Lecture 1: Quantum Annealing, Quantum Walks, Adiabatic Quantum Computing

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1 Overview: what I am going to cover

- This lecture: some of the theory behind quantum annealing and related algorithms, why we expect they could do better than classical
- Next lecture: problem mapping and some important complexity theory, essentially all classical, but important background for understanding quantum annealing
- Third lecture: Advanced topics, brief overview of more advanced aspects such as error correction, biased searching methods, shortcuts to adiabaticity

2 Before we do anything, why should we care: combinatorial optimisation (and sampling)

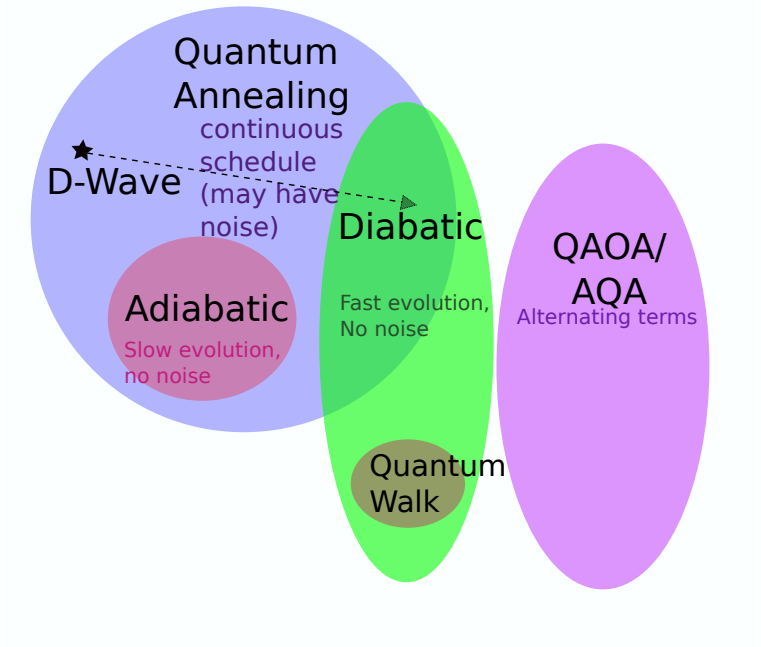
- These problems come up everywhere, logistics, design, biology, computing, probabilistic inference, machine learning etc...
- Better solutions to these problems could make a huge difference
- A finite (but large) number of possible solutions, can't practically check them all $\rightarrow$ combinatorial explosion

- Need clever tricks to find "good" solutions, but probably can't find a trick to always find the absolute best solution ($P? = NP$)
- Sampling, sometimes you want to find many "good" solutions (for example thermal distributions)

3 Terminology

- A warning: historical use of terminology is not consistent and still evolving, be careful when reading papers, check methods, don't just rely on the meaning of words
- Where it is seems to be converging to:
  1. Quantum Annealing=Anything using continuous time quantum evolution to solve problems which involved parameter "sweeps", usually finite temperature
  2. Adiabatic Quantum Computing=Quantum Annealing in the limit of slow evolution (where the adiabatic theorem applies) and closed systems
  3. Diabatic Quantum Computing= Quantum annealing with closed systems but with rapid quenches
  4. (continuous time) quantum walks=Specific algorithms which are based on evolution with constant Hamiltonians
  5. Quantum Approximate Optimisation Algorithm (QAOA)= (a.k.a. Quantum Alternating Operator Ansatz) A related protocol where operators are applied in an alternating way (often compiled to gate model), AQA= Approximate Quantum Annealing, a similar protocol but with parameters chosen in a different way

Where the language seems to be evolving to (involves some guesswork and not universal)



4 Reminder of continuous time quantum mechanics and how it can be used to compute

- Hamiltonians acting on qubits: n qubits and $N = 2^n$ possible states, states represented by bitstrings, Hamiltonians can be thought of as huge matrices because QM is linear
- Evolution wrt. Schrödinger equation ($\frac{\partial}{\partial t}|\psi\rangle = -iH(t)|\psi\rangle$) can be written $|\psi(t)\rangle = U(H,t)|\psi(0)\rangle$ For a time independent H

$$U(H,t) = \exp(-iH\,t) \tag{1}$$

In general, for a time dependent Hamiltonian the evolution needs to be represented by an infinite product of matrix exponentials:

$$U(H,t_{\max}) = \int_0^{t_{max}} Dt\,\mathcal{T}\exp(-iH(t)) = \lim_{q\to\infty}\mathcal{T}\prod_{j=1}^{q}\exp(-i\frac{t_{max}}{q}\,H(\frac{j\,t_{max}}{q})) \tag{2}$$

$\mathcal{T}$ indicates time ordering, path integral taken over multiplication rather than addition. This representation is useful for (small) numerical simulation since matrix exponentials can be calculated numerically.

- Combinatorial optimisation problems can be represented as Hamiltonians which are diagonal in the computational basis, → lower energy states=better solutions
- Adiabatic theorem of quantum mechanics, (look it up if you don't know what it is)
- Beyond adiabatic: diabatic and finite (low) temperature, not a lot of theory, diabatic is a recent "hot topic" theory developing rapidly [1]
- Can also simulate continuous time on a gate model machine (and recent QAOA work suggests this is the best way to solve optimization problems [2]), research on continuous time still valuable if gate model dominates

5 Why continuous time might be useful

- Unstructured search, only information is whether answer is right or wrong → continuous time analogue of Grover search

Two Hamiltonians, problem Hamiltonian $H_{\text{search}} = -|x\rangle\langle x|$, where $|x\rangle$ is the solution (classical bit-string). Driver Hamiltonian, $H_{\text{full}} = -|\omega\rangle\langle\omega|$, where $|\omega\rangle = \frac{1}{\sqrt{N}}\sum_i |i\rangle$, equal sum of all computational basis states. Start in equal superposition $|\omega\rangle$, unbiased initial guess.

By symmetry, all dynamics take place in the space spanned by $|x\rangle$ and $|\omega\rangle$. These aren't orthogonal, but we can choose an orthogonal basis made from these states, I choose $\{|x\rangle, |\tilde{\omega}\rangle = |\omega\rangle - \frac{1}{\sqrt{N}}|x\rangle\}$. In this reduced basis

$$H_{\text{search}} = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix} \tag{3}$$

and

$$H_{\text{full}} = \begin{bmatrix} -\frac{1}{N} & -\frac{\sqrt{N-1}}{N} \\ -\frac{\sqrt{N-1}}{N} & \frac{1}{N} - 1 \end{bmatrix} = \begin{bmatrix} 0 & -\frac{1}{\sqrt{N}} \\ -\frac{1}{\sqrt{N}} & -1 \end{bmatrix} + O(\frac{1}{N}) \tag{4}$$

Full matrix

$$\begin{aligned} H(\Gamma) = H_{\text{search}} + \Gamma H_{\text{full}} &\approx \begin{bmatrix} -1 & -\Gamma\frac{1}{\sqrt{N}} \\ -\Gamma\frac{1}{\sqrt{N}} & -\Gamma \end{bmatrix} \\ &= -\frac{1}{2}(1+\Gamma)\,\mathbf{1} + \frac{1}{2}(1-\Gamma)\,\sigma^z - \frac{\Gamma}{\sqrt{N}}\sigma^x \end{aligned} \tag{5}$$

where σ^z and σ^x are the respective Pauli matrices. Eigenvalues will be

$$E_\pm = -\frac{1}{2}(1+\Gamma) \pm \sqrt{\frac{1}{4}(1-\Gamma)^2 + \frac{\Gamma^2}{N}} \tag{6}$$

gap is therefore

$$\Delta(\Gamma) = E_+ - E_- = \sqrt{(1-\Gamma)^2 + 4\frac{\Gamma^2}{N}} \tag{7}$$

with a minimum gap at $\Gamma = 1$ of $\frac{2}{\sqrt{N}}$. Find (un-normalized) Eigenvectors $v_\pm$ by applying top line of the matrix in Eq. 5

$$-\langle v_\pm \mid x\rangle - \frac{\Gamma}{\sqrt{N}}\langle v_\pm \mid \tilde{\omega}\rangle = E_\pm \langle v_\pm \mid x\rangle . \tag{8}$$

solve to obtain

$$\frac{\langle v_\pm \mid x\rangle}{\langle v_\pm \mid \tilde{\omega}\rangle} = \frac{\sqrt{N}}{\Gamma}(1+E_\pm) = \frac{\sqrt{N}}{\Gamma}\left(\frac{1}{2}(1-\Gamma) \pm \sqrt{\frac{1}{4}(1-\Gamma)^2 + \frac{\Gamma^2}{N}}\right). \tag{9}$$

For every case except for $\Gamma \approx 1$, we find $\frac{\langle v_+|x\rangle}{\langle v_+|\omega\rangle} \propto \sqrt{N}$, eigenvector has a high overlap with $|x\rangle$ and therefore there are no search dynamics. At $\Gamma = 1$, the gap takes a minimum value of $\Delta(\Gamma = 1) = 2\sqrt{N}$ and $\langle v_+ \mid x\rangle = \langle v_+ \mid \tilde{\omega}\rangle$, $\langle v_- \mid x\rangle = -\langle v_- \mid \tilde{\omega}\rangle$. For large N, $|\omega\rangle = |\tilde{\omega}\rangle + O(\frac{1}{N})$, and therefore $\left\langle x\right| \exp\left[-iH(\Gamma=1)\pi\sqrt{N}\right] \left|\omega\right\rangle = 1 - O(\frac{1}{N})$ [3]. In other words, evolving for at time proportional to $\sqrt{N}$ can solve the problem, this is exactly the Grover speedup (quantum walk in this example)! All classical methods would take $O(N)$ to find the answer.

Also works with adiabatic but not with linear schedule! For linear schedule scales as $\frac{1}{\Delta^2} \rightarrow$ no better than classical. Non-linear schedule can get scaling with $\frac{1}{\Delta}$, same $\sqrt{N}$ speedup [4].

Can also interpolate between the two and get same speedup, in other words, I can make an algorithm which is 30% AQC and 70% quantum walk and it will also get a $\sqrt{N}$ speedup [5].

Other evidence:

- All quantum circuits can be mapped to (non-stoquastic) AQC, in other words it is a universal model → complicated to prove, I won't cover it here
- Other permutation symmetric models → efficient to simulate because of symmetry, can show exponential speedups
- Extrapolated numerical scaling from small sizes → suggests that perfect continuous. time will do very well
- D-Wave experiments, too complicated to discuss in detail here → mixed results but essentially whether future versions will be useful is an open question

6 What about real problems?

- Ising model

$$H_{\text{Ising}} = \sum_{ij} J_{ij} Z_i Z_j + \sum_i h_i Z_i \tag{10}$$

- Simplest possible problem: $\rightarrow$ max cut, take a graph G, for every edge set $J_{ij} = 1$, -1 unit of energy where pairs disagree $+1$ where they agree, minimum energy for maximum number of disagreements
- Slightly more complicated: maximum independent set, take a graph G, for each edge add -1 to h at each end, and set $J_{ij} = 1$, energy of -1 for $|00\rangle$, $|01\rangle$, $|10\rangle$, energy of $+3$ for $|11\rangle$, enforces independence, no adjacent ones, add an additional field of $0 < \lambda < 4$ to encourage maximum number of ones
- Next lecture will be the details of problem mappings!

7 Energy arguments for diabatic quantum computing

- Consider a quantum walk $H = \Gamma H_{\text{hop}} + H_{\text{problem}}$
- Start in the ground state of H_{hop}, energy expectation $\langle H_{\text{problem}} \rangle$ can only go down, why?
- Energy has to be conserved and $\langle H_{\text{hop}} \rangle$ can only go up [6, 7]
- Furthermore, if we take $\Gamma \rightarrow \Gamma'$ where $\Gamma' < \Gamma$ than $\langle H \rangle$ decreases (setting gs energy to zero w.l.o.g) while $\langle H_{\text{problem}} \rangle$ remains unchanged
- By rescaling time/energy we can always put the evolution in the form $H(t) = \Gamma(t) H_{\text{hop}} + H_{\text{problem}}$ therefore, diabatic energy evolution can never increase $\langle H_{\text{problem}} \rangle$ as long as Γ is non-increasing [8]
- Arguments can also be made based on modified adiabatic theorem, but require special structure [1]

8 Summary

- Quantum annealing is exciting because it can solve combinatorial optimisation problems, which come up everywhere
- Be careful when reading quantum annealing papers, terminology is not standardized
- Continuous time evolution expressed as an integral over multiplication rather than addition
- Continuous time versions of Grover's algorithm exist, show quantum speedup possible in this setting, + other bits of evidence
- Diabatic quantum computing (no noise but much too fast to be adiabatic) is a popular recent topic and the theory is just being established, too fast to rely on simple adiabatic theorem

References

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