Lecture 10

Last class we learned many properties of partial traces.

Here is another important fact.

Theorem Let H_1 and H_2 be finite dimensional (non-zero) complex Hilbert spaces.

i) For any $A \in B(H_1 \otimes H_2)$,

$$Tr[Tr_{H_2}[A]] = Tr[A] = Tr[Tr_{H_1}[A]].$$

ii) Let $A \in B(H_1 \otimes H_2)$. If $A \geq 0$, then

$$Tr_{H_2}[A] \geq 0 \quad \text{and} \quad Tr_{H_1}[A] \geq 0.$$

In words, this result shows that

i) => the partial trace preserves trace

ii) => the partial trace preserves non-negativity

We will prove this result in homework.

The above theorem shows us that the partial trace has an important physical interpretation.

Interpretation

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces corresponding to two quantum mechanical systems.

- Often the 1st Hilbert space $\mathcal{H}_1$ consists of some "degrees of freedom" that we are trying to measure. For example, this system may be directly coupled to some experimental apparatus.

- In this case, the 2nd Hilbert space $\mathcal{H}_2$ is often regarded as "the environment". This could, for example, be a "heat bath" or just some degrees of freedom that are not directly coupled to the measurement apparatus.

Now if ω is any state of the full system, then ω is in one-to-one correspondence with a density matrix ρ, i.e. there is some $\rho \in B(\mathcal{H}_1 \otimes \mathcal{H}_2)$ with $\rho \geq 0$ and $\mathrm{Tr}[\rho] = 1$ for which

$$\omega(A) = \mathrm{Tr}[\rho A] \quad \text{for all } A \in B(\mathcal{H}_1 \otimes \mathcal{H}_2).$$

Here again, $\omega(A)$ is the expected value of the observable A in the state ω.

The collection of observables on the full system having the form

$$A = B \otimes \mathbb{1} \quad \text{for some } B \in B(\mathcal{H}_1)$$

are clearly of interest. They correspond to observations on the 1st subsystem.

When we restrict the state to this collection of observables, i.e.

$$(B \otimes \mathbb{1}) \mapsto \omega(B \otimes \mathbb{1}) = \mathrm{Tr}[\rho(B \otimes \mathbb{1})]$$

we are considering expected values of observables that our apparatus might measure.

The above theorem tells us that the partial trace allows us to express this restriction in terms of a density matrix on the 1st subsystem.

In fact, as we have proven

$$\mathrm{Tr}[\rho(B \otimes \mathbb{1})] = \mathrm{Tr}[\mathrm{Tr}_{\mathcal{H}_2}[\rho]\, B] \quad \text{for all } B \in B(\mathcal{H}_1).$$

Moreover:

- $\mathrm{Tr}[\mathrm{Tr}_{\mathcal{H}_2}[\rho]] = \mathrm{Tr}[\rho] = 1$

  and

- $\mathrm{Tr}_{\mathcal{H}_2}[\rho] \geq 0$ since $\rho \geq 0$

$\Rightarrow$ $\mathrm{Tr}_{\mathcal{H}_2}[\rho]$ is a density matrix on $\mathcal{H}_1$.

It therefore corresponds to a state on $B(\mathcal{H}_1)$.

On the von Neumann Entropy

Let's recall our basic set-up.

Let $\mathcal{H}$ be the Hilbert space associated to a quantum system. Let $\mathcal{A} = B(\mathcal{H})$ be the algebra of observables associated to this quantum system.

A state ω on $\mathcal{A}$ is a normalized, positive linear functional on $\mathcal{A}$:

- $\omega: \mathcal{A} \to \mathbb{C}$ is linear
- $\omega(\mathbb{1}) = 1$
- $\omega(A^*A) \geq 0$ for all $A \in \mathcal{A}$.

Each unit vector $\psi \in \mathcal{H}$ corresponds to a state.

$\omega_\psi : \mathcal{A} \to \mathbb{C}$ given by

$$\omega_\psi(A) = \langle \psi, A\psi \rangle \quad \text{for all } A \in \mathcal{A} = B(\mathcal{H})$$

is a state. States of this form are called <u>vector states</u>.

In general, we saw that the collection of states on $\mathcal{A}$ is convex.

The extreme points of this convex set are called <u>pure states</u>.

In homework, we showed that if $\mathcal{H}$ is finite dimensional, i.e. there is an integer $d \geq 1$ for which $\mathcal{A} = B(\mathcal{H}) = M_d$, then

- ω is an extreme point of M_d $\iff$ ω is a vector state.

In this finite dimensional case, we also showed that:

each state ω on M_d corresponds to a density matrix $\rho \in M_d$ i.e. there is $\rho \in M_d$ with $\rho \geq 0$ and $Tr[\rho] = 1$ for which

$$\omega(A) = Tr[\rho A] \quad \text{for all } A \in M_d.$$

By the previous claim, ω is a pure state if and only if there is a vector $\psi \in \mathbb{C}^d$ with $\|\psi\| = 1$ and

$$\omega(A) = \langle \psi, A\psi \rangle \quad \text{for all } A \in M_d.$$

In this case, the corresponding density matrix ρ is the orthogonal projection onto the 1-dimensional subspace spanned by ψ, i.e.

$$\rho = P_\psi = |\psi\rangle\langle\psi| \quad \text{in Dirac Notation.}$$

More generally, any density matrix $\rho \in M_d$ is self-adjoint and therefore the spectral theorem implies that there exists an orthonormal basis $\{\psi_j\}_{j=1}^{d}$ in $\mathbb{C}^d$ for which

$$(*) \quad \rho = \sum_{j=1}^{d} \lambda_j P_{\psi_j} = \sum_{j=1}^{d} \lambda_j |\psi_j\rangle\langle\psi_j|$$

where $\lambda_j \geq 0$ and $Tr[\rho] = \sum_{j=1}^{d} \lambda_j = 1$.

If ω is a pure state (i.e. a vector state), then the corresponding density matrix ρ has the form $(*)$ and there is j_0 with $1 \leq j_0 \leq d$ for which $\lambda_{j_0} = 1$ and $\lambda_j = 0$ for all $j \neq j_0$. Thus $\rho = |\psi_{j_0}\rangle\langle\psi_{j_0}|$.

If ω is <u>not</u> a pure state, then the corresponding density matrix ρ has the form $(*)$ and

$$\max_{1 \leq j \leq d} \lambda_j < 1.$$

In this case, ω is called a mixed state.
The corresponding density matrix ρ is also said to be mixed.

<u>Note</u>: In the literature, it is not uncommon that the density matrix ρ is called a state. You may see ρ is a pure state or ρ is a mixed state. By the 1 to 1 correspondence, this can be easily understood.

In the homework, we will show that:

Let ρ be a density matrix on M_d.

- ρ is mixed $\iff \mathrm{Tr}[\rho^2] < 1$.

Von Neumann Entropy

It is an interesting question to ask:

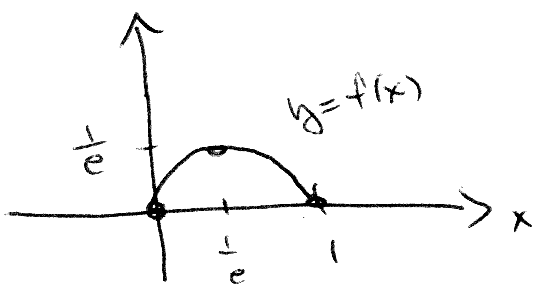
Are their quantities that allow one to distinguish between density matrices corresponding to pure states and those corresponding to mixed states?

The answer is yes. One such quantity is the von Neumann entropy.

Some calculus:

Define $f: [0,1] \to \mathbb{R}$ by setting

$$f(x) = \begin{cases} -x\ln(x) & \text{if } 0 < x \leq 1 \\ 0 & \text{if } x = 0. \end{cases}$$



One readily checks that

- $f(x) \geq 0$ is continuous for all $x \in [0,1]$. (Note: $x=0$ is included!)
- $f'(x) = -\ln(x) - 1$ for all $x \in (0,1]$ (Note: $x=0$ is not included)
- $f''(x) = -\frac{1}{x} < 0$ for all $x \in (0,1]$. "

Thus f is strictly concave for all $0 < x \leq 1$.
It is easy to check the claimed maximum. (see picture)

For any density matrix $\rho \in M_d$, we have that

$$\rho = \sum_{j=1}^{d} \lambda_j |\psi_j\rangle\langle\psi_j| \quad \text{where } \{\psi_j\}_{j=1}^{d} \text{ is an orthonormal basis}$$

of $\mathbb{C}^d$, $\lambda_j \geq 0$, and $\sum_{j=1}^{d} \lambda_j = 1$. Thus $\lambda_j \in [0,1]$ and so

$$-\rho \ln(\rho) = f(\rho) = \sum_{j=1}^{d} f(\lambda_j)\, |\psi_j\rangle\langle\psi_j|$$

(where f is the function described above) is well-defined using functional calculus. In fact, $f(\rho) \in M_d$ is non-negative.

The von-Neumann entropy of a density matrix $\rho \in M_d$ is

$$S(\rho) = -\operatorname{Tr}[\rho \ln(\rho)] = \operatorname{Tr}[f(\rho)]$$
$$= \sum_{j=1}^{d} f(\lambda_j)$$
$$= -\sum_{j=1}^{d} \lambda_j \ln(\lambda_j).$$

Some basic properties:

<u>Proposition</u>: Let $d \geq 1$ be an integer.

i) For any density matrix $\rho \in M_d$, $S(\rho) \geq 0$.

ii) $S(\rho) = 0$ if and only if ρ corresponds to a pure state.

iii) $\sup_{\rho} S(\rho) = \ln(d)$. This supremum over density matrices $\rho \in M_d$ is attained (i.e. it is a maximum) and

$$S(\rho) = \ln(d) \iff \rho = \frac{1}{d}\mathbb{1}.$$

Some comments

1) If ρ corresponds to a pure state, then $\rho = |\psi\rangle\langle\psi|$ for some $\psi \in \mathbb{C}^d$ with $\|\psi\| = 1$. In this case, from the probabilistic perspective, ρ is trivial. The system is in state ψ with probability 1. Such states correspond to zero entropy and these are the only states with zero entropy.

2) If ρ corresponds to a mixed state, then $S(\rho) > 0$. The largest possible value of $S(\rho)$ is $\ln(d)$ where d is the dimension ($\rho \in M_d$). This value is attained if and only if $\rho = \frac{1}{d}\mathbb{1}$. In this case, from the probabilistic perspective, ρ is uniformly distributed. All vectors are equally likely and the corresponding state is often referred to as "random".

Using this entropy as a quantifier, $\frac{1}{d}\mathbb{1}$ is the density matrix "furthest" away from those representing pure states.

$\rho = \frac{1}{d}\mathbb{1}$ is said to be maximally mixed.

Proof of the Proposition:

i) $S(\rho) = \sum_{j=1}^{d} \underbrace{-\lambda_j \ln(\lambda_j)}_{\geq 0} \Rightarrow S(\rho) \geq 0.$

Since this is just a finite sum, we conclude

$S(\rho) \in [0, \infty)$ for any $\rho \in M_d$ a density matrix.

ii) $S(\rho) = 0 \iff -\lambda_j \ln(\lambda_j) = 0$ for $1 \leq j \leq d$

$\iff \lambda_j \in \{0, 1\}$ for $1 \leq j \leq d$

$\iff$ there is some $1 \leq j_0 \leq d$ for which

$\lambda_{j_0} = 1$ and $\lambda_j = 0$ for $j \neq j_0$.

$\iff \rho = |\psi_{j_0}\rangle\langle\psi_{j_0}|.$

iii) One can prove this with the basic methods of Calculus. Write

$$F(\lambda_1, \lambda_2, \dots, \lambda_d) = \sum_{j=1}^{d} f(\lambda_j)$$

and maximize using Lagrange multipliers.

I prefer to use Jensen's inequality.

Theorem (Jensen's Inequality)

Let $f: \mathbb{R} \to \mathbb{R}$ be a convex function.

Let μ be a probability measure on $\mathbb{R}$, i.e. $\int_{\mathbb{R}} 1 \, d\mu = 1$.

Let $g: \mathbb{R} \to \mathbb{R}$ satisfy $\int |g| \, d\mu < \infty$.

Then

$$(**) \qquad f\left(\int_{\mathbb{R}} g \, d\mu \right) \leq \int_{\mathbb{R}} f \circ g \, d\mu .$$

Moreover, if f is strictly convex, then equality holds if and only if g is constant almost everywhere with respect to μ.

For a proof see Lieb-Loss Theorem 2.2.

Understanding $(**)$

Let $f \geq 0$ be a convex function.

Fix $[a,b] \subset \mathbb{R}$ and let μ correspond to the uniform distribution over $[a,b]$, i.e.

$$d\mu = \frac{\chi_{[a,b]}}{b-a} \, dx .$$

Let $g(x) = x$.

Clearly

$$\int_{\mathbb{R}} g(x) \, d\mu(x) = \frac{1}{b-a} \int_a^b x \, dx = \frac{b^2 - a^2}{2(b-a)} = \frac{a+b}{2}$$

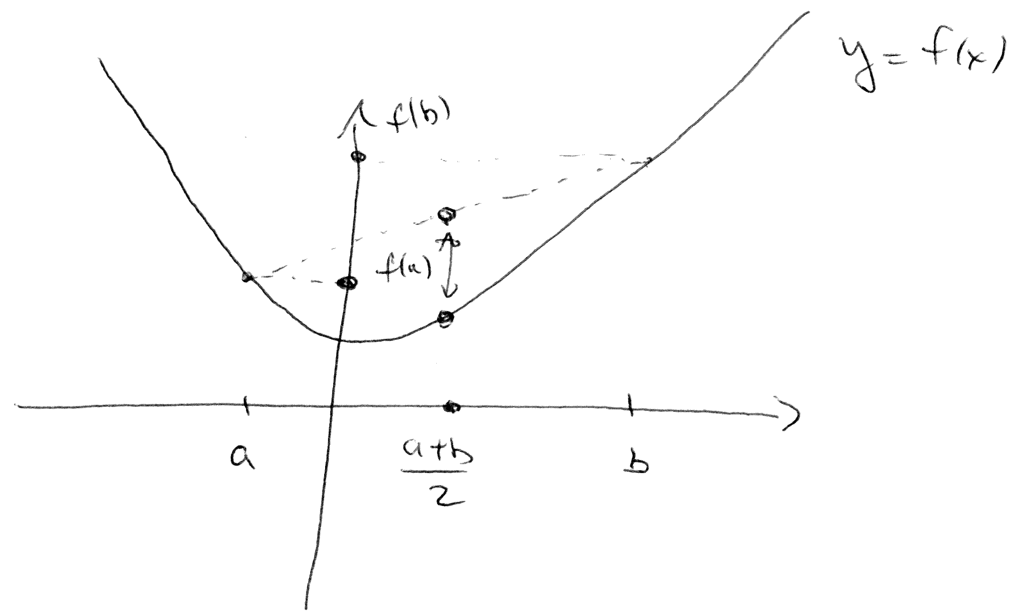
the mid point of $[a,b]$.

Further more,

$$\int_{\mathbb{R}} (f \circ g)(x)\, d\mu(x) = \frac{1}{b-a}\int_a^b f(x)\,dx$$

$\to$ The average value of f over $[a,b]$.

<u>Thus</u>



$(**)$ means that there is a generalization of this geometric picture

$$f\left(\frac{a+b}{2}\right) \le \frac{1}{b-a}\int_a^b f(x)\,dx$$

True for all convex functions.

Applying Jensen's Inequality to prove Proposition iii, i.e.

$$\sup_{\mathcal{P}} S(p) = \ln(d).$$

The function $f(x) = -x\ln(x)$ we introduced above is concave.

<u>But</u> $-f(x) = x\ln(x)$ is convex.

We will use $-f$.

Let $\mu = \frac{1}{d} \sum_{j=1}^{d} \delta_{\lambda_j}$.

This measure is the average of point masses (delta measures) supported on the eigenvalues of ρ.

Let $g(x) = \begin{cases} x & 0 \le x \le 1 \\ 0 & \text{otherwise.} \end{cases}$

Note that

$$\int_{\mathbb{R}} g(x)\, d\mu(x) = \int_{\mathbb{R}} |g(x)|\, d\mu = \int_0^1 x\, d\mu(x) = \frac{1}{d} \sum_{j=1}^{d} \lambda_j = \frac{1}{d}$$

$$\left(\text{since } \sum_{j=1}^{d} \lambda_j = 1 \right)$$

Thus

$$\frac{1}{d} \ln\left(\frac{1}{d}\right) = -f\left(\frac{1}{d}\right) = -f\left(\int_{\mathbb{R}} g(x)\, d\mu(x)\right)$$

$$\text{Jensen's} \neq \longrightarrow \quad \le \int_{\mathbb{R}} -(f \circ g)(x)\, d\mu(x)$$

$$= -\frac{1}{d} \sum_{j=1}^{d} (f \circ g)(\lambda_j)$$

$$= \frac{1}{d} \sum_{j=1}^{d} \lambda_j \ln(\lambda_j)$$

$$= -\frac{1}{d} S(\rho).$$

multiplying both sides by $-d$ we see that

$$S(\rho) \leq -\ln\left(\tfrac{1}{d}\right) = \ln(d).$$

as claimed.

Observing that the only "estimate" we used was the Jensen inequality, we see that:

since $-f$ is strictly convex

$$\begin{aligned}
S(\rho) = \ln(d) &\iff \text{equality happens above} \\
&\iff g(x) = x \text{ is constant for } \mu \text{ a.e. } x \\
&\iff \mu \text{ is concentrated at a single point } \lambda \text{ (since } g \text{ is not constant!)} \\
&\iff \lambda_j = \lambda \quad \text{for } 1 \leq j \leq d \\
&\iff \rho = \sum_{j=1}^{d} \lambda_j |\psi_j\rangle\langle\psi_j| \\
&\qquad = \lambda \sum_{j=1}^{d} |\psi_j\rangle\langle\psi_j| \\
&\qquad = \lambda \cdot \mathbb{1}
\end{aligned}$$

since $1 = \mathrm{Tr}[\rho] = \lambda d \implies \lambda = \frac{1}{d}$ and we are done.