CS 880: Quantum Information Processing 10/25/2010

Lecture 20: Density Operator Formalism

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So far in this course we have been working in the setting where the goal is to realize a relation by means of some computation. This involved only one "party" that was performing the computation. In today's lecture and several following lectures, we will focus on systems where multiple parties participate in the computation. We develop the *density operator formalism* which is suitable for describing multiparty systems. It turns out that we can use this formalism to describe the evolution of a quantum system, too, and that it is in some sense superior to our original way of describing things.

1 Density Operator

We start with the definition of the density operator, give some examples, and prove some properties of density operators. To conclude this section, we show how to represent the evolution of a quantum system using density operators.

Definition 1 (Density operator)**.** *For a pure state $|\psi\rangle$, the density operator is $\varrho = |\psi\rangle\langle\psi|$. For a mixed state $\{(p_i, |\psi_i\rangle)\}_i$, the density operator is $\varrho = \sum_i p_i |\psi\rangle\langle\psi|$.*

When we apply the density operator to a state ϕ, we get the projection of ϕ onto ψ, that is, $\varrho|\phi\rangle = |\psi\rangle\langle\psi|\phi\rangle$. Also note that the density operator corresponding to a mixed state is just a convex combination of density operators for the individual pure states that form the mixed state.

1.1 Examples of Density Operators

We now present some examples of density operators. As the next two examples show, two different mixed states can have the same density operator.

Example: Let's compute the density operator corresponding to $\{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$. The density operators for $|0\rangle$ and $|1\rangle$ are

$$\varrho_0 = (1,0)^T(1,0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \varrho_1 = (0,1)^T(0,1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Now we take their convex combination based on the probabilities describing our mixed state and get that $\varrho = \frac{1}{2}\varrho_0 + \frac{1}{2}\varrho_1 = \frac{1}{2}I$. ⊠

Example: Now we compute the density operator corresponding to $\{(\frac{1}{2}, |+\rangle), (\frac{1}{2}, |-\rangle)\}$. The density operators for $|+\rangle$ and $|-\rangle$ are

$$\varrho_+ = \frac{1}{\sqrt{2}}(1,1)^T\frac{1}{\sqrt{2}}(1,1) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \varrho_- = \frac{1}{\sqrt{2}}(1,-1)^T\frac{1}{\sqrt{2}}(1,-1) = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Now we take their convex combination based on the probabilities describing our mixed state and get that $\varrho = \frac{1}{2}\varrho_+ + \frac{1}{2}\varrho_- = \frac{1}{2}I$. ⊠

We see that the mixed states $\{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$ and $\{(\frac{1}{2}, |+\rangle), (\frac{1}{2}, |-\rangle)\}$ have the same corresponding density operators. As we will see later, this implies that no quantum procedure can distinguish between these two mixed states.

We conclude our list of examples with a density operator corresponding to a two-qubit state.

Example: The density operator corresponding to $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}}(1,0,0,1)^T$ is

$$\frac{1}{\sqrt{2}}(1,0,0,1)^T \frac{1}{\sqrt{2}}(1,0,0,1) = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

⊠

The state in the last example, $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, is called an EPR pair.

1.2 Properties of Density Operators

We use traces extensively when describing properties of density operators, so we start with some properties of the trace of a matrix. Afterwards, we state three properties of density operators.

Recall that the trace of a matrix M, denoted $\mathrm{Tr}\,(M)$, is the sum of the diagonal entries of M, i.e., $\mathrm{Tr}\,(M) = \sum_i M_{ii}$. It is easy to see that $\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA)$. Note, however, that it is not true in general that $\mathrm{Tr}\,(ABC) = \mathrm{Tr}\,(ACB)$. The equality holds only for cyclic shifts of a product of matrices. For example, $\mathrm{Tr}\,(ABC) = \mathrm{Tr}\,(CAB)$ holds.

An equivalent definition of the trace is $\mathrm{Tr}\,(A) = \sum_i \lambda_i$ where the λ_i are the eigenvalues of A. To see this for the case where A has a basis of eigenvectors, write V as the matrix whose columns are A's eigenvectors, and note that $AV = V\Lambda$. Since V's columns form a basis for A, V is invertible, and we have $A = V\Lambda V^{-1}$ where Λ is the matrix with $\Lambda_{ii} = \lambda_i$ and with zeros in the off-diagonal entries. Now $\mathrm{Tr}\,(A) = \mathrm{Tr}\left(V\Lambda V^{-1}\right) = \mathrm{Tr}\left(V^{-1}V\Lambda\right) = \mathrm{Tr}\,(\Lambda) = \sum_i \lambda_i$.

Also recall that a matrix is positive semi-definite if $\langle x| M |x\rangle \geq 0$ for all x.

Claim 1. *Let ϱ be a density operator. Then $Tr\,(\varrho) = 1$.*

Proof. First consider a pure state $|\psi\rangle = \sum_x \alpha_x |x\rangle$. Then the diagonal entry ϱ_{ii} of the corresponding density operator is α_x^2, and we know that $\sum_x \alpha_x^2 = 1$.

For a mixed state, just notice that the resulting density operator is a convex combination of matrices with trace 1. □

Claim 2. *The density operator is Hermitian.*

Proof. For a state $\sum_x \alpha_x |x\rangle$, the corresponding density operator is $\varrho = (\sum_x \alpha_x |x\rangle)(\sum_y \overline{\alpha_y} \langle y|)$. Then $\varrho_{xy} = \alpha_x \overline{\alpha_y}$, and $\varrho_{yx} = \alpha_y \overline{\alpha_x} = \overline{\alpha_x \overline{\alpha_y}} = \overline{\varrho_{yx}}$. This shows that ϱ is Hermitian for pure states. For mixed states, just note that a convex combination of Hermitian matrices is Hermitian. □

Claim 3. *The density operator is positive semi-definite.*

Proof. Consider a state $|\phi\rangle$. Then $\langle\phi| \varrho |\phi\rangle = \langle\phi| (\sum_i p_i |\psi_i\rangle \langle\psi_i|) |\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle \langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0$, where the inequality follows because $p_i \geq 0$ for all i. □

Exercise 1. *It turns out that we don't need Claim 2 because every positive semi-definite operator is Hermitian. Prove this assertion.*

The combination of the necessary conditions from Claim 1 and Claim 3 actually yields a sufficient condition for a matrix to be a density operator. We have the following theorem.

Theorem 1. *The matrix ϱ describes a density operator if and only if $Tr(\varrho) = 1$ and ϱ is positive semi-definite.*

Proof. We argued the forward direction in the proofs of Claims 1 and 3.

For the reverse direction, assume $\mathrm{Tr}(\varrho) = 1$ and ϱ is positive semi-definite. We need to find a mixed state whose density operator is described by ϱ. Since ϱ is positive semi-definite, it's Hermitian, and thus has an orthonormal basis of eigenvectors, say $|\psi_1\rangle, \ldots, |\psi_k\rangle$, with corresponding eigenvalues $\lambda_1, \ldots, \lambda_k$. This means that we can write $\varrho = \sum_i \lambda_i |\psi_i\rangle \langle\psi_i|$. Since ϱ is Hermitian, it has real eigenvalues. Since it's also positive semi-definite, all eigenvalues are non-negative. Finally, since the trace of ϱ is 1, the eigenvalues define a probability distribution, so ϱ is the density operator corresponding to the mixed state $\{(\lambda_i, |\psi_i\rangle)\}_i$. ∎

1.3 Describing the Evolution of a Quantum System

Now we show that we can describe quantum computation using density operators. For that, we need to describe the density operator ϱ' corresponding to the state $|\psi'\rangle$ obtained from state $|\psi\rangle$ either by applying a unitary operation to $|\psi\rangle$ or by making a measurement of $|\psi\rangle$.

Let's start with applying a unitary operation U to the state $|\psi\rangle$. The new state is $|\psi'\rangle = U|\psi\rangle$, so the corresponding density operator is $\varrho' = U|\psi\rangle (U|\psi\rangle)^* = U|\psi\rangle\langle\psi| U^* = U\varrho U^*$. We use linearity to get the density operator in the case of mixed states.

Now suppose we make a measurement of a state $|\psi\rangle$ whose density operator is ϱ. We measure with respect to some orthogonal basis $\{|\phi_1\rangle, \ldots, |\phi_k\rangle\}$. The state is a linear combination of the basis vectors, say $|\psi\rangle = \sum_i \alpha_i |\phi_i\rangle$. We observe the state $|\phi_i\rangle$ with probability $|\alpha_i|^2$, so the new state is a mixed state $\{(|\alpha_i|^2, |\phi_i\rangle)\}_i$, and its corresponding density operator is

$$\varrho' = \sum_i |\alpha_i|^2 |\phi_i\rangle\langle\phi_i| = \sum_i |\phi_i\rangle \alpha_i \overline{\alpha_i} \langle\phi_i| \tag{1}$$

Note that if we multiply ϱ on the right with $|\phi_j\rangle$ and on the left with $\langle\phi_j|$, we get the probability that we observe ϕ_j. This follows from the second summation in (1) because $\langle\phi_j|\phi_i\rangle = 1$ if $i = j$, and is zero otherwise. Thus, another way of writing (1) is $\varrho' = \sum_i \langle\phi_i|\varrho|\phi_i\rangle |\phi_i\rangle\langle\phi_i|$. Once again, we can apply linearity to get the resulting density operator when we observe a mixed state.

With this in hand, we can prove the following theorem.

Theorem 2. *Two states are distinguishable by some quantum process if and only if their density operators are different.*

Proof. Assume that two density operators are the same. We just showed in the previous paragraphs that we only need the density operator in order to describe the outcome of some quantum process, and gave an expression for the density operator corresponding to the next state of the system. Thus, any quantum process operating on two states with the same density operators evolves the same for both of the states, results in the same final density operator for the two final states, and, most importantly, the probability of observing a string x is the same for both states. Thus, since we rely on observations to decide on the output of quantum algorithms, we cannot tell from the distribution of the observations which state we were in at the beginning.

Now suppose the density operators of two states are different. Since they are both density operators, they have a different orthogonal basis of eigenvectors, or the eigenvalue corresponding to some eigenvector is different for the two density operators. In either case, we get a different distribution of observed basis vectors, and we can distinguish between the two states. $\square$

Exercise 2. *Make the second paragraph in the proof of Theorem 2 more formal.*

2 Two-Party Systems

In a two-party system, two parties, Alice and Bob, have access to two different parts of a quantum register. Alice applies unitary transformations and observations to her part of the register without affecting Bob's part, and vice versa. The general form of the state is $\sum_{s,t} \alpha_{s,t} |s\rangle |t\rangle$ where the first component (the state $|s\rangle$) belongs to Alice and the second component belogs to Bob. To Alice, the state of the system looks like a mixed state over all possible states that Bob's part of the quantum register could be in. Thus, Alice's state is

$$\left\{ \left(\Pr[t], \frac{\sum_s \alpha_{s,t} |s\rangle}{\sqrt{\Pr[t]}} \right) \right\}_t \quad \text{where} \quad \Pr[t] = \sum_s |\alpha_{s,t}|^2,$$

and there is a symmetric expression for Bob's state.

Let's now find the density operator ϱ_A for Alice. We call this the *reduced density operator.*

$$\begin{aligned} \varrho_A &= \sum_t \Pr[t] \cdot \frac{\sum_s \alpha_{s,t} |s\rangle}{\sqrt{\Pr[t]}} \cdot \frac{\sum_{s'} \overline{\alpha_{s',t}} \langle s'|}{\sqrt{\Pr[t]}} \\ &= \sum_{s,s'} \left(\sum_t \alpha_{s,t} \overline{\alpha_{s',t}} \right) |s\rangle \langle s'| \\ &= \sum_{s,s'} \left(\sum_t (\varrho_{AB})_{(s,t),(s',t)} \right) |s\rangle \langle s'| . \end{aligned} \tag{2}$$

where the inner sum in (2) is denoted $(\mathrm{Tr}_B(\varrho_{AB}))_{s,s'}$ and is called the *trace with respect to B*. The matrix ϱ_{AB} in (2) is the density operator for the whole system. It follows from (2) that for states (not superpositions) s, t, s', and t' we have $\mathrm{Tr}_B(|s\rangle\langle s'| \otimes |t\rangle\langle t'|) = \langle t|t'\rangle |s\rangle \langle s'|$, with $\langle t|t'\rangle = 1$ if $t = t'$ and zero otherwise, and we use linearity for superpositions. This may look a little confusing, so let's look at an example.

Example: Suppose Alice and Bob operate on a two-qubit system, where the first qubit belongs to Alice and the second qubit belongs to Bob. The density operator is

$$\varrho = \begin{pmatrix} \varrho_{00,00} & \varrho_{00,01} & \varrho_{00,10} & \varrho_{00,11} \\ \varrho_{01,00} & \varrho_{01,01} & \varrho_{01,10} & \varrho_{01,11} \\ \varrho_{10,00} & \varrho_{10,01} & \varrho_{10,10} & \varrho_{10,11} \\ \varrho_{11,00} & \varrho_{11,01} & \varrho_{11,10} & \varrho_{11,11} \end{pmatrix}.$$

Then the trace with respect to B is the matrix

$$\mathrm{Tr}_B(\varrho) = \begin{pmatrix} \varrho_{00,00} + \varrho_{01,01} & \varrho_{00,10} + \varrho_{01,11} \\ \varrho_{10,00} + \varrho_{11,01} & \varrho_{10,10} + \varrho_{11,11} \end{pmatrix}.$$

We see that $(\mathrm{Tr}_B(\varrho))_{(s,s')}$ is the trace of a submatrix of ϱ where Alice's part of the first index (i.e., the first bit of the first index in our case) is fixed to s and Alice's part of the second index is fixed to s'. Using this observation, we see that the trace with respect to A is the matrix

$$\mathrm{Tr}_A(\varrho) = \begin{pmatrix} \varrho_{00,00} + \varrho_{10,10} & \varrho_{00,01} + \varrho_{10,11} \\ \varrho_{01,00} + \varrho_{11,10} & \varrho_{01,01} + \varrho_{11,11} \end{pmatrix}.$$

⊠

Example: Let

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

be the density operator for the EPR pair. Then we have $\mathrm{Tr}_A(\varrho) = \mathrm{Tr}_B(\varrho) = \frac{1}{2}I$. ⊠

2.1 Schmidt Decomposition

Suppose we have a system where Alice can act on some part of it and Bob acts on the rest. The state is described by $|\psi_{AB}\rangle$. We can always write this state as a linear combination of the standard basis vectors. The next theorem states that we can do better. It is possible to write the state as a tensor product of two linear combinations of vectors coming from two orthonormal bases, one for Alice and one for Bob, that are potentially much smaller. Moreover, both bases have the same set of eigenvalues.

Theorem 3. *Given a state $|\psi_{AB}\rangle$, there exist orthonormal bases $\{|\psi_i\rangle\}_i$ for Alice's part of the state and $\{|\phi_i\rangle\}_i$ for Bob's part of the state, and $\lambda_i \in [0,1]$ such that $|\psi_{AB}\rangle = \sum_i \lambda_i |\psi_i\rangle |\phi_i\rangle$ with $\sum_i \lambda_i^2 = 1$.*

Before we prove Theorem 3, let's see how we can use it to obtain reduced density operators ϱ_A and ϱ_B for Alice and Bob. It turns out that we can use traces with respect to B and A, respectively. To see that, note $\varrho_{AB} = \sum_i \lambda_i^2 |\psi_i\rangle |\phi_i\rangle \langle\psi_i| |\psi_i\rangle = \sum_i \lambda_i^2 (|\psi_i\rangle\langle\psi_i|) \otimes (|\phi_i\rangle\langle\phi_i|)$, and if we trace out the B component we get $\varrho_A = \mathrm{Tr}_B\left(\sum_i \lambda_i^2 (|\psi_i\rangle\langle\psi_i|) \otimes (|\phi_i\rangle\langle\phi_i|)\right) = \sum_i \lambda_i^2 \langle\phi_i|\phi_i\rangle |\psi_i\rangle\langle\psi_i| = \sum_i \lambda_i^2 |\psi_i\rangle\langle\psi_i|$, where the last equality follows because $\langle\phi_i|\phi_i\rangle = 1$. Similarly, we get $\varrho_B = \mathrm{Tr}_A(\varrho_{AB}) = \sum_i \lambda_i^2 |\phi_i\rangle\langle\phi_i|$.

Proof Sketch for Theorem 3. Look at a superposition $\sum_{s,t} \alpha_{s,t} |s\rangle |t\rangle$. The values $\alpha_{s,t}$ form a matrix $A = (\alpha_{st})_{s,t}$, which we express using singular value decomposition as $A = U\Lambda V$ where U and V are orthogonal and Λ is the matrix containing the singular values of A on the diagonal. We now have $\alpha_{s,t} = \sum_i U_{si}\Lambda_{ii}V_{it}$, so we can use the columns of U and V as the bases for Alice's and Bob's parts of the state, respectively. □

2.2 Purification

We use the Schmidt decomposition to go from a density operator representing the state of the system to a reduced density operator correspodning to what is seen by one of the parties participating in the computation. Our goal here is the opposite. We start with a mixed state described by the density operator ϱ_A and want to construct from it a pure state $|\psi_{AB}\rangle$ of a bigger system so that $\varrho_A = \mathrm{Tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|)$. We have $\varrho_A = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, and let $|\psi_{AB}\rangle = \sum_i \sqrt{\lambda_i} |\psi_i\rangle |\psi_i\rangle$. As we can see, we are defining Bob's part of the state to be the same as Alice's part.

3 Next Time

In the following lectures, we will see some applications of density operators.