Modenizing Quantum Annealing using Local Search

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See full paper at: arXiv:1606.06833

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Outline

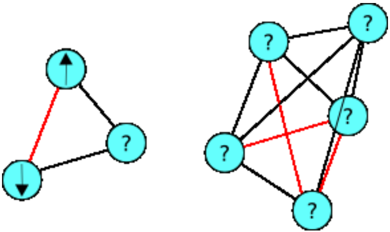
1. Energy Computing and the Ising Model
2. Quantum Annealing and Simulated Annealing
    - Better Classical Algorithms: Parallel Tempering and Population Annealing
    - Hybrid Computing: Gaining the Advantages of Advanced Algorithms
3. Search Range
    - Controlling Range
    - Parallel tempering and population annealing analogues
    - Controlling Problem mis-specification
4. A few slides about implementation
5. Thermal Sampling

Problem Statement: Ising Spin Glass Hamiltonian

$$H_{ISG} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

Goal is to find ground/low energy states

- 'Universal' in the sense that any classical Hamiltonian can be mapped to it De las Cuevas, Cubitt Science 351 6278
- Thermal/quantum distributions also useful for inference and machine learning tasks ex. Amin et. al. arXiv:1601.02036, Chancellor et. al. Scientific Reports 6, 22318 ...

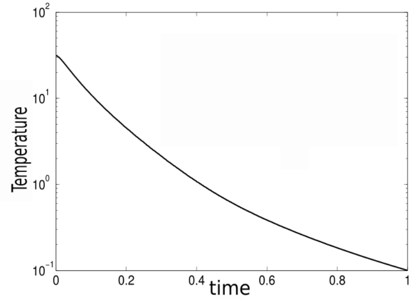


Simulated Annealing (classical)

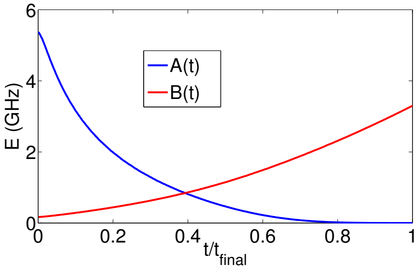
Updates drive toward thermal distribution with temperature T if they obey detailed balance

$$P(S(1) \to S(2)) = \exp(\frac{(E(1) - E(2))}{T})P(S(2) \to S(1))$$

Start at high T and lower over time



Quantum Annealing (QA)



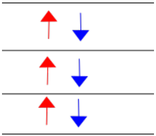
Add non-commuting transverse field terms

$$H(s) = -A(s)\sum_i \sigma_i^x + B(s)H_{ISG}$$

start at $\frac{A(s=0)}{B(s=0)} \gg 1$, go to $\frac{B(s=1)}{A(s=1)} \gg 1$
Quantum fluctuations + low temperature bath cause tunneling toward low energy states

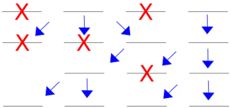
Beyond Simulated Annealing (classical)

Parallel Tempering



- Multiple replicas at different temperatures
- Swap replicas by rules which obey detailed balance
- $P_{swap}(i,j) = \min\left[1, \exp\left(\left(\frac{1}{T(i)} - \frac{1}{T(j)}\right)(E_i - E_j)\right)\right]$

Population Annealing



- Anneal multiple replicas
- Probabilistically remove poorly performing replicas and copy those which perform well
- Rules preserve average population and obey detailed balance
- $\bar{N}(E) = \frac{1}{Q}\exp\left(\left(\frac{1}{T_{old}} - \frac{1}{T_{new}}\right)E\right)$

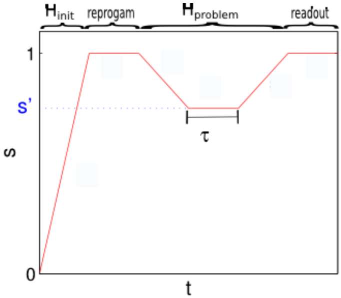
Can hybrid strategies combine these with calls to an annealer?

Can these strategies be used directly by a quantum annealer?

Difficulties in building new annealer strategies

- No cloning theorem $\rightarrow$ cannot copy quantum states
- Measurements (ex. energy) disturb state of system and likely experimentally difficult
- Usual QA is global search, no way of inserting information from previous runs

Solution $\rightarrow$ use annealer subroutine which starts and ends at $s = 1$ (recall $\frac{B(s=1)}{A(s=1)} \gg 1$) with programmed initial state



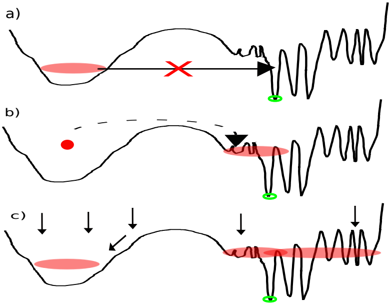
Hybrid computing using local search

Potential Strategies

1. Quantum and classical algorithms used together
   - Classical input and output means that annealer can be used alongside any classical algorithm
   - Google have started looking into these ideas, see Hartmut Neven talk at AQC 2016 [1]
2. Multiple local quantum searches controlled by classical algorithm
   - Analogues to parallel tempering and population annealing which use annealer only
   - Will return to this later

[1] Should be uploaded soon and viewable at: https://aqc2016.eventfarm.com

Cartoon example: energy landscape with rough and smooth features



a) QA gets stuck in broad local minima and cannot tunnel to correct minima

b) Classical algorithms can easily explore the broad features, while the annealer can explore the rough ones

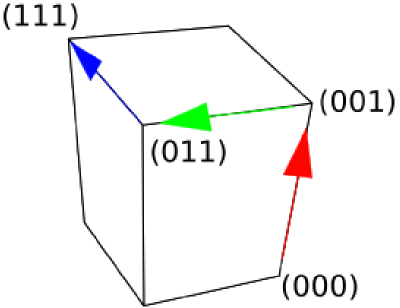
c) Even random initialization can improve solution probabilities, may hit rough region by chance

Range of local search

Define search range in terms of typical Hamming distance $\mathfrak{h}(s')$ from starting state

$\mathfrak{h}(s')$ will increase monotonically with decreasing s' but...

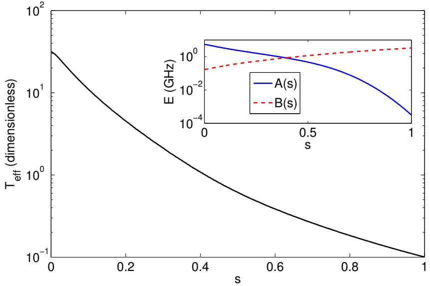
- Not easy to theoretically predict
- Will depend on both problem and starting state



Choosing the range of the search

Options:

1. Choose heuristically: use different ranges and take best and take best, typical $\mathfrak{h}(s')$ for problem type etc...
2. Measure search range and use bisection to get to desired range
3. Define effective temperature and construct analogues of known classical algorithms



Effective Temperature

1. Single qubit Hamiltonian with transverse and longitudinal components

$$H_1(s') = -A(s')\,\sigma^x + B(s')\,\sigma^z$$

2. Diagonalize 2x2 matrix by hand to get occupation ratio

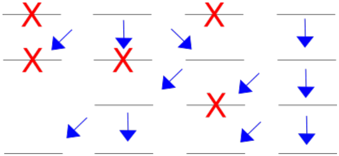
$$\frac{\psi(1)}{\psi(2)} = \frac{\sqrt{A(s')^2 + B(s')^2}}{A(s')} + \frac{B(s')}{A(s')}$$

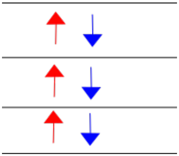
3. Invert Boltzmann equation to get effective temperature

$$T_{eff}(s') = 2\left[\ln\left(\left|\frac{\psi(1)}{\psi(2)}\right|^2\right)\right]^{-1}$$

Parallel tempering and population annealing analogues

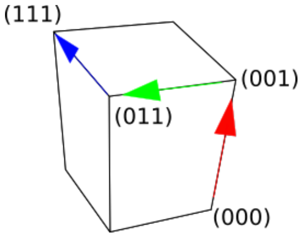
1. Replace metropolis updates with annealing runs consisting of calls to annealer
2. Define 'energy' and 'state' as the lowest energy solution found in an annealing run and the corresponding classical state
3. Replace $T \rightarrow T_{eff}$
4. Apply replica swapping/copying/deleting rules as usual





Problem mis-specification

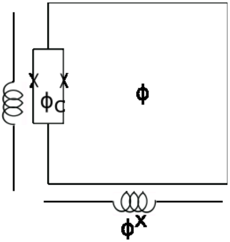
- Error in each energy proportional to $\sqrt{N_{qubit}}$
- Only energy differences within search matter
- Energy difference proportional to square root of Hamming distance
- $\therefore$ relevant error proportional to $\sqrt{\mathfrak{h}(s')}$ not $\sqrt{N_{qubit}}$ [2]



[2] Up to details about shape of the explored subspace, see arXiv:1606.06833

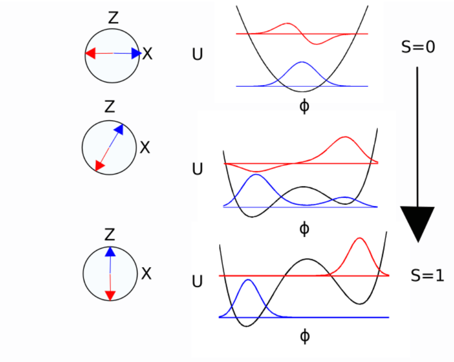
Implementation background: flux qubit circuit

Compound Compound Josephson Junction device like those used in D-Wave systems



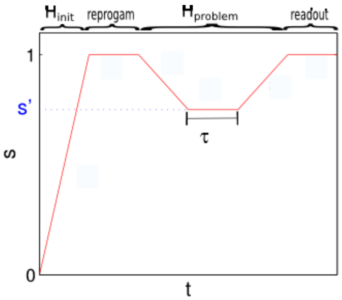
- ϕ is relevant variable
- ϕ_c Controls effective transverse field
- ϕ^x Acts as external bias
- Couple inductively between loops

Implementation Background: Single qubit potential



- Barrier width controlled by ϕ_c
- Energy difference between wells controlled by ϕ^x
- Quantum tunneling suppressed exponentially late in the anneal
- High barrier also blocks classical transitions

Runback protocol



1. Anneal forward using standard annealing protocol and trivial Hamiltonian to initialize state
2. Reprogram problem Hamiltonian to target problem
   - State protected due to high energy barrier
3. Anneal back to point s'
4. Possibly wait a period τ and anneal back to $s = 1$

One slide on sampling

Annealer calls will not obey detailed balance, but...

- Somtimes quantum distributions can act as an effective proxy for thermal distributions Otsubo et. al. Phys. Rev. E 86, 051138
- Quantum fluctuations may aid in machine learning tasks Amin et. al. arXiv:1601.02036
- Relative weights of local minima can be calculated though post processing: numerically calculate free energy with classical Monte Carlo

Acknowedgements

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- Work supported by EPSRC
- You $\rightarrow$ thanks for listening

You are encouraged to read the full paper: arXiv:1606.06833