CS 269Q: Section 3

Ensembles and Density Matrices

Jon Braatz
jfbraatz@stanford.edu

April 27, 2019

Mixed and Pure States

- Pure states are definite quantum states where there is no uncertainty as to which state the system is in. For example, if we know with 100% certainty that the state of the system is $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, that is a pure state.
- For a mixed state, there is some uncertainty in the state of the system, for example 50% odds of $|0\rangle$ and 50% odds of $|1\rangle$.
- What, experimentally is the difference between these states? Don't they both give 50/50 odds to measure $|0\rangle$ or $|1\rangle$.
- The difference is how they are affected by unitaries and their behavior when measuring in different bases.

Differences Between Mixed and Pure States

- Apply an $R_y(-\pi/2) = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$ gate to the mixed and pure states.
- The pure state in the $|+x\rangle$ direction on the Bloch sphere gets rotated to $|-z\rangle = |0\rangle$, while the mixed state goes from 50/50 in $|\pm z\rangle$ to 50/50 in $|\pm x\rangle$.
- Now measure in the computational basis. The pure state is $|0\rangle$ with probability 1 and the mixed state is still 50/50 between $|0\rangle$ and $|1\rangle$.
- So amplitude distributions (pure states) are measurably different from probability distributions over amplitude distributions (mixed states).
- We'd like a common notation to describe and manipulate both types of states.

Ensembles of Quantum States

- Consider a probability distribution over a set of pure states $|\psi_i\rangle$ each having a probability p_i.
- This distribution $\{p_i, |\psi_i\rangle\}$ is called an ensemble of pure states.
- Let's find the distribution over outcomes if we make a measurement.
- Let M_m denote the projection operator onto the subspace of states that give measurement outcome of m (namely the eigenspace of M_m with eigenvalue 1).
- Recall that the probability of actually getting measurement outcome m for state $|\psi_i\rangle$ is $||M_m|\psi_i\rangle||^2 = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle$

The Density Operator

- Probability $p(m|i)$ of getting result m if initial state was really $|\psi_i\rangle$ is just what we said before, and it's just a number so it's equal to its trace:

$$p(m|i) = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle = \mathrm{tr}(\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle)$$

- Marginalize over i to get total probability $p(m)$:

$$p(m) = \sum_i p(m|i)p_i = \sum_i p_i \mathrm{tr}(\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle)$$

- Simplify using the cyclic property of the trace ($\mathrm{tr}(ABC) = \mathrm{tr}(BCA)$) and its linearity:

$$p(m) = \sum_i p_i \mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|) = \mathrm{tr}(M_m^\dagger M_m(\sum_i p_i|\psi_i\rangle\langle\psi_i|))$$

- This shows that only the operator $\sum_i p_i|\psi_i\rangle\langle\psi_i|$ is observable, and we call this operator the density operator ρ of the ensemble.

Properties of the Density Operator

- An operator ρ is the density operator associated with some ensemble $\{p_i, \psi_i\}$ if and only if it satisfies the conditions:
  1. (Trace Condition) ρ has trace equal to one.

     Proof of $\rightarrow$: $\text{tr}(\rho) = \sum_i p_i \text{tr}(|\psi_i\rangle\langle\psi_i) = \sum_i p_i = 1$.
  2. (Positivity condition) ρ is a positive-semidefinite operator.

     Proof of $\rightarrow$: Suppose $|\phi\rangle$ is an arbitrary vector in state space. Then

     $$\langle\phi|\rho|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0$$

- Proofs of $\leftarrow$ are on Page 101-102 of Mike and Ike.

Measurement Operators for Density Operators

- We saw that probability that result m occurs after a measurement is $p(m) = \text{tr}(M_m^\dagger M_m \rho)$.
- For a pure state $|\psi\rangle$, we know that the state immediately after measuring and getting outcome m is $M_m|\psi\rangle/\sqrt{p(m)}$. This means that the density matrix becomes:

$$(\sum_i p_i (M_m|\psi\rangle)^\dagger (M_m|\psi\rangle))/p(m) = \frac{M_m^\dagger \rho M_m}{\text{tr}(M_m^\dagger M_m \rho)}$$

- Since we're guaranteed to get some measurement outcome, the measurement operators satisfy the completeness equation $\sum_m M_m^\dagger M_m = I$.

Pure vs Mixed Density Operators (Ex. 2.71)

Ex 2.71: (Criterion to decide if a state is mixed or pure) Let ρ be a density operator. Show that $\mathrm{tr}(\rho^2) \leq 1$ with equality if and only if ρ is a pure state.

- Since ρ is Hermitian, we can express it in terms of its spectral decomposition as $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.
- The trace is the sum of the eigenvalues p_i, which sum to 1.
- The trace of ρ^2 is the sum of the eigenvalues squared.
- $1 = (\sum_i p_i)^2 = \sum_i p_i^2 + \sum_{i \neq j} p_i p_j$.
- Thus $\sum_i p_i^2 = \mathrm{tr}(\rho^2) \leq 1$, with equality only when $\sum_{i \neq j} p_i p_j = 0$, which is to say there is only one non-zero probability p_i equal to 1, meaning the state is pure.

Bloch Sphere for Mixed States (Ex 2.72) Part 1

Ex 2.72: (Bloch sphere for mixed states) The Bloch sphere picture for pure states of single qubit was introduced in Section 1.2. This descriptions has an important generalization to mixed states as follows.

1. Show that an arbitrary density matrix for a mixed state qubit may be written as

$$\rho = \frac{I + \vec{r} \cdot \vec{\sigma}}{2} = \frac{1}{2}(I + r_x X + r_y Y + r_z Z),$$

   where $\vec{r}$ is a real three-dimensional vector such that $||\vec{r}|| \leq 1$. This vector is known as the *Bloch vector* for the state ρ.

Ex 2.72 Part 2

2. What is the Bloch vector representation for the state $\rho = I/2$?

Ex 2.72 Part 3

3. Show that a state ρ is pure if and only if $||\vec{r}|| = 1$.

Ex 2.72 Part 4

4. Show that for pure states the description of the Bloch vector we have given coincides with that in Sectton 1.2.

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Back to the First Example

- Let's revisit our motivating example of density matrices from the first slide using what we now know.
- Consider a pure state given by $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ and a mixed state that is 50/50 between $|0\rangle$ and $|1\rangle$.
- The density matrix for the pure state is

$$\begin{aligned}
\rho_{\text{pure}} &= (\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle)(\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}\langle 1|) \\
&= \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) \\
&= \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}
\end{aligned}$$

- Quiz: What is this state's Bloch vector?

Back to the First Example

- We can pattern match $\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$ onto $\frac{I+\vec{r}\cdot\vec{\sigma}}{2} = \frac{1}{2}(I + r_x X + r_y Y + r_z Z)$ by noticing that it's $1/2(I+X)$ and conclude that $\vec{r} = (1,0,0)$.
- If that wasn't obvious, we can get components of a vector in the usual way by using inner products with basis elements. In this case the basis elements are $\{I, X, Y, Z\}$ and the inner product between density matrices A and B is $\mathrm{tr}(AB)$.

$$r_x = \mathrm{tr}(\rho_{\text{pure}} X) = 1$$
$$r_y = \mathrm{tr}(\rho_{\text{pure}} Y) = 0$$
$$r_z = \mathrm{tr}(\rho_{\text{pure}} Z) = 0$$

Back to the First Example

- What about the density matrix for our mixed state?

$$\begin{aligned}\rho_{\text{mixed}} &= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \\ &= \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = I/2\end{aligned}$$

- So the mixed state's Bloch vector is apparently $(0, 0, 0)$. It is a point at the origin of the Bloch sphere.

Transformations of These States

- How do these states behave under unitary transformations like the $R_y(-\pi/2)$ gate that we considered earlier?
- Unitaries correspond to rotations on the Bloch sphere. A rotation of $-\pi/2$ around the y-axis sends the vector $(1,0,0)$ to $(0,0,-1)$, and the point at the origin stays at the origin.
- $(0,0,-1)$ corresponds to $|0\rangle$, so a measurement in the computational basis gives $|0\rangle$ with probability 1 as before.
- Since the mixed state is proportional to the identity, any unitary acting on it will give $U^\dagger \rho_{\text{mixed}} U = U^\dagger (I/2) U = I/2$, so the density matrix is unchanged. This is the maximally mixed state.