Capstone C: Quantum Computing Math

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Hilbert Spaces & Dirac Notation

Quantum mechanics is described in the mathematical framework of **Hilbert spaces**. For our purposes, a Hilbert space is a complex vector space with an inner product. It's the stage where quantum states live.

Dirac Notation (Bra-Ket Notation) is the standard language for linear algebra in quantum mechanics.

- **Ket `$|\psi⟩$`**: A column vector representing a quantum state.

$$|0> = \begin{pmatrix}1\\0\end{pmatrix}, \quad |1> = \begin{pmatrix}0\\1\end{pmatrix}, \quad |\psi\rangle = \alpha|0> + \beta|1> = \begin{pmatrix}\alpha\\\beta\end{pmatrix}$$

- **Bra `$\langle\psi|$`**: The conjugate transpose (Hermitian conjugate) of a ket. It's a row vector.

$$\langle 0| = \begin{pmatrix}1 & 0\end{pmatrix}, \quad \langle 1| = \begin{pmatrix}0 & 1\end{pmatrix}, \quad \langle\psi| = \alpha^*\langle 0| + \beta^*\langle 1| = \begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}$$

- **Bra-Ket `$\langle\phi|\psi\rangle$`**: The inner product between two states. It's a complex number.

$$\langle\phi|\psi\rangle = (\text{row vector}) \times (\text{column vector})$$

  The probability of measuring state $|\psi\rangle$ to be state $|\phi\rangle$ is $|\langle\phi|\psi\rangle|^2$.

- **Ket-Bra `$|\psi\rangle\langle\phi|$`**: The outer product. It's a matrix (an operator).

$$|0\rangle\langle 0| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} \quad \text{(A projection operator)}$$

Qubits and Superposition

A **qubit** is a two-level quantum system. Unlike a classical bit (0 or 1), a qubit can exist in a **superposition** of both states simultaneously.

- **State of a Qubit**: Represented by a unit vector $|\psi\rangle$ in a 2D complex Hilbert space.

$$|\psi\rangle = \alpha|0> + \beta|1>$$

- **Amplitudes**: α and β are complex numbers called probability amplitudes.

- **Normalization**: The probabilities must sum to 1, which means the state vector must have a norm of 1.

$$|\alpha|^2 + |\beta|^2 = 1$$

Operators and Gates

Quantum operations are linear transformations. In QC, these are called **gates**.

- **Operators**: Represented by matrices that act on state vectors.
- **Unitary Operators**: All quantum gates must be represented by **unitary matrices** (`U`). A unitary matrix is one whose inverse is its conjugate transpose: `U^† U = I`.
  - **Why?** Unitary transformations preserve the norm of vectors. This ensures that after applying a gate, the state vector is still normalized ($|\alpha'|^2 + |\beta'|^2 = 1$), so probabilities still make sense.

Common Single-Qubit Gates

- **Pauli-X (NOT gate)**: Flips the qubit.

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

- **Hadamard Gate**: Creates superposition.

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H|0> = \frac{1}{\sqrt{2}}(|0> + |1>) = | + >$$

$$H|1> = \frac{1}{\sqrt{2}}(|0> - |1>) = | - >$$

The Tensor Product: Combining Systems

How do we describe a system of multiple qubits (e.g., a 2-qubit system)? We can't just stack the vectors. We need the **tensor product** (or Kronecker product $\otimes$).

If we have two qubits, $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|\phi\rangle = \gamma|0\rangle + \delta|1\rangle$, the combined 2-qubit system is a vector in a 4D Hilbert space.

- **State Space**: The combined space is the tensor product of the individual spaces: $V_{\text{total}} = V_1 \otimes V_2$.

- **Basis States**: The basis states of the 2-qubit system are:

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

And so on for $|10\rangle$ and $|11\rangle$.

- **Entanglement**: The tensor product allows for states that cannot be written as a simple product of individual qubit states. These are **entangled states**. The most famous is the Bell state:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

This state cannot be factored into $|\psi\rangle \otimes |\phi\rangle$.

Gates on Multiple Qubits

- **CNOT Gate**: A 2-qubit gate that flips the second qubit (target) if the first qubit (control) is $|1\rangle$. It's a 4x4 matrix.

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

This is how we create entanglement: $CNOT\,(H \otimes I)\,|00\rangle$ produces the Bell state $|\Phi^+\rangle$.

Simple Quantum Algorithms

Deutsch-Jozsa Algorithm

- **Problem**: Given a function `f: {0, 1} -> {0, 1}`, determine if it is **constant** (output is always 0 or always 1) or **balanced** (output is 0 for half the inputs and 1 for the other half).
- **Quantum Advantage**: A classical computer needs two queries to the function. A quantum computer needs only **one**.
- **Linear Algebra**: The algorithm works by preparing a state in superposition using Hadamard gates, applying the function via a unitary operator `U_f`, and then applying more Hadamards to interfere the amplitudes, revealing the global property of the function.

Grover's Search Algorithm

- **Problem**: Find a specific item in an unsorted database of `N` items.
- **Quantum Advantage**: Classically, this takes `O(N)` queries on average. Grover's algorithm does it in $O(\sqrt{N})$ queries.
- **Linear Algebra**: The algorithm is a geometric rotation in a Hilbert space. It starts with an equal superposition of all states. Then, it iteratively applies an operator (the Grover operator `G`) that rotates the state vector slightly closer to the target state. The `G` operator is a product of two reflection matrices.

Practice Problems

1. Given $|\psi\rangle = (1/\sqrt{5})|0\rangle + (2i/\sqrt{5})|1\rangle$, write down $\langle\psi|$ and verify that $\langle\psi|\psi\rangle = 1$.
2. Calculate the result of applying the Hadamard gate H to the state $|+\rangle$. What does this mean?
3. Calculate the tensor product $|0\rangle \otimes |+\rangle$. Write the result as a column vector and in Dirac notation.
4. Show that the Pauli-X matrix is unitary.
5. **Conceptual**: If you have a 3-qubit system, what is the dimension of its Hilbert space? How many basis vectors are there?