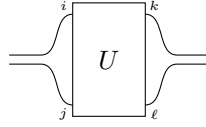


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Exercise 5.1 (Partial trace)

Let $U \in \mathbb{C}^{m \times n \times m \times n}$ be a tensor of degree 4, which we can interpret as $mn \times mn$ matrix by combining the first two and last two dimensions:



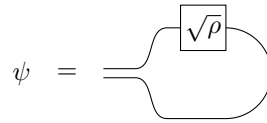
The *partial trace* is defined by “tracing out” (contracting) the subsystem corresponding to the upper two or lower two legs of U :

$$(\text{tr}_1[U])_{j\ell} = \sum_{i=1}^m U_{ij, i\ell} \hat{=} \text{Diagram}, \quad (\text{tr}_2[U])_{ik} = \sum_{j=1}^n U_{ij, kj} \hat{=} \text{Diagram}$$

The first diagram shows a box labeled U with legs j and ℓ on the bottom, and legs i and i on the top connected by a loop. The second diagram shows a box labeled U with legs j and j on the bottom connected by a loop, and legs i and k on the top.

Note that the partial trace yields a matrix: $\text{tr}_1[U] \in \mathbb{C}^{n \times n}$, $\text{tr}_2[U] \in \mathbb{C}^{m \times m}$.

- Show graphically that $\text{tr}_1[A \otimes B] = \text{tr}[A] B$ and $\text{tr}_2[A \otimes B] = \text{tr}[B] A$ for any square matrices A and B .
- Let $\rho \in \mathbb{C}^{n \times n}$ be a Hermitian, positive semidefinite matrix, such that its eigenvalues are non-negative and $\sqrt{\rho}$ is well defined. Let $\psi \in \mathbb{C}^{n^2}$ be the vectorization of $\sqrt{\rho}$:



Show that $\text{tr}_2[\psi \circ \psi^*] = \rho$.

Hint: $\psi \circ \psi^*$ plays the role of the above U interpreted as matrix. $\sqrt{\rho}$ inherits the Hermitian property from ρ .

Remark: In terms of quantum mechanics, ρ is a “density matrix” and ψ denoted “purification” of ρ . The outer product $\psi \circ \psi^*$ is written in bra-ket notation as $|\psi\rangle\langle\psi|$.

- Conversely, let $\psi \in \mathbb{C}^{n^2}$ be an arbitrary vector. Show that $\text{tr}_2[\psi \circ \psi^*]$ is Hermitian and positive semidefinite.

Hint: Revisit the proof of the SVD from the lecture to verify that AA^\dagger is positive semidefinite for any matrix A .

Solution

- For two square matrices A and B we can write

$$\text{tr}_1[A \otimes B] \hat{=} \text{Diagram} = \text{Diagram} = \text{Diagram} \hat{=} \text{tr}[A] B.$$

The first diagram shows a box labeled $A \otimes B$ with a loop on the top legs. The second diagram shows a box labeled A with a loop on its top legs, and a box labeled B with two legs on its bottom. The third diagram shows a box labeled A with a loop on its top legs, and a box labeled B with two legs on its bottom, with the A box's legs connected to the B box's legs.

An analogous proof shows that $\text{tr}_2[A \otimes B] = \text{tr}[B] A$.

- Since ρ is hermitian, we find that

$$\psi^* = \text{Diagram} = \text{Diagram}$$

The first diagram shows a box labeled $\sqrt{\rho}^\dagger$ with two legs, each of which is connected to a loop. The second diagram shows a box labeled $\sqrt{\rho}$ with two legs, each of which is connected to a loop.

Using the graphical depiction of both ψ and ψ^* we write

Therefore

$$\begin{aligned} \mathrm{tr}_2 [\psi \circ \psi^*] &= \text{diagram with two loops, each containing a box labeled } \sqrt{\rho}, \text{ connected by a curved line below.} \\ &= \text{diagram with two boxes labeled } \sqrt{\rho} \text{ in series.} = \text{diagram with one box labeled } \rho. \end{aligned}$$

(c) These properties can be shown without the graphical representation.

- *Hermitian*:

$$\mathrm{tr}_2[\psi \circ \psi^*] = \sum_j \psi_{ij} \psi_{kj}^* = \psi \psi^\dagger = (\psi \psi^\dagger)^\dagger = (\mathrm{tr}_2[\psi \circ \psi^*])^\dagger.$$

The first equality uses the definition of the parital trace and the third equality uses that for any square matrix A

$$(AA^\dagger)^\dagger = (A^\dagger)^\dagger A^\dagger = AA^\dagger.$$

- *Positive semidefinite:*

$$\langle v | \text{tr}_2 [\psi \circ \psi^*] | v \rangle = \langle v | \psi \psi^\dagger | v \rangle = \langle \psi^\dagger v | \psi^\dagger v \rangle = ||\psi^\dagger v||^2 \geq 0$$

for all $v \in \mathbb{C}^d$.