# Exercise Sheet 1 for the 'Quantum Machine Learning' Course

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This first set of exercises is aimed at recalling some of the basic principles of quantum mechanics that will be used throughout the course.

## I. Pauli Matrices

*In quantum mechanics, Pauli matrices are related to the operators that take into account the interaction of the spin of a particle with an external electromagnetic field.*

The set of Pauli matrices $X$, $Y$, $Z$, are $2\times 2$ complex Hermitian unitary matrices that form a basis for the Lie algebra $\mathfrak{su}(2)$. Explicitly, the Pauli matrices are

$$X=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad Y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad Z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1}$$

**Exercise 1** (Properties of the Pauli Matrices). *Prove that:*

- $X^2=Y^2=Z^2=I$, *where $I$ is the $2\times 2$ identity matrix.*
- $\mathrm{Tr}[X]=\mathrm{Tr}[Y]=\mathrm{Tr}[Z]=0$.
- $[\sigma_i,\sigma_j]=2i\epsilon_{ijk}\sigma_k$, *where $\epsilon_{ijk}$ is the Levi-Civity symbol (see below), and where $\sigma_i,\sigma_j,\sigma_k\in\{X,Y,Z\}$.*
- $\{\sigma_j,\sigma_k\}=2\delta_{jk}I$, *where $\delta_{ij}$ is the Kronecker delta (see below), and where $\sigma_i,\sigma_j\in\{X,Y,Z\}$.*

We recall here that

$$\varepsilon_{ijk}=\begin{cases}+1 & \text{if } (i,j,k) \text{ is } (1,2,3),(2,3,1),\text{ or } (3,1,2),\\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1),(1,3,2),\text{ or } (2,1,3),\\ 0 & \text{if } i=j,\text{ or } j=k,\text{ or } k=i\end{cases} \tag{2}$$

and

$$\delta_{ij}=\begin{cases}0 & \text{if } i\neq j,\\ 1 & \text{if } i=j.\end{cases} \tag{3}$$

Finally, we also recall that for two matrices $A$ and $B$, their commutator is defined as $[A,B]=AB-BA$ and their anti-commutator as $\{A,B\}=AB+BA$.

## II. Single Qubit States

*In quantum mechanics, all of the dynamical information of a system is contained within a mathematical entity called the wavefunction, often denoted in Dirac notation as $|\psi\rangle$.*

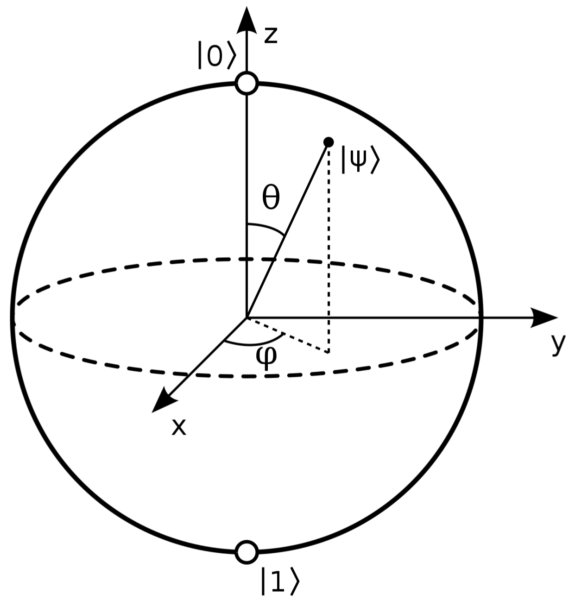


FIG. 1. **Bloch Sphere**. The state of a qubit can be represented as a point in the Bloch sphere. Pure states belong in the surface, while mixed states belong inside of the sphere.

A *"qubit"* represents a quantum mechanical system that can be in one of two possible states: $|0\rangle$, and $|1\rangle$. The more general *pure* qubit state can be expressed as a linear combination of these two states:

$$|\psi\rangle=\alpha|0\rangle+\beta|1\rangle, \tag{4}$$

where $\alpha$ and $\beta$ are complex numbers such that $|\alpha|^2+|\beta|^2=1$.

In vector representation, we usually adhere to the convention that

$$|0\rangle=\begin{pmatrix}1\\0\end{pmatrix},\quad\text{and}\quad |1\rangle=\begin{pmatrix}0\\1\end{pmatrix}, \tag{5}$$

are the eigenvectors of the $Z$-Pauli operator. we refer to the basis $\{|0\rangle,|1\rangle\}$ as the *computational basis.*

**Exercise 2** (Rotations on the Bloch Sphere). *Prove that $Z|0\rangle=|0\rangle$ and $Z|1\rangle=-|1\rangle$.*

Put another way, the state of a qubit is a vector in a two-dimensional complex vector space called the *Hilbert space*, and denoted by $\mathcal{H}$. Because of the normalization condition, it is also usually convenient to express

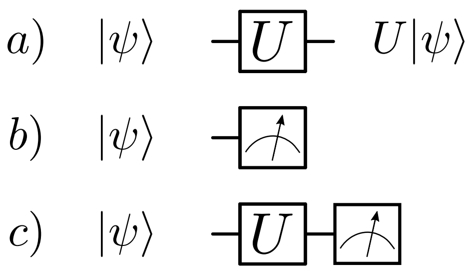


FIG. 2. a) Circuit implementing a unitary $U$. b) Circuit for measuring in the computational basis. c) Circuit for applying a unitary $U$, and then measuring in the computational basis.

the state of a qubit as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle, \tag{6}$$

with $\theta$, $\phi$, real numbers. As seen in Fig. 1, the state of a qubit can be represented as a point in the Bloch sphere.

So far, we have described the state of quantum systems by state vectors. An alternate formulation is possible using a tool known as the *density matrix*. For pure states, the density matrix is defined as $\rho = |\psi\rangle\langle\psi|$. The formulation of state vectors or density matrices is mathematically equivalent, but as we will see later, density matrices will allow us to describe quantum systems beyond that which is possible with the vector state formalism.

**Exercise 3** (Density matrix)**.** *Prove that the density operator $\rho = |\psi\rangle\langle\psi|$ for the state in Eq. (6) is*

$$\rho = \begin{pmatrix} \cos^2\left(\frac{\theta}{2}\right) & e^{-i\phi}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) & \sin^2\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{7}$$

*Then, explicitly show that* $\mathrm{Tr}[\rho^2] = 1$*, indicating that the state is pure.*

## III. Unitary Operations

*The evolution of a closed quantum system is described by a unitary transformation $U$ obtained from the solution of the Schrödinger equation.*

A rotation on the Bloch sphere about one of the principal axes ($x$, $y$ or $z$) can be expressed as

$$U(\theta) = e^{-i\theta\sigma/2}, \tag{8}$$

where $\sigma \in \{X, Y, Z\}$. For instance, we denote a rotation about the $x$-axis as $U_y(\theta) = e^{-i\theta Y/2}$. As shown in Fig. 2(a), rotating a quantum state $|\psi\rangle$ is then expressed as $U(\theta)|\psi\rangle$, while the rotation of a matrix $A$ is given by $U(\theta)AU^\dagger(\theta)$. Note that the latter includes as special case the rotation of a quantum state $\rho$ in the density matrix representation. Thus, rotating a quantum state $\rho$ is expressed as $U(\theta)\rho U^\dagger(\theta)$,

**Exercise 4** (Rotations on the Bloch Sphere)**.** *Prove that Eq. (8) can be explicitly expressed as*

$$U(\theta) = \cos\left(\frac{\theta}{2}\right) I + i\sin\left(\frac{\theta}{2}\right)\sigma, \tag{9}$$

*for any $\sigma \in \{X, Y, Z\}$.*

Then, prove the following (also, think about the geometrical interpretation from the Bloch sphere!):

**Exercise 5** (Rotations about the $y$-axis.)**.** *Prove that*

- *$U_y(\pi/2)|0\rangle = |+\rangle$, where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is an eigenvector of $X$ such that $X|+\rangle = |+\rangle$.*
- *$U_y(\pi/2)ZU_y^\dagger(\pi/2) = X$.*

From the previous, answer the following questions:

**Exercise 6** (Change of basis.)**.**

- *What rotation is needed to change from the $Z$ basis to the $X$ basis?*
- *What rotation is needed to change from the $Z$ basis to the $Y$ basis?*

## IV. Measurements

*Measurements describe the physical process in which an experimentalists interacts with a quantum state to find out what information about the system.*

Let us recall the measurement postulate of quantum mechanics. Suppose we perform a projective measurement described by the operator $M_m$. If the initial state was $|\psi\rangle$, then the probability of getting result $m$ is

$$p(m) = \langle\psi|M_m|\psi\rangle = \mathrm{Tr}[M_m|\psi\rangle\langle\psi|] = \mathrm{Tr}[M_m\rho]. \tag{10}$$

The state after obtaining the result $m$ is

$$|\psi^m\rangle = \frac{M_m|\psi\rangle}{\sqrt{p(m)}}. \tag{11}$$

As shown in Fig. 2(b), in quantum computing, one usually measures in the computational basis, and obtains the probability of the qubit measurement being '0' or '1'. That is, defining the projective measurement operators

$$M_0 = |0\rangle\langle 0|, \quad \text{and} \quad M_1 = |1\rangle\langle 1|, \tag{12}$$

we usually compute

$$p(0) = \mathrm{Tr}[M_0\rho] = |\langle 0|\psi\rangle|^2 = |\alpha|^2, \tag{13}$$
$$p(1) = \mathrm{Tr}[M_1\rho] = |\langle 0|\psi\rangle|^2 = |\beta|^2. \tag{14}$$

**Exercise 7** (Expectation value)**.** *Prove that*

$$\langle Z\rangle = \mathrm{Tr}[\rho Z] = p(0) - p(1). \tag{15}$$

**Exercise 8** (Expectation value and change of basis)**.** *Using the result in Exercise 6, how does one compute the expectation value $\langle X \rangle$? In other words, what rotation U in Fig. 2(c) do we have to apply before the measurement so that one measures in the basis of $X$.*

In practice, however, when using a quantum computer, one estimates $p(0)$ and $p(1)$ by finite sampling. That is, we measure $N$ times, count the number of times $N_0$ and $N_1$ that outcome '0' and '1', respectively appear, and approximate the probabilities by the frequencies

$$p(0) \sim \frac{N_0}{N}\,, \quad p(1) \sim \frac{N_1}{N}\,. \tag{16}$$

We know (statistical uncertainty) that sampling $N$ times from a probability distribution yields a statistical error of $1/\sqrt{N}$. Thus, in order to obtain a precision $\varepsilon$ when estimating the observable one needs a number of shots $N = 1/\varepsilon^2$.

## V. Hamiltonians, or Hermitian Operators

*Hamiltonians play a key role in quantum mechanics, as they describe the underlying interactions of a quantum system.*

Let $H$ be a $2 \times 2$ Hamiltonian, that is, a Hermitian operator, or a complex-valued matrix such that $H^\dagger = H$.

**Exercise 9** (Expectation values)**.** *Prove that for any state $|\psi\rangle$, the expectation value $\langle H \rangle = \mathrm{Tr}[|\psi\rangle\langle\psi| H]$ is real.*

Let $\{E_i\}$ and $\{|E_i\rangle\}$ respectively be the sets of eigenvalues and associated eigenvectors of $H$ (note that $E_i$ are real-valued). Then, we can expand $H$ in its eigenbasis as

$$H = \sum_i E_i |E_i\rangle\langle E_i|\,. \tag{17}$$

There always exists a change of basis matrix $V$ that maps the state $|\psi\rangle$ of Eq. (6) to the eigenbasis of $H$. That is, by writing

$$|0\rangle = c_{00}|E_0\rangle + c_{01}|E_1\rangle\,, \quad |1\rangle = c_{10}|E_0\rangle + c_{11}|E_1\rangle\,, \tag{18}$$

we explicitly find

$$V = \begin{pmatrix} c_{00} & c_{10} \\ c_{01} & c_{11} \end{pmatrix}. \tag{19}$$

**Exercise 10** (Change of basis)**.** *Using Eq. (4) and Eq. (18), write the state $|\psi\rangle$ in the basis of $H$.*

**Exercise 11** (Change of basis and expectation value)**.** *From the previous result, explicitly compute the expectation value $\langle H \rangle = \mathrm{Tr}[|\psi\rangle\langle\psi| H]$. How can we interpret this result as occupancy probabilities?*

## VI. Mixed Single Qubit States

*Quantum mechanical systems are usually not perfectly isolated from their environment, thus their states are not pure, but rather mixed.*

We have seen that the density matrix of a *pure state* is $\rho = |\psi\rangle\langle\psi|$. In general, however, when the state cannot be expressed in this form, we say that the state is *mixed*. In this general case, the state $\rho$ can be expanded as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|\,, \tag{20}$$

where $\{|\psi_i\rangle\}$ form an orthonormal basis ($\langle\psi_i\,|\,\psi_j\rangle = \delta_{ij}$), and $\sum_i p_i = 1$.

**Exercise 12** (Mixed States)**.** *Prove that a density matrix $\rho$ is pure if and only if $\rho^2 = \rho$.*

The density matrix of a general mixed state can be expanded in the Pauli basis as

$$\rho = \frac{1}{2}\left(I + \boldsymbol{r}\cdot\boldsymbol{\sigma}\right)\,, \tag{21}$$

where $\boldsymbol{r} = r_x, r_y, r_z$ is an arbitrary vector such that $|\boldsymbol{r}| \leqslant 1$ and $\boldsymbol{\sigma} = (X, Y, Z)$.

**Exercise 13** (Mixed States 1)**.** *Find the eigenvalues of $\rho$ in Eq. (21) and determine the cases for which $\rho$ is pure.*

**Exercise 14** (Mixed States 2)**.** *Express $\boldsymbol{r}$ in terms of $\langle\sigma\rangle = \mathrm{Tr}[\rho\sigma]$ for $\sigma \in \{X, Y, Z\}$.*