Week 6: Optimization-I

Hybrid Algorithms

- Hybrid algorithms utilize both classical and quantum computers to perform certain computational tasks.
- We prepare a trial quantum state. Encode the cost function into Qubit Hamiltonian. Measure its expectation and feed the energy answer to a classical optimizer which minimizes the energy by supplying the new variational parameters. This process is repeated till convergence.

Hybrid Algorithm-I: Variational Quantum Eigensolver (Step-1)

- Based on Variational Principle $\left\langle \hat{H} \right\rangle \equiv \left\langle \psi | \hat{H} | \psi \right\rangle \geq E_g$

  If you choose a trial state, the Hamiltonian expectation gives a value which is greater than or equal to ground state energy.

- If you can carefully prepare the trial state, one can encode the solution of the problem in the ground state of the system. This is the crux of the first step in VQE.

Step-2 (a):
Form the Classical Hamiltonian

- We first map the cost function to a classical Ising model whose Hamiltonian operator is given by

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

  Where C and h represent the coupling matrix between two neighboring spins and the magnetic field strength respectively.

- This is the Classical Ising Hamiltonian. For a ferromagnetic substance, the particles tend to align in the same direction. Hence, C matrix has elements which have positive values so as to decrease the overall energy.

Step-2 (b):
Form the Quantum Hamiltonian

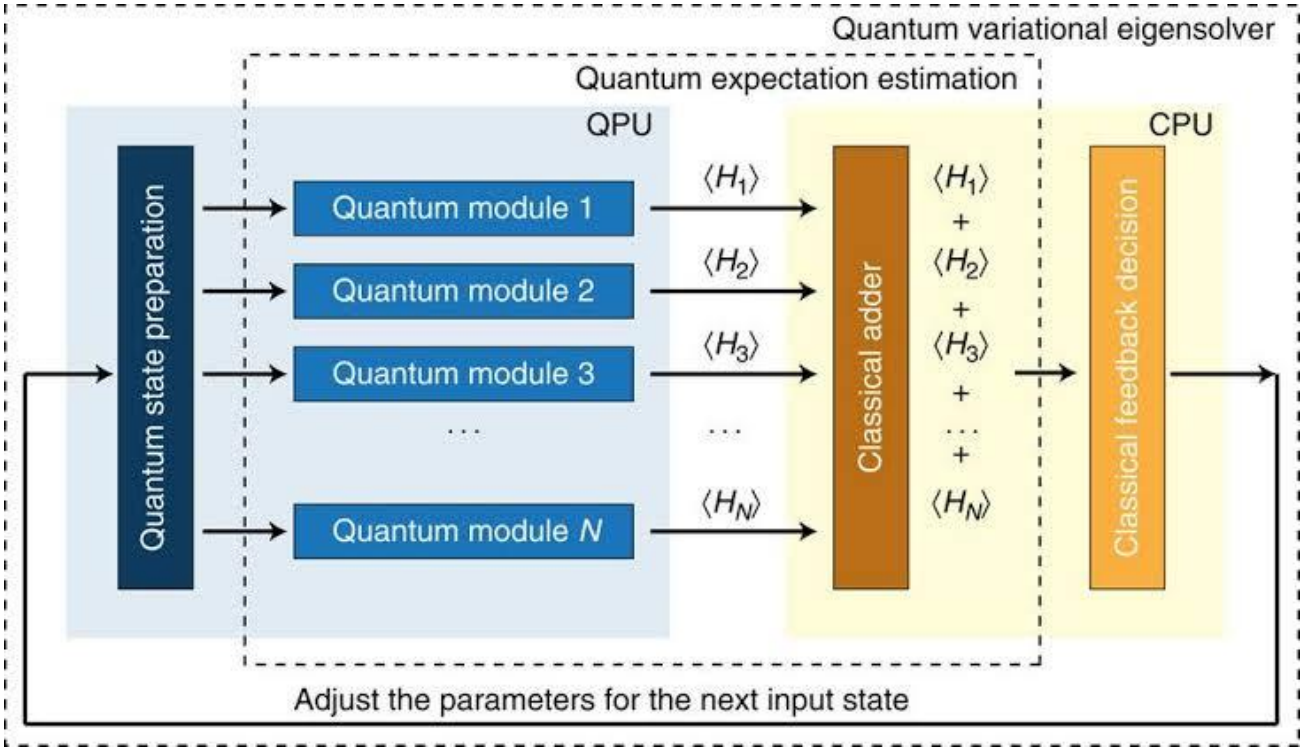
- We nowmap the classical Ising Hamiltonian to a quantum Ising Hamiltonian given by

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

Where Z is a pauli-Z matrix. This mapping is done as the Z matrix has +1 and -1 eigenvalues which is representative of the values of the spin variables.

- For computer science problems, our spins take the values of 1 and 0. Hence, we map the spins to (1-Z)/2 since it has 0 and 1 energy eigenvalues.

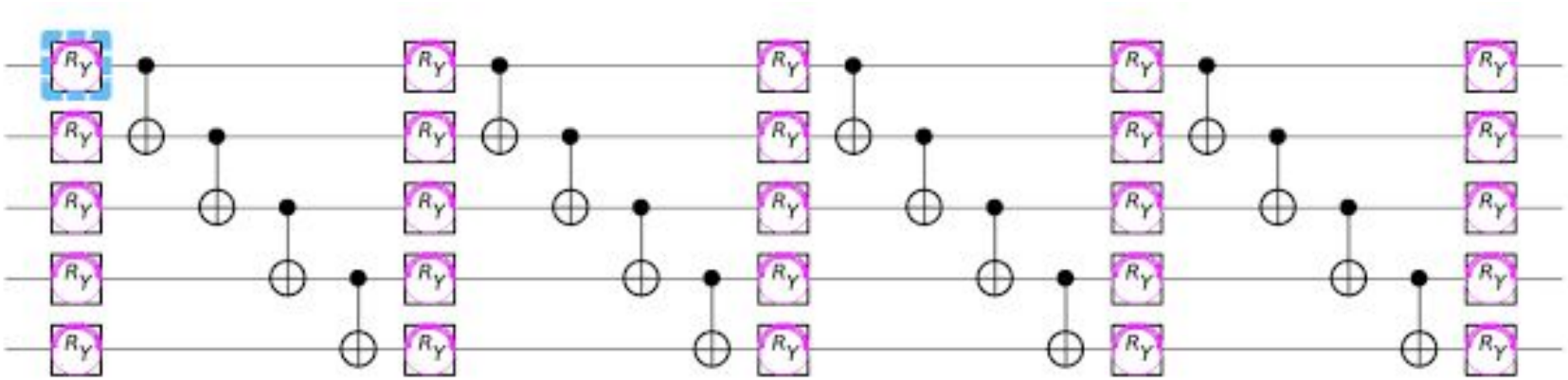
Step-3:
Implementation



Algorithm Explanation

- Quantum Subroutine: We prepare a trial parametrized quantum circuit using rotation and entangling gates. We measure the expectation value of the individual terms in the Hamiltonian operator on N quantum modules simultaneously so as to speed up the process.
- Classical Computer: The individual expectation values are fed to a classical adder and then sent to a non-linear optimizer to minimize the energy landscape by finding the next set of parameters of the rotation gates.
- Repeat till convergence to obtain the approximate ground state energy

Popular Heuristic Ansatz

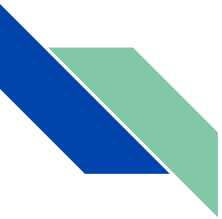


- In this ansatz, we have RY rotation gates which have the variational parameters that we were earlier talking about. These are optimized to find the lowest energy eigenvalue. In this ansatz, the entanglement is linear.

Transverse Ising Model

- Quantum Tunneling helps to come out of the local minima and drive the system towards obtaining a global minima. This is an essential part of quantum tunneling which we shall cover in the next week.
- To achieve quantum tunneling, we need to modify our classical Ising Hamiltonian to include one more term which is formed of Pauli-X unitaries to give the transverse Ising model.

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



For more detailed description, study this week's handout.

References are given in handouts.

Solve theory and Qiskit exercises given in the handout.