Principal components and linear mixed models

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(joint w/ Iain Johnstone, Yi Sun, Zhichao Wang)

Random Matrices and Related Topics
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This talk will describe some applications of random matrix theory to understand spectral behavior and principal components analysis for classical covariance estimates in these models.

Outline

Model and motivation

Example: A twin study

Measure p quantitative traits in $n/2$ pairs of twins. For $i = 1, \ldots, n/2$, model this with two "levels" of variation as

$$Y_{i,1} = \alpha_i + \varepsilon_{i,1} \in \mathbb{R}^p$$
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$$\alpha_i \overset{iid}{\sim} \mathcal{N}(0, \Sigma_A), \qquad \varepsilon_{i,j} \overset{iid}{\sim} \mathcal{N}(0, \Sigma_E)$$

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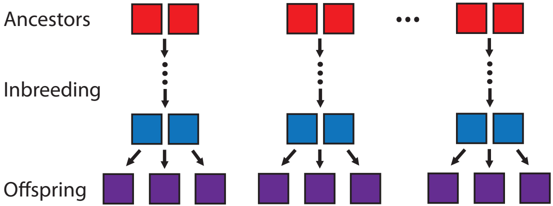
Only the $Y_{i,j}$'s (not the α_i's or $\varepsilon_{i,j}$'s) are observed. From this, we wish to separately understand Σ_A and Σ_E.

Example: Mutations in fruit flies [McGuigan et al '14]



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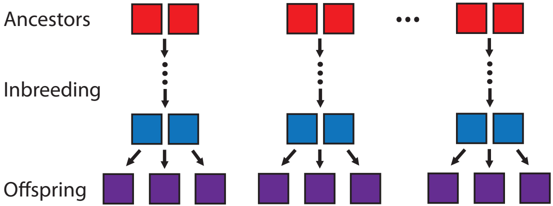

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Model traits (gene expression measurements) in the j^{th} offspring of the i^{th} inbred line as

$$Y_{i,j} = \alpha_i + \varepsilon_{i,j}.$$

The covariance Σ_A of α_i's is the mutational variation of interest.

Example: Genome-wide association studies

In n individuals, measure:

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The covariance Σ_A of α_i's is the (additive) genetic covariance.
The relative size of Σ_A to Σ_E provides a measure of heritability.

The linear mixed model

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($k = 1$, $U_1 = \mathrm{Id}$ is the setting of n independent observations in $\mathbb{R}^p$)

The MANOVA covariance estimator

For $r \in \{1, \ldots, k\}$, a classical estimator for Σ_r is the MANOVA estimator. This is a matrix

$$\widehat{\Sigma} = Y^{\mathsf{T}} B Y.$$

Here, $B \in \mathbb{R}^{n \times n}$ is symmetric and chosen so that $\mathbb{E}[\widehat{\Sigma}] = \Sigma_r$.

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- For $k = 2$ and the twin study, we take $B = \frac{1}{n}(\pi - \pi^{\perp})$ where $\pi, \pi^{\perp}$ are orthogonal projections onto the column span of U_1 and its complement.

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2. What is the behavior of principal components in spiked settings?

Aside: The case of isotropic noise

A simple statistical null hypothesis in this model is

$$\Sigma_r = \sigma_r^2 \, \mathrm{Id}$$

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This setting is special: We may write $\widehat{\Sigma} = G^\top F G$ where

$$G = \begin{pmatrix} G_1 \\ \vdots \\ G_k \end{pmatrix}, \quad F = (\sigma_r F_{rs} \sigma_s)_{r,s=1}^{k}.$$

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Here, $\widehat{\Sigma}$ is related to the sample covariance model. We've obtained more refined results in this setting than in the general case, due a known local law [Knowles, Yin '17].

Results on spectral behavior

Empirical spectral distribution

Theorem (Fan, Johnstone '16)

As $n, n_1, \ldots, n_k, p \to \infty$ *proportionally, the e.s.d.* $\hat{\mu}$ *of* $\widehat{\Sigma}$ *is approximated (weakly a.s.) by a deterministic equivalent measure* μ_0*.*

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$$a_r(z) = -n_r^{-1} \operatorname{Tr} \left((z \operatorname{Id} + b \cdot \Sigma)^{-1} \Sigma_r \right)$$
$$b_r(z) = -n_r^{-1} \operatorname{Tr}_r \left((\operatorname{Id} + FD(a))^{-1} F \right)$$
$$m_0(z) = -p^{-1} \operatorname{Tr} \left((z \operatorname{Id} + b \cdot \Sigma)^{-1} \right)$$

for $r = 1, \ldots, k$. Here,

$$b \cdot \Sigma \equiv b_1(z)\Sigma_1 + \ldots + b_k(z)\Sigma_k, \qquad F \equiv (F_{rs})_{r,s=1}^k$$
$$D(a) \equiv \operatorname{diag}(a_1(z) \operatorname{Id}_{n_1}, \ldots, a_k(z) \operatorname{Id}_{n_k}),$$

and Tr_r is the trace of the (r, r) block, of size n_r.

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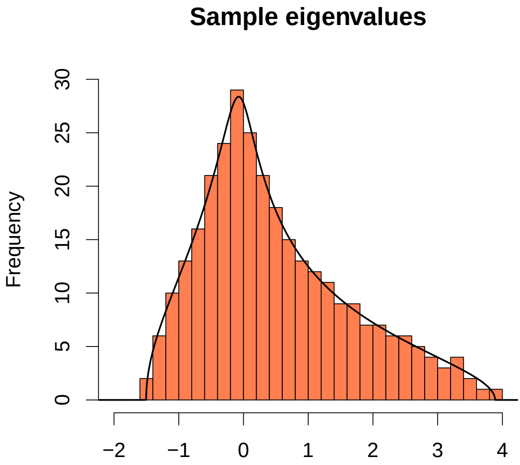

Spectrum of $\widehat{\Sigma}_A$ in a twin study design, 300 twin pairs, 300 traits.

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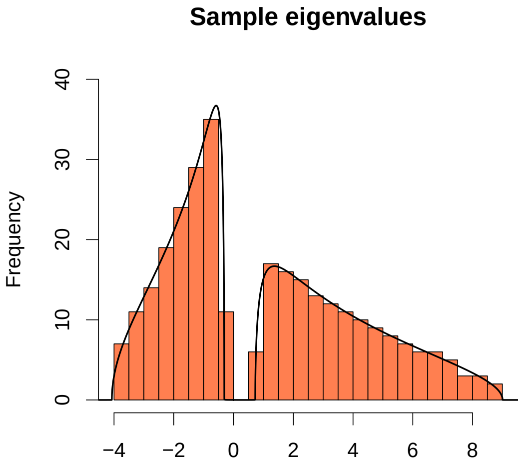

Spectrum of $\widehat{\Sigma}_A$ in a twin study design, 150 twin pairs, 600 traits.

A free approximation

The measure μ_0 is the τ-law of an operator

$$w = \sum_{r=1}^{k} \sum_{s=1}^{k} h_r^* g_r^* f_{rs} g_s h_s$$

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- Each $g_r^* g_r$ has Marcenko-Pastur moments under τ.
- The families $\{h_r : r = 1, \ldots, k\}$, $\{f_{rs} : r, s = 1, \ldots, k\}$, and elements $g_1, \ldots, g_k$ are free with amalgamation over a diagonal sub-algebra of projections. [Benaych-Georges '09]

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We show that this approximation is asymptotically correct, due to the independence and rotational invariance of $G_1, \ldots, G_k$.

Computation of fixed-point equations

In $(\mathcal{A}, \tau)$, let $\tau^{\mathcal{H}} : \mathcal{A} \to \mathcal{H}$ be the conditional expectation onto the subalgebra $\mathcal{H} = \langle h_1, \ldots, h_k \rangle \subset \mathcal{A}$, and similarly for $\tau^{\mathcal{G}}, \tau^{\mathcal{F}}$.

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We relate the $\tau^{\mathcal{H}}$ Stieltjes-transform of w, $\tau^{\mathcal{G}}$ Stietjes-transform of v, and $\tau^{\mathcal{F}}$ Stieltjes-transform of u using conditional cumulant relations, and compute $\tau \circ \tau^{\mathcal{H}}((z - w)^{-1})$. [Speicher, Vargas '12]

All eigenvalues stick to the support

Theorem (Fan, Sun, Wang '19)

For any fixed $\delta > 0$, *almost surely for all large* n

$$\mathrm{spec}(\widehat{\Sigma}) \subset \mathrm{supp}(\mu_0)_\delta \equiv \{x \in \mathbb{R} : \mathrm{dist}(x, \mathrm{supp}(\mu_0)) < \delta\}.$$

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This is a distinct analytic argument specific to the isotropic setting. Establishing Tracy-Widom for general Σ_r is interesting and open.

Spiked model and outliers

For understanding principal components analysis in these models, we are interested in spiked settings

$$\Sigma_r = \mathring{\Sigma}_r + \Gamma_r^T \Gamma_r$$

where $\Gamma_r \in \mathbb{R}^{p \times \ell_r}$, and $\Gamma_r^T \Gamma_r$ is a perturbation of fixed rank ℓ_r.

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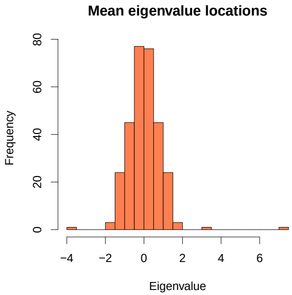

$\widehat{\Sigma}_A$ in a twin-study design, where each Σ_A and Σ_E is a rank-1 perturbation of Id. The spike-to-outlier mapping is not 1-to-1, and Σ_E produces outliers in $\widehat{\Sigma}_A$.

Spiked model and outliers

Define μ_0 by the bulk components $\mathring{\Sigma}_1, \ldots, \mathring{\Sigma}_k$. Recall $b_1(z), \ldots, b_k(z)$ from the fixed-point equations for μ_0, and set

$$T(z) = \mathrm{Id} + \left(\Gamma_r^\mathsf{T} \left(z \, \mathrm{Id} + b \cdot \mathring{\Sigma} \right)^{-1} \Gamma_s b_s(z) \right)_{r,s=1}^{k} \in \mathbb{C}^{\ell_+ \times \ell_+}$$

where $\ell_+ = \ell_1 + \ldots + \ell_k$ and $b \cdot \mathring{\Sigma} = b_1 \mathring{\Sigma}_1 + \ldots + b_k \mathring{\Sigma}_k$.

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Theorem (Fan, Sun, Wang '19)

Eigenvalues $\widehat{\lambda}$ *of* $\widehat{\Sigma}$ *separated from* $\mathrm{supp}(\mu_0)$ *are in correspondence with roots of* $0 = \det T(\lambda)$*, such that* $\widehat{\lambda} - \lambda \to 0$.

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Eigenvalues $\widehat{\lambda}$ *of* $\widehat{\Sigma}$ *separated from* $\operatorname{supp}(\mu_0)$ *are in correspondence with roots of* $0 = \det T(\lambda)$, *such that* $\widehat{\lambda} - \lambda \to 0$. *If* λ *is an isolated root, then the eigenvector* $\widehat{v}$ *and unit vector* $u \in \ker T(\lambda)$ *satisfy*

$$(\Gamma_1^\mathsf{T} \widehat{v}, \ldots, \Gamma_k^\mathsf{T} \widehat{v}) - \alpha^{-1/2} u \to 0.$$

Spiked model and outliers

Define μ_0 by the bulk components $\mathring{\Sigma}_1, \ldots, \mathring{\Sigma}_k$. Recall $b_1(z), \ldots, b_k(z)$ from the fixed-point equations for μ_0, and set

$$T(z) = \mathrm{Id} + \left(\Gamma_r^\top \left(z\,\mathrm{Id} + b \cdot \mathring{\Sigma} \right)^{-1} \Gamma_s b_s(z) \right)_{r,s=1}^{k} \in \mathbb{C}^{\ell_+ \times \ell_+}$$

where $\ell_+ = \ell_1 + \ldots + \ell_k$ and $b \cdot \mathring{\Sigma} = b_1 \mathring{\Sigma}_1 + \ldots + b_k \mathring{\Sigma}_k$.

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For $\mathring{\Sigma}_r = \sigma_r^2\,\mathrm{Id}$, we established also in [Fan, Johnstone, Sun '18] a Gaussian CLT for $\widehat{\lambda} - \lambda$.

Bias and phase transition of eigenvalues

The number of outlier eigenvalues is predicted by

$$|\{\lambda \notin \mathrm{supp}(\mu_0) : 0 = \det T(\lambda)\}|.$$

This is 0 if all population spikes are small.

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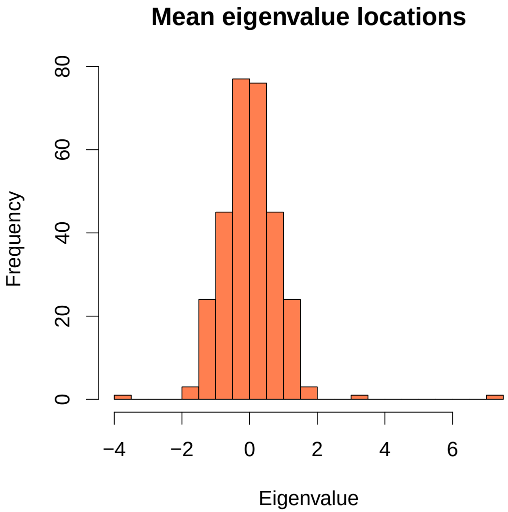
Qualitatively, for the twin-study design:

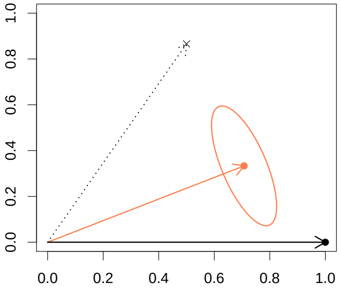
- Large spikes in Σ_E generate two outliers of opposite sign in $\widehat{\Sigma}_A$
- Large eigenvalues in Σ_A are observed with upward bias in $\widehat{\Sigma}_A$, where the bias is larger if this eigenvector of Σ_A is aligned with eigenvectors of Σ_E.

Bias and phase transition of eigenvalues



Bias of principal eigenvectors

In contrast to the sample covariance setting of $k = 1$, here there may also be bias in the outlier *eigenvectors*:



In high dimensions, principal component eigenvectors of $\widehat{\Sigma}_A$ may be biased towards eigenvectors of Σ_E.

Debiasing the principal components

For $\mathring{\Sigma}_r = \sigma_r^2 \,\mathrm{Id}$, we developed in [Fan, Johnstone, Sun '18] an algorithm to estimate the population eigenvalues, and also debias the estimated principal eigenvectors:

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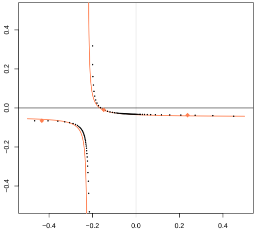
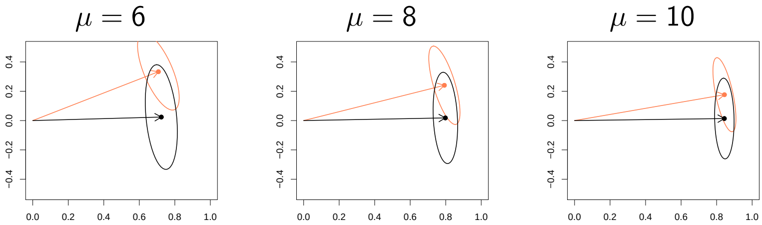


Debiasing the principal components

Mean and 90%-ellipsoid of MANOVA and debiased principal eigenvector estimates, for true eigenvector $(1, 0)$ and eigenvalue μ:



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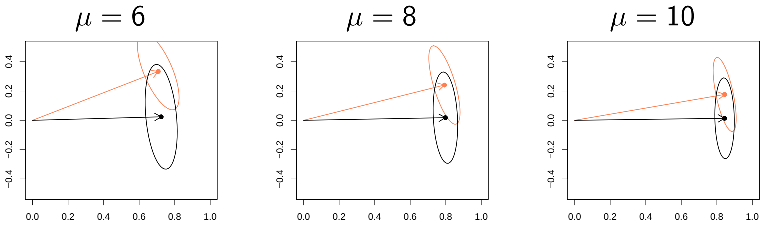

Mean and st. dev. of MANOVA and debiased eigenvalue estimates:

	$\mu = 6$	$\mu = 8$	$\mu = 10$
MANOVA	10.57 (1.74)	11.98 (1.85)	13.59 (1.99)
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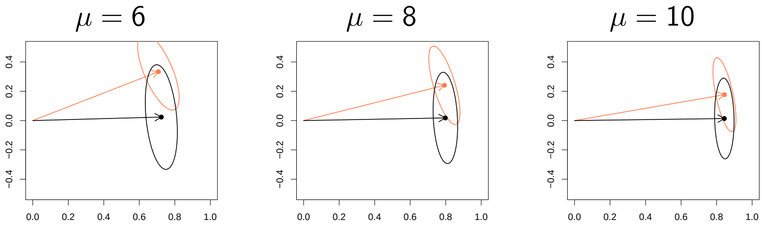

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Developing estimation procedures for general $\mathring{\Sigma}_r \neq \sigma_r^2 \,\mathrm{Id}$ is open.

A few general tools

1. ℓ_2 fluctuation averaging

In the setting $\Sigma_r = \sigma_r^2 \,\mathrm{Id}$, recall that $\widehat{\Sigma} = G^\mathsf{T} F G$.

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has a deterministic approximation $R_0(z)$ in the form of an anisotropic local law [Knowles, Yin '17].

For z separated from the spectral support, $\mathrm{dist}(z, \mathrm{supp}(\mu_0)) > \delta$, and any deterministic unit vectors u and v, this says

$$u^*(R(z) - R_0(z))v \prec 1/\sqrt{n}.$$

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To approximate other combinations of resolvent entries, e.g. $\operatorname{Tr} R(z)$, one may apply weak dependence of these entries and "fluctuation averaging" techniques [Erdös, Yau, Yin '11].

1. ℓ_2 fluctuation averaging

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be independent random quantities. For $\mathcal{Y}$ a scalar function of $\mathbf{x}_1, \ldots, \mathbf{x}_n$, denote

$$\mathcal{P}_i[\mathcal{Y}] = \mathbb{E}_{\mathbf{x}_i}[\mathcal{Y}], \quad \mathcal{Q}_i[\mathcal{Y}] = \mathcal{Y} - \mathcal{P}_i[\mathcal{Y}], \quad \mathcal{Q}_S[\mathcal{Y}] = \left(\prod_{i \in S} \mathcal{Q}_i \right) [\mathcal{Y}]$$

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Suppose $\mathcal{Y}_1, \ldots, \mathcal{Y}_n$ satisfy $\mathcal{P}_i[\mathcal{Y}_i] = 0$, $\mathcal{Y}_i \prec 1$, and the weak dependence $\mathcal{Q}_S[\mathcal{Y}_i] \prec n^{-|S|/2}$ for $i \notin S$.

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Compared with existing results that I'm aware of, this does not require $u_i \equiv 1/n$ or use an upper bound on $\|u\|_\infty$.

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For z with $\operatorname{dist}(z, \operatorname{supp}(\mu_0)) > \delta$, we obtain from these and the entrywise local law, for any deterministic matrix M, that

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This recovers the anisotropic local law for rank-one $M = vu^*$, but provides a strengthened guarantee when $\operatorname{rank}(M) \gg 1$. We use this to establish the CLT for fluctuations of outlier eigenvalues.

2. Anisotropic resolvent approximation

For $\Sigma_r \neq \sigma_r^2 \operatorname{Id}$, we still wish to approximate $u^* R(z) v$ to analyze outliers by a "master equation" approach [Benaych-Georges, Nadakuditi '12], but we currently don't have a local law.

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Note: R_0 is not necessarily isotropic. The approximation is not $u^* R(z) v \approx u^* v \cdot m_0(z)$ if u, v are aligned with $R_0(z)$.

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Let

- $H_1, \ldots, H_q \in \mathbb{C}^{n\times n}$ be deterministic matrices,
- $G_1, \ldots, G_p \in \mathbb{C}^{n\times n}$ be random and jointly orthogonally invariant in law.

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Define the von Neumann algebras

- $(\mathcal{A}_1, \tau_1) \equiv (\mathbb{C}^{n \times n}, n^{-1} \operatorname{Tr})$, containing $H_1, \ldots, H_q$,
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Let $\tau^{\mathcal{H}} : \mathcal{A} \to \mathcal{H} \equiv \langle H_1, \ldots, H_q \rangle$ be the conditional expectation.
Note: For any $a \in \mathcal{A}$, $\tau^{\mathcal{H}}(a) \in \mathcal{H} \subset \mathcal{A}_1$ is an $n \times n$ matrix!

2. Anisotropic resolvent approximation

Theorem (Fan, Sun, Wang '19)

Fix a self-adjoint $*$-polynomial Q and $\delta > 0$. Let

$$W = Q(G_1, \ldots, G_p, H_1, \ldots, H_q) \in \mathbb{C}^{n \times n},$$
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Let $R(z) = (W - z\,\mathrm{Id})^{-1}$, and define a deterministic approximation

$$R_0(z) = \tau^{\mathcal{H}}((w - z)^{-1}) \in \mathbb{C}^{n \times n}.$$

Then for any deterministic unit vectors $u, v \in \mathbb{C}^n$, as $n \to \infty$,

$$u^*(R(z) - R_0(z))v \to 0$$

uniformly over $\{z \in \mathbb{C} : \mathrm{dist}(z, \mathrm{spec}(W) \cup \mathrm{spec}(w)) > \delta\}$.

3. Augmented Cauchy and $\mathcal{R}$-transforms

Our computations in the approximating free model use relations between (conditional) Cauchy and $\mathcal{R}$-transforms:

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Let $\kappa_\ell(a_1, \ldots, a_\ell)$ be the ℓ^{th} order non-crossing cumulant, and

$$G_a(z) = \tau((z-a)^{-1}) = \sum_{\ell=0}^{\infty} z^{-(\ell+1)}\tau(a^\ell),$$

$$\mathcal{R}_a(z) = \sum_{\ell=1}^{\infty} z^{\ell-1}\kappa_\ell(a, \ldots, a).$$

The moment-cumulant relations for non-crossing partitions give

$$G_a(z) = (z - \mathcal{R}_a(G_a(z)))^{-1}.$$

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for certain (random) matrices A. We introduce augmented transforms and some associated moment-cumulant relations:

$$G_{a,w}(z) = \tau(a(z-w)^{-1}) = \sum_{\ell=0}^{\infty} z^{-(\ell+1)}\tau(aw^{\ell}),$$

$$\mathcal{R}_{a,w}(z) = \sum_{\ell=1}^{\infty} z^{\ell-1}\kappa_{\ell}(a,w,\ldots,w).$$

Lemma (Fan, Sun, Wang '19)

$$G_{a,w}(z) = \mathcal{R}_{a,w}(G_w(z))G_w(z)$$

4. Strong asymptotic freeness for GOE

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$$\mathrm{spec}(Q(\{W_i\}_{i=1}^p, \{H_j\}_{j=1}^q)) \subset \mathrm{spec}(Q(\{w_i\}_{i=1}^p, \{H_j\}_{j=1}^q))_\delta.$$

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We follow proof ideas of these works, and of [Schultz '05] in the pure GOE setting.

References

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Thank you!