PHYS379: Group Project - Quantum Computer Simulator Topic

Edward McCann

Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK

Keywords: quantum computer; quantum information; Hadamard gate; Grover's search algorithm; Shor's factoring algorithm; quantum teleportation

Introduction

In PHYS379, you should undertake an open-ended group project and submit a group report describing the project. The group project is worth twenty credits. Please see the document "PHYS379-group-project-notes.pdf" for details about organisation and assessment.

Open-ended project

Your task in the project is to simulate a quantum computer using a regular pc. Precisely what you do is your choice - the project is open-ended. You will need to formulate a research question (or questions) that is more specific than simply "simulate a quantum computer". What are you trying to discover? You should do some research in the library or on the internet to find out what the interesting questions are. It may be that you will not finalise the research question until the latter stages of the project, once you have found what is (or is not) interesting. Remember that this is group work - it will make sense to plan for parallel tasks in order to use your personnel effectively. For example, you might want parallel numerical and analytic investigations, investigations looking at different aspects of the same problem, or you might deliberately duplicate effort in order to check important results (in the "real" world, results should always be checked before publication, getting different people to work independently is the best way to do this). There are some ideas below, you can follow some or all of them, or you can follow your own ideas.

Getting started

N-qubit register

This follows Ref.[1], please read this paper for more details. A qubit [1,2] is a quantum system with two basis vectors in its Hilbert space. An example is a spin-1/2 particle like an electron, for which an arbitrary state can be written as

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are states with eigenvalues $S_z = \pm 1/2$. Complex amplitudes a and b obey the normalisation condition $|a|^2 + |b|^2 = 1$. The basis states $|\uparrow\rangle$ and $|\downarrow\rangle$ can be used to represent information 0 and 1:

$$|0\rangle \equiv |\uparrow\rangle; \quad |1\rangle \equiv |\downarrow\rangle$$

An N-qubit register is N of these 2-state qubits, considered together to be one quantum system. We'll consider a state with $N = 3$ qubits, it has $2^N = 8$ different basis states:

$$|000\rangle = |\uparrow\rangle|\uparrow\rangle|\uparrow\rangle; \quad |001\rangle = |\uparrow\rangle|\uparrow\rangle|\downarrow\rangle; \quad |010\rangle = |\uparrow\rangle|\downarrow\rangle|\uparrow\rangle; \quad |011\rangle = |\uparrow\rangle|\downarrow\rangle|\downarrow\rangle$$
$$|100\rangle = |\downarrow\rangle|\uparrow\rangle|\uparrow\rangle; \quad |101\rangle = |\downarrow\rangle|\uparrow\rangle|\downarrow\rangle; \quad |110\rangle = |\downarrow\rangle|\downarrow\rangle|\uparrow\rangle; \quad |111\rangle = |\downarrow\rangle|\downarrow\rangle|\downarrow\rangle \quad (1)$$

An arbitrary state is a superposition of the eight basis states,

$$|\psi\rangle = a|000\rangle + b|001\rangle + c|010\rangle + d|011\rangle + e|100\rangle + f|101\rangle + g|110\rangle + h|111\rangle \quad (2)$$

with normalisation

$$|a|^2 + |b|^2 + |c|^2 + |d|^2 + |e|^2 + |f|^2 + |g|^2 + |h|^2 = 1$$

We'll consider a quantum computer that works with three stages: (i) initiate the N-qubit register in a certain state [of the form of Eq.(2)]; (ii) apply a series of quantum gate operations; (iii) measure the N-qubit register.

Step 1: Initiate the N-qubit register in a certain state

For a given initial state, the amplitudes a-h must be stored in the computer as a column vector

$$|\psi\rangle = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \end{pmatrix}$$

Step 3: Measure the N-qubit register

The aim is to measure S_z for each of the N qubits, each measurement should give $S_z = \pm 1/2$, i.e. the result of the measurement will be to find the register in one of the 2^N basis states Eq.(1). The probability of measuring each basis state is given by the square magnitude of the corresponding amplitude, for example

$$P(|010\rangle) = |\langle 010|\psi\rangle|^2 = |c|^2$$

Simulate a measurement of S_z for the three qubits using the computer's random number generator to simulate quantum probability by picking a random number r with $0 \leq r \leq 1$:

1. Fix r.
2. Set $q = |a|^2$. If $r < q$ the result is $|000\rangle$; otherwise proceed to the next step.
3. Set $q = q + |b|^2$. If $r < q$ the result is $|001\rangle$; otherwise proceed to the next step.
4. Set $q = q + |c|^2$. If $r < q$ the result is $|010\rangle$; otherwise proceed to the next step.
5. Continue with three similar steps.
6. Set $q = q + |g|^2$. If $r < q$ the result is $|110\rangle$; otherwise the result is $|111\rangle$.

To do this you could use a series of IF statements, but it's better to use a loop, ideally for arbitrary N. Repeat the measurements many times (with different r values) to see which results are most frequent.

- Set the initial state to one of the basis states, for example, $|010\rangle$. With this initial state, every measurement should give the result $|010\rangle$.
- Set the initial state to the "cat" state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\0\\0\\0\\0\\1\end{pmatrix}$$

At random, either all of the qubits should be 0 or 1, i.e the result should be $|000\rangle$; or $|111\rangle$;.

- Set the initial state to an equal superposition of all 2^N basis states,

$$|\psi\rangle = \frac{1}{\sqrt{8}}\begin{pmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{pmatrix}$$

All possible results should occur, each with equal frequency within random fluctuations.

Step 2: Apply a series of quantum gate operations

An example of a quantum gate is the Hadamard gate which acts on a single qubit. Applying a Hadamard gate to one basis state (of a single qubit) gives a superposition of both basis states. Applying the Hadamard gate to the second qubit (for $N = 3$) is represented by a matrix:

$$H_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\0 & 1 & 0 & 1 & 0 & 0 & 0 & 0\\1 & 0 & -1 & 0 & 0 & 0 & 0 & 0\\0 & 1 & 0 & -1 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 1 & 0 & 1 & 0\\0 & 0 & 0 & 0 & 0 & 1 & 0 & 1\\0 & 0 & 0 & 0 & 1 & 0 & -1 & 0\\0 & 0 & 0 & 0 & 0 & 1 & 0 & -1\end{pmatrix}$$

Applying this Hadamard gate to the N-qubit register can be done by matrix multiplication $H_2|\psi\rangle$. For initial state $|000\rangle$, this Hadamard gate puts qubit 2 in an equal superposition $|0\rangle$ and $|1\rangle$. Therefore, the result of the calculation should vary randomly between the two possibilities, $|000\rangle$ and $|010\rangle$. This is project 2(a) on p692 of Ref.[1]. You should also complete projects 2(b), 2(c), 2(d).

Open-ended part

Please note:

1. **The aim is for your group to do its own, original calculations.** A literature review and, perhaps, reproduction of other people's results may be important steps along the way, but these are not the final aim.

2. The quantum computer topic has run in PHYS379 for four years and it has generally been very successful. It is very interesting, but will require you to invest energy and enthusiasm in learning about the topic. Another difficulty is finding original calculations to do: sometimes groups spend a lot of energy simulating complicated algorithms without doing anything new.
3. You might be able to find software on the web that creates a simulation for you. Be very wary of doing this, because (i) if someone else has written the simulation, how much credit will you get in PHYS379? (ii) possibly more importantly, if someone else has written the simulation, to what extent do you understand what it actually does?

Ideas include:

- Continue working through the projects in Ref.[1], particularly Grover's search algorithm (p692); CNOT gates (p694); an arbitrary number of qubits (p695); Shor's factoring algorithm (p696).
- Estimate the uncertainty of your simulator, e.g. for a circuit for which the probabilities of certain outcomes are known, check how the value of the average measurement varies after many repetitions of the measurement. What is the effect of using different datatypes for your numerical values? How does run time depend on the number of qubits?
- Quantum Fourier transform [3].
- Deutsch algorithm, Deutsch-Jozsa algorithm [4].
- Quantum teleportation [5].
- Quantum eraser experiment using qubits [6,7].
- Look at other simulators (e.g. [8-12]), you can use these to "benchmark" your simulator and to get new ideas.
- For a given quantum circuit, is it possible to check it works as it should? If one gate is missing, is it possible to determine which gate?

Bibliography

[1] D. Candela, Am. J. Phys. **83**, 688 (2015).

[2] "Quantum computing" Wikipedia, http://en.wikipedia.org/wiki/Quantum_computing

[3] "Quantum Fourier transform", Wikipedia, https://en.wikipedia.org/wiki/Quantum_Fourier_transform

[4] "Deutsch-Jozsa algorithm", Wikipedia, https://en.wikipedia.org/wiki/Deutsch\%E2\%80\%93Jozsa_algorithm

[5] "Quantum teleportation", Wikipedia, https://en.wikipedia.org/wiki/Quantum_teleportation

[6] "Quantum eraser experiment", Wikipedia, https://en.wikipedia.org/wiki/Quantum_eraser_experiment

[7] "Delayed choice quantum eraser", Wikipedia, https://en.wikipedia.org/wiki/Delayed_choice_quantum_eraser

[8] Quantiki, https://quantiki.org/wiki/list-qc-simulators

[9] Quantum Computing Playground, http://www.quantumplayground.net/\#/home

[10] LIQ*U*i|⟩, http://stationq.github.io/Liquid/

[11] Quirk, http://algassert.com/2016/05/22/quirk.html

[12] Davy Wybiral, http://davywybiral.blogspot.co.uk/2012/12/quantum-circuit-simulator.html