Introduction to Quantum Information Science
Recitation, week 6

Outer products and The Trace

1. Outer Products We have seen that products of a bra and ket of the form $\langle\psi|\phi\rangle$ correspond to inner products, which result in scalars as output. Show that if instead we multiply a ket and bra together like $|\psi\rangle\langle\phi|$, then the result is a matrix. This new type of product is called the *outer product*.

Solution: This follows directly from the rules of matrix multiplication. $|\psi\rangle$ is a column vector and $\langle\phi|$ is a row vector so their product is of the form:

$$\begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{n-1} \end{bmatrix} \begin{bmatrix} \phi_0 & \phi_1 & \cdots & \phi_{n-1} \end{bmatrix} = \begin{bmatrix} \psi_0\phi_0 & \psi_0\phi_1 & \psi_0\phi_2 & \cdots \\ \psi_1\phi_0 & \psi_1\phi_1 & \psi_1\phi_2 & \cdots \\ \psi_2\phi_0 & \psi_2\phi_1 & \psi_2\phi_2 & \cdots \\ \vdots & & & \ddots \end{bmatrix}$$

2. The Trace You may recall from your linear algebra course that the trace of a square $n \times n$ matrix A, denoted $\mathrm{Tr}(A)$, can be defined in several equivalent ways. Here are a few:

1. The sum of the diagonal elements: $\mathrm{Tr}(A) = \sum_i^n A_{i,i}$.
2. The sum of the eigenvalues: $\mathrm{Tr}(A) = \sum_i^n \lambda_i$.
3. For any orthonormal basis of n elements $|\psi_i\rangle$, $\mathrm{Tr}(A) = \sum_i^n \langle\psi_i| A |\psi_i\rangle$.

Some important properties of the trace include that it's *linear* and that it's *cyclic*. See e.g. Wikipedia for more.

a) Write the matrix

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

in the form

$$\sum_{i,j} \alpha_{i,j} |i\rangle\langle j|$$

Solution:

$$1\,|0\rangle\langle 0| + 2\,|0\rangle\langle 1| + 3\,|1\rangle\langle 0| + 4\,|1\rangle\langle 1|$$

b) Write the matrix from part (a) using Hadamard basis instead (a.k.a. the $|+\rangle\,/\,|-\rangle$ basis).

Solution: We can start with the matrix we found in part (a). Recall that a change of basis can be accomplished using a transition matrix, which is the matrix where the columns are the coordinate vectors (in the original basis) of the new basis vectors. The transition matrix here is not-so-coincidentally the Hadamard matrix. We have to update both the kets and the bras, so we multiply on both sides.

$$\begin{aligned} H(1\,|0\rangle\,\langle 0| + 2\,|0\rangle\,\langle 1| + 3\,|1\rangle\,\langle 0| + 4\,|1\rangle\,\langle 1|)H^\dagger &= 1\,|+\rangle\,\langle +| + 2\,|+\rangle\,\langle -| + 3\,|-\rangle\,\langle +| + 4\,|-\rangle\,\langle -| \\ &= \begin{bmatrix} 5 & -1 \\ -2 & 0 \end{bmatrix} \end{aligned}$$

where we use the fact that $H^\dagger = H$ to simplify our multiplication from the right.

c) Write the CNOT gate in the form

$$\sum_{i,j} \alpha_{i,j}\,|i\rangle\langle j|$$

Solution: Begin with any orthonormal basis for the right vectors / for the bras / for the inputs. Then, write the corresponding left vectors / kets / outputs.

$$|00\rangle\,\langle 00| + |01\rangle\,\langle 01| + |11\rangle\,\langle 10| + |10\rangle\,\langle 11|$$

d) Using the definition of CNOT in terms of outer product notation you found in part (c), apply CNOT to the state $|\psi\rangle = \frac{1}{2}(|00\rangle + e^{-i\pi/4}\,|01\rangle + e^{i\pi/4}\,|10\rangle - |11\rangle)$.

Solution: All of the resulting inner products become 0 or 1:

$$\begin{aligned} &(|00\rangle\,\langle 00| + |01\rangle\,\langle 01| + |11\rangle\,\langle 10| + |10\rangle\,\langle 11|)\,\frac{1}{2}(|00\rangle + e^{-i\pi/4}\,|01\rangle + e^{i\pi/4}\,|10\rangle - |11\rangle) \\ &= \frac{1}{2}(|00\rangle\,\langle 00|\,|00\rangle + e^{-i\pi/4}\,|01\rangle\,\langle 01|\,|01\rangle + e^{i\pi/4}\,|11\rangle\,\langle 10|\,|10\rangle - |10\rangle\,\langle 11|\,|11\rangle) \\ &= \frac{1}{2}(|00\rangle + e^{-i\pi/4}\,|01\rangle - |10\rangle + e^{i\pi/4}\,|11\rangle) \end{aligned}$$

where in the second line, we dropped any terms which were 0, and in the final line we dropped any factors which equal 1.

e) Let $|\psi\rangle = \sum_{i=0}^{n-1} v_i\,|i\rangle$ be a unit-length vector and let $\rho = |\psi\rangle\,\langle\psi|$. Compute $\mathrm{Tr}(\rho)$ by summing the diagonal entries of ρ.

Solution: The i-th diagonal entry of ρ is $v_i v_i^* = |v_i|^2$, so the sum of the diagonal entries is $\sum_i |v_i|^2 = 1$ because $|\psi\rangle$ is a unit length vector.

So, the trace of any density matrix corresponding to a pure state is 1. In fact, the trace of any mixed state is also 1.

f) In the next two exercises, we'll prove some of the properties of the trace that we mentioned earlier. Show that $\mathrm{Tr}(A{\cdot}B) = \mathrm{Tr}(B{\cdot}A)$. Generalize this to show the *cyclic property* of the trace $\mathrm{Tr}(A_1{\cdot}A_2 \dots A_n) = \mathrm{Tr}(A_2 \dots A_n \cdot A_1)$.
Hint: Begin by writing A and B using outer product notation.

Solution: Let $A = \sum_{ij} a_{ij} |i\rangle\langle j|$ and $B = \sum_{ij} b_{ij} |i\rangle\langle j|$.

$$
\begin{aligned}
\mathrm{Tr}(A \cdot B) &= \sum_i \langle i| (\sum_{jk} a_{jk} |j\rangle\langle k|)(\sum_{lm} b_{lm} |l\rangle\langle m|) |i\rangle \\
&= \sum_i \langle i| (\sum_{jkl} a_{jk} b_{kl} |j\rangle\langle l|) |i\rangle \\
&= \sum_{ij} a_{ij} b_{ji} \\
&= \sum_{ji} a_{ji} b_{ij} && \text{(Change variable names)} \\
&= \sum_{ij} b_{ij} a_{ji} && \text{(Addition and multiplication are commutative)} \\
&= \mathrm{Tr}(B \cdot A) && \text{(By symmetry)}
\end{aligned}
$$

For the cyclic property, let $B = A_2 \cdot ... \cdot A_n$.

$$\mathrm{Tr}(A_1 \cdot A_2 \cdot ... \cdot A_n) = \mathrm{Tr}(A_1 \cdot B) = \mathrm{Tr}(B \cdot A) = \mathrm{Tr}(A_2 \cdot ... \cdot A_n \cdot A_1)$$

g) We can write the trace as $\mathrm{Tr}(M) = \sum_i \langle i| M |i\rangle$. Would the same be true if we replaced $\{|i\rangle\}$ with any other orthonormal basis $\{|v_i\rangle\}$? Prove it.

Solution: Let U be the unitary such that $\forall i\colon U|i\rangle = |v_i\rangle$.

$$\sum_i \langle v_i| M |v_i\rangle = \sum_i \langle i| U^\dagger M U |i\rangle$$

So the trace with respect to the new basis is the same as the trace of $U^\dagger M U$ in the standard basis. But from the cyclic invariance of the trace:

$$\mathrm{Tr}(U^\dagger M U) = \mathrm{Tr}(U U^\dagger M) = \mathrm{Tr}(M)$$

We can do the trace with respect to any orthonormal basis we want.