Fluctuations of the spectrum of random quantum states

Joint work with David Grzybowski and Elizabeth Meckes

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Discrete probability with quantum terminology

- A state on $\Omega_n = \{1, \ldots, n\}$ is a vector $p \in \mathbb{R}^n_+$ with $\sum_i p_i = 1$.
- An observable is a function $f : \Omega_n \to \mathbb{R}$.
- f is observed to be $f(i)$ with probability p_i.

Discrete probability as ~~non~~commutative probability

- $F = \begin{bmatrix} f(1) & & 0 \\ & \ddots & \\ 0 & & f(n) \end{bmatrix} = \sum_i f(i) e_i e_i^*$

- $P = \begin{bmatrix} p_1 & & 0 \\ & \ddots & \\ 0 & & p_n \end{bmatrix} = \sum_i p_i e_i e_i^*$

- F is observed to be the eigenvalue $f(i)$ with probability $\langle Pe_i, e_i \rangle$.

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$P \in M_n$ is diagonal, PSD, with $\operatorname{Tr} P = 1$.

Pure quantum states and observables

- A pure state on $\mathbb{C}^n$ is a unit vector $\psi \in \mathbb{C}^n$.

- An observable is a Hermitian matrix $A \in M_n(\mathbb{C})$.

  A has a spectral decomposition $A = \sum_i \lambda_i u_i u_i^*$.

- A is observed to be the eigenvalue λ_i with probability $|\langle \psi, u_i \rangle|^2 = \langle \psi\psi^* u_i, u_i \rangle$.

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  $\psi\psi^* \in M_n(\mathbb{C})$ is PSD with $\operatorname{Tr} \psi\psi^* = 1$ and rank 1.

Marginals in ~~non~~commutative probability

Suppose

- p is a state on $\Omega_n \times \Omega_m$.
- f is an observable on Ω_n only.

The probability of observing $f(i)$ is $q_i = \sum_j p_{ij}$.

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$q \in \mathbb{R}_+^n$ with $\sum_i q_i = 1$.

Matrix version:

- $P \in M_n \otimes M_m \cong M_{n \times m}$.
- $\sum_j p_{ij} = \langle (\mathrm{Tr}_2\, P) e_i, e_i \rangle$, where

$$\mathrm{Tr}_2 = \mathrm{Id} \otimes \mathrm{Tr} : M_n \otimes M_m \to \mathbb{C}$$

is the partial trace.

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$\mathrm{Tr}_2\, P \in M_n$ is diagonal, PSD, with $\mathrm{Tr}(\mathrm{Tr}_2\, P) = 1$.

Quantum marginals

Suppose

- ψ is a pure state on $\mathbb{C}^n \otimes \mathbb{C}^m \cong \mathbb{C}^{n\times m}$
- $A = \sum_i \lambda_i u_i u_i^* \in M_n$ is an observable on $\mathbb{C}^n$ only.
- The probability of observing λ_i is

$$\sum_{j=1}^{m} \left|\langle \psi, u_i \otimes v_j \rangle\right|^2 = \sum_j \langle \psi\psi^*(u_i \otimes v_j), u_i \otimes v_j \rangle$$
$$= \langle (\mathrm{Tr}_2\, \psi\psi^*) u_i, u_i \rangle \,.$$

Here $\{v_j\}$ is any ONB of $\mathbb{C}^m$.

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$\operatorname{Tr}_2 \psi\psi^* \in M_n$ is PSD with $\operatorname{Tr}(\operatorname{Tr}_2 \psi\psi^*) = 1$, but now generically has rank $\min\{m, n\}$.

Induced distributions

A PSD matrix $\rho \in M_n$ with $\operatorname{Tr} \rho = 1$ is a mixed state or density matrix.

There is a canonical (Haar) distribution on simple states $\psi \in \mathbb{C}^n$.

For each m, the Haar distribution on simple states $\psi \in \mathbb{C}^n \otimes \mathbb{C}^m$ induces a distribution on density matrices

$$\rho = \operatorname{Tr}_2(\psi\psi^*) \in M_n.$$

These distributions are widely studied in quantum information theory.

Induced distributions

Unitary invariance of $\psi \rightsquigarrow$ unitary invariance of ρ.

$$\psi \overset{D}{=} (V \otimes U)\psi \qquad \Rightarrow \qquad \rho \overset{D}{=} V\rho V^{*}.$$

To understand the induced distribution we want to understand the eigenvalues of ρ.

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Concrete random matrix representation:

Under the identification

$$\mathbb{C}^n \otimes \mathbb{C}^m \cong \mathbb{C}^{n\times m} \cong M_{n\times m}$$

we can write

$$\rho = XX^*$$

where X is uniformly distributed in the Hilbert–Schmidt unit sphere of $M_{n\times m}$.

Spectral measure

The spectral measure of a Hermitian $A \in M_n$ is

$$\mu_A = \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(A)}.$$

For $f : \mathbb{R} \to \mathbb{R}$,

$$\int f \, d\mu_A = \frac{1}{n} \sum_{i=1}^{n} f(\lambda_i(A)) = \frac{1}{n} \operatorname{Tr} f(A).$$

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Note

$$\mathbb{E} \int x \, d\mu_{nXX^*} = \operatorname{Tr} XX^* = 1,$$

so $A = nXX^*$ is the right normalization to look for a large-n limit for μ_A.

Limiting spectral measure

Theorem (Nechita '07)

Suppose that $\frac{m}{n} \xrightarrow{n\to\infty} \alpha \geq 1$. *Then* μ_{nXX^*} *approaches a deterministic limit measure* μ_α *almost surely.*

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Idea of proof:

$X \overset{D}{=} \frac{Z}{\|Z\|_{HS}}$ where $Z \in M_{n\times m}$ is standard Gaussian.

$\|Z\|_{HS} \approx \sqrt{mn}$ with high probability

$\Rightarrow \mu_{nXX^*} \approx \mu_{\frac{\alpha}{n}ZZ^*}$

$\mu_{\frac{1}{n}ZZ^*}$ is known to have a limit μ_α (Marčenko–Pastur law). $\square$

Main theorem of this talk — rough statement

Theorem (DG–EM–MM '23+)

Suppose that $\frac{m}{n} \xrightarrow{n\to\infty} \alpha \geq 1$. *Linear eigenvalue statistics*

$$\operatorname{Tr} f(nXX^*) = \sum_{i=1}^{n} f(\lambda_i(nXX^*))$$

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The corresponding result for $\frac{1}{n}ZZ^*$ is known (Bai–Silverstein '04, etc.).

But the same trick doesn't work — the fluctuations of $\|Z\|_{HS}$ aren't small enough in this setting.

We need a different approach.

Stein's method for functions of stationary distributions

Theorem (Grzybowski '23)

Let $X \in S$ be in the stationary distribution for a nice Markov process with infinitesimal generator L and carré du champ operator Γ, and let $F : S \to \mathbb{R}^d$ such that $\mathbb{E}F(X) = 0$.
Suppose that

- $LF(X) = -\Lambda F(X) + E$ *and*
- $[\Gamma(F_i(X), F_j(X))]_{ij} = \Lambda\Sigma + E'$

for deterministic $\Lambda, \Sigma \in M_d$ and random centered $E \in \mathbb{R}^d$, $E' \in M_d$.
If Σ is positive definite, then

$$d_W\big(F(X), \mathcal{N}(0, \Sigma)\big) \leq c \left\|\Lambda^{-1}\right\|_{op} \left(\mathbb{E}\left\|E\right\|_2 + \left\|\Sigma^{-1/2}\right\|_{op} \mathbb{E}\left\|E'\right\|_{HS}\right).$$

Stein's method for functions of stationary distributions

Theorem (Grzybowski '23, continued)

Moreover, if Λ is upper triangular with distinct positive entries and $\Lambda\Sigma$ is diagonal, then Σ is indeed both positive definite and diagonal.

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The first part follows by applying the multivariate infinitesimal version of Stein's method of exchangeable pairs (Chatterjee–E. Meckes '08, E. Meckes '09) with the pair $(F(X_t), F(X_0))$.

(Similar approaches in Ledoux, Nourdin–Zhen, Du...).

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The second part is linear algebra.

First warm-up result

Theorem (Johansson '98)

Let $A \in M_n^{sa}(\mathbb{C})$ be a GUE matrix (standard normal distribution on the space of Hermitian matrices). For each k let

$$Y_k = \operatorname{Tr} T_k\left(\tfrac{1}{\sqrt{2n}} A\right) - \mathbb{E} \operatorname{Tr} T_k\left(\tfrac{1}{\sqrt{2n}} A\right),$$

where $T_k(x)$ are the Chebyshev polynomials of the first kind. Then

$$d_W\left((Y_1, \ldots, Y_d), \mathcal{N}\left(0, \tfrac{1}{2}\operatorname{diag}(1, 2, \ldots, d)\right)\right) \le \frac{C_d}{n}.$$

Analogous results hold for the GOE and GSE.
(More general results by many authors.)

First warm-up result

Sketch of proof (Grzybowski ’23):

A is stationary for the Ornstein–Uhlenbeck process on M_n^{sa}:

- $Lf(x) = \Delta f(x) - \langle \nabla f(x), x \rangle$
- $\Gamma(f, g) = \langle \nabla f, \nabla g \rangle$

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For a polynomial p, $\nabla \operatorname{Tr} p(A) = p'(A)$, so
$\langle \nabla \operatorname{Tr} p(A), A \rangle = \operatorname{Tr}(p'(A)A)$

$\Rightarrow \Lambda$ will be upper triangular with distinct positive diagonal entries.

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This reasoning holds for any sequence of polynomials p_k with $\deg p_k = k$.

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Why Chebyshev polynomials of the first kind?

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$$\begin{aligned}\mathbb{E}\left\langle \nabla \operatorname{Tr} p\big(\tfrac{1}{\sqrt{2n}}A\big), \nabla \operatorname{Tr} q\big(\tfrac{1}{\sqrt{2n}}A\big)\right\rangle &= \mathbb{E}\frac{1}{2n}\operatorname{Tr}\left(p'\big(\tfrac{1}{\sqrt{2n}}A\big)q'\big(\tfrac{1}{\sqrt{2n}}A\big)\right)\\ &= \frac{1}{2}\mathbb{E}\int p'q'\ d\mu_{\frac{1}{\sqrt{2n}}A}.\end{aligned}$$

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The orthogonal polynomials w.r.t. σ are the Chebyshev polynomials of the second kind U_k, and $T_k' = kU_{k-1}$.

Error terms can be bounded via measure concentration (M–Szarek '12). □

Second warm-up result

Now let $A \in M_n^{sa}$ be uniformly distributed in the Hilbert–Schmidt unit sphere S.

A is stationary for Brownian motion on S:

- $Lf(x) = \Delta_S f(x) = r^2 \Delta f(x) - r^2 \frac{\partial^2 f}{\partial r^2} - r(\dim S) \frac{\partial f}{\partial r}$
- $\Gamma(f, g)(x) = \langle \nabla_S f(x), \nabla_S g(x) \rangle$
  $= \langle \nabla f(x), \nabla g(x) \rangle - \langle \nabla f(x), x \rangle \langle \nabla g(x), x \rangle$

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  $= \langle \nabla f(x), \nabla g(x) \rangle - \langle \nabla f(x), x \rangle \langle \nabla g(x), x \rangle$

Λ will be nice as before.

We want to pick polynomials so that

$$\mathbb{E}\Gamma\big(\operatorname{Tr} p_i(\sqrt{n}A), \operatorname{Tr} p_j(\sqrt{n}A)\big)$$

is asymptotically diagonal.

Second warm-up result

$$\begin{aligned}
&\mathbb{E}\Gamma\big(\operatorname{Tr} p(\sqrt{n}A), \operatorname{Tr} q(\sqrt{n}A)\big) \\
&\quad = n\mathbb{E}\operatorname{Tr}\big(p'(\sqrt{n}A)q'(\sqrt{n}A)\big) \\
&\qquad - \mathbb{E}\left(\operatorname{Tr}\big(p'(\sqrt{n}A)\sqrt{n}A\big)\right)\left(\operatorname{Tr}\big(q'(\sqrt{n}A)\sqrt{n}A\big)\right)
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&\quad = n^2\mathbb{E}\Bigg[\int p'q' \; d\mu_{\sqrt{n}A}\\
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$\Rightarrow \Sigma$ will be diagonal when the derivatives of our polynomials are orthogonal w.r.t. σ to each other and to $U_1(x) = 2x$.

Second warm-up result

Theorem (EM–MM '21, DG–EM–MM '23+)

Let $A \in M_n^{sa}(\mathbb{C})$ be a uniformly distributed in the Hilbert–Schmidt unit sphere. For each k let

$$Y_k = \operatorname{Tr} T_k(\sqrt{n}A) - \mathbb{E} \operatorname{Tr}(\sqrt{n}A).$$

Then

$$d_W \left((Y_1, Y_3, Y_4 \dots, Y_d), \mathcal{N}\big(0, \tfrac{1}{2} \operatorname{diag}(1, 3, 4, \dots, d)\big) \right) \leq \frac{C_d}{n}.$$

Third warm-up result

Now let $Z \in M_{n \times m}$ be standard Gaussian, and $m = \lfloor \alpha n \rfloor$.

We again use the Ornstein–Uhlenbeck semigroup.

We have

$$\nabla \operatorname{Tr} p\left(\tfrac{1}{n} ZZ^*\right) = \frac{2}{n} p'\left(\tfrac{1}{n} ZZ^*\right) Z$$

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and so

$$\mathbb{E}\Gamma\left(\operatorname{Tr} p\big(\tfrac{1}{n}ZZ^*\big), \operatorname{Tr} q\big(\tfrac{1}{n}ZZ^*\big)\right) \approx 4\int p'(x)q'(x)x \, d\mu_\alpha.$$

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We thus want to work with derivatives of orthogonal polynomials w.r.t. $x \, d\mu_\alpha(x)$.

Third warm-up result

Theorem (Cabanal-Duvillard '01, Kusalik–Mingo–Speicher '07)

Let $Z \in M_{n\times m}$ be standard Gaussian, and $m = \lfloor \alpha n \rfloor$. For each k let

$$Y_k = \operatorname{Tr} \widetilde{T}_k\left(\tfrac{1}{n} ZZ^*\right) - \mathbb{E}\widetilde{T}_k\left(\tfrac{1}{n} ZZ^*\right),$$

where $\widetilde{T}_k$ are shifted Chebyshev polynomials of the first kind, which have the form

$$\widetilde{T}_k(x) = a_{\alpha,k} T_k(b_\alpha k + c_\alpha) + d_{\alpha,k}.$$

Then

$$d_W\left((Y_1, \ldots, Y_d), \mathcal{N}\big(0, \operatorname{diag}(s_{\alpha,1}, \ldots, s_{\alpha,d})\big)\right) \leq \frac{C_{d,\alpha}}{n}.$$

Main theorem, finally

Return to the first setting:

$X \in M_{n \times m}$ is uniformly distributed in the Hilbert–Schmidt unit sphere S, $m = \lfloor \alpha n \rfloor$.

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In this case it is only when p and q are linear that the latter integrals are nonzero.

Main theorem, finally stated

Theorem (DG–EM–MM ’23+)

Let $\rho \in M_n$ be a random density matrix with the m^{th} induced distribution, with $m = \lfloor \alpha n \rfloor$. For each k let

$$Y_k = \operatorname{Tr} \widetilde{T}_k(n\rho) - \mathbb{E} \operatorname{Tr} \widetilde{T}_k(n\rho).$$

Then

$$d_W \left((Y_2, \dots, Y_d), \mathcal{N}\big(0, \operatorname{diag}(s_{\alpha,2}, \dots, s_{\alpha,d})\big) \right) \le \frac{C_{d,\alpha}}{n}.$$

The end

Thank you!