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 theorem

Definition (Normal operator)

$A \in \mathcal{L}(\mathcal{X})$ is said to be normal if $AA^\dagger = A^\dagger A$.

Hermitian matrix ($H^\dagger = H$) and unitary matrix ($UU^\dagger = I$) are normal.

Theorem (Spectral decomposition theorem)

$A \in \mathcal{L}(\mathbb{C}^n)$ is normal if and only if there exist orthonormal basis $\{|\psi_j\rangle\}$ of $\mathbb{C}^n$ and complex numbers $\{\lambda_j\}$ such that

$$A = \sum_j \lambda_j |\psi_j\rangle \langle\psi_j| .$$

Any complex matrix has an eigenvalue

For any $A \in \mathcal{L}(\mathbb{C}^n)$ and non-zero $|\psi\rangle \in \mathbb{C}^n$,

$$|\psi\rangle\,,\ A|\psi\rangle\,,\ A^2|\psi\rangle\,,\ \ldots\,,\ A^n|\psi\rangle$$

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

$$\begin{aligned} 0 &= a_0|\psi\rangle + a_1 A|\psi\rangle + \cdots + a_n A^n|\psi\rangle \\ &= a_m(A - \lambda_1 I)(A - \lambda_2 I)\cdots(A - \lambda_m I)|\psi\rangle \end{aligned}$$

where m is the largest i such that $a_i \neq 0$.
This means that there exist $i \in \{1, 2, \ldots, m\}$ and non-zero $|\varphi\rangle \in \mathbb{C}^n$ such that

$$(A - \lambda_i I)|\varphi\rangle = 0.$$

Orthogonal projection

For linear space V and its subspace W, the orthogonal projection onto W is defined by

$$P = \sum_j |\psi_j\rangle \langle\psi_j|$$

where $(|\psi_j\rangle)_j$ forms an orthonormal basis of W.

- P is Hermitian
- $P^2 = P$
- $P|\psi\rangle \in W$ for any $|\psi\rangle \in V$
- $P|\psi\rangle = |\psi\rangle$ for any $|\psi\rangle \in W$
- $I - P$ is the orthogonal projection onto $W_\perp$

Any normal matrix has a spectral decomposition

Induction on the dimension n. Spectral decomposition theorem obviously holds for $n = 1$. A has a eigenvalue λ and corresponding eigenspace W. Let P be the orthogonal projection onto W. Let $Q = I - P$.

$$A = (P + Q)A(P + Q) = PAP + PAQ + QAP + QAQ$$

- $PAP = \lambda P$.
- $QAP = Q\lambda P = 0$.
- For $|\psi\rangle \in W$, $AA^\dagger |\psi\rangle = A^\dagger A |\psi\rangle = \lambda A^\dagger |\psi\rangle$ which means $A^\dagger |\psi\rangle \in W$. This implies $(PAQ)^\dagger = QA^\dagger P = 0$.

Hence, $A = \lambda P + QAQ$. Since $QA = QA(P + Q) = QAQ$ and $QA^\dagger = QA^\dagger(P + Q) = QA^\dagger Q$,

$$\begin{aligned}(QAQ)(QA^\dagger Q) &= QAA^\dagger Q \\ &= QA^\dagger AQ = QA^\dagger QQAQ\end{aligned}$$

Hence, QAQ is normal linear operator on $W_\perp$. From the hypothesis of induction, QAQ 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.

- State vector: A complex unit vector $|\psi\rangle$ that represents a pure state $\rho = |\psi\rangle\langle\psi|$.

- Mixed state: A state that is not a pure state.

- 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 $\rho_1, \dots, \rho_k$ 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

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

for $(\lambda_i \geq 0)_i$ can be regarded as an ensemble $(\lambda_i, |\psi_i\rangle \langle\psi_i|)_i$ of pure states.

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

for

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

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 $\mathrm{Tr}_W : \mathcal{L}(V \otimes W) \to \mathcal{L}(V)$ is linear map defined by

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

for all $A \in \mathcal{L}(V)$ and $B \in \mathcal{L}(W)$.

For $A \in \mathcal{L}(V \otimes W)$, A is a linear combination of the orthonormal basis $(|a\rangle \langle b| \otimes |c\rangle \langle d|)_{a,b,c,d}$

$$A = \sum_{a,b,c,d} A_{a,b,c,d} |a\rangle \langle b| \otimes |c\rangle \langle d|$$

$$\begin{aligned}\mathrm{Tr}_W(A) &= \sum_{a,b,c,d} A_{a,b,c,d} |a\rangle \langle b| \, \mathrm{Tr}\left(|c\rangle \langle d|\right) \\ &= \sum_{a,b,c} A_{a,b,c,c} |a\rangle \langle b|\end{aligned}$$

$$\mathrm{Tr}(\mathrm{Tr}_W(A)) = \sum_{a,c} A_{a,a,c,c} = \mathrm{Tr}(A)$$

Local tomography

For measurements $\{P_a\}_a$ of quantum system on V and $\{Q_b\}_b$ of quantum system on W, a measurement $\{P_a \otimes Q_b\}_{a,b}$ in the joint system is said to be local.

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

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, $\mathrm{Tr}_W(\rho)$ 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)

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

$$|\Phi\rangle\langle\Phi| = \frac{1}{2}(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|)$$

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

$$\rho = \sum_i \lambda_i |\psi_i\rangle_V \langle\psi_i|_V$$

let

$$|\psi\rangle_{V\otimes W} := \sum_i \sqrt{\lambda_i}\, |\psi_i\rangle_V |\psi_i\rangle_W .$$

Then,

$$\mathrm{Tr}_W(|\psi\rangle_{V\otimes W} \langle\psi|_{V\otimes W}) = \rho. \qquad \square$$

$|\psi\rangle_{V\otimes W}$ is called a purification of ρ.

Quantum states discrimination

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

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

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

$\langle\psi_k^{(i)}| P_j |\psi_k^{(i)}\rangle = \delta_{i,j}$ implies $|\psi_k^{(i)}\rangle$ is an eigenvector of P_j with eigenvalue $\delta_{i,j}$. Hence, $\langle\psi_k^{(i)}|\psi_\ell^{(j)}\rangle = \delta_{i,j}$ which implies $n \leq m$.

Superdense coding

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

$$
\begin{aligned}
|\Phi_{00}\rangle &= \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B) & \\
|\Phi_{01}\rangle &= \frac{1}{\sqrt{2}}(|1\rangle_A |0\rangle_B + |0\rangle_A |1\rangle_B), & \text{by } X \\
|\Phi_{10}\rangle &= \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B - |1\rangle_A |1\rangle_B), & \text{by } Z \\
|\Phi_{11}\rangle &= \frac{1}{\sqrt{2}}(|1\rangle_A |0\rangle_B - |0\rangle_A |1\rangle_B), & \text{by } XZ
\end{aligned}
$$

These are orthogonal.

Assignments

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

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

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

2. For a single-qubit density matrix $\rho = \sum_{i,j=0}^{1} \rho_{i,j} \left| i \right\rangle \left\langle j \right|$, show the density matrix of an ensemble of quantum states ρ and $Z\rho Z$ chosen with probabilities $1/2$.

3. Show a purification of $\rho = \frac{3}{4} \left| 0 \right\rangle \left\langle 0 \right| + \frac{1}{4} \left| 1 \right\rangle \left\langle 1 \right|$.