Quantum computing seminar - Density matrix

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Slides can be found in
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A probability distribution on qubits

The n-qubit model : $|\psi\rangle = \sum_x c_x|x\rangle$ for $x \in \{0, \ldots, 2^n - 1\}$.

c_x - amplitudes

$$\mathbb{P}[|\psi\rangle = |x\rangle \text{ after an observation }] = |c_x|^2$$

Physical transformations of $|\psi\rangle$ **have to be** unitary transformations.

Consider the identification $|\psi\rangle \mapsto \rho_{|\psi\rangle} = |\psi\rangle\langle\psi|$

$$\mathbb{DM}(\mathcal{N}) = \{\pi \in \mathrm{End}(\mathcal{N}) | \pi = \pi^\dagger, \langle\eta|\pi|\eta\rangle \geq 0, \mathrm{Tr}(\pi) = 1\}$$

Mapping vectors $|\psi\rangle$ to operators $\rho_{|\psi\rangle}$ takes unit vectors to density matrices.

Motivations for using a density matrix

A **pure state** is a density matrix ρ that results from some $|\psi\rangle$, that is $\rho = \rho_{|\psi\rangle}$.

- Distinction between pure and mixed states.
- Important to understand **measurement operators.**
- Describing **physically realizable operators**.
- Reliable quantum circuits (coding theory in quantum computing).

Overview

Quantum probability model in $\mathcal{N}$

Event A = Linear subspaces of $\mathcal{N}$.
Probability distribution = density matrix $\rho \in \mathbb{DM}(\mathcal{N})$.

$$\mathbb{P}[\rho, A] := \mathrm{Tr}(\rho \Pi_A)$$

Coherent with the interpretation that if $|\psi\rangle = \sum_x c_x |x\rangle$, then $\mathbb{P}[\rho, x] = |c_x|^2$:

$$\mathbb{P}[\rho_{|\psi\rangle}, \mathbb{C}x] = \mathrm{Tr}(|\psi\rangle\langle\psi|\Pi_x) = \mathrm{Tr}(|\psi\rangle\langle\psi||x\rangle\langle x|) = |c_x|^2$$

For pure states and $\mathcal{M} \subseteq \mathcal{N}$, $\mathbb{P}[|\psi\rangle, \mathcal{M}] = \langle\psi|\Pi_M|\psi\rangle$.
A diagonal density matrix ρ corresponds to a classical probability model on the basis vectors.

The partial trace

Consider a density matrix ρ over $\mathcal{N} \otimes \mathcal{F}$, which can be written as

$$\rho = \sum_m A_m \otimes B_m \,,$$

A_m and B_m are operators $\mathcal{N}$ and $\mathcal{F}$, resp. (motivation: $\mathrm{End}(\mathcal{B}) \cong \mathcal{B} \otimes \mathcal{B}^*$)

Definition (The partial trace)

$$\mathrm{Tr}_{\mathcal{F}}(\rho) = \sum_m A_m \, \mathrm{Tr}(B_m) \,.$$

If $\mathcal{F} = \mathbb{C}$, then $\mathrm{Tr}_{\mathcal{F}} = \mathrm{Id}$. If $\mathcal{N} = \mathbb{C}$, then $\mathrm{Tr}_{\mathcal{F}} = \mathrm{Tr}$.

Example of partial trace

Consider $\mathcal{N} = \mathcal{F} = \mathcal{B}$, so that $\mathcal{N} \otimes \mathcal{F}$ is a four dimensional vector space, and $|\psi\rangle = \dfrac{|0,0\rangle + |1,1\rangle}{\sqrt{2}}$.

$$\rho_{|\psi\rangle} = \frac{1}{2} \sum_{a,b} |a,a\rangle\langle b,b| = \frac{1}{2} \sum_{a,b} |a\rangle\langle b| \otimes |a\rangle\langle b|$$

$$\mathrm{Tr}_{\mathcal{F}}(\rho_{|psi\rangle}) = \frac{1}{2} \sum_{a} |a\rangle\langle a|$$

Observe that $\rho_{|psi\rangle}$ is a **pure state**, whereas $\mathrm{Tr}_{\mathcal{F}}(\rho_{\psi})$ is mixed (has rank > 1).

Properties of quantum probability - 1

In classical probability, if $A \cap B = \emptyset$, then

$$\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$$

In quantum probability, if $\mathcal{M}_1 \perp \mathcal{M}_2$ then

$$\mathbb{P}(\rho, M_1) + \mathbb{P}(\rho, M_2) = \mathbb{P}(\rho, M_1 \oplus M_2)$$

	Properties of quantum probability
1	If $\mathcal{M}_1 \perp \mathcal{M}_2$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2)$
2	
3	
4	

Properties of quantum probability - 2

In classical probability, we have that

$$\mathbb{P}(A \cup B) + \mathbb{P}(A \cap B) = \mathbb{P}(A) + \mathbb{P}(B)$$

In quantum probability, if $\Pi_{\mathcal{M}_1}\Pi_{\mathcal{M}_2} = \Pi_{\mathcal{M}_2}\Pi_{\mathcal{M}_1}$ $(\star)$ then

$$\mathbb{P}(\rho, M_1) + \mathbb{P}(\rho, M_2) = \mathbb{P}(\rho, M_1 \oplus M_2) + \mathbb{P}(\rho, M_1 \cap M_2)$$

	Properties of quantum probability
1	If $\mathcal{M}_1 \perp \mathcal{M}_2$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2)$
2	If $\star$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2) + \mathbb{P}(M_1 \cap M_2)$
3	
4	

Properties of quantum probability - 3

Product probability spaces become density matrices on tensor products

	Properties of quantum probability
1	If $\mathcal{M}_1 \perp \mathcal{M}_2$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2)$
2	If $\star$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2) + \mathbb{P}(M_1 \cap M_2)$
3	$\mathbb{P}(\rho_1 \otimes \rho_2, \mathcal{M}_1 \otimes \mathcal{M}_2) = \mathbb{P}(\rho_1, \mathcal{M}_1)\mathbb{P}(\rho_2, \mathcal{M}_2)$
4	

Properties of quantum probability - 4

The trace helps us disregard unnimportant bits of information. In classical probability, a probability distribution in $N \times F$ satisfies

$$\mathbb{P}(A \times F) = \sum_{i \in A} \mathbb{P}(i \times F)$$

	Properties of quantum probability
1	If $\mathcal{M}_1 \perp \mathcal{M}_2$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2)$
2	If $\star$ then $\mathbb{P}(M_1) + \mathbb{P}(M_2) = \mathbb{P}(M_1 \oplus M_2) + \mathbb{P}(M_1 \cap M_2)$
3	$\mathbb{P}(\rho_1 \otimes \rho_2, \mathcal{M}_1 \otimes \mathcal{M}_2) = \mathbb{P}(\rho_1, \mathcal{M}_1)\mathbb{P}(\rho_2, \mathcal{M}_2)$
4	$\mathbb{P}(\rho, \mathcal{M}_1 \otimes \mathcal{F}) = \mathbb{P}(\mathrm{Tr}_{\mathcal{F}}(\rho), \mathcal{M}_1)$

Properties of quantum probability - 4

Proof of property 4: if $\rho = \sum_m A_m \otimes B_m$ is a density matrix in $\mathcal{N} \otimes \mathcal{F}$, goal: $\mathbb{P}(\rho, \mathcal{M}_1 \otimes \mathcal{F}) = \mathbb{P}(\mathrm{Tr}_{\mathcal{F}}(\rho), \mathcal{M}_1)$

$$\mathbb{P}(\rho, \mathcal{M}_1 \otimes \mathcal{F}) = \mathrm{Tr}(\rho \Pi_{\mathcal{M}_1 \otimes \mathcal{F}}) =$$
$$\sum_m \mathrm{Tr}((A_m \otimes B_m)(\Pi_{\mathcal{M}_1} \otimes \mathrm{Id}_{\mathcal{F}})) = \sum_m \mathrm{Tr}(A_m \Pi_{\mathcal{M}_1}) \, \mathrm{Tr}(B_m)$$

$$\mathbb{P}(\mathrm{Tr}_{\mathcal{F}}(\rho), \mathcal{M}_1) = \mathrm{Tr}(\mathrm{Tr}_{\mathcal{F}}(\rho) \Pi_{\mathcal{M}_1}) = \sum_m \mathrm{Tr}(A_m \Pi_{\mathcal{M}_1} \, \mathrm{Tr}(B_m))$$
$$= \sum_m \mathrm{Tr}(A_m \Pi_{\mathcal{M}_1}) \, \mathrm{Tr}(B_m)$$

Purification

Proposition (Purification of a state)

For any density matrix ρ over $\mathcal{N}$, there exists $\mathcal{F}$ and $|\psi\rangle \in \mathcal{N} \otimes \mathcal{F}$ such that $\rho = \mathrm{Tr}_{\mathcal{F}}(|\psi\rangle\langle\psi|)$.
*To ψ we call a **purification** of ρ.*

In the example above, we found that $|\psi\rangle = \frac{1}{\sqrt{2}} \sum_a |a, a\rangle$ is a purification of $\rho = \frac{1}{2} \sum_a |a\rangle\langle a|$, as $\mathrm{Tr}_{\mathcal{F}}(|\psi\rangle\langle\psi|) = \rho$.

Fact: two purifications $|\psi_1\rangle, |\psi_2\rangle$ of a density matrix ρ differ by a unitary operation on $\mathcal{F}$.

From the *Schmidt decomposition*: $\rho = \sum_a \lambda_a |\eta_a\rangle\langle\zeta_a|$.

Physically realizable transformations

Physical transformations act on density matrices, so we encode these as operators on density matrices $\mathbb{DM}(\mathcal{N})$. And call them **superoperators**.

- If U is an unitary operator on $\mathcal{N}$, then consider the superoperator

$$S_U : \rho \mapsto U^\dagger \rho U$$

- The partial trace $\mathrm{Tr}_{\mathcal{F}} : \mathbb{DM}(\mathcal{N} \otimes \mathcal{F}) \to \mathbb{DM}(\mathcal{N})$ is a superoperator.
- Adding trivial bits is also a superoperator:

$$A^N : \rho \mapsto \rho \otimes |0^N\rangle\langle 0^N|$$

The most natural postulate in the world

We postulate: A **physically realizable superoperator** (PRS) T is a composition of the operators $S_U, \mathrm{Tr}_{\mathcal{F}}$ and A^N.

Theorem

For any PRS T there is an isometric embedding V such that

$$T : \rho \mapsto \mathrm{Tr}_{\mathcal{F}}(V \rho V^{\dagger})$$

Theorem

For any PRS T there are can be written as

$$T : \rho \mapsto \sum_m A_m \rho A_m^{\dagger}$$

such that $\sum_m A_m A_m^{\dagger} = \mathrm{Id}$

The totally mixed state vs the uniform diagonal state

Take $\mathcal{N}$ an n-dimensional vector space with orthonormal basis B. Let

$$\rho_H = \frac{1}{n} \sum_{a,b \in B} |a\rangle\langle b|$$

$$\rho_d = \frac{1}{n} \sum_{a \in B} |a\rangle\langle a|$$

The state $\rho_H = |\frac{1}{\sqrt{n}} \sum_{a \in B} |a\rangle\rangle\langle \frac{1}{\sqrt{n}} \sum_{a \in B} |a\rangle|$ is a pure state.On the other hand, for any PRS T:

$$T(\rho_d) = \rho_d \text{ because } T : \rho \mapsto \sum_m A_m \rho A_m^\dagger$$

The partial trace working as intended

Compare two situations:
A DM $\rho \in \mathbb{DM}(\mathcal{N} \otimes \mathcal{F})$ is given. We disregard the information on $\mathcal{F}$ (putting it in the trash) and compute a probability in the remaining state, say $\mathcal{M} \subseteq \mathcal{N}$, obtaining:

$$\mathbb{P}(\mathrm{Tr}_{\mathcal{F}}(\rho), \mathcal{M}) = \mathbb{P}(\rho, \mathcal{M} \otimes \mathcal{F})$$

On another situation, something happens to the information on $\mathcal{F}$, being affected by a unitary operator U, obtaining

$$\mathbb{P}((\mathrm{Id} \otimes U)\rho(\mathrm{Id} \otimes U^\dagger), \mathcal{M} \otimes \mathcal{F})$$

Because we find that these values are the same, we can safely say that the trace has this physical meaning of *disregarding information*.

No observation without effect

Theorem

Suppose $T : \mathbb{DM}(\mathcal{N}) \to \mathbb{DM}(\mathcal{N} \otimes \mathcal{F})$ *is a physically realizable operator such that* $\mathrm{Tr}_{\mathcal{F}}(T|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|$ *for any vector* $|\psi\rangle \in \mathcal{N}$*. Then there exists some* $|\gamma\rangle \in \mathcal{F}$ *such that*

$$TX = X \otimes |\gamma\rangle\langle\gamma|\,.$$

$\mathcal{F}$ represents a ledger for the state of $\mathcal{N}$.

Decoherence

Physical irreversible degradation of a state
The decoherence superoperator $\mathcal{D}$ is defined with respect to a basis:

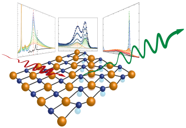
$$\rho = \sum_{a,b} \rho_{a,b} |a\rangle\langle b| \mapsto \sum_{a} \rho_{a,a} |a\rangle\langle a| \, .$$

This is a physically realizable superoperator that results in a classical density matrix.
Recall that $\Lambda(\sigma^x) : |a, b\rangle \mapsto |a, a \oplus b\rangle$

$$\rho \mapsto \rho \otimes |0\rangle\langle 0| \mapsto^{\Lambda(\sigma^x)} \sum_{a,b} \rho_{a,b} |a, b\rangle\langle a, b| \mapsto^{\mathrm{Tr}_{\mathcal{B}}} \sum_{a} \rho_{a,a} |a\rangle\langle a| \, .$$

The physical meaning of decoherence - Take a picture

Is decoherence reversible? Physically no, but mathematically yes.

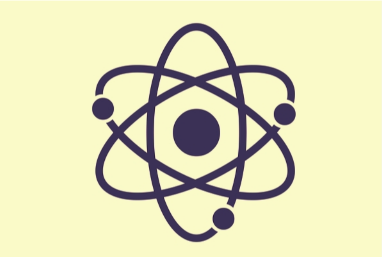


Copying the state of the photon to the chemical lattice corresponds to a copy

$$\rho \otimes |0\rangle\langle 0| \mapsto^{\Lambda(\sigma^x)} \sum_{a,b} \rho_{a,b} |a,b\rangle\langle a,b|$$

The quantum / classical computing model

Let $\mathcal{N}$ describe the quantum part of our computer that is in a state ρ, and $\mathcal{K}$ the classical part that is affected by ρ.



$\mathcal{N} = \oplus_j \mathcal{L}_k$ orthogonal decomposition, we want to record on $\mathcal{K}$ in which space $\{\mathcal{L}_1, \dots\}$ is the state ρ.

Projective measurements

This is called the **projective measurement** (with respect to the decomposition $\mathcal{N} = \oplus_j \mathcal{L}_j$) and maps $\mathbb{DM}(N) \to \mathbb{DM}(\mathcal{N} \otimes \mathcal{F})$.

$$R : \rho \mapsto \sum_j \Pi_{\mathcal{L}_j} \rho \Pi_{\mathcal{L}_j} \otimes |j\rangle\langle j|$$

is the only physically realizable operator that satisfies $R|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| \otimes |j\rangle\langle j|$ whenever $|\psi\rangle \in \mathcal{L}_j$.
After disregarding (i.e. taking the partial trace of) the quantum part, we get a **destructive** POV measurement

$$\mathbb{DM}(N) \to \mathbb{DM}(\mathcal{N} \otimes \mathcal{F}) \to^{\mathrm{Tr}_{\mathcal{N}}} \mathbb{DM}(\mathcal{F}) .$$

POVM measurements - generalization of POV measurements

Empirical observations brings a generalization.
For a given set of Hamiltonian operators, $\{X_k\}$ that satisfy the equality $\sum_k X_k = \mathrm{Id}$, we define the corresponding POVM measurement as:

$$R_{\{X_k\}} : \rho \mapsto \sum_k \mathrm{Tr}(\rho X_k)|k\rangle\langle k|\,.$$

For $X_k = \Pi_k$ we obtain the projective measurements earlier introduced.

Measuring operators

Given a decomposition $\mathcal{N} = \oplus_j \mathcal{L}_j$, a **measurement operator** is a choice of unitary operators U_j for each space $\mathcal{L}_j$, giving

$$R = \sum_j \Pi_{\mathcal{L}_j} \otimes U_j$$

Measuring operators - examples

For a unitary operator U in $\mathcal{N}$, the operator $\Lambda(U) = \Pi_0 \otimes \text{Id} + \Pi_1 \otimes U$ acting on $\mathcal{B} \otimes \mathcal{N}$ is a measurement operator with respect to $\mathcal{B}$.
Finding the eighenspaces $\mathcal{L}_j$ of $U = \sum_j \Pi_{\mathcal{L}_j} \lambda_j$ also gives us that $\Lambda(U)$ is a measurement operator with respect to $\mathcal{N}$

$$\Lambda(U) = \sum_j (\Pi_0 + \lambda \Pi_1) \otimes \Pi_{\mathcal{L}_j} .$$

The transformation $\Pi_0 + \lambda \Pi_1$ is unitary because $|\lambda_j| = 1$.

Summary

- Probability distributions - Density matrices
- Classical probability - Quantum probability

$$\mathbb{P}(\rho, \mathcal{M}) = \mathrm{Tr}(\rho \Pi_{\mathcal{M}})$$

- Properties of clasical probability - properties of quantum probability
- Pure and mixed states - The purification process
- Physically realizable transformations
- Observation paradox
- Decoherence in physics
- Quantum/Classical computing model - Projective measurements and measurement operators

The end