Spectral decomposition, purification

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Pauli matrices in braket notation

- $$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$$

- $|+\rangle := (|0\rangle + |1\rangle)/\sqrt{2}, \quad |-\rangle := (|0\rangle - |1\rangle)/\sqrt{2}.$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = |+\rangle\langle +| - |-\rangle\langle -|$$

- $|a\rangle := (|0\rangle + i\,|1\rangle)/\sqrt{2}, \quad |b\rangle := (|0\rangle - i\,|1\rangle)/\sqrt{2}.$

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = |a\rangle\langle a| - |b\rangle\langle b|$$

Spectral decomposition of Hermitian operator

Theorem (Spectral decomposition theorem)

$H \in L(\mathbb{C}^n)$ is Hermitian if and only if there exist orthonormal basis $\{|\psi_i\rangle\}$ of $\mathbb{C}^n$ and real numbers $\{\lambda_i\}$ such that

$$H = \sum_i \lambda_i |\psi_i\rangle \langle\psi_i| .$$

Outline of the proof.

- Any complex matrix H has an eigenvalue and eigenvector.
- All eigenvalues of any Hermitian matrix H are real.
- Any Hermitian matrix H has a spectral decomposition.

$\square$

Any complex matrix has an eigenvalue

For any $L \in L(\mathbb{C}^n)$ and non-zero $v \in \mathbb{C}^n$,

$$v,\ Lv,\ L^2v,\ \dots,\ L^nv$$

are linearly dependent. There exist $a_0, \dots, a_n$ that are not all-zero satisfying

$$\begin{aligned} 0 &= a_0 v + a_1 Lv + \cdots + a_n L^n v \\ &= c(L - \lambda_1 I)(L - \lambda_2 I) \cdots (L - \lambda_m I)v \end{aligned}$$

which means at least one $L - \lambda_i I$ is not injective, i.e., there exists non-zero $w \in \mathbb{C}^n$ such that

$$(L - \lambda_i I)w = 0 \iff Lw = \lambda_i w.$$

All eigenvalues of Hermitian matrix are real

Assume that Hermitian matrix H has an eigenvalue λ and a corresponding eigenvector v.

$$\lambda\langle v, v\rangle = \langle \lambda v, v\rangle = \langle Hv, v\rangle = \langle v, Hv\rangle = \langle v, \lambda v\rangle = \lambda^*\langle v, v\rangle.$$

Hence, λ is real.

Any Hermitian matrix has a spectral decomposition

Induction on the dimension n. Spectral decomposition theorem obviously holds for $n = 1$. H has real eigenvalue λ and corresponding (normalized) eigenvector $|\psi\rangle$. Let $P = |\psi\rangle \langle\psi|$ and $Q = I - P$.

$$H = (P + Q)H(P + Q) = PHP + PHQ + QHP + QHQ$$

$$QHP = Q\lambda P = 0$$

$PHQ = (QHP)^{\dagger} = 0$ since H is Hermitian.

$PHP = \lambda P$.

QHQ is Hermitian since H is Hermitian. QHQ is a linear map on linear subspace of dimension $n - 1$.
From the induction hypothesis, QHQ has a spectral decomposition.

Terminology

- Density matrix, density operator: A Hermitian matrix ρ that represents a state, i.e., $\rho \succeq 0$, $\mathrm{Tr}(\rho) = 1$.
- Pure state: A state that cannot be written as a convex combination of other states. Equivalently, its a density operator with rank one.
- Mixed state: A state that is not a pure state.
- State vector: A complex unit vector $|\psi\rangle$ that represents a pure state $\rho = |\psi\rangle \langle\psi|$.
- Positive operator-valued measurement (POVM): A tuple $\{P_j\}$ of Hermitian matrices that represents a measurement, i.e., $P_j \succeq 0$ and $\sum_j P_j = I$.

Ensemble of states

Let $\rho_1, \ldots, \rho_k$ be density matrices. If ρ_i is prepared with probability p_i, and POVM $\{P_j\}$ is applied, outcome j is obtained with probability

$$\sum_{i=1}^{k} p_i \mathrm{Tr}(\rho_i P_j) = \mathrm{Tr}\left(\sum_{i=1}^{k} p_i \rho_i P_j\right).$$

Hence, this ensemble of states is represented by $\rho := \sum_i p_i \rho_i$.

Ensemble of pure states

Any quantum state

$$\rho = \sum_i \lambda_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

can be regarded as an ensemble $\{\lambda_i, \left|\psi_i\right\rangle \left\langle\psi_i\right|\}$ of pure states.

$$\begin{aligned}\rho &= \frac{3}{4} \left|0\right\rangle \left\langle 0\right| + \frac{1}{4} \left|1\right\rangle \left\langle 1\right| \\ &= \frac{1}{2} \left|a\right\rangle \left\langle a\right| + \frac{1}{2} \left|b\right\rangle \left\langle b\right|\end{aligned}$$

for

$$\begin{aligned}\left|a\right\rangle &:= \sqrt{\frac{3}{4}} \left|0\right\rangle + \sqrt{\frac{1}{4}} \left|1\right\rangle \\ \left|b\right\rangle &:= \sqrt{\frac{3}{4}} \left|0\right\rangle - \sqrt{\frac{1}{4}} \left|1\right\rangle .\end{aligned}$$

Observable

Let $\{P_j\}$ be a POVM. If we assign real value a_j for each outcome j, its expectation is

$$\mathbb{E}[A] = \sum_j a_j \mathrm{Tr}(\rho P_j) = \mathrm{Tr}\left(\rho \sum_j a_j P_j\right) = \mathrm{Tr}(\rho A).$$

Here, Hermitian operator $A := \sum_j a_j P_j$ is called a observable.

If $\{P_j\}$ is a projective measurement, i.e., $P_j P_k = \delta_{j,k} P_j$,

$$\mathbb{E}[A^n] = \sum_j a_j^n \mathrm{Tr}(\rho P_j) = \mathrm{Tr}\left(\rho \sum_j a_j^n P_j\right) = \mathrm{Tr}(\rho A^n).$$

For example, X and Z are observables for POVMs $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ and $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ with the assignments ± 1, respectively.

Decoherence

For orthonormal basis $\{|\psi_i\rangle\}$, POVM $\{|\psi_i\rangle\langle\psi_i|\}$ is performed to a quantum state ρ. If outcome is i, the quantum state ρ is transformed into $|\psi_i\rangle\langle\psi_i|$. If we don't see the measurement outcome, the state after the measurement is

$$\sum_i \mathrm{Tr}(\rho\,|\psi_i\rangle\langle\psi_i|)\,|\psi_i\rangle\langle\psi_i| = \sum_i \langle\psi_i|\,\rho\,|\psi_i\rangle\,|\psi_i\rangle\langle\psi_i|$$

$$\rho = \sum_{i,j} \rho_{i,j}\,|\psi_i\rangle\langle\psi_j| \longmapsto \sum_i \rho_{i,i}\,|\psi_i\rangle\langle\psi_i|$$

This phenomenon is called decoherence.

Partial trace

The partial trace $\mathrm{Tr}_W : H(V \otimes W) \to H(V)$ is defined by

$$A \otimes B \mapsto \mathrm{Tr}(B)A$$

for all $A \in H(V)$ and $B \in H(W)$.

Marginal distribution and reduced density matrix

A probability of outcome of local measurement in a joint system is

$$P(a, b) = \mathrm{Tr}(\rho(P_a \otimes Q_b)).$$

$$\begin{aligned}\sum_b P(a, b) &= \sum_b \mathrm{Tr}(\rho(P_a \otimes Q_b)) \\ &= \mathrm{Tr}\left(\rho\left(P_a \otimes \sum_b Q_b\right)\right) \\ &= \mathrm{Tr}\left(\rho\left(P_a \otimes I\right)\right) \\ &= \mathrm{Tr}(\mathrm{Tr}_W(\rho) P_a).\end{aligned}$$

Here, $\mathrm{Tr}_W(r)$ is called a reduced density matrix.

Reduced state of a pure state is not necessarily pure

A two-qubit pure state (called Bell state, Bell pair or EPR pair)

$$|\varphi\rangle := \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

$$\begin{aligned} |\varphi\rangle\langle\varphi| = \frac{1}{2}(&|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| \\ &+ |1\rangle\langle 0| \otimes |1\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|) \end{aligned}$$

By taking the partial trace for the second qubit, we obtain a reduced density matrix $I/2$.

Purification

Theorem

For any density matrix ρ on V, there exists a pure state $|\psi\rangle$ of a joint system on $V \otimes W$ for some W such that $\mathrm{Tr}_W(|\psi\rangle\langle\psi|) = \rho$.

Proof.

For a spectral decomposition of ρ

$$\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

let

$$|\psi\rangle := \sum_i \sqrt{\lambda_i} |\psi_i\rangle |\psi_i\rangle .$$

Then,

$$\mathrm{Tr}_W(|\psi\rangle\langle\psi|) = \rho. \qquad \square$$

$|\psi\rangle$ is called a purification of ρ.

Quantum states discrimination

Alice encodes her classical information $\{1, 2, \dots, n\}$ into quantum states $\rho_1, \rho_2, \dots, \rho_n \in H(\mathbb{C}^m)$, and send it to Bob. Bob performs a POVM $\{P_1, \dots, P_n\}$ for estimating $i \in \{1, \dots, n\}$ that Alice encoded. Assume Bob could estimate i without error. Then,

$$\mathrm{Tr}(\rho_i P_j) = \delta_{i,j}.$$

$$\begin{aligned}\mathrm{Tr}(\rho_i P_j) &= \mathrm{Tr}\left(\sum_k \lambda_k^{(i)} |\psi_k^{(i)}\rangle \langle\psi_k^{(i)}| P_j\right) \\ &= \sum_k \lambda_k^{(i)} \langle\psi_k^{(i)}| P_j |\psi_k^{(i)}\rangle\end{aligned}$$

From $\sum_k \lambda_k = 1$ and $\langle\psi| P |\psi\rangle \leq 1$, we can replace ρ_i with $|\psi_k^{(i)}\rangle \langle\psi_k^{(i)}|$ for any k with $\lambda_k > 0$.

$\langle\psi^{(i)}| P_j |\psi^{(i)}\rangle = \delta_{i,j}$ implies $\{|\psi^{(i)}\rangle\}$ is orthonormal. Hence $n \leq m$.

Superdense coding

Alice can send two bits to Bob by sending a single qubit and using a shared Bell state.

$$
\begin{aligned}
|\varphi_{00}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) && \\
|\varphi_{01}\rangle &= \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle), && \text{by } X \\
|\varphi_{10}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), && \text{by } Z \\
|\varphi_{11}\rangle &= \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle), && \text{by } XZ
\end{aligned}
$$

These are orthogonal.

Assignments [Deadline is the next next Friday]

1. Show the reduced density matrix $\rho_V \in H(V)$ of

$$\sum_{i,j} \rho_{i,j} \left|i\right\rangle \left\langle j\right| \otimes \left|i\right\rangle \left\langle j\right| \in H(V \otimes W)$$

   where $\{\left|i\right\rangle\}$ is a orthonormal basis of V and W.

2. For a density matrix $\begin{bmatrix} \rho_{1,1} & \rho_{1,2} \\ \rho_{2,1} & \rho_{2,2} \end{bmatrix} \in H(\mathbb{C}^2)$, show the density matrix for a ensemble of quantum states ρ and $Z\rho Z$ with probabilities $1/2$.