CPEN 400Q Lecture 22
Mixed states and density matrices

Wednesday 3 April 2024

Announcements

- See updated lecture schedule on Piazza
- Literacy assignment 3 available, due 10 April (last assignment!)
- Quiz 10 (last quiz) next class on today's content

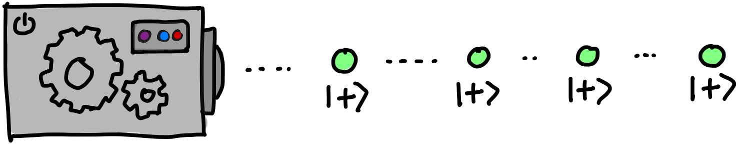
Learning outcomes

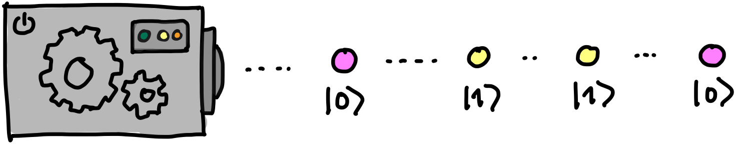
- Define a *mixed state*, and express quantum states using density matrices
- Identify mixed states using the Bloch sphere representation
- Perform quantum computation in the density matrix formalism
- Define and apply metrics for comparing two density matrices

These topics will be helpful for many of your project papers!

Mixed states

Suppose we have two different “boxes” that shoot particles:

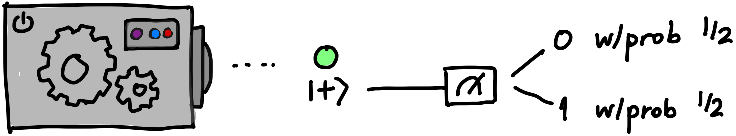


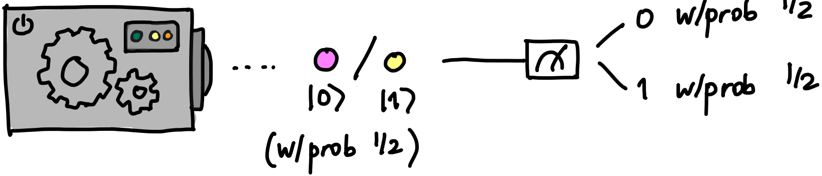


Are these the same?

Mixed states

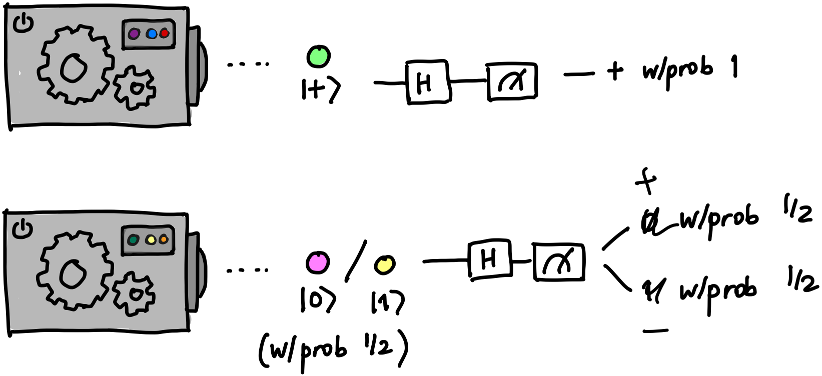
If we measure in the computational basis, it looks like they are.





Mixed states

But if we measure in the Hadamard basis, they are not!



What is the second box doing?

Mixed states

The second box prepares a **mixed state**.

A **pure state** can be expressed as a single ket vector, e.g.,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

A **mixed state** is a *probabilistic mixture of pure states*.

$$\cancel{|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)}$$

can't be expressed as a ket!

Density matrices

Mixed states are represented by **density matrices**.

The density matrix of a pure state $|\psi\rangle$ is

$$\rho = |\psi\rangle\langle\psi|$$

Exercise: what are the density matrices for $|0\rangle$ and $|1\rangle$?

$$\rho_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\rho_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \implies \rho_\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}\begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}$$

Hermitian

probs.

Trace 1

Density matrices of mixed states are linear combinations of density matrices of pure states:

$$\rho = \sum_i p_i \underbrace{|\psi_i\rangle\langle\psi_i|}_{\rho_{\psi_i}} , \quad \sum_i p_i = 1$$

Exercise: A system prepares $|+\rangle$ with probability $1/3$, and $|0\rangle$ with probability $2/3$. What is its state?

$$\rho = \frac{2}{3}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{3}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{5}{6} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{6} \end{pmatrix}$$

trace 1

Density matrices

Density matrices have some nice properties.

- they are Hermitian
- they have trace 1
- they are positive semi-definite (all eigenvalues are ≥ 0)
- (for pure states only) they are projectors, i.e., $\rho^2 = \rho$

$$\rho = |\psi\rangle\langle\psi| \quad \Rightarrow \quad \rho^2 = |\psi\rangle \underbrace{\langle\psi|\psi\rangle}_{=1} \langle\psi|$$

$$= |\psi\rangle\langle\psi|$$

Density matrices

Check with our example:

$$\rho = \begin{pmatrix} \frac{5}{6} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{6} \end{pmatrix}$$

- clearly Hermitian
- $\mathrm{Tr}\rho = 5/6 + 1/6 = 1$
- eigenvalues are 0.872678 and 0.127322, both ≥ 0
- not pure, so $\rho^2 \neq \rho$

Fun activity: show properties hold for general $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$

Working with density matrices and mixed states

We can do all the normal things we do to pure states (i.e., operations, measurements) with mixed states as well.

For a pure state $|\psi\rangle$ and operation U,

$$\rho_\psi = |\psi\rangle\langle\psi|$$

As ~~mixed states,~~
density matrix

$$\rho' = U\rho_\psi U^\dagger = \underbrace{U|\psi\rangle}_{|\psi'\rangle = U|\psi\rangle}\overbrace{\langle\psi|U^\dagger}^{\langle\psi'| = \langle\psi|U^\dagger}$$

$$= |\psi'\rangle\langle\psi'|$$

More generally,

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

$$\Rightarrow \rho' = \sum_i p_i \, U|\psi_i\rangle\langle\psi_i|U^\dagger$$

$$= U\left[\sum_i p_i |\psi_i\rangle\langle\psi_i|\right]U^\dagger$$

$$= U\rho U^\dagger$$

Working with density matrices and mixed states

Exercise: what is the output of applying H to our mixed state from the previous exercises? ($|+\rangle$ w/prob. $1/3$, $|0\rangle$ w/prob. $2/3$)

$$\rho = \frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|0\rangle\langle 0|$$

$$\rho' = H\rho H^\dagger = H\rho H$$

$$= \frac{1}{3}H|+\rangle\langle+|H + \frac{2}{3}H|0\rangle\langle 0|H$$

$$= \frac{1}{3}|0\rangle\langle 0| + \frac{2}{3}|+\rangle\langle+|$$

Recall that for a pure state $|\psi\rangle$, the probability of measuring and observing it in state $|\varphi\rangle$ is

$$\Pr(|\varphi\rangle) = |\langle\varphi|\psi\rangle|^2$$

We can rewrite this...

$$= \langle\varphi|\psi\rangle\langle\psi|\varphi\rangle$$

$$= \langle\psi\boxed{|\varphi\rangle\langle\varphi|}\psi\rangle$$

$$= \langle\psi|\rho_\varphi|\psi\rangle$$

$|\varphi\rangle\langle\varphi|$ is the density matrix of $|\varphi\rangle$, which is a *projector*. We are projecting $|\psi\rangle$ onto $|\varphi\rangle$, and then measuring the overlap with $|\psi\rangle$.

Measurement is performed w.r.t. a basis $\{|\varphi_i\rangle\}$; there are multiple possible outcomes:

$$\Pr(\text{outcome } i) = |\langle \varphi_i | \psi \rangle|^2$$

what if mixed?

For mixed states, measurement outcome probabilities follow the **Born rule**:

$$\Pr(\text{outcome } i) = \operatorname{Tr}(\Pi_i \rho)$$

where the set $\{\Pi_i\}$ is called a **positive operator-valued measure (POVM)**. The elements of the POVM satisfy

$$\sum_i \Pi_i = I$$

This reduces to a projective measurement when ρ is pure:

$$\{\Pi_i\} = \{|\varphi_i\rangle\langle\varphi_i|\}$$

$$\text{Prob}(\text{outcome } i) = \text{Tr}(\Pi_i \rho)$$

$$= \text{Tr}(\Pi_i |\psi\rangle\langle\psi|)$$

For an $m \times m$ matrix A,

$$I = \sum_k |k\rangle\langle k|$$

$$\text{Tr}(A) = \sum_{k=0}^{m-1} \langle k|A|k\rangle$$

$$A|k\rangle \quad \begin{pmatrix} * & * & * \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} |k\rangle \to \langle k| \begin{array}{c} \begin{array}{ccc} & k & \\ & \downarrow & \end{array} \\ \begin{pmatrix} 0 & * & 0 \\ 0 & * & 0 \\ \cdot & * & 0 \\ \cdot & - & \end{pmatrix} \end{array}$$

This reduces to a projective measurement when ρ is pure:

$$\Pr(\text{outcome } i) = \mathrm{Tr}\left(\Pi_i |\psi\rangle\langle\psi|\right)$$

$$= \sum_{k=0}^{N-1} \underbrace{\langle k|\Pi_i|\psi\rangle}\underbrace{\langle\psi|k\rangle}$$

$$= \sum_{k=0}^{N-1} \langle\psi|\underbrace{k\rangle\langle k|}\Pi_i|\psi\rangle$$

$$= \langle\psi|\underbrace{\left(\sum_k |k\rangle\langle k|\right)}_{= I}\Pi_i|\psi\rangle$$

$$= \langle\psi|\Pi_i|\psi\rangle$$

$\hookrightarrow \Pi_i = |\varphi_i\rangle\langle\varphi_i|$

Example: $\{|+\rangle\langle+|, |-\rangle\langle-|\}$.

The Born rule tells us that, given a state ρ,

$$Pr(+) = Tr(|+\rangle\langle+| \cdot \rho)$$
$$Pr(-) = Tr(|-\rangle\langle-| \cdot \rho)$$

Exercise: Show that $\{|+\rangle\langle+|, |-\rangle\langle-|\}$ form a legit POVM.

$$\sum_i \Pi_i = I$$

Exercise: Suppose we prepare our system in $|+\rangle$ with probability $1/3$ and $|0\rangle$ with probability $2/3$. What is the probability of obtaining the POVM outcome ~~$\Pi_+ = |+\rangle\langle+|$~~? $\Pi_- = |-\rangle\langle-|$

$$Pr = 1/3$$

$$\Rightarrow \quad Pr(-) = \mathrm{Tr}\left(|-\rangle\langle-| \cdot \left(\frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|0\rangle\langle 0|\right)\right)$$

$$= \mathrm{Tr}\left(\cancel{\frac{1}{3}|-\rangle\underbrace{\langle-|+\rangle}\langle+|} + \frac{2}{3}|-\rangle\langle-|0\rangle\langle 0|\right)$$

$$= \mathrm{Tr}\left(\frac{2}{3}|-\rangle\underbrace{\langle-|0\rangle}_{\frac{1}{\sqrt{2}}}\langle 0|\right)$$

$$= \mathrm{Tr}\left(\frac{2}{3}\cdot\frac{1}{\sqrt{2}}|-\rangle\langle 0|\right)$$

$$= \frac{2}{3}\cdot\frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}$$

$$= \frac{1}{3}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

Mixed states and measurements

Recall how to compute expectation values from samples:

$$\langle X \rangle = \frac{1 \cdot (\#\,{+1}\text{ samples}) + (-1)(\#\,{-1}\text{ samples})}{\text{num samples}}$$

$$= 1 \cdot \Pr(+1) + (-1) \cdot \Pr(-1)$$

$$= 1 \cdot \Pr(|+\rangle) + (-1) \cdot \Pr(|-\rangle)$$

We can compute these probabilities in terms of the trace and ρ...

$$\langle X \rangle = 1 \cdot \mathrm{Tr}\left(|+\rangle\langle+| \cdot \rho\right) + (-1) \cdot \mathrm{Tr}\left(|-\rangle\langle-| \cdot \rho\right)$$

$$= \mathrm{Tr}\left[|+\rangle\langle+| \cdot \rho - |-\rangle\langle-| \rho \right]$$

$$= \mathrm{Tr}\left[\underbrace{\left(|+\rangle\langle+| - |-\rangle\langle-|\right)}_{= X} \rho \right]$$

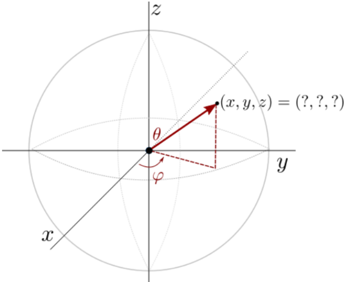
$$= \mathrm{Tr}\left[X \rho \right]$$

We can do the same for Y and Z: We can compute these probabilities in terms of the trace and ρ...

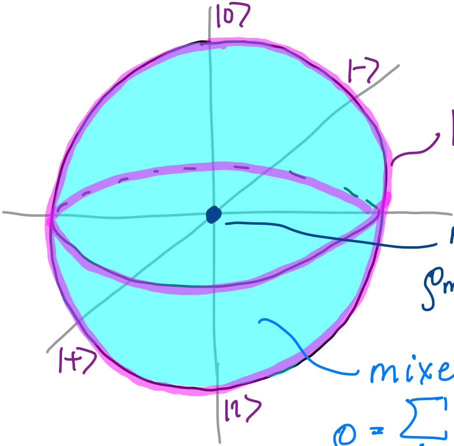
$$\langle Z \rangle = \mathrm{Tr}(Z\rho)$$
$$\langle Y \rangle = \mathrm{Tr}(Y\rho) \quad \ldots$$

Remember from assignment 1:

Write a function that uses quantum measurements to extract its Bloch vector, i.e., its coordinates in 3-dimensional space, as demonstrated by the following graphic:



Mixed states live *in* the Bloch sphere!



pure states

$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

maximally mixed state

$\rho_{max} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\mathbb{1}$

mixed states

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

More formally, we can write any ρ as

where $a_P = \mathrm{Tr}(P\rho) = \langle P \rangle$.

The case where $a_x = a_y = a_z = 0$ is the **maximally mixed state**.

(Note that all of this generalizes to multiple qubits as well)

Comparing density matrices

We use the inner product to tell us how close two pure states $|\psi\rangle$ and $|\phi\rangle$ were:

What can we do for mixed states?

Comparing density matrices

How close are two mixed states σ, ρ?

One common metric is the **trace distance**:

Value of trace distance is bounded by $0 \leq T(\rho, \sigma) \leq 1$, and *lower* trace distance is better.

Comparing density matrices

Another is the **fidelity**:

Value of fidelity is bounded by $0 \leq F(\rho, \sigma) \leq 1$, and *higher* fidelity is better.

Comparing density matrices

Exercise: Suppose both σ and ρ are pure states. What does the expression for fidelity reduce to?

Comparing density matrices

Exercise: Suppose ρ is pure but σ is not. What does the expression for fidelity reduce to?

Next time

Last few classes:

- Noise and quantum channels
- Noisy, intermediate-scale quantum computing

Action items:

1. Work on project; due 12 April
2. Literacy assignment 3

Recommended reading:

- Codebook module N