COL7160 : Quantum Computing

Lecture 25: Mixed States, Density Matrix, and Measurements

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1 Pure States vs. Mixed States

So far, we have worked exclusively with *pure states*: quantum states that are fully specified by a single state vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$. However a system may have been prepared by a classical process that produces $|\psi_i\rangle$ with probability p_i. In either case the state is *mixed*: a classical probability distribution over pure states.

Definition 1 (Ensemble)**.** An *ensemble* is a set $\{(p_i, |\psi_i\rangle)\}$ where each $|\psi_i\rangle$ is a (normalized) pure state and $\{p_i\}$ is a probability distribution, i.e. $p_i \geq 0$ for all i and $\sum_i p_i = 1$.

Example 2. A source emits $|0\rangle$ with probability $\frac{1}{2}$ and $|1\rangle$ with probability $\frac{1}{2}$. The ensemble is

$$\left\{ \left(\tfrac{1}{2}, |0\rangle\right),\ \left(\tfrac{1}{2}, |1\rangle\right) \right\}.$$

This is *not* the same as the pure superposition $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, even though the measurement probabilities in the computational basis agree.

2 Density Matrix (Density Operator)

The density matrix provides a unified mathematical description of both pure and mixed states.

Definition 3 (Density Operator)**.** The *density operator* (or *density matrix*) associated with an ensemble $\{(p_i, |\psi_i\rangle)\}$ is

$$\rho \;=\; \sum_i p_i \, |\psi_i\rangle\langle\psi_i|.$$

Proposition 4 (Characterization of Density Operators)**.** *A linear operator ρ on $\mathcal{H}$ is a valid density operator if and only if*

1. $\rho \succeq 0$ *(positive semi-definite),*
2. $\mathrm{tr}(\rho) = 1$ *(unit trace).*

Proof. ($\Rightarrow$) For any $|\varphi\rangle$, $\langle\varphi|\rho|\varphi\rangle = \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0$, so $\rho \succeq 0$. Moreover, $\mathrm{tr}(\rho) = \sum_i p_i \, \mathrm{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i \langle\psi_i|\psi_i\rangle = \sum_i p_i = 1$.
($\Leftarrow$) Any positive semi-definite, unit-trace operator has a spectral decomposition $\rho = \sum_j \lambda_j |e_j\rangle\langle e_j|$ with $\lambda_j \geq 0$ and $\sum_j \lambda_j = 1$, so $\{(\lambda_j, |e_j\rangle)\}$ is a valid ensemble. ☐

3 Evolution of Density Operators

Suppose a closed quantum system evolves by a unitary U. If the system is in state $|\psi_i\rangle$, it evolves to $U|\psi_i\rangle$. Therefore the density operator transforms as

$$\rho \;\longmapsto\; U \rho U^\dagger.$$

This is the *unitary conjugation* rule, and it follows immediately from the linearity of the density operator construction.

Homework. Show that unitary conjugation preserves positive semi-definiteness and unit trace.

4 Measurements and the Density Operator

Projective Measurements

Let $\{P_m\}$ be a complete set of orthogonal projectors:

$$P_m P_{m'} = \delta_{mm'} P_m, \qquad \sum_m P_m = I.$$

Proposition 5 (Born Rule for Mixed States)**.** *Given a system with density operator ρ, the probability of outcome m is*

$$\Pr[m] = \operatorname{tr}(P_m \rho),$$

and the post-measurement state is

$$\rho_m = \frac{P_m \rho P_m}{\operatorname{tr}(P_m \rho)}.$$

Proof. If the system is in state $|\psi_i\rangle$ with probability p_i, then by the standard Born rule,

$$\Pr[m \mid |\psi_i\rangle] = \langle \psi_i | P_m | \psi_i \rangle = \operatorname{tr}(P_m |\psi_i\rangle\langle\psi_i|).$$

Averaging over the ensemble,

$$\Pr[m] = \sum_i p_i \operatorname{tr}(P_m |\psi_i\rangle\langle\psi_i|) = \operatorname{tr}\Big(P_m \sum_i p_i |\psi_i\rangle\langle\psi_i|\Big) = \operatorname{tr}(P_m \rho).$$

The post-measurement state follows from Bayes' rule applied to each branch. □

Positive Operator-Valued Measures (POVMs)

A more general measurement is described by a *POVM*: a set of positive semi-definite operators $\{M_m\}$ satisfying $\sum_m M_m = I$.

Definition 6 (POVM)**.** A *positive operator-valued measure* is a collection $\{M_m\}$ with $M_m \succeq 0$ for all m and $\sum_m M_m = I$.

The probability of outcome m when measuring ρ is

$$\Pr[m] = \operatorname{tr}(M_m \rho).$$

A POVM does not specify the post-measurement state; for that one needs a *measurement model* (a set of Kraus operators $\{K_m\}$ with $M_m = K_m^\dagger K_m$).

Remark 7. Projective measurements are a special case of POVMs with $M_m = P_m$ (idempotent elements).