CMSC 657: Introduction to Quantum Information Processing
Lecture 3

Instructor: Daniel Gottesman

Fall 2024

1 Density Matrices

1.1 Properties and Decompositions

What are the properties of a density matrix? Which matrices can be density matrices of some mixed state?

Theorem 1. *Any density matrix ρ has the following properties:*

1. $\mathrm{Tr}\,\rho = 1$
2. $\rho = \rho^\dagger$ *(i.e., ρ is* Hermitian*)*
3. *ρ is a positive semi-definite matrix*

Moreover, any $D \times D$ matrix with these properties is a density matrix; that is, there exists an ensemble of states that has this matrix as a density matrix.

Proof. It is easy to see that $\mathrm{Tr}\,\rho = 1$ for any density matrix:

$$\mathrm{Tr}\,\rho = \sum_a \rho_{aa} = \sum_{i,a} p_i |c_{i,a}|^2. \tag{1}$$

But $\sum_a |c_{i,a}|^2 = 1$ because $|\psi_i\rangle$ is normalized and $\sum_i p_i = 1$ because we have a probability distribution, and therefore $\mathrm{Tr}\,\rho = 1$.

It is equally easy to show that ρ is Hermitian:

$$\rho^\dagger = \sum_i p_i (|\psi_i\rangle\langle\psi_i|)^\dagger = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \rho. \tag{2}$$

To see that ρ is postive semi-definite, we look at

$$\langle\phi|\rho|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0. \tag{3}$$

Thus, ρ is positive semi-definite.

To see that any $D \times D$ matrix ρ with these two properties can be realized as a density matrix, note that any positive semi-definite matrix can be diagonalized with a unitary change of basis. In this choice of basis $\{|a\rangle\}$, we write $\rho = \sum_a \rho_{aa}|a\rangle\langle a|$, and since ρ is Hermitian, $\rho^*_{aa} = \rho_{aa}$, that is, the diagonal elements are real. Because ρ_{aa} is positive semi-definite, $\rho_{aa} \geq 0$. Moreover, $\mathrm{Tr}\,\rho = \sum_a \rho_{aa}$, so we can let $p_a = \rho_{aa}$, and $\{p_a\}$ form a probability distribution. Thus, we have the ensemble which, with probability p_a gives us the state $|a\rangle$, and this ensemble has density matrix ρ.

□

Note that the decomposition of a mixed state as a mixture of pure states need not be unique. Even disregarding trivial decompositions where we get the same state $|\psi_i\rangle$ appearing more than once in the mixture, the only states which have a unique decomposition are pure states. There is always one choice of decomposition where the mixed state is a mixture of basis states, but we don't always consider this a "classical" mixture, because the basis states might be very weird (e.g., entangled states).

Note that a density matrix represents a pure state if and only if $\rho^2 = \rho$. Why is this? We can diagonalize ρ as in the proof of thm. 1, and ρ is pure if and only if it has only one non-zero eigenvalue (which must be 1 because $\operatorname{Tr}\rho = 1$), which is also equivalent to $\rho^2 = \rho$.

Example of decompositions: The mixture composed of 50% $|0\rangle$ and 50% $|1\rangle$ has density matrix

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|. \tag{4}$$

Now consider the mixture of 50% $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and 50% $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The density matrix of this mixture is

$$\begin{aligned}\rho =& \frac{1}{4}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) && (5)\\ &+ \frac{1}{4}(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|) && (6)\\ =& \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|). && (7)\end{aligned}$$

The other way to get a mixed state is to discard part of a larger quantum state. Suppose we have a bipartite system whose pure states live in the tensor product Hilbert space $A \otimes B$. To understand what happens in such a system, let us first consider the classical special case, where ρ_{AB} is diagonal. In this case, ρ_{AB} represents a *joint* probability distribution p_{ab}. If we only care about the *marginal* distribution for the ourcomes of A, we would find $p_a = \sum_b p_{ab}$.

The quantum analog of this is the *partial trace*: Given a mixed state ρ_{AB} on the tensor product space, we can find the density matrix of part of it by tracing over the other part, $\rho_A = \operatorname{Tr}_B \rho_{AB}$. If

$$\rho_{AB} = \sum_{a,a',b,b'} \rho_{aba'b'} |a\rangle_A |b\rangle_B \langle a'|_A \langle b'|_B, \tag{8}$$

then

$$\rho_A = \operatorname{Tr}_B \rho_{AB} = \sum_{a,a'} \left(\sum_c \rho_{aca'c} \right) |a\rangle_A \langle a'|_A. \tag{9}$$

Here's an example. Let us take the pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Then it has the density matrix

$$\rho = \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}. \tag{10}$$

The rows and columns are indexed, in order, by the basis states $|0\rangle_A|0\rangle_B$, $|0\rangle_A|1\rangle_B$, $|1\rangle_A|0\rangle_B$, $|1\rangle_A|1\rangle_B$. We can write ρ with block matrices representing the different states of B for a fixed state of A. Then to trace over B, we just trace over each of the block matrices, getting

$$\operatorname{Tr}_B \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}. \tag{11}$$

This is the maximally mixed state, the result of mixing equal amounts of 0 and 1 or really any two orthonormal basis states. You can also get it by mixing an equal amount of all pure states.

Note that if you trace over part of a tensor product pure state, the resulting state is still pure. It turns out that if you trace over one subsystem of an entangled pure state, the resulting state is always mixed, so this is a way of telling if a pure state is entangled or not. We will discuss this criterion more later in the class.

People often talk about a *proper* mixture as a density matrix formed by a probabilistic mixture of states, whereas an *improper* mixture is made by discarding (tracing over) a subsystem of an entangled pure state. However, there is no actual physical way to distinguish the two.

1.2 Density Matrices and Unitary Operations

Suppose we perform a unitary transformation U on a mixed state with density matrix ρ. What do we get? If $\rho = |\psi\rangle\langle\psi|$ is a pure state, we know we get the density matrix

$$U(\rho) = U|\psi\rangle\langle\psi|U^\dagger = U\rho U^\dagger. \tag{12}$$

corresponding to the pure state $U|\psi\rangle$. If we have a mixed state, we began with the state $|\psi_i\rangle$ with probability p_i, so after the unitary, we should have $U|\psi_i\rangle$ with probability p_i. That is,

$$U(\rho) = \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger \tag{13}$$

once again.

1.3 Density Matrices and Projective Measurements

When we make a projective measurement on a density matrix, the measurement is still defined by a set of projectors $\{\Pi_i\}$. The probability of outcome i when the state ρ is measured is

$$\mathrm{Prob}(i) = \mathrm{Tr}(\Pi_i \rho). \tag{14}$$

This is consistent with the rule for pure states: Consider a pure state $|\psi\rangle = \sum_a \alpha_a |a\rangle$. It has density matrix $\rho = |\psi\rangle\langle\psi|$. Then

$$\begin{aligned}
\mathrm{Prob}(i) =& \sum_a \langle a|(\Pi_i|\psi\rangle\langle\psi|)|a\rangle & (15)\\
=& \sum_{a,b,c} \alpha_b \alpha_c^* \langle a|\Pi_i|b\rangle\langle c|a\rangle & (16)\\
=& \sum_{a,b} \alpha_a^* \alpha_b \langle a|\Pi_i|b\rangle & (17)\\
=& \langle\psi|\Pi_i|\psi\rangle. & (18)
\end{aligned}$$

There is a quicker way to see this calculation, because

$$\mathrm{Tr}(M|\psi\rangle\langle\phi|) = \langle\phi|M|\psi\rangle \tag{19}$$

in general. This is an example of the cyclicity of the trace: The kets and bras are column and row vectors, which are also non-square matrices. Therefore, we can do a cyclic rotation of the argument of the trace and move the bra into the front. The product of the matrices then just gives us a scalar number, which is a 1×1 matrix, so the trace returns that number.

When we have a mixture of pure states, $|\psi_j\rangle$ with probability p_j, then

$$\mathrm{Prob}(i)(\rho) = \mathrm{Tr}(\Pi_i \rho) = \sum_j p_j \,\mathrm{Tr}(\Pi_i |\psi_j\rangle\langle\psi_j|) = \sum_j p_j \mathrm{Prob}(i)(|\psi_j\rangle). \tag{20}$$

That is, the probability of an outcome i is the average over the probabilities of getting i for the pure states in the ensemble. This is what we should expect and it validates the use of density matrices for mixed states. This formula lets us see immediately that the measurement outcomes of projective measurements only depends on the density matrix and not on the way it is formed, or indeed, whether it is a proper or improper mixture. This is why the density matrix is a good way of representing mixed states — it contains all the relevant information about the state.

Recall that if we make a partial measurement, there is some residual state left over. How does that work with density matrices? Let $\rho = \sum p_i |\psi_i\rangle\langle\psi_i|$. Then if we make the partial projective measurement $\{\Pi_a\}$, we can imagine that we happen to have the state $|\psi_i\rangle$, which happens with probability p_i. We get the outcome a with probability $q_{i,a} = \langle\psi_i|\Pi_a|\psi_i\rangle$. In this case, the residual state is

$$\frac{1}{\sqrt{q_{i,a}}}\Pi_a|\psi_i\rangle. \tag{21}$$

Since we initially have state $|\psi_i\rangle$ with probability p_i and get outcome a with probability $q_{i,a}$, the net probability of this outcome is $p_i q_{i,a}$. (Note here that we have just have a classical mixture, $q_{i,a}$ i the *conditional* probability of getting a conditioned on having had i.) We can get the overall density matrix after measurement by averaging over i that give this a:

$$\begin{aligned}
\rho'_a =& \frac{1}{\sum_i p_i q_{i,a}} \sum_i p_i q_{i,a} \frac{1}{q_{i,a}} \Pi_a |\psi_i\rangle\langle\psi_i|\Pi_a & (22)\\
=& \frac{1}{\sum_i p_i q_{i,a}} \sum_i p_i \Pi_a |\psi_i\rangle\langle\psi_i|\Pi_a & (23)\\
=& \frac{1}{\sum_i p_i q_{i,a}} \Pi_a \left(\sum_i p_i |\psi_i\rangle\langle\psi_i|\right) \Pi_a & (24)\\
=& \frac{1}{\sum_i p_i q_{i,a}} \Pi_a \rho \Pi_a. & (25)
\end{aligned}$$

Note that $\sum_i p_i q_{i,a} = p_a$ is the marginal probability of getting outcome a, averaged over states i in the mixture. This is thus the natural generalization of the pure state formula.

Note that one parameter of the pure state disappeared when we wrote the density matrix, which is the overall phase. Consider: The density matrix for $e^{i\phi}|\psi\rangle$ is

$$e^{i\phi}|\psi\rangle\langle\psi|e^{-i\phi} = |\psi\rangle\langle\psi| \tag{26}$$

because the $+$ and $-$ phases cancel. This, however, is OK, precisely because that global phase has no physical significance.

1.4 The density matrix is subjective

The density matrix has a subjective element to it. Consider: Suppose I flip a coin but do not look at the result. What is the state of the coin? It is a mixed state: Probability 1/2 of heads and probability 1/2 of tails. But now suppose I look and see one or the other, say heads. I know the state is actually heads, with 100% probability. And now suppose you want to know the result of the coin, but I don't tell you. You will still consider the state to be 1/2 heads and 1/2 tails, even though I know that the state is actually heads. This is what I mean when I say that the density matrix can be subjective.

If youre familiar with the Bayesian approach to probability, this is the same sort of idea. There's a philosophy that goes with Bayes' Theorem, and it says that probabilities simply quantify lack of knowledge about the true state of affairs. You don't have to believe this philosophy to use Bayes' Thm., but regardless, it is sensible to use probabilities if you have a situation like with the flipped coin where the outcome is definite but unknown.