Notes 8.370/18.435 Fall 2022

Lecture 12 Prof. Peter Shor

Today we started on density matrices.

Suppose we have a probabilistic mixture of quantum states. That is, suppose somebody prepares the state $|\, v_1 \rangle$ with probability p_1, the state $|\, v_2 \rangle$ with probability p_2, the state $|\, v_3 \rangle$ with probability p_3, and so on. How can we describe it? It turns out that a very good way to describe it is with something called a *density matrix*. If we have a system that is in state $|\, v_i \rangle$ with probability p_i, then the density matrix is

$$\rho = \sum_i p_i \,|\, v_i \rangle\langle v_i \,|\,.$$

Density matrices are customarily denoted by the variable ρ.

The density matrix ρ is a Hermitian positive semi-definite trace 1 matrix. Here, *trace 1* means that $\mathrm{Tr}\,\rho = 1$. It is easy to see that it is trace 1 because

$$\mathrm{Tr}\sum_i p_i \,|\, v_i \rangle\langle v_i \,| = \sum_i p_i \mathrm{Tr}\,|\, v_i \rangle\langle v_i \,| = \sum_i p_i = 1$$

The word $positive$ means that it has all non-negative eigenvalues. This is equivalent to the condition $\langle v \,|\, \rho \,|\, v \rangle \geqslant 0$ for all $|\, v \rangle$. It is also easy to see that it is positive because for any $|\, w \rangle$, we have $\langle w | v_i \rangle\langle v_i | w \rangle \geqslant 0$. This means that

$$\langle w \,|\, \rho \,|\, w \rangle = \sum_i p_i \langle w | v_i \rangle\langle v_i | w \rangle \geqslant 0 \;\forall \,|\, w \rangle\,.$$

In fact, any Heritian positive semidefinite trace 1 matrix ρ is a density matrix for some probabilistic mixture of quantum states, One way to see this is to use the eigenvectors of ρ for the quantum states and the eigenvalues for the probabilities.

The difference between a *superposition* of states and a *mixture* of states is important. A superposition of states is something like

$$\frac{1}{\sqrt{2}}\,|\, 0 \rangle + \frac{1}{\sqrt{2}}\,|\, 1 \rangle\,,$$

while a mixed state is

$$|\, 0 \rangle\langle 0 \,| \text{ with probability } \frac{1}{2} \quad \text{and} \quad |\, 1 \rangle\langle 1 \,| \text{ with probability } \frac{1}{2},$$

which would be represented by the density matrix

$$\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2}. \end{pmatrix}$$

For these two states, if you measure either one in the basis $\{|\, 0 \rangle, |\, 1 \rangle\}$, you get $|\, 0 \rangle$ with probability $\frac{1}{2}$ and $|\, 1 \rangle$ with probability $\frac{1}{2}$. But they don't behave the same. Consider what happens if you apply the Hadamard gate $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and then measure them in the basis $\{|\,0\rangle\,,|\,1\rangle\}$. (This is equivalent to measuring in the basis $\{|\,+\rangle\,,|\,-\rangle\}$.) The first one is taken to the state $|\,0\rangle$, and you observe the outcome $|\,0\rangle$ with probabiity 1. The second is taken to the state

$$|\,+\rangle \text{ with probability } \frac{1}{2} \quad \text{and} \quad |\,-\rangle \text{ with probability } \frac{1}{2},$$

and you observe the outcomes $|\,0\rangle$ and $|\,1\rangle$. with probabiity $\frac{1}{2}$ each.

There is another way of computing this result. To apply a unitary U to a density matrix ρ, you take $U\rho U^\dagger$. Thus, for the calculation above, we have

$$H\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} H^\dagger = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} HH^\dagger = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

since H commutes with the identity matrix.

One thing to notice is that two different probabilistic ensembles of quantum states can give the same density matrix. For example, suppose you have the ensembles

(a)	$\frac{4}{5}\,|\,0\rangle + \frac{3}{5}\,|\,1\rangle$	with probability	$\frac{1}{2}$	and	$\frac{4}{5}\,|\,0\rangle - \frac{3}{5}\,|\,1\rangle$	with probability	$\frac{1}{2}$,
(b)	$|\,0\rangle$	with probability	$\frac{16}{25}$	and	$|\,1\rangle$	with probability	$\frac{9}{25}$.

These both give the density matrix

$$\begin{pmatrix} \frac{16}{25} & 0 \\ 0 & \frac{9}{25} \end{pmatrix}.$$

So why use density matrices if they don't give a complete description of the quantum state? The reason is that if you know the density matrix, this is sufficient information to tell you the outcome of any experiment on the quantum state. Let's now give a demonstration of this fact.

Suppose we use the basis $\left\{\frac{2}{\sqrt{5}}\,|\,0\rangle + \frac{1}{\sqrt{5}}\,|\,1\rangle\,, -\frac{1}{\sqrt{5}}\,|\,0\rangle + \frac{2}{\sqrt{5}}\,|\,1\rangle\right\}$ to measure the probabilistic ensemble (a) above. The probability of observing the first basis state is

$$\frac{1}{2}\left|\left(\tfrac{2}{\sqrt{5}}\,\langle 0\,| + \tfrac{1}{\sqrt{5}}\,\langle 1\,|\right)\left(\tfrac{4}{5}\,|\,0\rangle + \tfrac{3}{5}\,|\,1\rangle\right)\right|^2 + \frac{1}{2}\left|\left(\tfrac{2}{\sqrt{5}}\,\langle 0\,| + \tfrac{1}{\sqrt{5}}\,\langle 1\,|\right)\left(\tfrac{4}{5}\,|\,0\rangle - \tfrac{3}{5}\,|\,1\rangle\right)\right|^2,$$

which is

$$\frac{1}{2}\left(\frac{11}{5\sqrt{5}}\right)^2 + \frac{1}{2}\left(\frac{5}{5\sqrt{5}}\right)^2 = \frac{73}{125}$$

If we do this for the probabilistic ensemble (b), we get

$$\frac{16}{25}\left|\left(\tfrac{2}{\sqrt{5}}\,\langle 0\,| + \tfrac{1}{\sqrt{5}}\,\langle 1\,|\right)|\,0\rangle\right|^2 + \frac{9}{25}\left|\left(\tfrac{2}{\sqrt{5}}\,\langle 0\,| + \tfrac{1}{\sqrt{5}}\,\langle 1\,|\right)\ |\,1\rangle\right|^2 = \frac{64}{25} + \frac{9}{25} = \frac{73}{125}$$

We will see that the formula for the probability of obtaining $|\,v\rangle$ in a von Neumann measurement on state ρ is $\langle v\,|\,\rho\,|\,v\rangle$. For the example above,

$$\langle v\,|\,\rho\,|\,v\rangle = \left(\tfrac{2}{\sqrt{5}}, \tfrac{1}{\sqrt{5}}\right)\begin{pmatrix} \frac{16}{25} & 0 \\ 0 & \frac{9}{25} \end{pmatrix}\begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix} = \frac{73}{125}.$$

To show that the outcome of any experiment depends only on the density matrix, we need to prove that if you apply a unitary U to a mixture of quantum states with density matrix ρ, you get a mixture of quantum states with density matrix $U\rho U^\dagger$, and that if you perform a measurement on a mixture of quantum states, the density matrix is enough to predict the outcome. We now show these two facts.

Suppose you have a mixture of quantum states, where $|\, v_i\rangle$ has probability p_i. Applying U gives the mixture where $U\,|\, v_i\rangle$ has probability p_i. Computing the density matrix of this mixture gives

$$\sum_i p_i U\,|\, v_i\rangle\langle v_i\,|\, U^\dagger = U\left(\sum_i p_i\,|\, v_i\rangle\langle v_i\,|\right)U^\dagger = U\rho U^\dagger,$$

as we wanted.

Now, suppose we have a mixture of quantum states with density matrix ρ, and we measure it with the von Neumann measurement corresponding to the basis $\{|\, w_i\rangle\}$. The probability that we see $|\, w_j\rangle$ if we started with state $|\, v_i\rangle$ is $|\langle w_j|v_i\rangle|^2 = \langle w_j|v_i\rangle\langle v_i|w_j\rangle$, so the total probability that we see $|\, w_j\rangle$

$$\begin{aligned}\sum_i p_i\langle w_j|v_i\rangle\langle v_i|w_j\rangle &= \langle w_j\,|\left(\sum_i p_i\,|\, v_i\rangle\langle v_i\,|\right)|\, w_j\rangle \\ &= \langle w_j\,|\,\rho\,|\, w_j\rangle\,,\end{aligned}$$

which depends only on ρ and not the p_i's and $|\, v_i\rangle$s.

Do these calculations show that density matrices are sufficient to predict all experimental outcomes from mixed quantum states? Not quite—we haven't shown that results of the more general type of von Neumann measurements, with projections onto subspaces of rank greater than 1, can be predicted from the density matrix. Let's do that now.

Recall that a von Neumann measurement has Hermitian projection matrices Π_1, $\Pi_2, \ldots, \Pi_r$ with $\sum_i \Pi_r = I$. When applied to a quantum state $|\, \phi\rangle$, we observe the rth outcome with probability

$$|\Pi_r\,|\,\psi\rangle|^2 = \langle\psi\,|\,\Pi_r\,|\,\psi\rangle$$

and the state after the measurement is

$$\frac{1}{|\Pi_r\,|\,\psi\rangle|}\Pi_r\,|\,\psi\rangle\,.$$

So what is the probability of observing the rth outcome if we have a probabilistic ensemble of quantum states where $|\, v_i\rangle$ appears with probabiity p_i. It's just the weighted sum of the probability of each outcome:

$$\begin{aligned}
\sum_i |\Pi_r \,|\, v_i\rangle|^2 &= \sum_i p_i \langle v_i \,|\, \Pi_r \,|\, v_i\rangle \\
&= \sum_i p_i \mathrm{Tr}\, \langle v_i \,|\, \Pi_r \,|\, v_i\rangle \\
&= \sum_i p_i \mathrm{Tr}\, \Pi_r \,|\, v_i\rangle\langle v_i \,| \\
&= \mathrm{Tr}\, \Pi_r \left(\sum_i p_i \,|\, v_i\rangle\langle v_i \,| \right) \\
&= \mathrm{Tr}\, \Pi_r \rho,
\end{aligned}$$

which depends only on the density matrix. For the second and third steps of this calculation, we used the fact that the trace of a scalar, i.e., a 1×1 matrix, is just the scalar, and the cyclic property of the trace:

$$\mathrm{Tr}\, ABC = \mathrm{Tr}\, BCA = \mathrm{Tr}\, CAB$$

(which is actually a straightforward consequence of $\mathrm{Tr}\, AB = \mathrm{Tr}\, BA$).

What we will do now is compute the residual state we get if we start with v_i and observe the rth outcome, and then compute the conditional probability of having started with v_i, given that we observe the rth outcome. These last two quantities will let us compute the density matrix, conditional on having observed the rth outcome.

First, the residual state is

$$\frac{\Pi_r \,|\, v_i\rangle}{|\Pi_r \,|\, v_i\rangle|} = \frac{\Pi_r \,|\, v_i\rangle}{\langle v_r \,|\, \Pi_r \,|\, v_i\rangle^{1/2}}.$$

The conditional probability that we started with $|\, v_i\rangle$, given that we observe the rth outcome, can be calculated using Bayes' rule. This gives:

$$\frac{p_i \langle v_i \,|\, \Pi_r \,|\, v_i\rangle}{\sum_i p_i \langle v_i \,|\, \Pi_r \,|\, v_i\rangle} = \frac{p_i \langle v_i \,|\, \Pi_r \,|\, v_i\rangle}{\mathrm{Tr}\ (\Pi_r \rho)}$$

The conditional density matrix, given that we observe the rth outcome, is thus.

$$\begin{aligned}
\rho_r &= \sum_i \frac{p_i \langle v_i \,|\, \Pi_r \,|\, v_i\rangle}{\mathrm{Tr}\ (\Pi_r \rho)} \cdot \frac{\Pi_r \,|\, v_i\rangle}{\langle v_r \,|\, \Pi_r \,|\, v_i\rangle^{1/2}} \frac{\langle v_i \,|\, \Pi_r}{\langle v_r \,|\, \Pi_r \,|\, v_i\rangle^{1/2}} \\
&= \frac{\Pi_r \left(\sum_i p_i \,|\, v_i\rangle\langle v_i \,|\right) \Pi_r}{\mathrm{Tr}\ (\Pi_r \rho)} \\
&= \frac{\Pi_r \rho \Pi_r}{\mathrm{Tr}\, (\Pi_r \rho)},
\end{aligned}$$

which depends only on ρ, so we are done. Note that $\mathrm{Tr}\ (\Pi_r \rho \Pi_r) = \mathrm{Tr}\ (\Pi_r \rho)$, so this indeed has trace 1, and so is a valid density matrix.