Exercise Sheet 2 for the 'Quantum Machine Learning' Course

TA: Subadra Echeverria, TA: Felipe Choi, and Teacher: M. Cerezo²

¹Escuela de Ciencias Físicas y Matemáticas, Universidad de San Carlos de Guatemala, Guatemala 01004, Guatemala ²Information Sciences, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

This second set of exercises is aimed at introducing basic multi-qubit quantum circuit results that will be used throughout the course.

Tensor Product I.

The tensor product is a way of putting vector spaces together to form larger vector spaces.

Let \mathcal{H}_A be the Hilbert space associated with a quantum system labeled with the letter "A", and let \mathcal{H}_B be the Hilbert space associated with a quantum system labeled with the letter "B". Assume that \mathcal{H}_A is of dimension d_A , while \mathcal{H}_B is of dimension d_B . As mentioned in the previous exercise sheet, Hilbert spaces are complex vector spaces. The tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$ is a Hilbert space that described the joint quantum system "A + B" that is in itself a complex vector space of dimension $d_A \times d_B$. If $\{|v_A\rangle\}$ and $\{|w_B\rangle\}$ are basis of \mathcal{H}_A and \mathcal{H}_B , respectively, then the space $\mathcal{H}_A \otimes \mathcal{H}_B$ has basis elements $\{|v_A\rangle \otimes |w_B\rangle\}$. Usually, we denote these simply as $\{|v_A w_B\rangle\}$.

By definition, the tensor product satisfies the following properties

- Let z be a scalar, let $|v\rangle \in \mathcal{H}_A$ and $|w\rangle \in \mathcal{H}_B$, then $z(|v\rangle \otimes |w\rangle) = (z|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z|w\rangle).$
- Let $|v_1\rangle, |v_2\rangle \in \mathcal{H}_A$ and $|w\rangle \in \mathcal{H}_B$ then $(|v_1\rangle +$ $|v_2\rangle \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle.$
- Let $|v\rangle \in \mathcal{H}_A$ and $|w_1\rangle, |w_2\rangle \in \mathcal{H}_B$ then $|v\rangle \otimes (|w_1\rangle \otimes |w_1\rangle \otimes |w_2\rangle \otimes |w_1\rangle \otimes |w_2\rangle \otimes |w_1\rangle \otimes |w_2\rangle \otimes$ $|w_2\rangle = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle.$

Explicitly, the entries of the vector $|v\rangle \otimes |w\rangle$ are given by

$$(|v\rangle \otimes |w\rangle)_{ij} = v_i w_j. \tag{1}$$

The simplest operators that act on $\mathcal{H}_A \otimes \mathcal{H}_B$ are obtained from local operators acting on each Hilbert space. For instance, given operators $V: \mathcal{H}_A \to \mathcal{H}_A$ and $W: \mathcal{H}_B \to \mathcal{H}_B$, then, the tensor product operator $V \otimes W$ acts on the elements of $\mathcal{H}_A \otimes \mathcal{H}_B$ as

$$(V \otimes W)|v\rangle \otimes |w\rangle = V|v\rangle \otimes W|w\rangle. \tag{2}$$

Explicitly, let V and W be 2×2 matrices:

$$V = \begin{bmatrix} v_{1,1} & v_{1,2} \\ v_{2,1} & v_{2,2} \end{bmatrix}, \tag{3}$$

$$V = \begin{bmatrix} v_{1,1} & v_{1,2} \\ v_{2,1} & v_{2,2} \end{bmatrix},$$

$$W = \begin{bmatrix} w_{1,1} & w_{1,2} \\ w_{2,1} & w_{2,2} \end{bmatrix}$$

$$(3)$$

then,

$$(V \otimes W) = \begin{bmatrix} v_{1,1}w_{1,1} & v_{1,1}w_{1,2} & v_{1,2}w_{1,1} & v_{1,2}w_{1,2} \\ v_{1,1}w_{2,1} & v_{1,1}w_{2,2} & v_{1,2}w_{2,1} & v_{1,2}w_{2,2} \\ v_{2,1}w_{1,1} & v_{2,1}w_{1,2} & v_{2,2}w_{1,1} & v_{2,2}w_{1,2} \\ v_{2,1}w_{2,1} & v_{2,1}w_{2,2} & v_{2,2}w_{2,1} & v_{2,2}w_{2,2} \end{bmatrix}.$$
(5)

More generally, an arbitrary operator $C: \mathcal{H}_A \otimes \mathcal{H}_B \to$ $\mathcal{H}_A \otimes \mathcal{H}_B$ is of the form

$$C = \sum_{i} c_i V_i \otimes W_i \,, \tag{6}$$

with $\{V_i\}$ and $\{W_i\}$ operators respectively acting on \mathcal{H}_A and \mathcal{H}_B .

Exercise 1 (Tensor Product of Pauli matrices). Let X, Y and Z be Pauli matrices, and let I be the 2×2 identity matrix. Explicitly compute the 4×4 matrices $Z\otimes I$, $I\otimes Z$, $X \otimes X$.

Exercise 2 (Transpose, conjugate and dagger of tensor products). Show that $(V \otimes W)^* = V^* \otimes W^*$, $(V \otimes W)^t =$ $V^t \otimes W^t$, and $(V \otimes W)^{\dagger} = V^{\dagger} \otimes W^{\dagger}$.

Exercise 3 (Tensor product of unitary matrices). Show that the tensor product of two unitary matrices, is unitary.

Exercise 4 (Tensor product of Hermitian matrices). Show that the tensor product of two Hermitian matrices, is Hermitian.

II. Composite systems

The state space of a composite physical system is the tensor product of the state spaces of the component physical systems.

Let us consider a two qubit system, where one qubit is labeled with the letter "A", and the other labeled with the letter "B". Then, the computational basis of the Hilbert space $\mathcal{H}_{AB} = \mathcal{H}^{\otimes 2} := \mathcal{H} \otimes \mathcal{H}$ (where \mathcal{H} here denoted the Hilbert space of a single qubit) describing the composite two qubit system is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

Exercise 5 (Vector representation of the basis). Using Eq. (1) and recalling that $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, find the vector representation of each element in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}.$

Exercise 6 (n-qubit systems). How many elements are there in the basis of the Hilbert space $\mathcal{H}^{\otimes n}$ describing a $composite \ n$ -qubit system?

The general pure state of two qubit $|\psi\rangle \in \mathcal{H}^{\otimes 2}$ can be expressed as

$$|\psi\rangle = \sum_{ij=0.1} c_{ij}|ij\rangle \tag{7}$$

$$= c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle, \qquad (8)$$

where $\sum_{ij=0,1} |c_{ij}|^2 = 1$.

Exercise 7 (Expectation value). Let $|\psi\rangle$ be the general state in Eq. (8). Compute the expectation value $\langle Z \otimes Z \rangle = \langle \psi | Z \otimes Z | \psi \rangle$.

Similarly to measuring single qubit states, we can write the projective measurement operators for the computational basis as

$$M_{00} = |00\rangle\langle 00|, \quad M_{01} = |01\rangle\langle 01|,$$
 (9)

$$M_{10} = |10\rangle\langle 10|, \quad M_{11} = |11\rangle\langle 11|.$$
 (10)

So that

$$p(00) = \text{Tr}[M_{00}\rho] = |\langle 00 | \psi \rangle|^2 = |c_{00}|^2,$$
 (11)

$$p(01) = \text{Tr}[M_{01}\rho] = |\langle 01 | \psi \rangle|^2 = |c_{01}|^2,$$
 (12)

$$p(10) = \text{Tr}[M_{10}\rho] = |\langle 10 | \psi \rangle|^2 = |c_{10}|^2,$$
 (13)

$$p(11) = \text{Tr}[M_{11}\rho] = |\langle 11 | \psi \rangle|^2 = |c_{11}|^2.$$
 (14)

where $\rho = |\psi\rangle\langle\psi|$.

Recall from probability theory that given the joint probability of two discrete variables $p(x_i, y_j)$, the marginal probability $p(x_i) = \sum_j p(x_i, y_j)$. Use Eq. (8) to explicitly show that the probability of measuring just the first qubit in zero, or one, are

$$p_A(0) = p(00) + p(01), \quad p_A(1) = p(10) + p(11). \quad (15)$$

Performing a local measurement, e.g., measuring only the first qubit, and not measuring the second qubit can be obtained from the projective measurement operators

$$M_0^A = |0\rangle\langle 0| \otimes \mathbb{1}$$
, $M_1^B = |1\rangle\langle 1| \otimes \mathbb{1}$. (16)

Exercise 8 (Marginal Probability). First, show that $I = |0\rangle\langle 0| + |1\rangle\langle 1|$, with I the 2×2 identity matrix. Then, how can we interpret the marginal probability as just performing a local measurement and not measuring the other qubit?

Exercise 9 (Expectation value 2). Let $|\psi\rangle$ be the general state in Eq. (8). Show that the expectation value $\langle Z \otimes Z \rangle$ can be expressed as

$$\langle Z \otimes Z \rangle = p(00) + p(11) - p(01) - p(10).$$
 (17)

Given the state $\rho = |\psi\rangle\langle\psi|$ of a two-qubit composite system $\rho \in \mathcal{H}_{AB}$, sometimes we are interested in only the state of a *single qubit* without much regards for the second qubit. Here, there is a simple way in which we can describe the state of a single qubit via the so-called

FIG. 1. Quantum circuit examples. a) Non-entangling quantum circuit. b) Entangling quantum circuit.

 $reduced\ density\ matrix.$ The reduced density matrix of qubit A is defined as

$$\rho_A = \text{Tr}_B[\rho] \,, \tag{18}$$

where Tr_B is an operator map known as the partial trace over system B. Explicitly, the partial trace is computed as

$$\operatorname{Tr}_{B}\left[|v_{1}\rangle\langle v_{2}|\otimes|w_{1}\rangle\langle w_{2}|\right] = |v_{1}\rangle\langle v_{2}|\operatorname{Tr}\left[|w_{1}\rangle\langle w_{2}|\right],$$
(19)

where here $|v_1\rangle$ and $|v_2\rangle$ are vectors of the Hilbert space describing qubit A, and $|w_1\rangle$ and $|w_2\rangle$ are vectors of the Hilbert space describing qubit B.

Exercise 10 (Partial Trace). Let $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ be a quantum state on two qubits. First, compute its density matrix $\rho = |\psi\rangle\langle\psi|$. Then, compute the reduced states ρ_A and ρ_B .

III. Quantum Entanglement

Entanglement refers to non-classical correlations in quantum states. They are a key resource for quantum computation and one of, if not the, defining properties of quantum mechanics.

Consider a bipartite quantum system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The state $|\psi\rangle \in \mathcal{H}$ is said to be *separable* (or non-entangled) if $|\psi\rangle = |i\rangle \otimes |j\rangle$. Alternatively, the state $|\psi\rangle$ is said to be entangled if it cannot be written as a product form, that is, if $|\psi\rangle \neq |i\rangle \otimes |j\rangle$.

Exercise 11 (Local unitaries). Let $|\psi\rangle = |00\rangle$ be a separable state. Prove that an entangled state cannot be created by local single-qubit unitaries that are of the form $U \otimes V$ (see Fig. 1(a)).

Exercise 12 (Reduced States of pure states). Show that the reduced state of any pure separable state is pure. That is, given a state $\rho = |\psi\rangle\langle\psi|$, with $|\psi\rangle = |v\rangle\otimes|w\rangle$, then $\rho_A^2 = \rho_A$ and $\rho_B^2 = \rho_B$.

The previous exercise gives us an easy way to check if a bipartite pure quantum state is entangled or not. We simply compute the reduced states and check if they are pure. The latter can be achieved by computing their purity. The purity of a quantum state ρ is defined as $\mathcal{P}(\rho) = \text{Tr}[\rho^2]$. For pure states $\rho = |\psi\rangle\langle\psi|$, $\mathcal{P}(\rho) = \text{Tr}[\rho^2] = \text{Tr}[\rho] = 1$.

Exercise 13 (Maximally entangled state). The state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ is known as the Bell state, and it is known to be maximally entangled. Using the results of Exercise 10, compute $\mathcal{P}(\rho_A)$ and $\mathcal{P}(\rho_B)$. How can we interpret this result in terms of knowledge of the reduced state of a maximally entangled state?

IV. Quantum Circuit Computation

A quantum computer is built from a quantum circuit containing wires and elementary quantum gates to carry around and manipulate the quantum information.

When working with quantum systems, we want to apply a general unitary U to an n-qubit state $|\psi\rangle$. However, usually we need to obtain a circuit description of U in terms of simple gates that we can implement in our quantum computer. For this purpose, it is very useful to determine universal sets of quantum gates. A set $\mathcal S$ of quantum gates is said to be universal if any unitary U can be express as a finite product of gates in $\mathcal S$. Mathematically, this translates onto

$$U = \prod_{j} W_j$$
, where $W_j \in \mathcal{S}$. (20)

For instance, a famous universal gate set is composed of the gates

$$S = \{R_x(\theta), R_y(\theta), R_z(\theta), P(\varphi), \text{CNOT}\},$$
 (21)

where $R_{\mu}(\theta)$ with with $\mu = x, y, z$ is a single qubit rotation about the μ -axis, $P(\varphi)$ is single-qubit gate known as the phase shift gate

$$P(\varphi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix},\tag{22}$$

and CNOT is two qubit gate called the *controlled-NOT*, or CNOT gate given by

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$
 (23)

Exercise 14 (Gates are unitary). Prove that $P(\varphi)$ and CNOT are unitaries.

Exercise 15 (CNOT action). Prove using matrix multiplication, that

$$CNOT \cdot |00\rangle = |00\rangle \tag{24}$$

$$CNOT \cdot |01\rangle = |01\rangle$$
 (25)

$$CNOT \cdot |10\rangle = |11\rangle$$
 (26)

$$CNOT \cdot |11\rangle = |10\rangle$$
 (27)

Exercise 16 (Bell Circuit). Show that the output state $|\psi\rangle$ of the circuit in Fig. 1(b) is the maximally entangled Bell state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Here, H is the Hadamard gate defined as

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}. \tag{28}$$