Week 7: Optimization-II

Adiabatic Theorem

- Based on Adiabatic Theorem: In an adiabatic process, the external conditions change very slowly such that if the system starts in its ground state, it remains in its ground state. The eigenstates become instantaneous and we find out that the wave function picks up a geometric phase in addition to dynamic phase.
- It remains an open question whether AQC will provide any advantage over its classical counterpart.

Adiabatic Quantum Computing

- We start with some initial Hamiltonian and reach our target Hamiltonian adiabatically using an evolution parameter s=t/T where T is the total time of evolution. The time-dependent Hamiltonian becomes

$$\hat{H} = (1-s)\hat{H}_{init} + s\hat{H}_{target}$$

- How does one decide the value of T? The answer lies in the fact that it is sensitive to g(t) which is the energy gap between the ground state and the first excited state. $T \propto \frac{1}{min(g(t))^2}$

Metropolis Monte Carlo Algorithm (1/2)

Algorithm 1: Metropolis Monte Carlo Algorithm

1. Assign initial ansatz x_0 to explain the molecular structure.
2. **Loop**
   (a) Randomly perturb to get the state $x_{i+1} = x_i + \triangle x_{rand}$. Calculate E_{i+1}.
   (b) **If**: $E_{i+1} \leq E_i$, accept x_{i+1} as the new state.
   Else: With probability $\exp\left(-\frac{\triangle E}{K_B T}\right)$, accept x_{i+1}.[2]
   Otherwise keep x_i as the current state.

MMC Explanation (2/2)

- We do biased sampling in this algorithm. We never reject any subspace of the solution. We accept it with a certain probability. For the physics students, they can understand this in terms of Ising modelling in which if we flip a spin and the energy increases, we accept it with a certain probability which is proportional to $\exp\left(-\frac{E(\mathbf{r})}{K_B T}\right)$
- Using this approach, we drive our landscape to the solution. This is not an optimal approach.

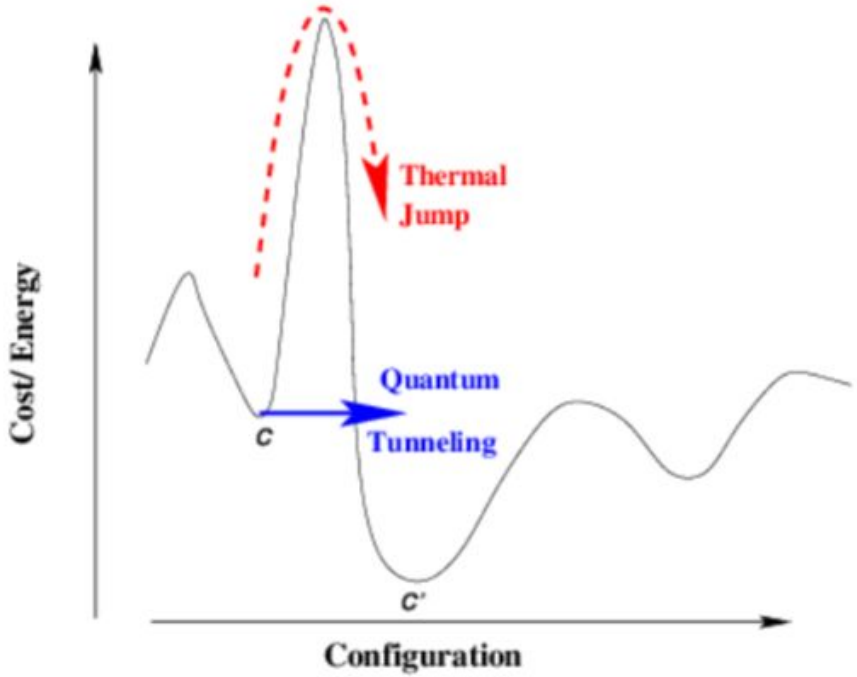
Simulated Annealing (1/2)

- Using Annealing, we control the number of iterations of the loop in Algorithm 1. We reduce the value of the temperature variable slowly as the simulation proceeds, i.e. with each iteration. The algorithm initializes the temperature parameter to a high value, and then it is decremented with each loop according to the rules specified by the algorithm.
- The stopping condition is generally T=0, but in our case, we add an extra condition which states that the algorithm may also halt if the lowest energy configuration has been found.

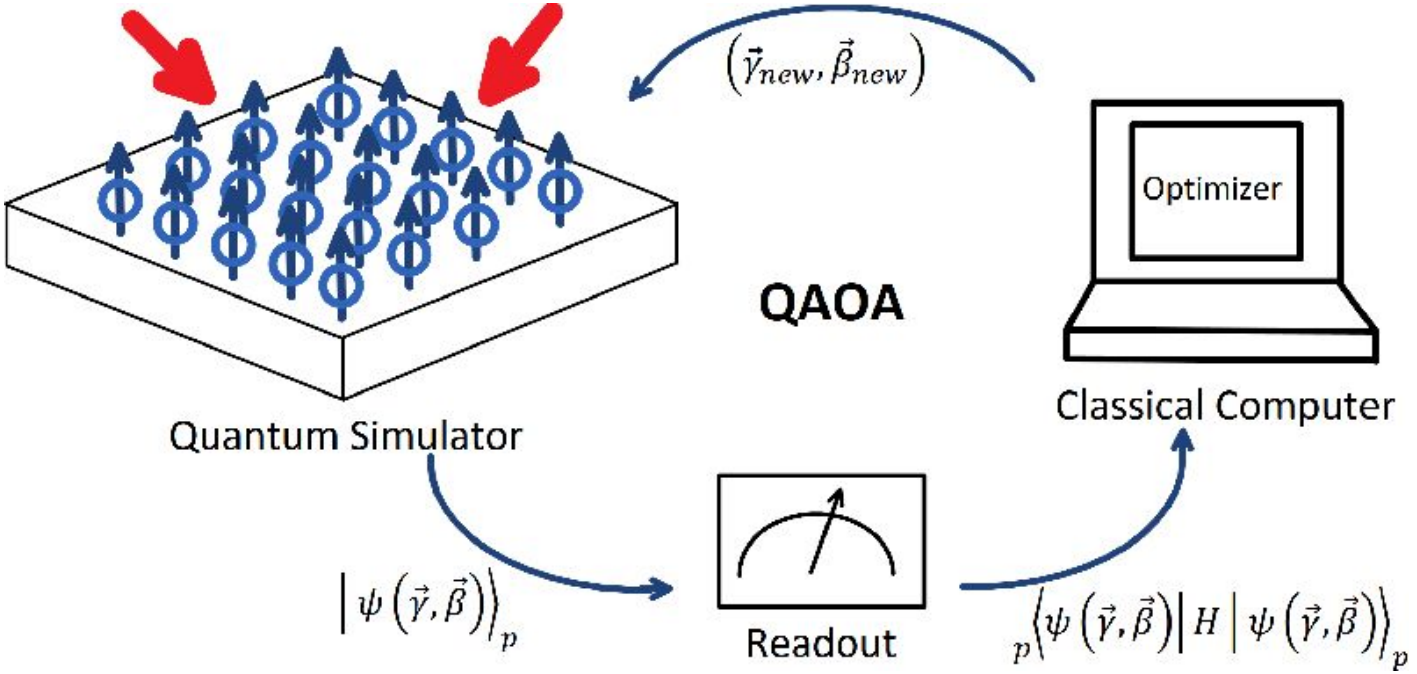
Simulated Annealing (2/2)

- Although combining Simulated Annealing with the Metropolis Monte Carlo algorithm helps us explore fruitful areas of the search space, there still exists some pitfalls of this approach.
- When T is low, our algorithm only accepts the bad choice with very low probability.
- When the change in energy is low, our algorithm only accepts the bad choice with very low probability. Thus, there is a scope for improvement.

Quantum Annealing



Quantum Approximate Optimization Algorithm Flowchart



QAOA Logic

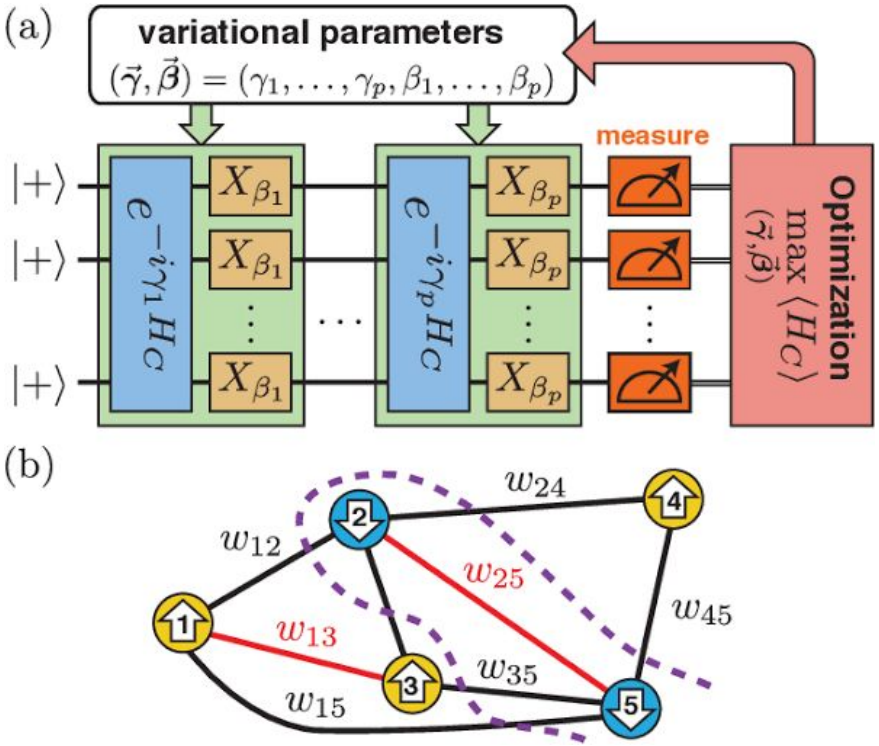
- We take our time dependent adiabatic Hamiltonian.
- Perform Trotterization to get the following unitary with 2p angles where

$$U = U(\hat{H}_{init}, \beta_0)U(\hat{H}_{targ}, \gamma_0)U(\hat{H}_{init}, \beta_1)U(\hat{H}_{targ}, \gamma_1).....U(\hat{H}_{init}, \beta_p)U(\hat{H}_{targ}, \gamma_p)$$

p is the precision of the algorithm.

- It is a polynomial time algorithm which has the capability of finding correct solutions to a given optimization algorithm

QAOA Variational Circuit and application In MaxCut



Thank-You