

Week 7: Optimization-II (a)

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1 Quantum Annealing

1.1 Metropolis Monte Carlo

¹ To solve a molecular mechanics problem, we usually carry out the following steps-

1. Initially give an ansatz to explain the molecule structure.
2. Calculate the resultant energy of this structure.
3. Adjust internal properties of our chosen configuration.
4. Repeat steps 2 and 3 till we reach the lowest energy configuration.

Monte Carlo simulations aim to explore the system in order to determine the equilibrium average of some property A . The form of a Monte Carlo integral is

$$\langle A \rangle = \int A(\mathbf{r})P(\mathbf{r})d\mathbf{r} \quad (1)$$

where $\langle A \rangle$ refers to the expectation of the property A , \mathbf{r} refers to the coordinates of our system (and can be generalized to represent the various structures), and

$$P(\mathbf{r}) = \frac{\exp\left(-\frac{E(\mathbf{r})}{K_B T}\right)}{\int \exp\left(-\frac{E(\mathbf{r})}{K_B T}\right) d\mathbf{r}} \quad (2)$$

Instead of solving the integral directly, we choose the configurations uniformly at random, to be the evaluation points for the integral. Sampling could give us a reasonable representation of all the states. At each step we calculate the resultant energy, estimate $A(\mathbf{r})P(\mathbf{r})$ and find $\langle A \rangle$.

This approach fails because we have assumed all configurations have equal contribution to the equilibrium average. Intuitively we can say this assumption is false since low energy configurations have the most contribution to the global equilibrium. Mathematically, we see that $P(\mathbf{r})$ is proportional to the Boltzmann factor $e^{-E/K_B T}$, which expresses the probability of a state of energy E relative to the probability of a state of zero energy. As E increases, $P(\mathbf{r})$ decreases and hence only low energy configurations make a significant contribution to the integral.

Hence we conclude that Monte Carlo algorithms in general are not biased towards any particular configuration of the system, and we need a modified version that caters to low energy configurations in general. This is known as the **Metropolis Monte Carlo algorithm**, and is detailed in Algorithm 1.

¹Adapted from [1]

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 $x_{i+1} = x_i + \Delta x_{rand}$. Calculate E_{i+1} .
 - (b) **If:** $E_{i+1} \leq E_i$, accept x_{i+1} as the new state.
Else: With probability $\exp\left(-\frac{\Delta E}{K_B T}\right)$, accept x_{i+1} .²
Otherwise keep x_i as the current state.
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1.2 Simulated Annealing

Annealing is a physical process in which we heat a metal till it starts glowing, and then slowly cool it in still air at room temperature. Without going into the gritty details, we state that entropy increases with temperature and therefore higher the the energy of the system, the higher is its entropy.

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 T 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. 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. Recall that with probability $\exp\left(-\frac{\Delta E}{K_B T}\right)$, we accept a bad choice. This means that there exists conditions in which we can get stuck in local minima (when the probability is very low). Let us see these cases in a bit more detail.

- When T is low, our algorithm only accepts the bad choice with very low probability since $\text{Pr} \propto e^{-1/T}$. This is shown in figure 1.

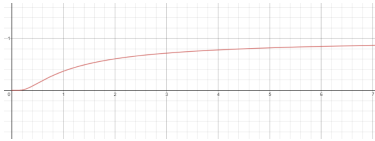


Figure 1: Graph of $e^{-\frac{1}{T}}$. When Temperature $T \rightarrow 0$, $e^{-\frac{1}{T}} \rightarrow 0$. Note that $T \geq 0$ in our model.

- When ΔE is high, our algorithm only accepts the bad choice with very low probability since $\text{Pr} \propto e^{-\Delta E}$. This is shown in figure 2.

These pitfalls indicate to us that there exists some scope for improvement upon the classical model.

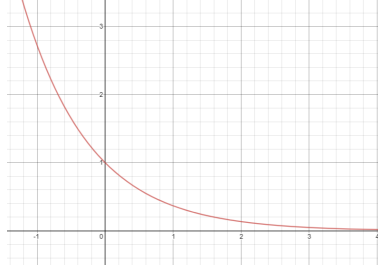


Figure 2: Graph of $e^{-\Delta E}$. When $\Delta E \rightarrow \infty$, $e^{-\Delta E} \rightarrow 0$.

1.3 Quantum Annealing

At the core of Quantum Annealing lies a physical phenomenon known as **Quantum Tunneling**. Quantum tunnelling is an entirely quantum phenomenon where a subatomic particle passes through a potential barrier (which are classically impenetrable), without having enough potential energy. Therefore, this phenomenon naturally lends itself as an alternative to simulated annealing when the latter fails.

In quantum annealing, we try to optimize a Hamiltonian (classical or quantum). As seen in previous lectures this is equivalent to optimizing the energy of state configurations. We add a kinetic energy term to this Hamiltonian and reduce it from a very high initial value to zero eventually. The reduction is assured to reach the ground state of the classical Hamiltonian, if carried out adiabatically.

$$\mathbb{H}_{\text{quantum}} = \mathbb{H}_{\text{classical}} + \mathbb{H}_{\text{kinetic}} \quad (3)$$

While CA uses only $\mathbb{H}_{\text{classical}}$ as a cost function, QA requires $\mathbb{H}_{\text{kinetic}}$ for the purpose of introducing artificial quantum fluctuations, which are used to try to escape local minima[2].

Simulations clearly demonstrate [2] that quantum annealing algorithms converge much faster than the corresponding classical annealing. What sets quantum annealing apart from simulated annealing, is the non-local nature and its higher tunneling ability as seen in figure 3.

References

- [1] D. L. G. Cheung, “Structures and properties of liquid crystals and related molecules from computer simulation,” Ph.D. dissertation, Durham University, 2002.
- [2] O. Titiloye and A. Crispin, “Quantum annealing of the graph coloring problem,” *Discrete Optimization*, vol. 8, no. 2, pp. 376 – 384, 2011. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S1572528610000721>
- [3] A. Das and B. K. Chakrabarti, “Colloquium: Quantum annealing and analog quantum computation,” *Reviews of Modern Physics*, vol. 80, no. 3, p. 1061–1081, Sep 2008. [Online]. Available: <http://dx.doi.org/10.1103/RevModPhys.80.1061>

³Image and explanation by Das et.al [3].

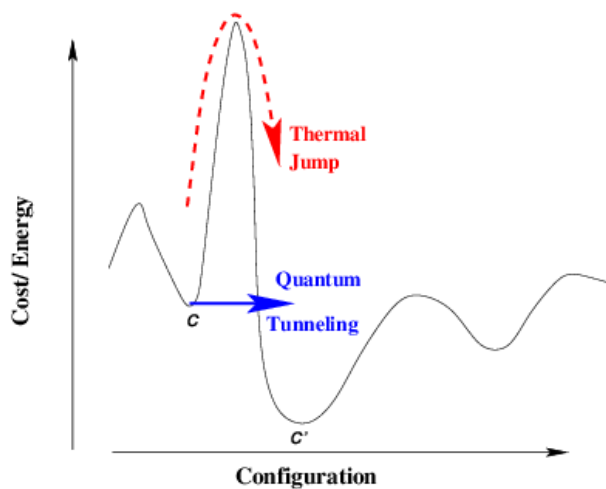


Figure 3: While optimizing the cost function of a computationally hard problem, we have to discard the local minimum like the configuration C , to reach a deeper (possibly global) minimum C' . This requires jumps or tunneling like fluctuations in the dynamics. If the barrier is high enough, thermal jump becomes very difficult (due to the probability being very low). However, if the barrier is narrow enough, quantum tunneling often becomes quite easy. ³