Quantum states, Unitary Brownian motion and Jacobi polynomials on the simplex

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Facts from Quantum theory

Pure states

- Pure state Q: rank-one projection acting on $\mathbb{C}^N \Leftrightarrow$

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- Qubit $\in \mathbb{C}^2$ (Dirac notations for the basis vectors):

$$\alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1.$$

Density Matrices

- Density matrix (non negative Hermitian matrices of unit trace):
  - $\rho = \rho^\star$.
  - $$\rho = \sum_{i=1}^{N} \lambda_i Q_i, \quad \sum_{i=1}^{N} \lambda_i = 1,\ \lambda_i \geq 0.$$

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- Observable: Hermitian operator A (more general?).
- Measurement (expectation) of A in the state ρ:

$$A \mapsto \mathrm{tr}(\rho A) = \sum_{i=1}^{N} \lambda_i \underbrace{\mathrm{tr}(Q_i A Q_i)}_{\text{Measurement of A in the state } Q_i}.$$

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- **Partial trace** with respect to $\mathbb{C}^K$:

$$\rho := \mathrm{tr}_K[XX^\star] \in \mathbb{C}^{N\times N} : \text{Induced Mixed state.}$$

Explicitly

- Take pure state

$$X = \sum_{i=1}^{N} \sum_{j=1}^{K} X_{ij} e_i \otimes v_j \quad \in \mathbb{C}^N \otimes \mathbb{C}^K,$$

- Identify

$$X \hookrightarrow (X_{ij})_{\substack{1 \leq i \leq N \\ 1 \leq j \leq K}} \in \mathbb{C}^{N \times K}.$$

- Partial trace:

$$\rho = XX^\star \in \mathbb{C}^{N \times N}.$$

- X: non normalised $\Rightarrow$

$$\rho = \frac{XX^\star}{\operatorname{tr}(XX^\star)}.$$

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2. Uniqueness: up to unitary transformations of the Ancilla.

Randomness

Purification of a Gaussian state

- Pick iid Gaussian $(X_{ij})_{1\leq i\leq N, 1\leq j\leq K}$.
- Gaussian vector:

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- X: complex $N \times K$ Gaussian matrix.
- $XX^\star$: **Complex Wishart matrix**.

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Proposition

1. *Induced state $XX^\star / tr(XX^\star)$: Complex Wishart matrix normalised to have unit trace.*
2. *$X/||X||$: uniform distribution on the sphere S^{NK-1}.*

Density

Let

$$\Sigma_N \triangleq \left\{ \sum_{j=1}^{N-1} \lambda_j < 1 \quad \& \quad \lambda_j > 0, j = 1, \ldots, N-1 \right\},$$

be the standard simplex. Then for any $K \geq N$, Let

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Theorem

The eigenvalues density of the induced state reads:

$$\left[\underbrace{(1 - \lambda_1 - \cdots - \lambda_{N-1})}_{\lambda_N} \prod_{j=1}^{N-1} \lambda_j \right]^{K-N} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 1_{\Sigma_N}(\lambda),$$

with respect to Lebesgue measure on Σ_N.

Dirichlet distribution from Haar unitaries

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- $(|U_\infty^{11}|^2, \ldots, |U_\infty^{N1}|^2)$ is uniformly distributed on Σ_N.
- $(|U_\infty^{11}|^2, \ldots, |U_\infty^{k1}|^2) \overset{d}{\sim} \mathrm{Dir}(\underbrace{1, \ldots, 1}_{k}, N-k)$:

$$(1 - u_1 - \cdots - u_k)^{N-1-k} 1_{\Sigma_k}(u) \prod_{j=1}^{k} du_j.$$

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- Invariance of U_∞ under $\mathrm{diag}(1, \cdots, e^{i\theta}, \cdots, 1)$:

$$\arg(U_\infty^{k1}) \overset{d}{=} \mathrm{uniform\ on\ } S^1, \quad k \in \{1, \cdots, N\}.$$

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$$V\psi_t = (VU_t)e_1 \overset{d}{\sim} (U_t V)e_1 = \psi_t.$$

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- Describe the joint distribution of

$$(|U_t^{11}|^2, \ldots, |U_t^{k1}|^2),\ k \in \{1, \ldots, N-1\}?$$

Approach via stochastic calculus on $\mathcal{U}_N$

1. For $1 \leq k \leq N-1, \lambda = (\lambda_i)_{i=1}^{k} \in \mathbb{R}^k$, set

$$\phi_t(\lambda) \triangleq \mathbb{E}\left[\exp\left\{\sum_{i=1}^{k} \lambda_i |U_t^{i1}|^2\right\}\right].$$

pde for the Laplace transform

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Proposition (Nechita-Pellegrini, 2013)

The function ϕ satisfies the pde

$$\partial_t \phi = \sum_{i=1}^{k} \lambda_i \phi + \sum_{i=1}^{k} (\lambda_i^2 - N\lambda_i)\partial_{\lambda_i}\phi - \sum_{i,j=1}^{k} \lambda_i \lambda_j \partial_{\lambda_i \lambda_j}\phi.$$

The single-variable case

- $(SU_tS)_{t\geq 0} \stackrel{d}{\sim} (U_t)_{t\geq 0}, S \in \mathcal{S}_N$:

$$\lambda_2 = \cdots = \lambda_k = 0.$$

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- The pde reduces to

$$\partial_t \phi = \lambda\phi + (\lambda^2 - N\lambda)\partial_\lambda \phi - \lambda^2 \partial_{\lambda\lambda}\phi.$$

Separation of variables

Proposition (Pellegrini-Nechita)

There exists a sequence of real numbers $(a_n)_n$ *depending on* N *and* $|U_0^{11}|^2$ *such that*

$$\phi_t(\lambda) = \sum_{n=0}^{\infty} a_n e^{-n(n+N-1)t} \lambda^n {}_1F_1(n+1, N+2n, \lambda).$$

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Remark (Pellegrini-Nechita)

$(a_n)_n$ *is determined when* $|U_0^{11}|^2 \in \{0, 1\}$.

Computing $(a_n)_n$

The sequence $(a_n)_{n\geq 0}$ is uniquely determined by $a_0 = 1$ and

$$\sum_{n=0}^{p} a_n \binom{p}{n} \frac{1}{(N+2n)_{p-n}} = \frac{c^p}{p!}, \quad p \geq 1.$$

where $c \triangleq |U_0^{11}|^2$.

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Proposition (D)

For any $c \in [0,1]$,

$$a_n = \frac{1}{(N+n-1)_n} P_n^{N-2,0}(2c-1),$$

where $P_n^{N-2,0}$ is the n-th Jacobi polynomial.

Sketch of the proof

1. Neumann series for Bessel functions:

$$\sum_{n\geq 0} \frac{a_n}{n!}\Gamma(N+2n)(-1)^n J_{2n+N-1}(x) = J_0(\sqrt{c}x)\left(\frac{x}{2}\right)^{N-1}$$

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2. Expansion of the right-hand side into a Neuman series:

$$(x/2)^{N-1}J_0(\sqrt{c}x) = \sum_{n\geq 0}(2n+N-1)$$

$$\sum_{p=0}^{n}\frac{(-1)^p c^p}{(p!)^2}\frac{\Gamma(p+n+N-1)}{(n-p)!}J_{2n+N-1}(x).$$

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3. Orthogonality of Bessel functions with different parameters:

$$\int_0^{\infty} J_{\nu+2n+1}(x)J_{\nu+2m+1}(x)\frac{dx}{x} = \frac{1}{2\nu+4n+2}\delta_{mn}, \;\; \nu > -1.$$

Inverting the Laplace transform

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Corollary

The density of $|U_t^{11}|^2$ *reads*

$$f_t(u) = \left[\sum_{n=0}^{\infty} e^{-n(n+N-1)t} \frac{P_n^{0,N-2}(1-2c)P_n^{0,N-2}(1-2u)}{||P_n^{0,N-2}||_2^2}\right] s_1(u)$$

where $s_1(u) = (1-u)^{N-2}$.

Jacobi operator

1. $(u \mapsto P_n^{0,N-2}(1-2u))_n$ is a complete set of eigenfunctions of

$$\mathscr{L}_u \triangleq u(1-u)\partial_u^2 + [1 - Nu]\partial_u.$$

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3. IPP on the pde:
$$\partial_t g_t = \mathscr{L}_u g_t.$$
4. $\mathscr{L}_u$ is the radial part of $\Delta_{\mathbb{C}P^{N-1}}$ (compact symmetric space of rank one).

Set

$$f_t(u_1, \ldots, u_k) = g_t(u_1, \ldots, u_k)(1 - u_1 - \cdots - u_k)^{N-k-1}.$$

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IPP leads to the heat equation:

$$\begin{aligned} \mathscr{L}_k g_t &\triangleq \left[\sum_{i=1}^{k}(u_i - u_i^2)\partial_{ii} - \sum_{i \neq j} u_i u_j \partial_{ij} + \sum_{i=1}^{k}[1 - Nu_i]\partial_i\right] g_t \\ &\approx \partial_t g_t. \end{aligned}$$

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$$\approx \partial_t g_t.$$

Problems

1. Boundary terms (vanish for $1 \leq k \leq N-2$).
2. Many (polynomial) orthonormal eigenbases of $\mathscr{L}_k$.

Direct approach

Spherical harmonics

1. Real vs Complex variables:

$$(x_1, \ldots, x_N, y_1, \ldots, y_N) \Leftrightarrow (z_1, \ldots, z_N, \overline{z}_1, \ldots, \overline{z}_N).$$

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2. $\mathrm{Pol}(x_1, \ldots, x_N, y_1, \ldots, y_N) \Leftrightarrow \mathrm{Pol}(z_1, \ldots, z_N, \overline{z}_1, \ldots, \overline{z}_N).$

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4. $\mathcal{H}_{x,y}(n)$: Harmonic homogeneous polynomials of degree n.

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4. $\mathcal{H}_{x,y}(n)$: Harmonic homogeneous polynomials of degree n.
5. Restrictions to S^{2N-1}: Eigenpolynomials of $\Delta_{S^{2N-1}}$.
6. Weierstrass Theorem:
$$\oplus_{n=0}^{\infty} \mathcal{H}_{x,y}(n) = C(S^{2N-1}).$$

Spherical harmonics of $\mathbb{C}P^{N-1}$

1. $\mathcal{H}_{x,y}(n) = \oplus_{i=0}^{n}\mathcal{H}_{z,\overline{z}}(i, n-i)$.

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2. $\mathbb{C}P^{N-1} = S^{2N-1}/S^1 \Rightarrow$

$$C(\mathbb{C}P^{N-1}) = \oplus_{n=0}^{\infty} \underbrace{\mathcal{H}_{z,\overline{z}}(n,n)}_{\text{homogeneous of degree zero}} .$$

Heat kernel on $\mathbb{C}P^{N-1}$

- $w, z \in \mathbb{C}P^{N-1}$.
- $d(n, N) = \mathrm{dim}\mathcal{H}_{z,\overline{z}}(n, n)$.
- $(Y_j)_{j=1}^{d(n,N)}$: orthonormal basis of $\mathcal{H}_{z,\overline{z}}(n, n)$.

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Proposition

The heat kernel on $\mathbb{C}P^{N-1}$ is given by

$$R_t(w, z) = \sum_{n=0}^{\infty} e^{-n(n+N-1)t} \sum_{j=1}^{d(n,N)} Y_j(w)\overline{Y_j}(z)$$

$$= \sum_{n=0}^{\infty} e^{-n(n+N-1)t} \frac{d(n, N)}{vol(\mathbb{C}P^{N-1})} \frac{P_n^{N-2,0}(2|\langle w, z\rangle|^2 - 1)}{P_n^{N-2,0}(1)}.$$

Distribution of $|U_t^{11}|^2$

- Decomposition of the variables

$$\begin{aligned} w &= \cos\theta_1 e_1 + \sin\theta_1 \xi_1, \quad e_1 \perp \xi_1 \in S^{2N-3}, \\ z &= \cos\theta_2 e_1 + \sin\theta_2 \xi_2, \quad , e_1 \perp \xi_2 \in S^{2N-3}. \end{aligned}$$

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- $\langle w, z\rangle = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \langle \xi_1, \xi_2\rangle$.
- Decomposition of the volume measure

$$\mathrm{vol}_{\mathbb{C}P^{N-1}}(dz) = [\cos\theta_2 (\sin\theta_2)^{2N-3} d\theta_2]\mathrm{vol}_{S^{2N-3}}(d\xi_2).$$

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Integrate over ξ_2?

-

Koornwinder product formula

- Action of $U(N-1)$ on S^{2N-3}:

$$\xi_1 \to e_2.$$

Koornwinder product formula

- Action of $U(N-1)$ on S^{2N-3}:

$$\xi_1 \to e_2.$$

- We are left with integration over $\xi_2^{(1)} = (r, \zeta) \in \mathbb{C}$:

$$r(1-r^2)^{N-3} 1_{[0,1](r)} dr 1_{[0,2\pi](\zeta)} d\zeta.$$

Koornwinder product formula:

$$\frac{(N-2)}{\pi} \int_0^1 \int_0^{2\pi} \frac{P_n^{N-2,0}(2|\langle w, z\rangle|^2 - 1)}{P_n^{N-2,0}(1)} dr d\zeta = \frac{P_n^{N-2,0}(\cos 2\theta_1)}{P_n^{N-2,0}(1)} \frac{P_n^{N-2,0}(\cos 2\theta_2)}{P_n^{N-2,0}(1)}.$$

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Definition (Koornwinder OP in the simplex)

With the convention $\nu_{k+1} = 0, u_{(0)} = 0$, *the polynomials*

$$R_\nu(u) = (-1)^{|\nu|} \prod_{j=1}^{k} (1 - |u_{(j)}|)^{\nu_{j+1}} P_{\nu_j}^{0,a_j} \left[1 - \frac{2u_j}{1 - |u_{(j-1)}|}\right]$$

form a complete set of OP in the simplex Σ_k. *If* $|\nu| = n$ *then*

$$\mathscr{L}_k R_\nu = -n(n + N - 1) R_\nu.$$

-

Example and remark

$k = 2, \nu = (n - j, j), 0 \leq j \leq n$:

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Remark

The construction of R_ν reflects the independence of the increments of the Dirichlet distribution:

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Remark

The construction of R_ν reflects the independence of the increments of the Dirichlet distribution:

If $(X_1, \ldots, X_k) \in \Sigma_k \hookrightarrow D(\alpha_1, \ldots, \alpha_k)$ then

$$\frac{X_j}{1 - |X_{(j-1)}|}, \quad 1 \leq j \leq k,$$

are mutually independent (complete neutrality).

Distribution of $(|U_t^{11}|^2, |U_t^{21}|^2)$

- Decomposition of variables:

$$
\begin{aligned}
w &= \cos\theta_1 e_1 + \sin\theta_1 \cos\beta_1 e^{i\phi_1} e_2 + \sin\theta_1 \sin\beta_1 \eta_1, \\
z &= \cos\theta_2 e_1 + \sin\theta_2 \cos\beta_2 e^{i\phi_2} e_2 + \sin\theta_2 \sin\beta_1 \eta_2,
\end{aligned}
$$

$$\eta_1, \eta_2 \in S^{2N-5}$$

- Decomposition of variables:

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$$\eta_1, \eta_2 \in S^{2N-5}$$

- Decomposition of the volume measure

$$\mathrm{vol}_{\mathbb{C}P^{N-1}}(dz) = \left(\cos\theta_2 \sin^{2N-3}\theta_2 \cos\beta_2 \sin^{2N-5}\beta_2 d\theta_2 d\beta_2 d\phi_2\right) \mathrm{vol}_{S^{2N-5}}(d\eta_2).$$

Integration over η_2

- Decomposition of spherical harmonics under $\mathcal{U}_{N-1}$-action into spherical harmonics of lower dimensions.
- Splitting of the reproducing kernel: $(\theta_2, \beta_2, \phi_2)|\eta_2$.

Result

$R_{n-j,j}$: Jacobi polynomial on the simplex Σ_2.

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Proposition (D)

The distribution of $(|U_t^{11}|^2, |U_t^{21}|^2)$ *admits the following expansion*

$$\left[\sum_{n=0}^{\infty} e^{-n(n+N-1)t} \sum_{j=0}^{n} \frac{R_{n-j,j}(c_1, c_2) R_{n-j,j}(u_1, u_2)}{||R_{n-j,j}||_2^2}\right] s_2(u_1, u_2),$$

where $(c_1, c_2) \triangleq (|U_0^{11}|^2, |U_0^{12}|^2) \in \Sigma_2$ *and*

$$s_2(u_1, u_2) \triangleq (1 - u_1 - u_2)^{N-3} 1_{\Sigma_2}(u_1, u_2).$$

Concluding remarks

1. Distribution of $(|U_t^{11}|^2, \ldots, |U_t^{k1}|^2)$: decompose the spherical harmonics under the action of the subgroup $\mathcal{U}(N-k+1)$.

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1. Distribution of $(|U_t^{11}|^2, \ldots, |U_t^{k1}|^2)$: decompose the spherical harmonics under the action of the subgroup $\mathcal{U}(N-k+1)$.
2. $(|U_t^{11}|^2, \ldots, |U_t^{k1}|^2)_{t\geq 0}$ is a Markov process:

$$\rho : \mathcal{U}_N \to \mathcal{U}_N/\mathcal{U}_{N-1}$$

is a Riemannian submersion and

$$h : S^{2N-1} \to \mathbb{C}P^{N-1}$$

is a (Hopf) fibration.

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Thank you for your attention