Expectation Values

Quantum Information and Computing Seminar

January 27, 2020

Qubits

A **classical bit** is an abstraction of a classical binary event (such as electricity flowing or not flowing through a wire). We label one of the events as 0 and the other as 1.

A **qubit**, or quantum bit, is an abstraction of a quantum binary events (such as an electron being spin-up or spin-down). Therefore, they are represented as discrete quantum states as opposed to just the numbers 0 and 1. Mathematically they are

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The **quantum state** of a qubit is represented by a complex-valued, 2×1 vector. It can be written as a linear combination of $|0\rangle$ and $|1\rangle$ as follows

$$|q\rangle = \begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} = a\,|0\rangle + b\,|1\rangle$$

where $a, b \in \mathbb{C}$.

Products

The **Hermitian conjugate** of a quantum state is its complex transpose and is represented as follows: If

$$|q\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

then

$$\langle q| \equiv |q\rangle^\dagger = \begin{pmatrix} a^* & b^* \end{pmatrix}$$

The **inner product** of two states $|\phi\rangle$ and $|\psi\rangle$ is given by $\langle \phi|\psi\rangle$.

Problem 1

Complete the following:

$$\langle 0|0\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1$$
$$\langle 0|1\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$
$$\langle 1|0\rangle = \begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} =$$
$$\langle 1|1\rangle =$$

As a general rule:

- $\langle a|b\rangle = 1$ if $a = b$
- $\langle a|b\rangle =$

The **outer product** of two states ψ and ϕ is given by $|\psi\rangle\,|\phi\rangle$.

Problem 2

Complete the following:

$$|0\rangle\langle 0| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$
$$|0\rangle\langle 1| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$$
$$|1\rangle\langle 0| = \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix}$$
$$|1\rangle\langle 1| =$$

Problem 3

Finish the following mixed products by using the results of Problem 1:

$$(|0\rangle\langle 0|)\,|0\rangle = |0\rangle\,(\langle 0|0\rangle) = |0\rangle\,(1) = |0\rangle$$
$$(|0\rangle\langle 0|)\,|1\rangle = |0\rangle\,(\langle 0|1\rangle) = |0\rangle\,(0) = 0$$
$$(|1\rangle\langle 0|)\,|0\rangle = |1\rangle\,(\langle 0|0\rangle) =$$
$$(|1\rangle\langle 0|)\,|1\rangle =$$

Now finish complete the following rules:

- When multiplying the outer-product $|0\rangle\langle 0|$ by the state $|x\rangle$, the outer-product "checks" if $x = 0$ because
  - if $x = 0$, the state remains unaffected
  - if $x = 1$, the state is destroyed

- When multiplying the outer-product $|1\rangle\langle 1|$ by the state $|x\rangle$, the outer-product "checks" if $x = 1$ because
  - if $x = 0$,
  - if $x = 1$,
- The outer-product $|1\rangle\langle 0|$ can be though of as a "raising" operator because, when multiplied by the state $|x\rangle$
  - if $x = 0$, the outer-product "raises" the state from $|0\rangle$ to $|1\rangle$
  - if $x = 1$, the state is destroyed as 1 cannot be raised.
- The outer-product $|0\rangle\langle 1|$ can be though of as a "lowering" operator because, when multiplied by the state $|x\rangle$
  - if $x = 0$,
  - if $x = 1$,

The **tensor product** of two $n \times n$ matrices

$$A = \begin{pmatrix} a_{00} & a_{01} & \dots & a_{0n} \\ a_{10} & a_{11} & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n0} & \dots & \dots & a_{nn} \end{pmatrix}, \; B = \begin{pmatrix} b_{00} & b_{01} & \dots & b_{0n} \\ b_{10} & b_{11} & & \vdots \\ \vdots & & \ddots & \vdots \\ b_{n0} & \dots & \dots & b_{nn} \end{pmatrix}$$

is defined to be

$$A \otimes B = \begin{pmatrix} a_{00}B & a_{01}B & \dots & a_{0n}B \\ a_{10}B & a_{11}B & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n0}B & \dots & \dots & a_{nn}B \end{pmatrix}$$

Problem 4

The tensor product can be used to form a larger space of qubits. Using the notation $|ab\rangle = |a\rangle \otimes |b\rangle$ we can create a 2-qubit space by taking the tensor products of the single qubits. For example, if

$$|a\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \quad |b\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$$

then

$$|ab\rangle = |a\rangle \otimes |b\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \\ a_1 \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$

Complete the following

$$
\begin{aligned}
|00\rangle &= \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix}1\\0\end{pmatrix} \\ 0\begin{pmatrix}1\\0\end{pmatrix} \end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \\
|01\rangle &= \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix}0\\1\end{pmatrix} \\ 0\begin{pmatrix}0\\1\end{pmatrix} \end{pmatrix} = \\
|10\rangle &= \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \\
|11\rangle &=
\end{aligned}
$$

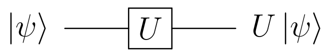
An important property of tensor products is the following

$$(A_1 \otimes A_2)(B_1 \otimes B_2) = A_1 B_1 \otimes A_2 B_2$$

Gates

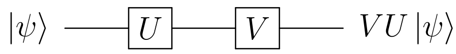
A quantum algorithm can be written in terms of a **quantum circuit** which shows how qubits are manipulated by **quantum gates**, which are 2×2, unitary matrices.

A gate U is represented in a quantum circuit as



which means $|\psi\rangle \to U|\psi\rangle$.

Applying U to the state and then V



is the same as $|\psi\rangle \to VU|\psi\rangle$. Note the switched order.

The **Pauli gates** correspond to the Pauli matrices.

$$
\begin{aligned}
I &= \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \\
X &= \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \\
Y &= \begin{pmatrix}0 & -i\\i & 0\end{pmatrix} \\
Z &= \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}
\end{aligned}
$$

To see how Pauli-gates are used to take expectation values, we'll write them in terms of outer-products.

Problem 5

Complete the following:

Let's see how the X gate affects qubits.

$$X|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$
$$X|1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

We've discovered that X "flips" the qubit that it acts on, from $|0\rangle$ to $|1\rangle$ and vice-verse. Therefore, we can write X in terms of outer-products as follows:

$$X = |1\rangle\langle 0| + |0\rangle\langle 1|$$

because then

$$X|0\rangle = (|1\rangle\langle 0| + |0\rangle\langle 1|)|0\rangle = |1\rangle\langle 0|0\rangle + |0\rangle\langle 1|0\rangle = |1\rangle(1) + |0\rangle(0) = |1\rangle$$
$$X|1\rangle = (|1\rangle\langle 0| + |0\rangle\langle 1|)|1\rangle = |1\rangle\langle 0|1\rangle + |0\rangle\langle 1|1\rangle = |1\rangle(0) + |0\rangle(1) = |0\rangle$$

Now let's look at the Y gate

$$Y|0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i|1\rangle$$
$$Y|1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} =$$

Therefore, we can write Y in terms of outer-products as follows:

$$Y = i|1\rangle\langle 0| - i|0\rangle\langle 1|$$

because then

$$Y|0\rangle = (i|1\rangle\langle 0| - i|0\rangle\langle 1|)|0\rangle = i|1\rangle\langle 0|0\rangle - i|0\rangle\langle 1|0\rangle =$$
$$Y|1\rangle = (i|1\rangle\langle 0| - i|0\rangle\langle 1|)|1\rangle =$$

Finally, let's look at the Z gate

$$Z|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} =$$
$$Z|1\rangle =$$

Therefore, we can write Z in terms of outer-products as follows:

$$Z =$$

because then

$$Z|0\rangle =$$
$$Z|1\rangle =$$

Bonus: I can be written in terms of outer-products as follows:

$$I =$$

We'll introduce two more gates, the Haddamard gate H and the phase gate S. They are defined as follows:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

Problem 6

Prove that $HZH = X$

$$\begin{aligned} HZH &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\ &= \end{aligned}$$

Prove that $SXS^\dagger = Y$

$$\begin{aligned} SXS^\dagger &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}^\dagger \\ &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \\ &= \end{aligned}$$

Show that $Y = \left(HS^\dagger\right)^\dagger Z \left(HS^\dagger\right)$ using the previous two results and the identity $(AB)^\dagger = B^\dagger A^\dagger$.

Measurement

If a qubit is in the state

$$|q\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

then, when the qubit is measured

- the probability that $|0\rangle$ is measured is $P_{|\psi\rangle}(0) = |\langle 0|q\rangle|^2 = \left|\begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}\right|^2 = |a|^2$
- the probability that $|1\rangle$ is measured is $P_{|\psi\rangle}(1) = |\langle 1|q\rangle|^2 = \left|\begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}\right|^2 = |b|^2$

Expectation Value

Every observable (thing one can observe) has a corresponding operator O. If particle is in a state $|q\rangle$ then the expected value of the observable corresponding to the operator O is given by

$$\langle q|O|q\rangle$$

Expectation Values

The following will demonstrate how to find the expectation value of a tensor string of Pauli spin matrices.

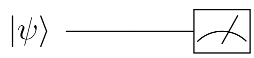
Expectation Value of Z

The expectation value of Z in state $|\psi\rangle$ is give by

$$\begin{aligned} E_\psi(Z) &= \langle\psi|Z|\psi\rangle \\ &= \langle\psi|\left(|0\rangle\langle 0| - |1\rangle\langle 1|\right)|\psi\rangle \\ &= \langle\psi|0\rangle\langle 0|\psi\rangle - \langle\psi|1\rangle\langle 1|\psi\rangle \\ &= |\langle 0|\psi\rangle|^2 - |\langle 1|\psi\rangle|^2 \\ &= P_{|\psi\rangle}(0) - P_{|\psi\rangle}(1) \end{aligned}$$

where $P_{|\psi\rangle}(x)$ is the probability that state $|\psi\rangle$ is measured to be $|x\rangle$.

So one creates the circuit



which means prepare the state ψ and measure. One does this over and over, counting C_0, the number of times one measures 0 and C_1, the number of times one measures 1. From these numbers, on can estimate the probability of measuring 0 and 1 as

$$\begin{aligned} P_{|\psi\rangle}(0) &= \frac{C_0}{C_0 + C_1} \\ P_{|\psi\rangle}(1) &= \frac{C_1}{C_0 + C_1} \end{aligned}$$

To find the expectation value of Z, one simply subtracts the probabilities as above:

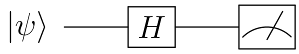
$$P_{|\psi\rangle}(0) - P_{|\psi\rangle}(1) = \frac{C_0 - C_1}{C_0 + C_1}$$

Expectation Value of X

To find the expectation value of X, we are going to rotate our computation basis. Recall that $X = HZH$. Thus

$$\begin{aligned} E_\psi(X) &= \langle\psi|X|\psi\rangle \\ &= \langle\psi|HZH|\psi\rangle \\ &= \left\langle H^\dagger\psi\middle|Z\middle|H\psi\right\rangle \\ &= \langle H\psi|Z|H\psi\rangle \\ &= E_{H\psi}(Z) \\ &= P_{H|\psi\rangle}(0) - P_{H|\psi\rangle}(1) \end{aligned} \tag{1}$$

So one creates the circuit



estimates the probabilities, and subtracts them, as above.

Problem 7

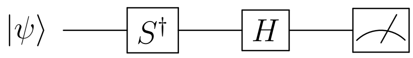
Complete the following:

Expectation Value of Y

To find the expectation value of Y, recall that $Y = SXS^\dagger$. Therefore $Y = \left(HS^\dagger\right)^\dagger Z \left(HS^\dagger\right)$. Thus

$$\begin{aligned} E_\psi(Y) &= \langle\psi|Y|\psi\rangle \\ &= \end{aligned}$$

So one creates the circuit



estimates the probabilities, and subtracts them, as above.

To summarize

$$\begin{cases} \text{Expectation value of:} & \text{Apply:} \\ Z & I \\ X & H \\ Y & HS^\dagger \end{cases} \tag{2}$$

String of Pauli's

Let's work out how to take the expectation value of a tensor-product string of Pauli matrices. For example, let's work out how to take the expectation value of $X \otimes Z$.

$$
\begin{aligned}
E_\psi(X \otimes Z) =& \; \langle\psi|X \otimes Z|\psi\rangle \\
=& \; \langle\psi|(HZH) \otimes (IZI)|\psi\rangle \\
=& \; \langle\psi|(H \otimes I)(Z \otimes Z)(H \otimes I)|\psi\rangle \\
=& \; \big\langle (H \otimes I)^\dagger\psi \big| (Z \otimes Z) \big| (H \otimes I)\psi \big\rangle \\
=& \; \langle (H \otimes I)\psi | Z \otimes Z | (H \otimes I)\psi\rangle \\
=& \; \langle\psi'|(|0\rangle\langle 0| - |1\rangle\langle 1|) \otimes (|0\rangle\langle 0| - |1\rangle\langle 1|)|\psi'\rangle \\
=& \; \langle\psi'|(|00\rangle\langle 00| - |01\rangle\langle 01| - |10\rangle\langle 10| - |11\rangle\langle 11|)|\psi'\rangle \\
=& \langle\psi'|00\rangle\langle 00|\psi'\rangle - \langle\psi'|01\rangle\langle 01|\psi'\rangle \\
& - \langle\psi'|10\rangle\langle 10|\psi'\rangle + \langle\psi'|11\rangle\langle 11|\psi'\rangle \\
=& |\langle 00|\psi'\rangle|^2 - |\langle 01|\psi'\rangle|^2 - |\langle 10|\psi'\rangle|^2 + |\langle 11|\psi'\rangle|^2 \\
=& P_{\psi'}(00) - P_{\psi'}(01) - P_{\psi'}(10) + P_{\psi'}(11)
\end{aligned}
$$

where I've defined $\psi' = (H \otimes I)\psi$.

Problem 8

Work out the following expectation value:

$$E_\psi(I \otimes X) = \langle\psi|I \otimes X|\psi\rangle$$

This can be extended to tensor-strings of arbitrary length. We can also extend this to sums of tensor-strings because expectation value is linear. For example:

$$\langle\psi|(X + Z)|\psi\rangle = \langle\psi|X|\psi\rangle + \langle\psi|Z|\psi\rangle$$

The power of this is that, if one can write a Hamiltonian H in terms of a linear combination of tensor-strings of Pauli matrices, one can use a quantum computer to estimate the expectation values of H (the energy) of the system for a given state $|\psi\rangle$.

We are now equipped to learn about the **variation quantum eigensolver**.