Today's outline - March 30, 2023

- Properties of density operators
- Geometry of mixed states
- von Neumann entropy
- Bipartite entanglement
- Examples

Reading assignment: Chapter 10.3–10.4

Homework Assignment #06:
Due Thursday, April 06, 2023

The density operator

Density operators are observables that act on a subsystem of a larger quantum system

By measuring a complete set of density operators on each subsytem making up the entire quantum space, it is possible to know all about the subsystems but information about entanglement between subsystems is completely lost

For a state $|x\rangle$ on the $n = m + l$ qubit space $X = A \otimes B$ with density matrix ρ_x^X, the density matrix ρ_x^A on the A subspace is computed using the partial trace over B of ρ_x^X

$$\rho_x^A = \sum_{u=0}^{M-1} \sum_{v=0}^{M-1} \sum_{w=0}^{L-1} \overline{x_{vw}} x_{uw} |\alpha_u\rangle\langle\alpha_v| = \mathrm{Tr}_B(\rho_x^X)$$

$$\mathrm{Tr}_B(\rho_x^X) = \sum_{u=0}^{M-1} \sum_{v=0}^{M-1} \left[\sum_{w=0}^{L-1} \langle\alpha_u|\langle\beta_w|\rho_x^X|\alpha_v\rangle|\beta_w\rangle \right] |\alpha_u\rangle\langle\alpha_v|$$

$$\rho_x^X = |x\rangle\langle x| = \sum_{i=0}^{M-1} \sum_{j=0}^{L-1} \sum_{k=0}^{M-1} \sum_{l=0}^{L-1} \overline{x_{ij}} x_{kl} |\alpha_k\rangle|\beta_l\rangle\langle\alpha_i|\langle\beta_j|$$

Example 10.1.1

Alice controls the first qubit of an EPR pair, $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

The density matrix for the pure state $|\psi\rangle \in A \otimes B$ is

$$\rho_\psi = |\psi\rangle\langle\psi| = \tfrac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

The density matrix which holds all information that can be obtained from Alice's qubit is given by $\rho_\psi^A = \mathrm{Tr}_B(\rho_\psi)$ with components $a_{ij} = \sum_k \overline{x_{jk}} x_{ik} = \sum_k \langle jk|\psi\rangle\langle\psi|ik\rangle$

$$a_{00} = \sum_{k=0}^{1} \langle 0k|\psi\rangle\langle\psi|0k\rangle = \frac{1}{\sqrt{2}}(\langle 00|00\rangle + \cancel{\langle 00|11\rangle})\frac{1}{\sqrt{2}}(\langle 00|00\rangle + \cancel{\langle 11|00\rangle})$$

$$+ \frac{1}{\sqrt{2}}(\cancel{\langle 01|00\rangle} + \cancel{\langle 01|11\rangle})\frac{1}{\sqrt{2}}(\cancel{\langle 00|01\rangle} + \cancel{\langle 11|01\rangle}) = \tfrac{1}{2} + 0 = \tfrac{1}{2}$$

Example 10.1.1 (cont.)

$$a_{01} = \sum_{k=0}^{1} \langle 0k|\psi\rangle\langle\psi|1k\rangle = \frac{1}{\sqrt{2}}(\langle 00|00\rangle + \cancel{\langle 00|11\rangle})\frac{1}{\sqrt{2}}(\cancel{\langle 00|10\rangle} + \cancel{\langle 11|10\rangle})$$

$$+ \frac{1}{\sqrt{2}}(\cancel{\langle 01|00\rangle} + \cancel{\langle 01|11\rangle})\frac{1}{\sqrt{2}}(\cancel{\langle 00|11\rangle} + \langle 11|11\rangle) = 0 + 0 = 0$$

$$a_{10} = \sum_{k=0}^{1} \langle 1k|\psi\rangle\langle\psi|0k\rangle = \frac{1}{\sqrt{2}}(\cancel{\langle 10|00\rangle} + \cancel{\langle 10|11\rangle})\frac{1}{\sqrt{2}}(\langle 00|00\rangle + \cancel{\langle 11|00\rangle})$$

$$+ \frac{1}{\sqrt{2}}(\cancel{\langle 11|00\rangle} + \langle 11|11\rangle)\frac{1}{\sqrt{2}}(\cancel{\langle 00|01\rangle} + \cancel{\langle 11|01\rangle}) = 0 + 0 = 0$$

$$a_{11} = \sum_{k=0}^{1} \langle 1k|\psi\rangle\langle\psi|1k\rangle = \frac{1}{\sqrt{2}}(\cancel{\langle 10|00\rangle} + \cancel{\langle 10|11\rangle})\frac{1}{\sqrt{2}}(\cancel{\langle 00|10\rangle} + \cancel{\langle 11|10\rangle})$$

$$+ \frac{1}{\sqrt{2}}(\cancel{\langle 11|00\rangle} + \langle 11|11\rangle)\frac{1}{\sqrt{2}}(\cancel{\langle 00|11\rangle} + \langle 11|11\rangle) = 0 + \frac{1}{2} = \frac{1}{2}$$

The density operators for the individual qubits subsystems are

$$\rho_\psi^A = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \rho_\psi^B = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

More properties of density operators

Any density operator, ρ_x^A, is Hermitian and $\text{Tr}(\rho_x^A) = \sum_j \overline{x_{ij}} x_{ij} \equiv 1$ when $|x\rangle$ is a unit vector

For a density operator $\rho_x^A : A \to A$ and $|v\rangle \in A$, we can write

$$\langle v|\rho_x^A|v\rangle = \sum_{i=0}^{M-1}\sum_{k=0}^{M-1}\sum_{j=0}^{L-1}\langle v|(\overline{x_{ij}}x_{kj}|\alpha_k\rangle\langle\alpha_i|)|v\rangle = \sum_{i=0}^{M-1}\sum_{k=0}^{M-1}\sum_{j=0}^{L-1}\overline{x_{ij}}\langle\alpha_i|v\rangle x_{kj}\langle v|\alpha_k\rangle$$

$$= \sum_{j=0}^{L-1}\left(\sum_{i=0}^{M-1}\overline{x_{ij}\langle v|\alpha_i\rangle}\right)\left(\sum_{k=0}^{M-1}x_{kj}\langle v|\alpha_k\rangle\right) = \sum_{j=0}^{L-1}\left|\sum_{i=0}^{M-1}x_{ij}\langle v|\alpha_i\rangle\right|^2 \geq 0$$

The fact that ρ_x^A is positive means that all its eigenvalues are real and non-negative

Given an orthonormal eigenbasis $\{|v_0\rangle, \ldots, |v_{M-1}\rangle\}$, the matrix for ρ_x^A is diagonalized with non-negative real entries λ_i such that

$$\sum_{i=0}^{M-1}\lambda_i \equiv 1, \qquad \rho_x^A = \sum_{i=0}^{M-1}\lambda_i|v_i\rangle\langle v_i|$$

More properties of density operators

Any operator which satisfies the three conditions must be a density operator

If ρ is an operator acting on A of dimension $M = 2^m$ with eigenbasis $\{|\psi_0\rangle, \dots, |\psi_{M-1}\rangle\}$ which satisfies all three conditions

$$\rho = \sum_{i=0}^{M-1} \lambda_i |\psi_i\rangle\langle\psi_i| = \lambda_0|\psi_0\rangle\langle\psi_0| + \cdots + \lambda_{M-1}|\psi_{M-1}\rangle\langle\psi_{M-1}|$$

Let B be a quantum system with a vector space of dimension $2^n > M$ and let $\{|\phi_0\rangle, \dots, |\phi_{M-1}\rangle\}$ be the first M elements of an orthonormal basis for B, define

$$|x\rangle = \sqrt{\lambda_0}|\psi_0\rangle|\phi_0\rangle + \sqrt{\lambda_1}|\psi_1\rangle|\phi_1\rangle + \cdots + \sqrt{\lambda_{M-1}}|\psi_{M-1}\rangle|\phi_{M-1}\rangle$$

$|x\rangle \in A \otimes B$ is a so-called pure state which satisfies $\rho_x^A = \rho$

The density operator $\rho_x^X = |x\rangle\langle x|$ for a pure state $|x\rangle$ is all zeros except for a 1 in the i^{th} diagonal element where $|x\rangle$ is the i^{th} element in a basis

The density operator of a pure state is a projection operator, such that $\rho_x^X \rho_x^X = \rho_x^X$

More properties of density operators

Projection operators of pure states also eliminate the issue associated with global phase differences

Consider the density operator for $|x\rangle = e^{i\theta}|y\rangle$

$$\rho_x = |x\rangle\langle x| = e^{-i\theta}|y\rangle\langle y|e^{i\theta} = |y\rangle\langle y|$$

The density matrix for mixed and pure states are very different

For the pure state $|+\rangle$ and the evenly mixed ensemble of $|0\rangle$ and $|1\rangle$ we have

$$\rho_{mixed} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \rho_{+} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Geometry of mixed states

It is possible to use the Bloch sphere to visualize single-qubit mixed states which are linear combinations of pure states with non-negative coefficients that sum to 1

A density operator for a single qubit must be Hermitian and self-adjoint with trace 1 and the general form

$$\rho = \begin{pmatrix} a & c - id \\ c + id & b \end{pmatrix}$$

The condition on the trace means that the matrix can be written with only 3 real parameters: x, y, z and expanded in terms of Pauli matrices

$$= \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix} = \frac{1}{2}(I + x\sigma_x + y\sigma_y + z\sigma_z)$$

$$\sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = -iY = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\det(\rho) = \begin{vmatrix} \frac{1+z}{2} & \frac{x-iy}{2} \\ \frac{x+iy}{2} & \frac{1-z}{2} \end{vmatrix} = \tfrac{1}{4}(1+z)(1-z) - \tfrac{1}{4}(x-iy)(x+iy) = \tfrac{1}{4}(1 - z^2 - x^2 - y^2)$$

Density matrix and the Bloch sphere

$$\det(\rho) = \frac{1}{4}(1 - z^2 - x^2 - y^2) = \frac{1}{4}(1 - r^2), \qquad r = \sqrt{|x|^2 + |y|^2 + |z|^2}$$

Because this is a density operator, its determinant must be real and non-negative so $0 \le r \le 1$

The values x, y, z can thus be interpreted as coordinates and the density matrix given by $\rho = \frac{1}{2}(I - x\sigma_x + y\sigma_y + z\sigma_z)$ can describe a vector which lies within the Bloch sphere

The density matrices which fall on the surface of the Bloch sphere have $r = 1$ and $\det(\rho) = 0$

The determinant is the product of its eigenvalues so states on the surface must be projectors and thus pure states

(x, y, z)	state	density matrix
$(1, 0, 0)$	$\lvert + \rangle$	$\frac{1}{2}(I + \sigma_x) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$
$(0, 1, 0)$	$\lvert i \rangle$	$\frac{1}{2}(I + \sigma_y) = \frac{1}{2}\begin{pmatrix} 1 & \bar{i} \\ i & 1 \end{pmatrix}$
$(0, 0, 1)$	$\lvert 0 \rangle$	$\frac{1}{2}(I + \sigma_z) = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$
$(0, 0, 0)$		$\rho_0 = \frac{1}{2} I = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Von Neumann entropy

Recall the density matrix for one of the qubits of an EPR pair, $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

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

This corresponds to the point in the center of the sphere, the furthest from a pure state possible

This state is maximally uncertain and will give the two possible answers with equal probability

For a pure state there is a basis in which a measurement gives a deterministic result

For an n-qubit system the uncertainty of measurement can be described by the von Neumann entropy

$$S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho) = -\sum_i \lambda_i \log_2 \lambda_i$$

Given that $0\log(0) \equiv 0$, the von Neumann entropy is zero for pure states where the density matrix is a projector, there is only one non-zero diagonal element and the determinant is zero

A maximally uncertain state for an n-qubit system has all the diagonal elements equal to 2^{-n} so $S(\rho) = n$

Entropy and the Bloch sphere

For a single qubit state with density operator ρ, what is the von Neumann entropy $S(\rho)$ and how does it relate to the Bloch sphere?

If λ_1 and λ_2 are the eigenvalues of ρ we have

$$\mathrm{Tr}(\rho) = 1 \quad \longrightarrow \quad \lambda_2 = 1 - \lambda_1$$

The determinant of ρ is

$$\det(\rho) = \lambda_1\lambda_2 = \lambda_1(1-\lambda_1) \quad \longrightarrow \quad \lambda^2 - \lambda + \det(\rho) = 0 \quad \longrightarrow \quad \lambda = \frac{1}{2} \pm \frac{\sqrt{1 - 4\det(\rho)}}{2}$$

Since $\det(\rho) = \frac{1}{4}(1-r^2)$

$$\lambda_1 = \frac{1+r}{2}, \qquad \lambda_2 = \frac{1-r}{2}$$

The entropy is therefore

$$S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho) = \sum_i \lambda_i \log_2 \lambda_i = -\left[\left(\frac{1+r}{2}\right)\log_2\left(\frac{1+r}{2}\right) + \left(\frac{1-r}{2}\right)\log_2\left(\frac{1-r}{2}\right)\right]$$

The von Neumann entropy for a single qubit system is just a function of the distance of the state from the center of the Bloch sphere

Bipartite entanglement

It is useful to find a good measure of entanglement for bipartite systems such as $X = A \otimes B$

The 2-qubit system is the simplest bipartite system with a maximally entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

For each of the two qubits, the density matrix ρ_{ME} has maximal von Neumann entropy

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

$$S(\rho) = -2\left[\tfrac{1}{2}\log_2\left(\tfrac{1}{2}\right)\right] = 2$$

An untangled state, such as $|00\rangle$ has minimal von Neumann entropy

$$\rho_{ME} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \longrightarrow S(\rho) = 0$$

It makes sense to use the von Neumann entropy of the partial trace as a measure of the entanglement if it can be assumed that the partial trace is the same for each of the two subsystems, A and B