form

$$\boldsymbol{G}_t = \frac{1}{n}\boldsymbol{X}^\top\left[\left(\frac{1}{\sqrt{N}}\left(\boldsymbol{y} - \frac{1}{\sqrt{N}}\sigma(\boldsymbol{X}\boldsymbol{W}_t)\boldsymbol{a}\right)\boldsymbol{a}^\top\right) \odot \sigma'(\boldsymbol{X}\boldsymbol{W}_t)\right],$$

From the proof of (Ba et al., 2022, Lemma 16), for each $t = 1, \dots, T$, this matrix $\boldsymbol{G}_t$ satisfies the same rank-one approximation

$$\left\|\sqrt{N}\,\boldsymbol{G}_t - \frac{b_\sigma}{n}\boldsymbol{X}^\top \boldsymbol{y}\boldsymbol{a}^\top\right\| \prec N^{-1/2}.$$

This implies (F.1) in light of (2.12), and the statements of (F.2) then follow from (Ba et al., 2022, Theorem 3). ■

We denote the columns of $\boldsymbol{W} \equiv \boldsymbol{W}_{\text{trained}} \in \mathbb{R}^{d\times N}$ and of the initialization $\boldsymbol{W}_0 \in \mathbb{R}^{d\times N}$ by

$$\boldsymbol{w}_i \in \mathbb{R}^d, \ \boldsymbol{w}_{i,0} \in \mathbb{R}^d \text{ for } i \in [N]$$

respectively. Fixing a large constant $B > 0$ and small constant $\varepsilon > 0$, define the event

$$\mathcal{E}(\boldsymbol{W}) = \Big\{\|\boldsymbol{W}\| < B,\ |\boldsymbol{w}_i^\top \boldsymbol{w}_j| < n^{-1/2+\varepsilon} \text{ and } |\|\boldsymbol{w}_i\|_2 - 1| < n^{-1/2+\varepsilon} \text{ for all } i \neq j \in [N]\Big\}.$$

Lemma 37 *Under Assumption 4, for some sufficiently large constant $B > 0$ and any fixed $\varepsilon > 0$, $\mathcal{E}(\boldsymbol{W})$ holds almost surely for all large n and any fixed $T \in \mathbb{N}$.*

Proof. By the assumption $[\boldsymbol{W}_0]_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1/d)$, it is immediate to check that $\mathcal{E}(\boldsymbol{W}_0)$ holds almost surely for all large n. To show that $\mathcal{E}(\boldsymbol{W})$ holds, we apply the approximation (F.1). Here, under Assumption 4, we have by standard tail bounds for Gaussian vectors and matrices that

$$\mathbf{1}\{\|\boldsymbol{X}^\top \boldsymbol{y}\| > Cn\} \leq \mathbf{1}\{\|\boldsymbol{X}\| \cdot (\lambda_{\sigma_*}\|\boldsymbol{X}\boldsymbol{\beta}_*\| + \|\boldsymbol{\varepsilon}\|_2) > Cn\} \prec 0, \qquad \mathbf{1}\{\|\boldsymbol{a}\|_2 > C\} \prec 0$$

for a sufficiently large constant $C > 0$, and also $\|\boldsymbol{a}\|_\infty \prec N^{-1/2}$. Then this implies

$$\max_{i=1}^{N} \|\boldsymbol{w}_i - \boldsymbol{w}_{i,0}\|_2 \leq \max_{i=1}^{N} \|\widetilde{\boldsymbol{w}}_i - \boldsymbol{w}_{i,0}\|_2 + \|\boldsymbol{W} - \widetilde{\boldsymbol{W}}\| \prec N^{-1/2} \tag{F.3}$$

and $\mathbf{1}\{\|\boldsymbol{W} - \boldsymbol{W}_0\| > C'\} \prec 0$ for a constant $C' > 0$. Then $\mathcal{E}(\boldsymbol{W})$ also holds almost surely for all large n, as claimed. ■

Analogous to the argument of Appendix E.1, we may now condition on $\boldsymbol{W}$, i.e. we assume that $\boldsymbol{W}$ is deterministic and satisfies $\mathcal{E}(\boldsymbol{W})$ for all large n, and we write $\mathbb{E}$ for the expectation over only the randomness of the new data $(\tilde{\boldsymbol{X}}, \tilde{\boldsymbol{y}})$. Defining

$$\boldsymbol{G} = \sqrt{\frac{N}{n}}(\boldsymbol{Y} - \mathbb{E}\boldsymbol{Y}) \in \mathbb{R}^{n \times N}, \quad \boldsymbol{u} = \frac{1}{\sqrt{n}}\tilde{\boldsymbol{y}} \in \mathbb{R}^n \quad \text{where} \quad \boldsymbol{Y} = \frac{1}{\sqrt{N}}\sigma(\tilde{\boldsymbol{X}}\boldsymbol{W}), \tag{F.4}$$

observe that $[\boldsymbol{u}, \boldsymbol{G}] \in \mathbb{R}^{n \times (N+1)}$ has centered i.i.d. rows with respect to the randomness of $(\tilde{\boldsymbol{X}}, \tilde{\boldsymbol{y}})$. We will write $\mathbb{E}_{\boldsymbol{x}}$ for the expectation with respect to a standard Gaussian vector $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_d)$.

Lemma 38 *Suppose $\boldsymbol{W}$ satisfies $\mathcal{E}(\boldsymbol{W})$ for all large n. Then*

$$\|\mathbb{E}_{\boldsymbol{x}}[\sigma(\boldsymbol{x}^\top \boldsymbol{W})]\|_2 \to 0, \qquad \|\mathbb{E}\boldsymbol{Y}\| \to 0, \qquad \|\boldsymbol{\Sigma} - \boldsymbol{\Sigma}_{\text{lin}}\| \to 0 \tag{F.5}$$

where

$$\boldsymbol{\Sigma} := \mathbb{E}_{\boldsymbol{x}}[\sigma(\boldsymbol{x}^\top \boldsymbol{W})^\top \sigma(\boldsymbol{x}^\top \boldsymbol{W})] - \mathbb{E}_{\boldsymbol{x}}[\sigma(\boldsymbol{x}^\top \boldsymbol{W})]^\top \mathbb{E}_{\boldsymbol{x}}[\sigma(\boldsymbol{x}^\top \boldsymbol{W})] \tag{F.6}$$

$$\boldsymbol{\Sigma}_{\text{lin}} := b_\sigma^2(\boldsymbol{W}^\top \boldsymbol{W}) + (1 - b_\sigma^2)\boldsymbol{I}_N. \tag{F.7}$$

Proof. The proof is the same as Lemmas 31 and 32. ■

Proof of Theorem 6. We condition on $\boldsymbol{W}$ satisfying $\mathcal{E}(\boldsymbol{W})$ for all large n, and we apply Theorem 13(c) for $[\boldsymbol{u}, \boldsymbol{G}] \in \mathbb{R}^{(n+1) \times N}$ (exchanging n and N). It may be checked that Assumption 5 holds for $[\boldsymbol{u}, \boldsymbol{G}]$ by the same argument as in Lemma 35.

By the convergence $\|\boldsymbol{\Sigma} - \boldsymbol{\Sigma}_{\text{lin}}\| \to 0$ in Lemma 38 and Proposition 36, if $\theta_1 > \gamma_0^{1/4}$, then Assumption 6 holds for $\boldsymbol{\Sigma}$ with $r = 1$ and

$$\nu = b_\sigma^2 \otimes \rho_{\gamma_0}^{\text{MP}} \oplus (1 - b_\sigma^2), \qquad \lambda_1 = b_\sigma^2 \frac{(1 + \theta_1^2)(\gamma_0 + \theta_1^2)}{\theta_1^2} + (1 - b_\sigma^2) \notin \operatorname{supp}(\nu),$$

where $\rho_{\gamma_0}^{\text{MP}}$ is the standard Marcenko-Pastur limit for the empirical eigenvalue distribution of $\boldsymbol{W}^\top \boldsymbol{W}$, hence ν is the limit empirical eigenvalue distribution of $\boldsymbol{\Sigma}$, and λ_1 is the limit of $\lambda_{\max}(\boldsymbol{\Sigma})$. If instead $\theta_1 \leq \gamma_0^{1/4}$, then Assumption 6 holds with $r = 0$.

Then Theorem 13(a,c) characterizes the outlier eigenvalue and eigenvector of $\boldsymbol{G}\boldsymbol{G}^\top$, showing:

- $\boldsymbol{G}\boldsymbol{G}^\top$ has a spike eigenvalue if and only if $\theta_1 > \gamma_0^{1/4}$ and $z'(-1/\lambda_1) > 0$, where $z(\cdot)$ is defined by (A.4) with $\gamma = \gamma_1$ and the measure ν given above. In this case, $\lambda_{\max}(\boldsymbol{G}\boldsymbol{G}^\top) \to z(-1/\lambda_1)$ almost surely.

- When $\theta_1 > \gamma_0^{1/4}$ and $z'(-1/\lambda_1) > 0$, letting $\boldsymbol{u}(\boldsymbol{G}), \boldsymbol{v}(\boldsymbol{\Sigma})$ be the leading unit-norm left singular vector of $\boldsymbol{G}$ and leading unit-norm eigenvector of $\boldsymbol{\Sigma}$, almost surely

$$|\boldsymbol{u}^\top \boldsymbol{u}(\boldsymbol{G})| - \frac{\sqrt{z(-1/\lambda_1)\varphi(-1/\lambda_1)}}{\lambda_1} \cdot \left|\mathbb{E}_{\boldsymbol{x}}[\sigma_*(\boldsymbol{\beta}_*^\top \boldsymbol{x})\sigma(\boldsymbol{x}^\top \boldsymbol{W})]\boldsymbol{v}(\boldsymbol{\Sigma})\right| \to 0.$$

  where $\varphi(\cdot)$ is defined by (B.6) also with $\gamma = \gamma_1$ and the above measure ν.

By an application of Weyl's inequality and the Davis-Kahan Theorem as in the proof of Theorem 4, this implies for $\boldsymbol{K} = \boldsymbol{Y}\boldsymbol{Y}^\top$ that if $\theta_1 > \gamma_0^{1/4}$ and $z'(-1/\lambda_1) > 0$, then its leading eigenvalue $\lambda_{\max}(\boldsymbol{K})$ and unit eigenvector $\widehat{\boldsymbol{u}}$ satisfy

$$\begin{aligned} &\lambda_{\max}(\boldsymbol{K}) \to \gamma_1^{-1} z(-1/\lambda_1), \\ &|\boldsymbol{u}^\top \widehat{\boldsymbol{u}}| - \frac{\sqrt{z(-1/\lambda_1)\varphi(-1/\lambda_1)}}{\lambda_1} \cdot \left|\mathbb{E}_{\boldsymbol{x}}[\sigma_*(\boldsymbol{\beta}_*^\top \boldsymbol{x})\sigma(\boldsymbol{x}^\top \boldsymbol{W})]\boldsymbol{v}(\boldsymbol{W})\right| \to 0, \end{aligned} \tag{F.8}$$

where $\boldsymbol{v}(\boldsymbol{W})$ is the leading unit eigenvector of $\boldsymbol{\Sigma}_{\text{lin}}$, i.e. the leading right singular vector of $\boldsymbol{W}$. If $\theta_1 \le \gamma_0^{1/4}$ or $z'(-1/\lambda_1) \le 0$, then all eigenvalues of $\boldsymbol{K}$ converge to the support of its limiting empirical eigenvalue law.

Finally, in the case of $\theta_1 > \gamma_0^{1/4}$ and $z'(-1/\lambda_1) > 0$, we may conclude the proof by showing

$$\left\|\mathbb{E}_{\boldsymbol{x}}[\sigma_*(\boldsymbol{\beta}_*^\top \boldsymbol{x})\sigma(\boldsymbol{x}^\top \boldsymbol{W})] - b_\sigma b_{\sigma_*} \boldsymbol{\beta}_*^\top \boldsymbol{W}\right\|_2 \to 0 \text{ a.s.} \tag{F.9}$$

For each column $i \in [N]$, we have from (F.3) that $\|\boldsymbol{w}_i - \boldsymbol{w}_{i,0}\|_2 \prec N^{-1/2}$, where $\boldsymbol{w}_{i,0} \sim \mathcal{N}(0, d^{-1}\boldsymbol{I})$ and $\boldsymbol{\beta}_*$ is deterministic. Hence $(\boldsymbol{w}_i, \boldsymbol{\beta}_*)$ satisfy the approximate orthonormality conditions $|\|\boldsymbol{w}_i\|_2 - 1| \prec N^{-1/2}$, $\|\boldsymbol{\beta}_*\|_2 - 1 = 0$, and $|\boldsymbol{w}_i^\top \boldsymbol{\beta}_*| \prec N^{-1/2}$. Then (Fan and Wang, 2020, Lemma D.3(a)) implies

$$\left|\mathbb{E}_{\boldsymbol{x}}[\sigma_*(\boldsymbol{\beta}_*^\top \boldsymbol{x})\sigma(\boldsymbol{x}^\top \boldsymbol{w}_i)] - b_\sigma b_{\sigma_*} \boldsymbol{\beta}_*^\top \boldsymbol{w}_i\right| \prec N^{-1}.$$

(We note that (Fan and Wang, 2020, Lemma D.3(a)) assumes $\sigma = \sigma_*$, but the proof is identical for $\sigma \neq \sigma_*$ both satisfying Assumption 3.) Applying this to each coordinate $i \in [N]$ yields (F.9). Observe that $\boldsymbol{\beta}_*^\top \boldsymbol{W}\boldsymbol{v}(\boldsymbol{W}) = s_{\max}(\boldsymbol{W}) \cdot \boldsymbol{\beta}_*^\top \boldsymbol{u}(\boldsymbol{W})$ where $s_{\max}(\boldsymbol{W})$ and $\boldsymbol{u}(\boldsymbol{W})$ are the leading singular value and left singular vector of $\boldsymbol{W}$, and recall from the definitions (F.4) that $\boldsymbol{u} = \frac{1}{\sqrt{n}}\tilde{\boldsymbol{y}}$. Then we can apply (F.9) and Proposition 36 to (F.8) to conclude that

$$\frac{1}{\sqrt{n}}|\tilde{\boldsymbol{y}}^\top \widehat{\boldsymbol{u}}| \to b_\sigma b_{\sigma_*} \frac{\sqrt{z(-1/\lambda_1)\varphi(-1/\lambda_1)}}{\lambda_1} \cdot \frac{\theta_2\sqrt{(\theta_1^4 - \gamma_0)(\gamma_0 + \theta_1^2)}}{\theta_1^3} > 0 \text{ a.s.}$$

■