Fast simulation of Grover’s quantum search on classical computer

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ABSTRACT

Over the last few decades, the research community have been actively working on the realization of quantum computer. While large scale commercial quantum computers are not a reality yet, quantum computing field has become richer by day with the advent of algorithms and the avenue of its application in multiple domains. Availability of efficient quantum simulators will enable the researchers to quickly verify their results and concepts, in order to establish a working proof of correctness. One important algorithm that has become one of the basic ingredients to build other algorithms and models is the Grover’s search algorithm, which is known to be the most compute intensive. This report highlights the design principles for the fast simulations of Grover’s search, which can be implemented on a general purpose personal computer. The performance obtained are encouraging when compared to the existing simulators.

Introduction

Grover’s search algorithm\textsuperscript{1} has found applications in multiple domains, like cryptography, AI, pattern matching, database search, etc to name a few. The algorithm demands CPU intensive operations for executing multiple iterations ($O(\sqrt{N})$, where $N$ is the dimension of the input state or size of the search space) of the Grover iterator. Essentially, the iterator constitutes (1) application of oracle, (2) Hadamard transformation, (3) phase inversion about mean and (4) Hadamard transformation.

The traditional implementation of this algorithm for $n$-qubits ($N = 2^n$), would require an $N \times N$ matrix operation on an $N \times 1$ state. The space and compute-time complexities can thereby be quantified as $O(N^2)$ and $O(4N^2 \sqrt{N} = 4N^{\frac{7}{2}})$ respectively, where $4N^2$ corresponds to the 4 operations of the Grover iterator. Simulation of this matrix approach will become extremely time consuming and huge space invasive on a general purpose computer, (COTS HW) CPU with limited RAM, due to the exponential increase in computations and memory with the increasing number of qubits. Till date, there have been various attempts to build simulators that can run on a general purpose computer with limited resources and scale efficiently. One such high performance simulator is QuEST\textsuperscript{2}, which can be configured to either run in a single CPU mode or utilize the parallel computing benefits on a multiple CPUs/threads architecture and distributed system.

Here, we will present two approaches to implement the Grover search algorithm to improve upon both the limitations of the matrix approach. The first approach is based on applying the basic 1 and 2 qubit Universal gates to compute all the unitary operations on an $n$-qubit input state, which is the commonly used approach; while the second one using the Diffusion operator and the selected state inversion operator for further optimizing the time complexity. We will also provide the performance results obtained on a general purpose classical computer using single CPU (single thread), along with a couple of existing simulators, as a comparison.

Results

Approach1: Simulation based on Universal gates

This approach is more inline with the practical quantum circuit implementation. The idea here is to apply the standard Universal gates to individual qubits in a way that directly maps to the actual quantum circuit and can be realizable on a quantum computer. A $2 \times 2$ Hadamard gate and a $4 \times 4$ controlled-pauli $Z$ gate will be sufficient to implement the algorithm for an $n$-qubit quantum system. Since the allocated memory space for these two unitary operators are fixed, space complexity will only depend upon dimension $N = 2^n$ of the input state with $n$-qubits.

The application of a unitary gate to a target qubit can be interpreted as follows. The unitary operator will be generically applied to the corresponding target qubit of all the basis states of the input superposition state (which is in the form of
\( |\psi\rangle = \sum_{i=0}^{N-1} |x\rangle \), similar to the theoretical calculation done using Dirac notation. The Hadamard operation will only update the probability amplitudes of the basis state that is operated on and the affected basis states. The outcome depends on whether the target qubit is in \( |0\rangle \) or \( |1\rangle \) state. For example, a Hadamard transformation on the first qubit (LSB) of state \( |000\rangle \) will result in \( \frac{1}{\sqrt{2}} (|000\rangle + |001\rangle) \). This not only reduced the probability amplitude of the input state \( |000\rangle \), but also introduced another basis state \( |001\rangle \) in superposition to the system. The number of complex arithmetic calculations per qubit per basis state will be \( 4(2 \text{ multiplications} + 2 \text{ additions}) \). This means the number of calculations for an \( n \)-qubit system in a complete superposition state will be \( 4N \) (\( N = 2^n \)) per qubit, which is to say \( 4nN \) for \( n \)-qubits. Compared to the matrix approach, where the number of arithmetic calculations are \( N^2 \), this is a significant reduction. The application of all other unitary operators (non-Hadamard) will only require updating the basis state that is being operated on, which will have lesser calculations compared to the Hadamard gate.

Overall time complexity for the Grover’s algorithm in this simulation would be \( O(CnN^{\frac{3}{2}}) \). This corresponds to \( \sqrt{N} \) Grover’s iterations \((O(\sqrt{N}))\), 4 main operations in each Grover iteration \((O(C = \text{constant}))\), \( n \)-qubits in each iteration \((O(n))\), and iterating through \( N \) basis states for each target qubit \((O(N))\).

**Approach 2: Simulation based on Diffusion operator**

This approach is targeted mainly for simulation because the calculations are directly based on the mathematical method rather than the actual circuit involving unitary gates. Thus, this algorithm cannot be executed on a quantum computer directly. Though this has similar space complexity as the first approach, the time complexity is significantly improved, which is very crucial when running the algorithm on general purpose classical computers with limited CPU and memory.

Here the Grover’s iterator is realized by implementing two mathematical operators, the selected state inversion (Oracle) using \( I - 2|i\langle i| \) and the Diffusion operator corresponding to the 2-Hadamard operations and the average phase inversion by \( 2|\psi\rangle\langle\psi| - I \). For computational speedup and to reduce the space footprint, the state inversion operator stores the position of state which would undergo phase inversion when acted upon. The time complexity is thus reduced to a near constant value as number of phase inversions would be very small compared to state dimension. Diffusion operator has the symmetry in structure and a mere \( 2 \times 2 \) matrix would be sufficient to operate on prepared state. Each diagonal element would carry matrix element of \( \frac{2}{N} - 1 \) and off diagonal element \( \frac{2}{N} \), where \( N = 2^n \) is the total state dimension. Similar to the previous approach, this operator too would act on the basis states of the overall superposed state. The time complexity to operate on the states would thus be \( O(\sqrt{N}) \) per Grover iteration, but space complexity is constant \( 2 \times 2 \).

The overall space complexity will be \( O(N) \) identical the the first approach, whereas time complexity will be \( O(\sqrt{N}^2) \). The reduction in time complexity by a factor \( O(nC) \) is observed to be significant for simulation involving more than 10 qubits. This approach, though may not be realizable on a quantum computer, significantly enhances the performance due to highly optimized computation.

**Simulation Results**

Table 1 below captures the performance comparison with QuEST and libquantum simulators. The simulations were performed with single CPU/thread on a laptop with Intel(R) Core(TM) i3-5005U CPU @ 2.00GHz 8GB RAM and -O4 compiler option.
Table 1. Performance of Grover’s algorithm

| Simulators | # qubits | minutes:seconds (approx) |
|------------|----------|--------------------------|
| Approach 1 |          |                          |
|            | 10       | 0:0.031                  |
|            | 16       | 0:9.026                  |
|            | 18       | 1:26.651                 |
|            | 20       | 12:38.643                |
| Approach 2 |          |                          |
|            | 10       | 0:0.025                  |
|            | 16       | 0:0.349                  |
|            | 18       | 0:2.579                  |
|            | 20       | 0:20.005                 |
| QuEST      |          |                          |
|            | 10       | 0:0.021                  |
|            | 16       | 0:9.401                  |
|            | 18       | 1:31.053                 |
|            | 20       | 12:51.286                |
| libquantum |          |                          |
|            | 10       | 0:0.055                  |
|            | 16       | 0:15.736                 |
|            | 18       | 2:56.230                 |
|            | 20       | 36:0.0                   |

Discussion

We have shown that the simulation efficiency, both space and time, of the Grover’s algorithm was significantly improved using the diffusion and phase inversion operator approach. The simulation results provided clearly indicate the performance improvement compared to the conventional approach and existing implementations. The performance can be further improved multiple folds on high performance computers with multiple CPUs and multi-threading.

References

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