Lecture 3: Advanced topics in quantum annealing

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1 Overview: what is in this lecture

- (non-)stoquasticity and path integral quantum Monte Carlo
  - Perron-Frobenius theorem and the PageRank algorithm (original algorithm which powered Google search)
  - Where non-stoquastic Hamiltonians arise: Electronic systems
  - The sign problem and path integral quantum Monte-Carlo
  - QMC does not simulate noisy QA (a common misconception)
- Reverse annealing and biased search
  - Core idea, use information from classical algorithms or previous runs to help the anneal
  - Coherent reverse annealing "Mexican hat" protocol
  - Dissipation driven reverse annealing (D-Wave)
  - Biased drivers
- Error correction
  - Naive translation of code to Hamiltonian: self correcting codes
  - Why this isn't practical
  - Brief overview of what has been tried
- Shortcuts to adibaticity

- Basic concept, counteract terms which take you out of the ground state
- Theoretical version, success probability 1 with tiny runtimes

2 (non-)stoquasticity

- Stoquastic[1] Hamiltonians → all off diagonal elements are negative (or zero) (or can be made negative or zero)
- Perron-Frobenius theorem: if all off-diagonal elements are negative than unique ground state with all positive weights
- Extension: if negative or zero than GS can be degenerate, but there is a state with all positive weights in the manifold
- Intuition, adding a phase can only increase energy if all are negative
- Application in classical computing: PageRank algorithm [1] edges represented probability to link to page, higher support in (all positive) ground state means higher rank
- Path integral quantum Monte Carlo: can find thermal state of a quantum system in one higher dimension:
  - Sketch of concept, want to approximate $\mathrm{Tr}(e^{-\frac{H}{T}})$ Trotterize

$$\sum_{\psi_1,\psi_2...\psi_m} \mathrm{Tr}(e^{-\frac{H}{mT}}|\psi_1\rangle\langle\psi_1|e^{-\frac{H}{mT}}|\psi_2\rangle\langle\psi_2|....|\psi_m\rangle\langle\psi_m|) \quad (1)$$

  - Diagonal parts of H become interactions within a classical "copy", off diagonal parts become couplings between copies
  - Thermal distribution of this classical Hamiltonian can be found with classical Monte Carlo
  - Can be made mathematically rigorous → in the limit $m \to \infty$, with enough equilibrated samples the distribution is the same as the real quantum Hamiltonian
- Seems too good to be true, there are some "catches":
  1. No guarantees on how long it takes to reach thermal equilibrium, could take lifetime of the universe
  2. For non-stoquastic Hamiltonians samples will all have phases, phases will mostly cancel and exponentially many samples may be required → sign problem

[1] nb: not at typo, related but different to stochastic

- Non-stoquastic Hamitonians tend to be hard in practice for QMC at low T
- This has lead to the misconception that non-stoquastic=hard therefore stoquastic=easy
- If all stoquastic were easy at all temperatures, than we could show that $P = NP$ by using QMC for annealing like protocols (see [2])
- Another persistent myth, highly dissipative stoquastic (think D-Wave) quantum annealers are no more powerful than QMC annealing
  - Theoretical counterexamples [3] (easier to understand arguments can be found in [4])
  - Very recent experimental evidence than annealer does in fact scale better [5]
- Non-stoquastic may still be useful, for instance needed to simulate electronic systems; electrons are fundamentally non-stoquastic due to exchange statistics
- Path integral quantum Monte-Carlo can still be interesting as a quantum inspired algorithm even if not as good as true quantum

3 Reverse annealing and biased searches

- Core idea: don't start "from zero", either start from solution from classical algorithm, or use as a subroutine in a hybrid quantum-classical algorithm
- One way to see how this is a good idea: quantum annealing is the quantum analogue of simulated annealing, but simulated annealing has been superseded by algorithms like parallel tempering, can win with parallel tempering analogues in annealing [6]
- Need a way to bias the search toward a desired solution, several ways to do this
  1. Have three Hamiltonians, unbiased starting Hamiltonian, bias Hamiltonian, and problem Hamiltonian, bias turns on in the middle [7] coherent reverse annealing
  2. Program starting state and use dissipation in dissipative annealers (implemented on D-Wave systems) dissipative reverse annealing [6]
  3. Start in a ground state of a biased search Hamiltonian [8, 9]
- Method 1 has been shown to change first order phase transitions to second order (allowing annealing to be much faster) [10]

- Method 2 is heavily used in quantum simulation on D-Wave devices (including in [5]) and has also been used to construct hybrid algorithms (example: [11])
- Method 3 was proposed by [8] in 2013, but only really popularized recently ([9]), not as much known, but it is the only of the three compatible with the energy arguments in [12] → likely to be very useful in diabatic settings

4 Hamiltonian based error correction

- Reminder: gate model error correction → measure stabilizer degrees of freedom, allow errors to be detected without disturbing quantum information, for a good introduction see [13]
- Gate model error correction requires errors to be actively corrected, but can be made fully fault tolerant
- Hamiltonian version, replace stabilizer measurements with Hamiltonian terms → errors raise energy, and dissipation lowers energy while correcting errors [14]
- Only works if Hamiltonian is "thermodynamically stable", in other words energetic factors outweigh entropic ones [15]
- Normal 2D surface code is not thermodynamically stable, defects can move with no additional energy cost 4D version is stable
- Require high weight (i.e. involving many terms $Z_iZ_j...Z_k$) operators so full error correction is not currently practical
- Some proof-of-concept demonstrations of error *suppression* on D-Wave devices [16]
- Dynamical decoupling, another technique where errors are removed by cancelling qubit rotations, not going to discuss more here, but more can be found here: [17]

5 Shortcuts to adiabaticity

- Key concept: imagine evolution in instantaneous energy eigenbasis of Hamiltonian
- Changing Hamiltonian over time create off diagonal elements in this basis
- What if we can create a Hamiltonian which cancels these elements, in principle we can stay in the ground state without being adiabatic

$$H_{CD} = \sum_m \sum_n \frac{|n(t)\rangle\langle n(t)|\dot{H}|m(t)\rangle\langle m(t)|}{E_n - E_m} \tag{2}$$

- Review can be found at [18]
- Caveats:
  - Hamiltonians will have to be of high weight to fully cancel the off diagonal elements
  - The faster the time evolution the stronger these Hamiltonians need to be scale as $\frac{1}{t_f}$
  - In general not possible to know the exact form for the whole evolution without knowing the answer
- In practice try to make a low order approximation see for example [19]

6 Summary and important points

- Myth that stoquastic AQC can be simulated by quantum Monte-Carlo
- Can only simulate thermal distribution and may take a very long time to get there
- Path integral quantum Monte-Carlo can be an interesting quantum inspired algorithm
- Reverse annealing and related techniques are a powerful tools for building hybrid algorithm
- Self correcting Hamiltonians can exist in theory, but involve terms which are not practical with current technology
- Error suppression has been demonstrated though
- Shortcuts to adiabaticity can potentially help as well, but are impractical to implement exactly

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