SENG 457/CSC 557
Lab 7: Expectation Values

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To-do list for today

- Expectation Values (math)
- Expectation Values (Pennylane)
- Numpy
- Add your name to the excel sheet!

Last week: Eigenvalues and Eigenvectors [M23]

- Computing the eigenvalues & eigenvectors of Hermitian and Unitary matrices is fundamental to QC & QM
- Computing eigenvalues & eigenvectors has an enormous number of applications in many different fields — especially science & engineering

Expectation values are not new!

$$E(X) = \frac{1}{6}(1) + \frac{1}{6}(2) + \frac{1}{6}(3) + \frac{1}{6}(4) + \frac{1}{6}(5) + \frac{1}{6}(6) = 3.5$$

Expectation Values in QM

- In Quantum Mechanics, the expectation value is the the expected value of the result or measurement of an experiment.
- As there are often multiple measurement outcomes, the expectation value can be thought of as an **average of all possible results** weighted by their probabilities of occurring.
- This is *NOT* the same thing as being the most probable outcome.

What are the possible results?

Observables

- An observable is a property of a system that can be determined by performing physical operations on the system.
- Observables represent measurable quantities associated with a quantum state
- Examples: position, momentum, energy, and spin.

Observables

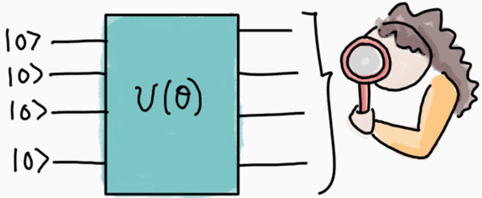
- In QM, every variable is associated with an observable
- This is represented by a matrix
- The **eigenvalues of this matrix** tell us what **possible values** the variable can take when we measure it in an experiment
- One of the most important observables is the **Hamiltonian**
- The Hamiltonian is associated with the energy which means the eigenvalues of the Hamiltonian tell us what possible values of energy we can measure in that system

Observables

One of the postulates of quantum mechanics is that for every observable A, there corresponds a linear Hermitian operator $\hat{A}$, and when we measure the observable A, we get an eigenvalue of $\hat{A}$ as the result.

Quantum States and Observables

- A quantum circuit uses gates to prepare a quantum state
- This state is measured in a basis of choice (e.g. computational basis)
- This orthonormal basis set is the collection of eigenvectors of the observable



Example

- For a single qubit system, the computational basis (or the Z basis) is $|0\rangle$, $|1\rangle$.
- $|0\rangle$, $|1\rangle$ are the eigenvectors of the observable Z:

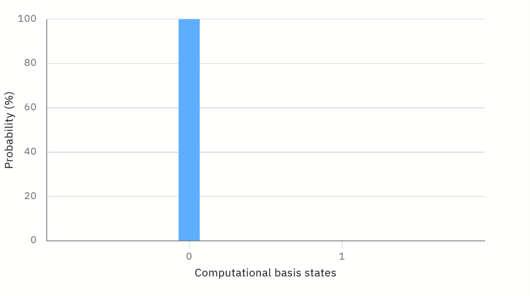
$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Eigenvalues and Eigenvectors of the Z-gate

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

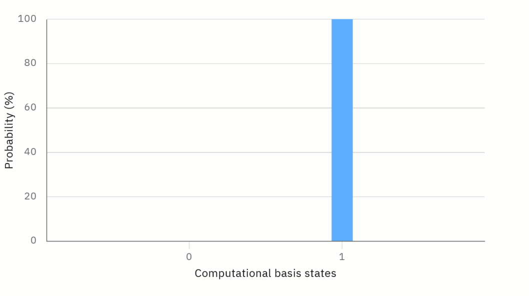
- has two eigenvalues $+1$ and -1
- corresponding to its eigenvectors $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Calculating the expectation value



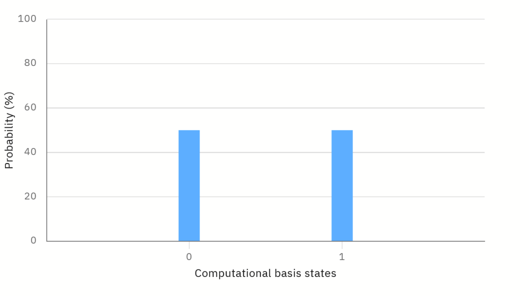
$$E = P(0) * \lambda_0 + P(1) * \lambda_1$$
$$= 1 * 1 + 0 * -1 = 1$$

Calculating the expectation value



$$E = P(0) * \lambda_0 + P(1) * \lambda_1$$
$$= 0 * 1 + 1 * -1 = -1$$

Calculating the expectation value



$$E = P(0) * \lambda_0 + P(1) * \lambda_1$$
$$= ?$$

Eigenvectors and eigenvalues of Pauli X

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- also has two eigenvalues $+1$ and -1
- corresponding to its eigenvectors $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ and $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$
- In Dirac Notation:
  - $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$
  - $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$

Expectation Values

If we have a quantum system $|\psi\rangle$, then the expectation value of the observable $\hat{O}$ is:

$$E(|\psi\rangle) = \langle\psi|\hat{O}|\psi\rangle$$

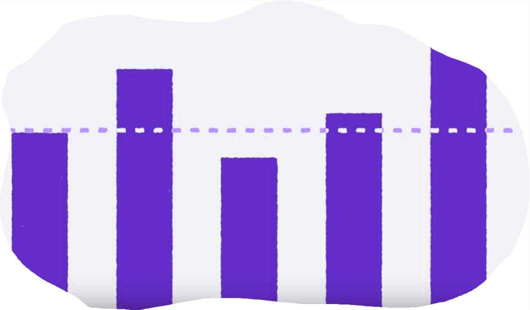
- When we calculate this expression, we will get the value that one would "expect" to find, according to the laws of probability.
- This is a weighted average of all possible outcomes; so a result that is more probable would contribute more to the expectation value.

Calculate Expectation Values

- Find the expectation value of the observable Z on the state $|1\rangle$
- Find the expectation value of the observable X on the state $|1\rangle$

Expectation Values $\langle\psi|\hat{O}|\psi\rangle$ or $\langle\hat{O}\rangle$

- There are multiple possible measurement outcomes in a quantum circuit
- The expectation value is the expected value of the result or measurement of a circuit
- This is the average of all possible results weighted by their probabilities of occurring
- **This is not the same as being the most probable outcome**



Eigenvalue/vector properties

Given a matrix, U, and a corresponding eigenvector $|\psi\rangle$,

$$U|\psi\rangle = \lambda|\psi\rangle$$

Expectation Values = Eigenvalues?

The expectation value for an any $|\psi\rangle$ is given by

$$E(|\psi\rangle) = \langle\psi|H|\psi\rangle^{\#}$$

The energy for an eigenstate $|\psi_\lambda\rangle$ is given by

$$\begin{aligned} E(|\psi_\lambda\rangle) &= \langle\psi_\lambda|\hat{H}|\psi_\lambda\rangle \\ &= \langle\psi_\lambda|\lambda|\psi_\lambda\rangle \\ &= \lambda\langle\psi_\lambda|\psi_\lambda\rangle \\ &= \lambda \end{aligned}$$

$^{\#}$Note that **observables are Hermitian and not usually unitary.** On a quantum computer, there exists a unitary transformation V such that $\hat{H} = V^\dagger \Lambda V$. More on this described in [IBM24] under cost functions.

Measurement

- Suppose we have a single qubit system in the $|0\rangle$ or the $|1\rangle$ state.
- Then, measuring the system gives us 0 or 1 with a 100% probability (since $|0\rangle$ and $|1\rangle$ are eigenvectors/eigenstates of the computational basis, i.e., Z)
- Now, if our qubit system was in the $|+\rangle$ state, then we no longer measure 0 or 1 with a 100% probability!

Expectation Value calculation in Numpy

Given an observable $\hat{O}$ and a quantum state $|\psi\rangle$, calculate

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle$$

Think about

- Conjugate transpose
- Tensor products
- matrix/vector multiplication

References

Variational Algorithm Design.
learning.quantum.ibm.com/course/variational-algorithm-design,
2024.

Hausi Müller.
Course lectures on Quantum computing (UVic), 2023.