MULT90063 Introduction to Quantum Computing

Lab Session 10

10.1 Introduction

Welcome to Lab 10 of MULT90063 Introduction to Quantum Computing. The purpose of this lab session is to get some experience with mapping and solving optimisation problems using hybrid approaches, e.g. Quantum Approximate Optimisation Algorithm (QAOA).

10.2 Programming quadratic forms

As you saw in lectures many optimisation problems can be cast into the "spin-glass" form where the task is to minimise the energy of a particular function E over variables $\{z_i\}$. The quadratic form (QUBO) involve products $z_i\, z_j$, so when we map the problem onto a quantum computer and convert variables z_i to operators Z_i we need to be able to program operator products $Z_i\, Z_j$ acting on a particular trial state.

Exercise 10.2.1 Consider the circuit below over two qubits: 1 (top) and 2 (bottom). For the case $\theta_{ij} = \pi$ (global phase $\pi/2$) verify that the circuit form below is equivalent to the operation Z_1Z_2. Hint – one way to do this is to write out the gates as 4x4 matrices over the two qubit space and multiply them out. Verify the action on the QUI.

$$H = \ldots + J_{ij}\, Z_i Z_j + \ldots$$

$$\theta_{ij} = -\frac{J_{ij}\alpha}{2}$$

10.3 Solving a number partitioning problem

Let's consider an instance of the number partitioning problem and solve it on the QUI. The problem is stated as follows: given a set S of numbers $\{w_i\}$, is there a partition of this set of numbers into two disjoint subsets R and S − R, such that the sum of the elements in both sets is the same? In lectures we saw the solution is equivalent to finding the basis state with the minimum energy in the system given by the "Hamiltonian" over qubit operators:

$$H = \left(\sum_i w_i Z_i\right)^2 = \sum_{i \neq j} 2 w_i w_j Z_i Z_j + \sum_i w_i^2 I$$

where and each number is assigned a qubit ($w_i \leftrightarrow q_i$) and the qubit value 0 or 1 indicates which of the two sets, R and S–R, the numbers are associated with.

We will solve the number partitioning problem for the set S = {1, 2, 3} using QAOA on the QUI.

Exercise 10.3.1 Classically solving the problem (i.e. in your head), what are the solution sets R and S–R?

Exercise 10.3.2 Convert classical solutions to quantum land. Assigning "R" ↔ "0" and "S–R" ↔ "1", translate the expected possible solutions from 10.3.1 into qubit form $|q_1 q_2 q_3\rangle$ where that values of each q_i = 0, 1 indicates which set the corresponding number w_i is assigned to in the solution. The solutions are:

_____ and _____

Exercise 10.3.3 The Hamiltonian of this number partitioning problem is

$$H = 4Z_1Z_2 + 6Z_1Z_3 + 12Z_2Z_3 + 14I$$

Make sure you understand how to get this from the general expression above. Show that the energy of this system is zero for the solution basis states $|q_1q_2q_3\rangle$ you found in 10.3.2, and non-zero for other states.

Exercise 10.3.4 Now we will program the QAOA circuit to solve this system. For the construction of the ZZ operators in the circuit we have from the Hamiltonian the individual energies: J_{12} = 4, J_{13} = 6, J_{13} = 12. Consider the basic QAOA circuit (k=1, i.e. one iteration), program this in the QUI for the choice $\alpha = 0.01\pi$ and $\beta = 0.3\pi$, and the values E_{ZZ}^{ij} given above for the problem. Run to compute the state $|\phi(\alpha,\beta)\rangle$.

To calculate the energy, we take the expectation value of the Hamiltonian H in the state $|\phi(\alpha,\beta)\rangle$ i.e.

$$\langle H\rangle_{\alpha\beta} = 4\langle Z_1Z_2\rangle_{\alpha\beta} + 6\langle Z_1Z_3\rangle_{\alpha\beta} + 12\langle Z_2Z_3\rangle_{\alpha\beta} + 14$$

where, $\langle\mathcal{O}\rangle_{\alpha\beta} = \langle\phi(\alpha,\beta)|\mathcal{O}|\phi(\alpha,\beta)\rangle$. Note that for a 3 qubit state written in terms of the basis states we have in general:

$$|\varphi\rangle = a_0|000\rangle + a_1|001\rangle + a_2|010\rangle + a_3|011\rangle + a_4|100\rangle + a_5|101\rangle + a_6|110\rangle + a_7|111\rangle,$$

The measurement of $\langle Z_1Z_2\rangle$ amounts to averaging the of Z_1Z_2 in each of the basis states (recall $Z|0\rangle = +|0\rangle$, $Z|1\rangle = -|1\rangle$ etc), weighted by the probabilities of the basis states,

$$\langle Z_1Z_2\rangle = \langle\varphi|Z_1Z_2|\varphi\rangle = (+1)|a_0|^2 + (-1)|a_1|^2 + (-1)|a_2|^2 + (+1)|a_3|^2$$
$$+ (-1)|a_4|^2 + (-1)|a_5|^2 + (+1)|a_6|^2 + (+1)|a_7|^2.$$

On a real QC we would have to run many times to get these expectation values. In the QUI we have the probabilities $|a_i|^2$ for each basis state (i = decimal index), and can sum the expectation values of the terms in the Hamiltonian. Notice that we could also work out the expectation value of the sum of terms in the Hamiltonian with respect to each of the basis states and sum those over the basis states (which we will do in the next exercise).

Exercise 10.3.5 From the QUI, let's break down the expectation values over the individual basis states. The table you want to fill out from the QUI output is given below. Best to do this in excel because you will be repeating it for other choices of α and β (yes, it's one of those labs, but we'll try to make it as painless as possible).

Basis state, i	$\langle Z_1Z_2\rangle_i$	$\langle Z_1Z_3\rangle_i$	$\langle Z_2Z_3\rangle_i$	$E_i = 4\langle Z_1Z_2\rangle_i + 6\langle Z_1Z_3\rangle_i + 12\langle Z_2Z_3\rangle_i + 14$	QUI $\lvert a_i\rvert^2$ $\alpha = 0.01\pi$ $\beta = 0.3\pi$	$\lvert a_i\rvert^2 E_i$
$\lvert 000\rangle$	1	1	1	36	0.215	7.74
$\lvert 001\rangle$						
$\lvert 010\rangle$						
$\lvert 011\rangle$						
$\lvert 100\rangle$						
$\lvert 101\rangle$						
$\lvert 110\rangle$						
$\lvert 111\rangle$						
					Total energy	20.16

Exercise 10.3.6 For the best values of parameter which you found: What does the QUI output state look like? Are the states corresponding to the solutions higher in probability?

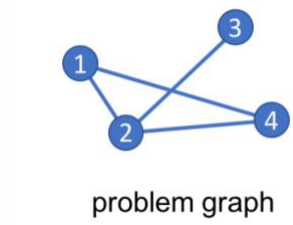
Exercise 10.3.7 From whatever is your best choice of α and β, add another QAOA iteration (see lectures: i.e. k=2) and see if you can get a better fidelity solution.

10.4 Graph partitioning

In this part of the lab you will be using a hybrid quantum variational method to solve a graph partitioning problem. We will divide this task into three stages (i) Write down the target Hamiltonian, (ii) encode a trial wavefunction (iii) measure the energy and the probability of success and (iv) optimize the parameters in the circuit to increase the probability of success.

The computational problem which we would like to solve is this: Given a graph, partition the vertices into two equal subsets with the minimum number of edges between the subsets.

Here is the example we will use in the lab:



problem graph

Exercise 10.4.1 Find the solution for the example given. Which two subsets, each with two vertices, which give the minimum number of edges between the two subsets? Draw answer here (there may be more than one).

Exercise 10.4.2 Quantum version of the solution. In the lecture we discussed how to map this to a QUBO (quadratic unconstrainted binary optimisation) problem – and its associated Hamiltonian/total energy. The first step is to associate each vertex with a particular qubit. If the qubit is in state 0, that indicates that vertex is in subset "0", if it is in state 1, that indicates the vertex is in subset "1".

Given your answer for 10.4.1, which two states correspond to correct solutions to this problem?

_____ and _____

Our next task is to find the Hamiltonian whose minimum energy encodes the answer to this optimization problem. We do this in two parts – considering vertices and edges. If there are an equal number of vertices in subset "0" and subset "1", we should have that the sum of the z-eigenvalues in our solution states will be zero:

$$\sum_{\substack{\text{vertices,}\\ i}} z_i = 0$$

Equivalently, if we can find a state is the lowest energy (ground state) of the operator form of the energy acting on qubits (each corresponding to a vertex):

$$H_A = \left(\sum_{\text{qubit, } i} Z_i \right)^2$$

then it will have an equal number of 0's as 1's in the solution, and hence an equal number of vertices in each subset.

Exercise 10.4.3 For the problem graph given, write out the (vertex) Hamiltonian, H_A:

We also need to minimize the number of edges which connect between the two. A Hamiltonian whose energy is equal to the number of edges between the two subsets is:

$$H_B = \sum_{i,j \in E} \frac{I - Z_i Z_j}{2}$$

where E is the set of edges (i.e. only include edges in the graph, and don't double count – the operators in the product commute).

Exercise 10.4.4 For the problem graph given, write out the (edge) Hamiltonian, H_B:

The final Hamiltonian is linear combination of these two Hamiltonians:

$$H = AH_A + BH_B$$

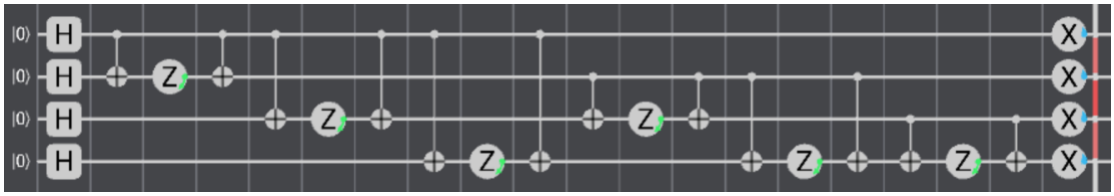
Exercise 10.4.5 If A=1 and B=1 (this choice works for our example), then write out the total Hamiltonian:

Evaluate the energy of all 16 computational basis states, and check that the ground state (lowest energy states) corresponds to a partitioning that does indeed match with your answer for 10.4.2 (again, exel might help). Don't forget to use Z eigenvalues.

Basis state, i	$E[H_A]$	$E[H_B]$	Basis state energy	Basis state, i	$E[H_A]$	$E[H_B]$	Basis state energy
$\|0000\rangle$	16	0	16	$\|1000\rangle$			
$\|0001\rangle$	4	2	6	$\|1001\rangle$			
$\|0010\rangle$				$\|1010\rangle$			
$\|0011\rangle$				$\|1011\rangle$			
$\|0100\rangle$				$\|1100\rangle$			
$\|0101\rangle$				$\|1101\rangle$			
$\|0110\rangle$				$\|1110\rangle$			
$\|0111\rangle$				$\|1111\rangle$	16	0	16

Now we will construct a trial wavefunction, using a method adapted from QAOA, in order to find the ground state(s) of this Hamiltonian, and hence solve the problem.

For this we will need to construct a circuit which initially has a set of Hadamard gates, then a series of phase operations, and finally a series of X-rotations, similar to that shown below (this circuit for H_A alone):



Exercise 10.4.6 First we will just attempt to find the ground-state of H_A alone. Note here the coefficients of the ZZ operators are all the same. Making each z-axis rotation angle of

$$\alpha = 0.3\pi$$

and final x-rotations by an angle of

$$\beta = \theta_X = 0.3\pi$$

construct the circuit above using the QUI. **NB. In the QUI you can highlight many R-gates at once and edit the rotation angles in one go (particularly useful when changing these angles later).**

a) Which states are most likely to be measured?

b) What is the probability that we measure a state with an equal number of vertices in each subset?

c) Optional. By systematically varying the angle of z-rotations, and x-rotations try to find α and β which give a higher probability of being in a state which has equal number of vertices in each subset (a balanced state).

α	β	Probability of being in any balanced state.

Now, let us attempt to find a solution to the problem by adding in the edge Hamiltonian H_B. We need to modify the circuit to accommodate the fact that the coefficients of ZZ terms are not all the same.

Exercise 10.4.7 Noting the coefficients in the Hamiltonian E_{ZZ}^{ij} modify the QUI circuit to the required rotations using

$$\alpha = 0.2\pi$$
$$\beta = 0.3\pi$$

a) Which two states are most likely to be measured?

_____ and _____

b) What is the probability that we measure a state corresponding to the correct solution?

c) What is the expectation value of the energy for this trial wavefunction?

d) Optional. By varying the angle of the z-rotations, and x-rotations through α and β (keeping each angle proportional to the corresponding term in the Hamiltonian) try to reduce the expectation value of the energy, and record the probability of a correct solution:

α	β	Energy	Probability

Exercise 10.4.8 If you got this far (well done!), try another graph partitioning problem with more vertices.