State Vector Simulation and Expectation Value Calculation

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1 Introduction

This document provides an explanation of the procedure for simulating a quantum circuit, obtaining samples from the final quantum state, and computing expectation values of operators on a quantum state. We will cover each of the following steps:

1. Initializing the quantum state in the standard state vector representation.
2. Applying quantum gates to the state vector.
3. Sampling outcomes from the final quantum state.
4. Computing expectation values of operators, specifically in the form $\langle\Psi|\mathrm{Op}|\Psi\rangle$.

2 Step 1: Initializing the Quantum State

To initialize an n-qubit quantum system in the $|0\ldots0\rangle$ state, we define the state vector to have length 2^n, where each element corresponds to an amplitude of one of the 2^n basis states. For the initial state, the amplitude for the $|0\ldots0\rangle$ basis state (corresponding to the index 0) is set to 1, and all other elements are set to 0.

3 Step 2: Applying Quantum Gates

We apply quantum gates by constructing an operator that acts on the entire n-qubit system. This is done using the Kronecker product:

- For each qubit in the system, we apply either the desired gate or an identity gate (if the qubit is not the target of the operation).
- The full operator is a tensor product of the gate and identity matrices, which expands the gate to act on the entire n-qubit space.

The gate is applied by performing a matrix multiplication between this expanded operator and the state vector.

4 Step 3: Sampling from the Final State

To sample measurement outcomes from the final quantum state:

1. First, we calculate the probability distribution over measurement outcomes by squaring the magnitudes of each element in the state vector. This gives the probability $p(i) = |\langle i|\Psi\rangle|^2$ of observing each basis state $|i\rangle$.

2. Using these probabilities, we can generate samples by drawing from the resulting distribution. Repeated sampling yields a frequency distribution over basis states, which simulates what would be observed in a real quantum measurement process.

5 Step 4: Computing Expectation Values

To compute the expectation value of an operator Op with respect to the state $|\Psi\rangle$, we calculate:

$$\langle\Psi|\mathrm{Op}|\Psi\rangle.$$

This expectation value is computed as follows:

- We first compute the conjugate transpose (or Hermitian transpose) of the state vector, $\langle\Psi|$.

- Next, we multiply the state vector, the operator Op, and the conjugate transpose vector in the sequence $\langle\Psi|\mathrm{Op}|\Psi\rangle$.

This operation yields the expectation value as a complex number. For a Hermitian operator, the expectation value is real, so we take only the real part of the result.

6 Example: Z Operator on the First Qubit

As an example, consider the Z operator acting on the first qubit of a 3-qubit system. To represent this in the system's Hilbert space:

- The Z operator acts on the first qubit, while the identity operator acts on the remaining two qubits.

- The combined operator is constructed as $\mathrm{Op} = Z \otimes I \otimes I$, where $\otimes$ denotes the Kronecker product.

Applying this operator to the final state allows us to calculate the expectation value $\langle\Psi|\mathrm{Op}|\Psi\rangle$, giving insight into the measurement statistics of the Z operator on the first qubit.

7 Conclusion

This process illustrates how a quantum state can be simulated in a classical environment and how measurements and expectation values are derived from the resulting state vector. The sampling technique mimics quantum measurement, while the expectation value calculation provides exact statistical information about observables in the system.