Random density matrices

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Lyon, 27 October 2006

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Why random density matrices ?

- Density matrices are central objects in quantum information theory, quantum computing, quantum communication protocols, etc.
- We would like to characterize the properties of *typical* density matrices $\Rightarrow$ we need a probability measure on the set of density matrices
- Compute averages over the important quantities, such as von Neumann entropy, moments, etc.
- Random matrix theory: after all, density matrices are positive, trace one complex matrices

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Two classes of measures

There are two main classes of probability measures on the set of density matrices of size n:

- *Metric* measures: define a distance on the set of density matrices and consider the measure that assigns equal masses to balls of equal radii. Example: the *Bures* distance

$$d(\rho, \sigma) = 2 \arccos \operatorname{Tr}(\rho^{1/2} \sigma \rho^{1/2})^{1/2}.$$

- *Induced* measures: density matrices are obtained by partial tracing a random pure state of larger size

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Introduction

- In physics, a pure state of a quantum state is a norm one vector $|\psi\rangle$ of a complex Hilbert space $\mathcal{H}$ with an undetermined phase:

$$|e^{i\theta}\psi\rangle = |\psi\rangle \quad \theta \in \mathbb{R}$$

- We introduce an equivalent definition

Definition

A pure state $|\psi\rangle$ is an element of $\mathcal{E}_n = \mathcal{H} \setminus \{0\}/\sim$, where $\sim$ is the equivalence relation defined by

$$x \sim y \Leftrightarrow \exists \lambda \in \mathbb{C}^* \; s.t. \; x = \lambda y.$$

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- Consider a quantum system $\mathcal{H}$ in interaction with another system $\mathcal{K}$. The Hilbert space of the compound system is given by the tensor poduct $\mathcal{H} \otimes \mathcal{K}$.
- One typical situation is that we have access to the system $\mathcal{H}$ only, for several possible reasons: $\mathcal{K}$ may not be accessible (e.g. $\mathcal{H}$ and $\mathcal{K}$ are in distant galaxies) or it can be too complicated to study (an unknown environemnt, a heat bath, a noisy channel, etc.).
- If the state of the compound system is pure, what can be said about the $\mathcal{H}$-part of $\mathcal{H} \otimes \mathcal{K}$?

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$$\Rightarrow \text{ density matrices}$$

Partial tracing

- One can measure for instance an observable X on $\mathcal{H}$, i.e. measure $X \otimes I_{\mathcal{K}}$ on the whole system.
- We can compute the probability of obtaining the result λ_i knowing that the state of $\mathcal{H} \otimes \mathcal{K}$ is $|\psi\rangle$:

$$Prob(X = \lambda_i) = \langle\psi|P_i \otimes I_{\mathcal{K}}|\psi\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|(P_i \otimes I_{\mathcal{K}})) = \mathrm{Tr}(\rho P_i),$$

  where λ_i is the eigenvalue corresponding to the eigenspace P_i and $\rho = \mathrm{Tr}_{\mathcal{K}}(|\psi\rangle\langle\psi|)$ is the partial trace of the pure system $|\psi\rangle$ over $\mathcal{K}$.
- The observer of $\mathcal{H}$ will not "see" $|\psi\rangle$, but only its partial trace ρ, the density matrix corresponding to $\mathcal{H}$.

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Density matrices and partial tracing

Definition

A *density matrix* on a Hilbert space $\mathcal{H}$ is a positive and unit trace matrix of size $n = \dim \mathcal{H}$. We note the convex set of density matrices of size n with $\mathcal{D}_n$.

We consider the partial trace map

$$\begin{aligned} T_{n,k} : \mathcal{E}_{nk} &\longrightarrow \mathcal{D}_n \\ |\psi\rangle &\longmapsto \mathrm{Tr}_{\mathcal{K}}(|\psi\rangle\langle\psi|). \end{aligned}$$

If we write ψ ($\|\psi\| = 1$) in a basis $e_i \otimes f_j$ of $\mathcal{H} \otimes \mathcal{K}$, then

$$T_{n,k}(|\psi\rangle)_{i,j} = \sum_{s=1}^{k} \psi_{is}\overline{\psi_{js}},$$

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Random pure states

- One would like to endow $\mathcal{E}_n$ with an uniform probability measure ν_n. But what does *uniform* mean ?
- As there is no preferred basis for this space, we will ask that the uniform probability measure ν_n should be invariant under any change of basis. As basis changes are realized via unitary matrices, ν_n should be invariant under the action of the unitary group $\mathcal{U}(n)$.

Definition

We call a measure ν_n on $\mathcal{E}_n$ *unitarily invariant* if

$$\nu_n(UA) = \nu_n(A),$$

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Existence and unicity - the general result

Definition

Let G be a topological group acting on a topological space X. We call the action

- *transitive* if for all $x, y \in X$, there is $g \in G$ such that $y = g \cdot x$
- *proper* if for all $g \in G$, the application $X \ni x \mapsto g \cdot x$ is proper, i.e. the pre-image of a compact set is compact

Theorem

Let G be a topological group that acts transitively and properly on a topological space X. Suppose that both G and X are locally compact and separable. Then there exists an unique (up to a constant) measure ν on X which is G-invariant.

Existence and unicity - uniform pure states

Theorem

The action of $\mathcal{U}(n)$ on $\mathcal{E}_n$ is transitive and proper and thus there exists an unique unitarily invariant probability measure ν_n on $\mathcal{E}_n$.

This measure can be obtained directly in two ways:

1. Let X be a random complex vector of law $\mathcal{N}_{\mathbb{C}}^n(0,1)$. Then the class $|X\rangle$ of X is distributed along ν_n.
2. Let U be a random unitary matrix distributed along the Haar measure on $\mathcal{U}(n)$ and let Y be the first column of U. Then the class $|Y\rangle$ has law ν_n.

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The induced measure

Choose a pure state on $\mathcal{H} \otimes \mathcal{K}$ distributed accordingly to the uniform measure ν_{nk}. The density matrix obtained by taking a partial trace is distributed along the image measure

$$\mu_{n,k} = T_{n,k\#}\nu_{nk},$$

where $T_{n,k}$ is the partial trace over the k-dimensional system.

Definition

We call $\mu_{n,k}$ the induced measure on $\mathcal{D}_n$ by partial tracing over an environment of size k.

- From now on, we will focus on the measures $\mu_{n,k}$ and their properties.

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Results at fixed size

Connection with the Wishart ensemble

- We have seen that if Z is a complex Gaussian vector in $\mathbb{C}^{nk}$ then the class $|Z\rangle$ is uniformly distributed on $\mathcal{E}_{nk}$.
- Thus, if we set $\rho = \mathrm{Tr}_{\mathcal{K}}(|Z\rangle\langle Z|)$, we obtain

$$\rho_{ij} = \frac{1}{\|Z\|^2} \sum_{s=1}^{k} Z_{is} \overline{Z_{js}}.$$

- Equivalently, if we arrange the components of Z in a $n \times k$ matrix X, then we obtain

$$\rho = \frac{X \cdot X^*}{\mathrm{Tr}(X \cdot X^*)}.$$

- Notice that in the previous formula, the matrix X has i.i.d. complex Gaussian entries

$$\Rightarrow \text{ the Wishart ensemble}$$

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Wishart random matrices

Definition

Let X be a $n \times k$ complex matrix such that the entries are i.i.d. $\mathcal{N}_{\mathbb{C}}(0,1)$ random variables. The $n \times n$ matrix $W = X \cdot X^*$ is called a Wishart (random) matrix of parameters n and k.

- The first model of random matrices; introduced in the 30's to study covariance matrices in statistics.
- Since, it has found many applications, both theoretical and practical: PCA, engineering, random matrix theory, etc.
- The preceding formula describing a random density matrix reads now

$$\rho = \frac{W}{\operatorname{Tr} W}$$

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The eigenvalues of Wishart matrices

Theorem

The distribution of the (unordered) eigenvalues $\lambda_1(W), \ldots, \lambda_n(W)$ has density with respect to the Lebesgue measure on $\mathbb{R}_+^n$ given by

$$\Phi_{n,k}^{(w)}(\lambda_1, \ldots, \lambda_n) = C_{n,k}^{(w)} \exp(-\sum_{i=1}^{n} \lambda_i) \prod_{i=1}^{n} \lambda_i^{k-n} \Delta(\lambda)^2,$$

where

$$C_{n,k}^{(w)} = \left[\prod_{j=0}^{n-1} \Gamma(n+1-j)\Gamma(k-j) \right]^{-1}$$

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Generalities

- One would like to know the distribution of the eigenvalues $(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$ of a random density matrix of law $\mu_{n,k}$.
- As the trace of a density matrix equals one, the (random) vector $(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$ is confined on the $(n-1)$-dimensional probability simplex

$$\Sigma_{n-1} = \{(x_1, \cdots, x_n) \in \mathbb{R}_+^n : \sum_{i=1}^n x_i = 1\}.$$

- Recall that if W is a Wishart matrix of parameters n and k, then $\rho = W/\operatorname{Tr}(W)$ has distribution $\mu_{n,k}$. It follows that if $(\lambda_1, \ldots, \lambda_n)$ are the eigenvalues of W and $(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$ are those of ρ, then we have

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$$\Sigma_{n-1} = \{(x_1, \cdots, x_n) \in \mathbb{R}_+^n : \sum_{i=1}^n x_i = 1\}.$$

- Recall that if W is a Wishart matrix of parameters n and k, then $\rho = W/\operatorname{Tr}(W)$ has distribution $\mu_{n,k}$. It follows that if $(\lambda_1, \ldots, \lambda_n)$ are the eigenvalues of W and $(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$ are those of ρ, then we have

$$\tilde{\lambda}_i = \frac{\lambda_i}{\sum_{j=1}^n \lambda_j} \quad \forall 1 \leq i \leq n.$$

The density function

Theorem

The distribution of the (unordered) eigenvalues $\tilde{\lambda}_1(\rho), \ldots, \tilde{\lambda}_{n-1}(\rho)$ has density with respect to the Lebesgue measure on Σ_{n-1} given by

$$\Phi_{n,k}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_{n-1}) = C_{n,k} \prod_{i=1}^{n} (\tilde{\lambda}_i)^{k-n} \Delta(\tilde{\lambda})^2,$$

where $\tilde{\lambda}_n$ is not itself a variable, but merely a function of the other eigenvalues:

$$\tilde{\lambda}_n = 1 - (\tilde{\lambda}_1 + \cdots + \tilde{\lambda}_{n-1}).$$

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Numerical simulations, $n = 2$

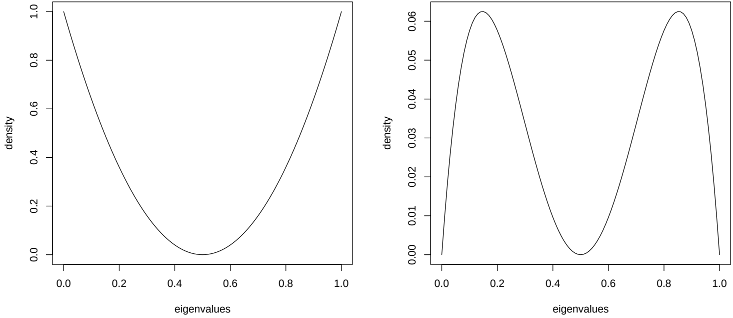


Figure: Theoretical eigenvalue distribution for $n = 2, k = 2$ (left) and $n = 2, k = 3$ (right)

Numerical simulations, $n = 2$

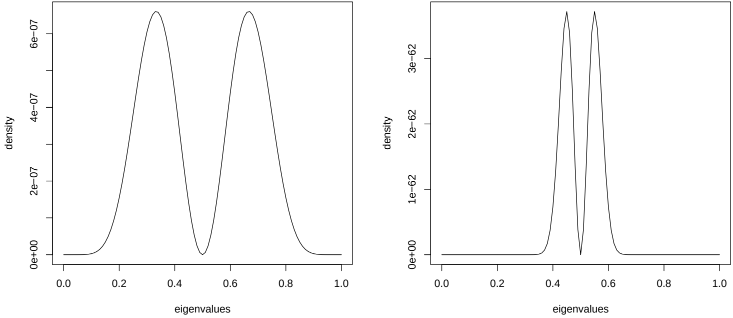
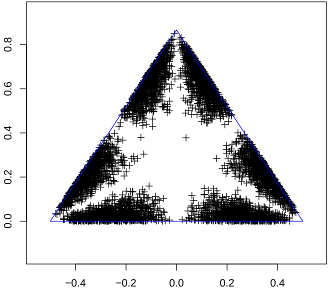


Figure: Theoretical eigenvalue distribution for $n = 2, k = 10$ (left) and $n = 2, k = 100$ (right)

Numerical simulations, $n = 3$



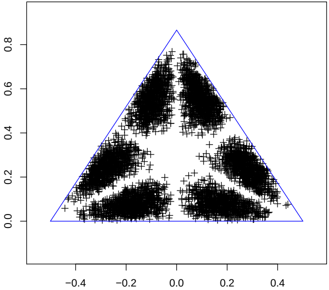


Figure: Empirical eigenvalue distribution for $n = 3, k = 3$ (left) and $n = 3, k = 5$ (right)

Numerical simulations, $n = 3$

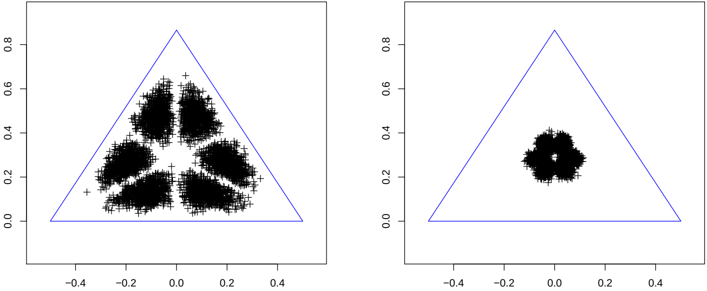


Figure: Empirical eigenvalue distribution for $n = 3, k = 10$ (left) and $n = 3, k = 100$ (right)

Asymptotics

Motivation

- Typically, quantum systems have a large number of degrees of freedom ⇒ large density matrices
- Properties of typical large density matrices can be expressed in function of the limit object
- There are a lot of results dealing with Wishart matrices in the large n and k limit

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Two models

We have studied two models, both motived by natural situations arising in physics:

1. n is constant and $k \to \infty$
   - describes typically a small system (a qubit, a pair of qubits, etc.) coupled to a much larger environment
   - we will show that in the limit $k \to \infty$, density matrices distributed along $\mu_{n,k}$ converge to the maximally mixed state Id/n
2. $n, k \to \infty$, $k/n \to c > 0$
   - describes a large system coupled to a large environment with constant ratio of size ($\dim \mathcal{K} / \dim \mathcal{H} \approx c$)
   - we show that the spectral measure of density matrices of law $\mu_{n,k}$ converge to a deterministic measure known in random matrix theory as the *Marchenko-Pastur distribution*
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The spectral measure

- permits to state results on the whole spectrum of a density matrix
- density matrices admit spectral decompositions:

$$\rho = \sum_{i=1}^{n} \lambda_i |\psi_i\rangle\langle\psi_i|,$$

where the eigenvalues $\lambda_1, \ldots, \lambda_n$ are positive and sum up to 1.

Definition

The *spectral measure* associated to a density matrix with spectrum $\{\lambda_1, \ldots, \lambda_n\}$ is the probability measure

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Dirichlet distributions

- Consider the probability distributions $\mu_{n,k}$ at fixed n and $k \to \infty$. It has density

$$\Phi_{n,k}(\lambda_1, \ldots, \lambda_{n-1}) = C_{n,k} \prod_{i=1}^{n} (\lambda_i)^{k-n} \Delta(\lambda)^2.$$

- Because n fixed, the Vandermonde factor $\Delta(\lambda)$ is constant; the other factor, properly normalized in order to get a probability density, is the Dirichlet measure of parameter $\alpha = k - n + 1$:

$$\Phi'_{n,k}(\lambda_1, \ldots, \lambda_{n-1}) = C'_{n,k} \prod_{i=1}^{n} (\lambda_i)^{\alpha-1}.$$

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It is a classical result in probability theory that

Theorem

The Dirichlet measure converges weakly as $\alpha \to \infty$ to the Dirac measure $\delta_{(1/n,\dots,1/n)}$

As the maximally mixed state Id/n is the unique state having spectrum $\{1/n, \dots, 1/n\}$, we get:

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Density matrices of the first model converge almost surely to the maximally mixed state Id/n.

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The Marchenko Pastur measure

The Marchenko-Pastur distribution arises naturally in random matrix theory and free probability.

Definition

For $c \in]0, \infty[$, we denote by μ_c the *Marchenko-Pastur* probability measure given by the equation

$$\mu_c = \max\{1 - c, 0\}\delta_0 + \frac{\sqrt{(x-a)(b-x)}}{2\pi x}\mathbf{1}_{[a,b]}(x)dx,$$

where $a = (\sqrt{c} - 1)^2$ and $b = (\sqrt{c} + 1)^2$.

An useful lemma

Lemma

Assume that $c \in]0, \infty[$, *and let* $(k(n))_n$ *be a sequence of integers such that* $\lim_{n\to\infty} \frac{k(n)}{n} = c$. *Consider a sequence of random matrices* $(W_n)_n$ *such that for all* n, W_n *is a Wishart matrix of parameters* n *and* $k(n)$. *Let* $S_n = \operatorname{Tr} W_n$ *be the trace of* W_n. *Then*

$$\frac{S_n}{nk(n)} \to 1 \quad \textit{almost surely}$$

and

$$\frac{S_n - nk(n)}{\sqrt{nk(n)}} \Rightarrow \mathcal{N}(0,1),$$

The main result

Theorem

Assume that $c \in]0, \infty[$, *and let* $(k(n))_n$ *be a sequence of integers such that* $\lim_{n\to\infty} \frac{k(n)}{n} = c$. *Consider a sequence of random density matrices* $(\rho_n)_n$ *such that for all* n, ρ_n *has distribution* $\mu_{n,k(n)}$. *Define the renormalized empirical distribution of* ρ_n *by*

$$L_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{cn\lambda_i(\rho_n)},$$

where $\lambda_1(\rho_n), \cdots, \lambda_n(\rho_n)$ *are the eigenvalues of* ρ_n. *Then, almost surely, the sequence* $(L_n)_n$ *converges weakly to the Marchenko-Pastur distribution* μ_c.

Proof

We know that the empirical distribution of eigenvalues for the Wishart ensemble

$$L_n^{(W)} = \frac{1}{n} \sum_{i=1}^{n} \delta_{n^{-1}\lambda_i(W_n)},$$

converges almost surely to the Marchenko-Pastur distribution of parameter c. Recall that the eigenvalues of the density matrix $\rho_n = W_n / \operatorname{Tr}(W_n)$ are those of W_n divided by the trace S_n of W_n; we have thus

$$L_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{cn\lambda_i(W_n)/S_n} = \frac{1}{n} \sum_{i=1}^{n} \delta_{n^{-1}\lambda_i(W_n) \cdot \frac{cn^2}{S_n}}.$$

Use the fact that $S_n / nk(n) \to 1$ almost surely to conclude.

Numerical simulations

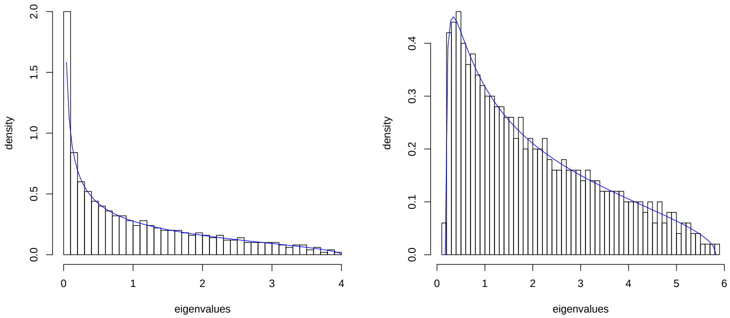

Figure: Empirical and limit measures for $n = 500, k = 500$ (left) and $n = 500, k = 1000$ (right)

Numerical simulations

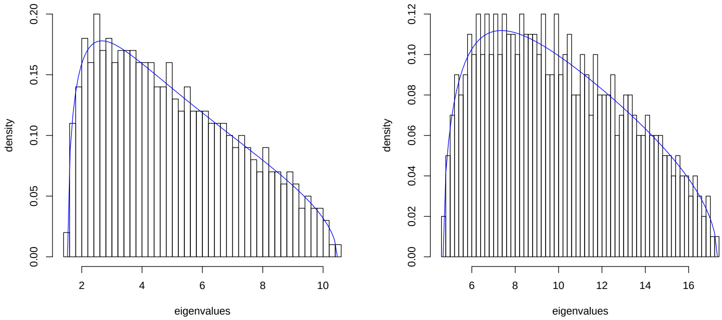

Figure: Empirical and limit measures for $n = 500, k = 2500$ (left) and $n = 500, k = 5000$ (right)

Random density matrices - largest eigenvalue

Theorem

Assume that $c \in]0,\infty[$, *and let* $(k(n))_n$ *be a sequence of integers such that* $\lim_{n\to\infty} \frac{k(n)}{n} = c$. *Consider a sequence of random matrices* $(\rho_n)_n$ *such that for all* n, ρ_n *has distribution* $\mu_{n,k(n)}$, *and let* $\lambda_{max}(\rho_n)$ *be the largest eigenvalue of* ρ_n. *Then, almost surely,*

$$\lim_{n\to\infty} cn\lambda_{max}(\rho_n) = (\sqrt{c}+1)^2.$$

Moreover,

$$\lim_{n\to\infty} \frac{n^{2/3}\left[cn\lambda_{max}(\rho_n) - (\sqrt{c}+1)^2\right]}{(1+\sqrt{c})(1+1/\sqrt{c})^{1/3}} = \mathcal{W}_2 \quad \textit{in distribution.}$$

Fin

Questions ?