Week-6: Optimization-I

Contents

1 Introduction to Hybrid Algorithms

Hybrid algorithms utilize both classical and quantum assets to tackle conceivably troublesome problems in computer science (NP-hard problems), chemistry, physics, finance and mathematics. This methodology is especially encouraging for current quantum computers of constrained size and power and especially due to decoherence. Variations of hybrid quantum algorithms have as of late been illustrated, for example, the Variational Quantum Eigensolver for quantum chemistry and related applications and the Quantum Approximate Optimization Algorithm for computer science problems. Hybrid quantum algorithms can likewise be utilized for generative models, which expect to learn representations of information to make consequent tasks simpler. These algorithms combine trial quantum state preparation and hamiltonian estimation in these states with a non-linear classical optimizer. These calculations for the most part expect to decide the ground state eigenvector and the corresponding eigenvalue of a Hermitian Operator in which our solution is encoded. The simple concept behind applying these algorithms is rooted in the fact that quantum computers have limited coherence time. We must perform optimization on a classical computer so as to use limited quantum resources and get correct results. In CS problems, the cost function is encoded in the Hamiltonian which is mapped to a qubit Hamiltonian using strings of Pauli operators. We now discuss the first hybrid technique VQE.

2 Variational Quantum Eigensolver

Present and near-term quantum computers experience the bad effects of decoherence, readout and gate errors. Qubits are very delicate and start losing information once the program is started. We can not stop the program and rectify errors. This is the reason we can't run long calculations, that is, deep circuits on quantum computers. Another type of calculations began to show up since 2013 that brought attention on getting an advantage from these defective quantum computers in this NISQ era. The fundamental thought is very straightforward: build the qubit hamiltonian, run a short circuit of gates where a few single qubit gates are parametrized (quantum subroutine). At that point read the outcome, make changes in accordance, with the parameters on a classical computer (optimization phase), and repeat the hamiltonian estimation calculation on the new quantum state (with the new updated parameters). Thus, we create an iterative loop between the quantum and classical processors till convergence, creating VQE.

2.1 Variational Principle

Variational technique in quantum physics is a technique to obtain approximate answers to ground state energies using variational principle. It states that $\left\langle \hat{H} \right\rangle \geq E_g$ whee E_g is the ground state energy of the system and expctation of $\hat{H}$ represents the total energy of the system as described in Week-5. We now give the proof of this theorem.

Theorem 1. $\left\langle \hat{H} \right\rangle \equiv \left\langle \psi | \hat{H} | \psi \right\rangle \geq E_g$

Proof.

$$\begin{aligned}
\left\langle \hat{H} \right\rangle \equiv \left\langle \psi | \hat{H} | \psi \right\rangle &= \left\langle \sum_m c_m \psi_m | \hat{H} | \sum_n c_n \psi_n \right\rangle \\
&= \sum_m \sum_n c_m^* c_n \left\langle \psi_m | \hat{H} | \psi_n \right\rangle \\
&= \sum_m \sum_n c_m^* c_n E_n \left\langle \psi_m | \psi_n \right\rangle \\
&= \sum_m \sum_n c_m^* c_n E_n \delta_{mn} \\
&= \sum_m |c|^2 E_n \qquad (1)
\end{aligned}$$

Since $E_n \geq E_g$, we can write $\sum_n |c|^2 E_n \geq \sum_n |c|^2 E_g$ which further means that $\left\langle \hat{H} \right\rangle \geq \sum_n |c|^2 E_g$. Since E_g is a constant, it can come out and the inequality simplifies to

$$\begin{aligned}
\left\langle \hat{H} \right\rangle &\geq E_g \sum_n |c|^2 \qquad (2) \\
&\geq E_g \qquad (3)
\end{aligned}$$

□

The recipe for obtaining the ground state energies using the variational principle is as follows:

1. Prepare a trial wave function $|\psi\rangle$ which is parametrized.
2. Measure the expectation value of the Hamiltonian $\hat{H}$ in this trial state i.e. perform $\langle \psi | \hat{H} | \psi \rangle$
3. Minimize the expectation with respect to parameters to obtain the minimum energy
4. Substitute the values of the parameters obtained in Step 3 in the trial wave function

2.2 Ising Model

Ising model helps to visualize the relation between solving a physical system and its computational hardness. A simple example of this is the travelling salesman problem. It is difficult to draw connections as to how to model this physical system since solving it is an NP-hard problem. This is where we use the Ising model.

2.2.1 Classical Ising Model

Look at the fig. 1. Consider 2 magnets. If they are brought closer to each other, they tend to anti-align themselves in order to lower the energy. For abstraction, we consider these two magnets as spins. Thus, spins tend to anti-align. We associate binary random variables σ to

these spins. If the spin is pointing up, we associate with it $\sigma = 1$ and if it is pointing down, we associate with it $\sigma = -1$. Thus two such spins on a 1-D lattice contribute to either a total energy of 1 or -1 which is given by the product of these variables.

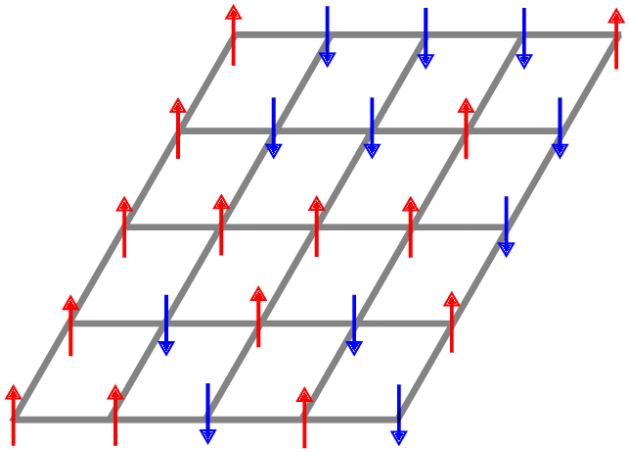


Figure 1: Spins on a lattice

If we go on to add more magnets (n magnets/spins) into the system and considering the interactions between any 2 magnets can be different, we introduce a coupling term and write the total Hamiltonian as

$$\hat{H} = -\sum_{j<k} C_{jk}\sigma_j\sigma_k \tag{4}$$

where C_{jk} represents the interaction term. If we have anti-ferromagnetic system, we will have all interaction terms to be negative. If we have ferromagnetic system, we will have all interaction terms to be positive. We can have mixed values as well depending upon the system under study. The aim is to find the lowest energy configuration. We shall take a simple example to demonstrate 4 spins on a 1-D lattice in an anti-ferromagnetic system.Let the interaction vector C=[-1.0,-2.0,-3.0]. We now calculate the lowest energy eigenvector and eigenvalue as given in Table 1.

Spin Configuration	Energy Eigenvalue
-1 -1 -1 -1	6.0
-1 -1 -1 1	0.0
-1 -1 1 -1	-4.0
-1 -1 1 1	2.0
-1 1 -1 -1	0.0
-1 1 -1 1	-6.0
-1 1 1 -1	-2.0
-1 1 1 1	4.0
1 -1 -1 -1	4.0
1 -1 -1 1	-2.0
1 -1 1 -1	-6.0
1 -1 1 1	0.0
1 1 -1 -1	2.0
1 1 -1 1	-4.0
1 1 1 -1	0.0
1 1 1 1	6.0

Table 1: Eigenvectors with their respective eigenvalues

We also add an external magnetic field such that now the classical Ising Hamiltonian is modified in this way

$$\hat{H} = -\sum_{j<k} C_{jk}\sigma_j\sigma_k - \sum_j h_j\sigma_j \tag{5}$$

where h_j is the strength of the external field. For quantum physicists and chemists, this Hamiltonian is representative of the energy. In computer science problems, we model our cost function in terms of this Hamiltonian. In Table 2, we look at some of these formulations.

Problem	Statement	Classical Ising Hamiltonian	Rationale
Vertex Cover	An NP-Hard problem, the aim is to find a minimum size vertex subset(vertex cover) of an un-directed graph G consisting of V vertices and E edges such that for every edge, atleast one of its incident vertices is in the subset(vertex cover). We formulate this problem in terms of graph coloring such that all the vertices in the vertex cover are given one color and the vertices which do not belong to the vertex cover are given another color or they are left uncolored.	$C\sum_i x_i$ $+ \mathrm{D}\sum_{ij\in E}(1-x_i)(1-x_j)$	The first term ensures that the size of the vertex cover remains minimum and the second term acts as the penalty such that that if both the vertices belonging to an edge are not colored, the energy is increased. $C < D$ should be chosen to account for the deviations from the correct solution.
Binary ILP	Given n binary variables, the aim is to minimize/maximize $\sum_{i=1}^{n} c_i x_i$ or $c^T x$ subject to the constraint that $Ax = b$ where c and x are vectors of size n, A is an $p \times n$ matrix and g is a p-dimensional vector. Here p represents the number of constraint equations. We discuss hereby the case of minimizing the cost function.	$C\sum_{i=1}^{n} c_i x_i$ $+\mathrm{D}\sum_{i=1}^{p}((\sum_{j=1}^{n} A_{ij}x_j) - b_i)^2$	The second term enforces the constraint equations. The second term is squared to account for both the overshooting and undershooting from the b_i.

Table 2: Classical Ising Hamiltonian for some instances of NP hard problems. ILP stands for integer linear programming

2.2.2 Quantum Ising Model

We now map the classical Hamiltonian to a qubit Hamiltonian. We replace the spin variables by pauli Z matrices since they also have 1 and -1 eigenvalues. The mapped qubit Hamiltonian becomes

$$\hat{H} = -\sum_{j<k} C_{jk} Z_j Z_k - \sum_j h_j Z_j \tag{6}$$

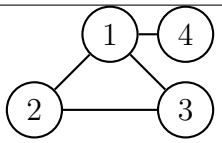
Problem	Example	Quantum Ising Hamiltonian
Vertex Cover		$2C + D + \left(\frac{D-2C}{4}\right)(\sigma_z \otimes I \otimes I \otimes I + \mathrm{I} \otimes \sigma_z \otimes I \otimes I + I \otimes I \otimes \sigma_z \otimes I + I \otimes I \otimes I \otimes \sigma_z) + \left(\frac{D}{4}\right)(\sigma_z \otimes \sigma_z \otimes I \otimes I + \sigma_z \otimes I \otimes \sigma_z \otimes I + \sigma_z \otimes I \otimes I \otimes \sigma_z + I \otimes \sigma_z \otimes \sigma_z \otimes I)$
Binary ILP	$c^T = [4, 2, 6]$ $\mathrm{x}^T = [x_1, x_2, x_3]$ $\mathrm{A} = \begin{bmatrix} 2 & 4 & 8 \\ 10 & 6 & 4 \end{bmatrix}$ $b^T = [25, 30]$	$6C + 424D - 2(C + 32D)(\sigma_z \otimes I \otimes I) + 2(-C + 8D)(I \otimes \sigma_z \otimes I) + (-C + 104D)(I \otimes I \otimes \sigma_z) + D(34(\sigma_z \otimes \sigma_z \otimes I) + 28(\sigma_z \otimes I \otimes \sigma_z) + 28(I \otimes \sigma_z \otimes \sigma_z))$

Table 3: Quantum Ising Hamiltonians for some instances of NP-hard problems (C and D are constants)

In Table 3, we give the qubit mapings of the instances of vertex cover and binary integer linear programming.

2.2.3 How to hop out of local minimum?

Nature drives towards the minimal energy microstate of a system. Envision that the energy difference between the ground state and the first excited state is little, but the energetic expense of going from one to the next is high. On the off chance that we start from a random distribution (of spins for example), we might never come out of the local minimum. This is the thing that occurs in metals in the event that they are chilled off too rapidly. A procedure called annealing helps in metallurgy by increasing the temperature, the possibility of overcoming the barrier (potential) increments and the crystal gets time to reconfigure itself. In the event that the barrier is high and the energy difference is little between the ground state and the next excited state, the likelihood of this incident drops. Hence, we switch to simulated annealing in which we use the concept of temperature to come out of the local minimum. We have given a separate handout for quantum annealing in which we see that for a graph coloring problem, as we lower the temperature , the chances of seeing the actual minimum increases. In quantum annealing, we use the concept of quantum tunneling to hop out of the local minimum.

2.2.4 Transverse Ising Model

In transverse ising model. we add an extra term to the Hamiltonian of pauli-X operators which facilitates quantum tunneling. Since we know the eigenvectors of the pauli-X matrix are the Hadamard basis, one can be simultaneously in all states if one uses pauli-X gates in the quantum circuit. This is the concept used in Adiabatic quantum computing in which the initial Hamiltonian is written in terms of Pauli-X operators. The modified Hamiltonian becomes

$$\hat{H} = -\sum_{j<k} C_{jk} Z_j Z_k - \sum_j h_j Z_j - \sum_j f_j X_j \tag{7}$$

where f_j are interaction strengths of some external field with the spins in the lattice.

2.3 VQE Algorithm

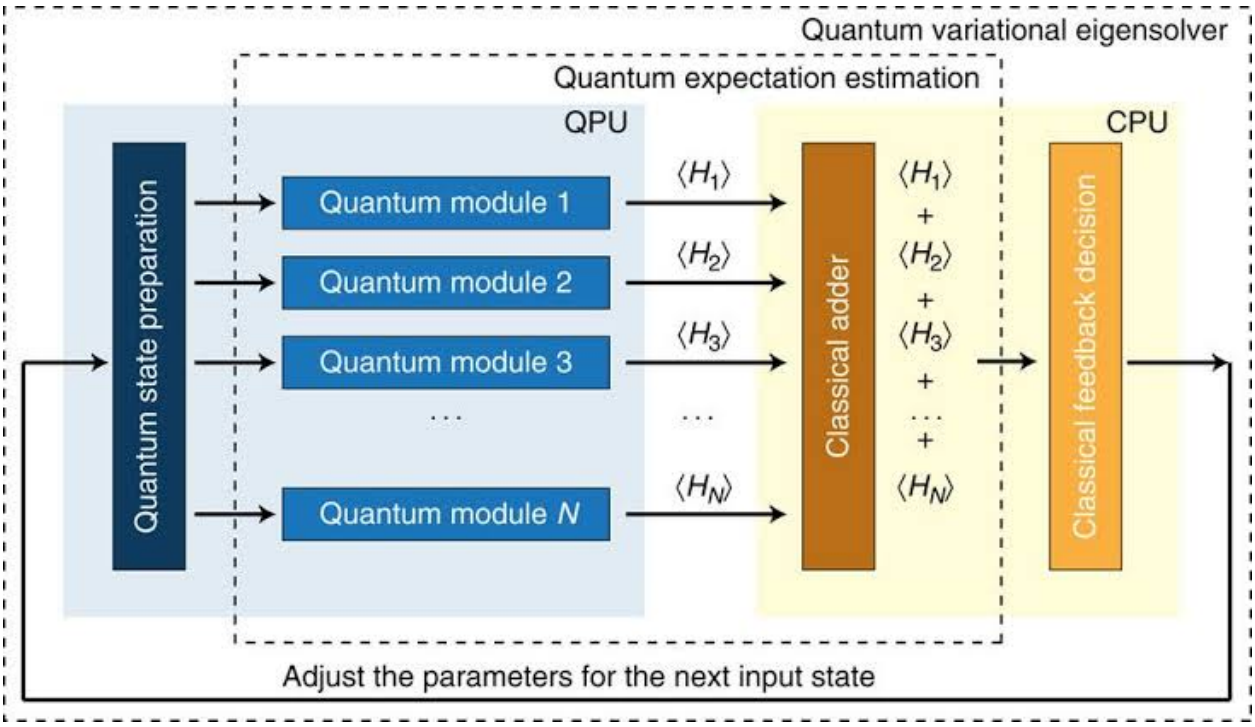


Figure 2: VQE Flowchart [1]

In Fig. 2, we give the general flowchart of the VQE algorithm. We first prepare a trial variational quantum state. This state must be carefully prepared to give correct results. We then measure the expectation of individual terms in the total Hamiltonian operator on this quantum circuit. We then add the answers from all such N modules on a classical computer using an adder which is then fed to a classical non-linear optimizer to generate the next set of variational parameters which are then fed to the quantum circuit. The new circuit is formed and the measurement process is carried out again. This process is repeated till convergence to obtain the lowest energy solution and its corresponding energy eigenvector.

2.4 Variational Circuit Example

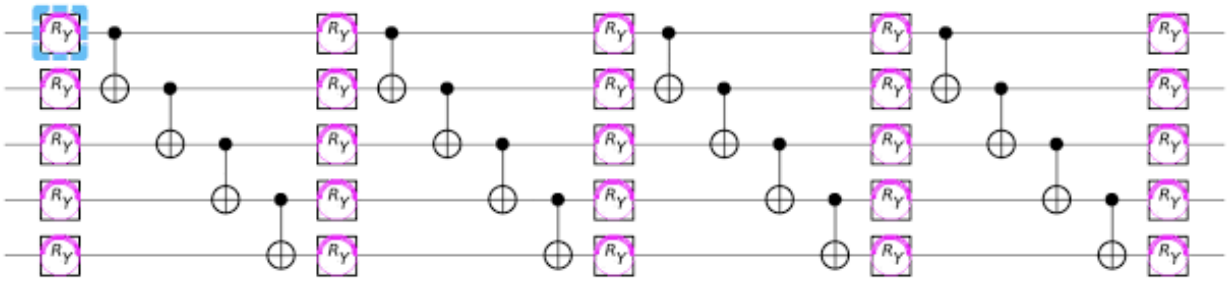


Figure 3: Linearly entangled C-NOT gates & RY rotation unitary based variational circuit [2]

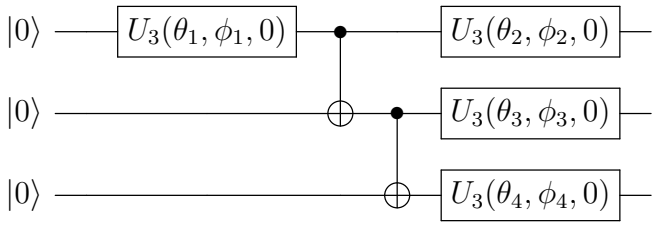
3 Exercises

3.1 Theory Exercises

1. **1-D Harmonic Oscillator**: Find the ground state energies to the following trial wave functions for a 1-dimensional quantum harmonic oscillator a) $Ae^{-\beta x^2}$ b) $Axe^{-\beta x^2}$. Verify that we have guessed the correct wave functions and they give the energies of the ground state and the first excited state respectively.

2. **Ising Formulations of NP-hard problems**: Formulate the Classical and Quantum Ising Hamiltonians for Maxcut Problem

3. What is the output of the given circuit?



4. **Application-Based Question**: Design an algorithm for efficient quantum circuit preparation with reduced variational parameters for a multi-electron system with n orbitals and m electrons. You must design the circuit while respecting particle number and time reversal symmetries.

5. k^{th} **Excited State**: Modify VQE algorithm such that it gives the energy of the k^{th} excited state. One of the popular algorithms to achieve this is the Weighted Subspace-Search VQE known as WSS-VQE. Think whether you can come up with your own algorithm.

3.2 Qiskit Exercises

1. **Minimal Vertex Cover Problem using VQE**: Implement VQE on an instance of minimal Vertex Cover problem using the Qiskit packages and verify the result.

2. Prove that the Pauli matrices do not commute.

3. For the example given for the classial Ising model with J=[-1.0,-2.0,-3.0], we now add magnetic field given as h=[3.0,2.0,1.0,0.5]. Using simulated annealing, find the optimal energy. Have 20 trials. Use the dimod package.

4. Calculate the energy corresponding to the following Hamiltonian operator on the state $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. We give the following transverse ising model

$$\hat{H} = -2Z_1Z_2 - Z_1 - 0.5Z_2 - 0.5X_1 - X_2$$

5. * Implement **WSS-VQE** on an instance of Heisenberg Ising Model.

References

[1] Coles, Patrick & Eidenbenz, Stephan & Pakin, Scott & Adedoyin, Adetokunbo & Ambrosiano, John & Anisimov, Petr & Casper, William & Chennupati, Gopinath & Coffrin, Carleton & Djidjev, Hristo & Gunter, David & Karra, Satish & Lemons, Nathan & Lin, Shizeng & Lokhov, Andrey & Malyzhenkov, Alexander & Mascarenas, David & Mniszewski, Susan & Nadiga, Balasubramanya & Zhu, Wei. (2018). Quantum Algorithm Implementations for Beginners.

[2] JAMES WEAVER. *Medium* [online]
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