Robust optimisation with quantum annealing and the domain wall encoding

AQC 2019

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June 26 2019

A brief note about terminology

For the purposes of this talk:

- Adiabatic quantum computation (AQC) $\rightarrow$ *closed system* protocols where an eigenstate is maintained via the adiabatic theorem of quantum mechanics
- Quantum Annealing (QA) $\rightarrow$ *dissipation* from open system effects is the dominant mechanism

The terminology is not standardized and different groups may use these terms differently

Our (Durham) group (underlined people are at AQC)

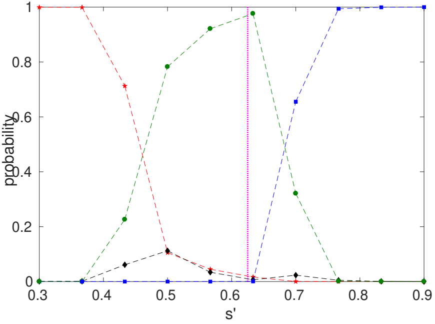
- Two PIs

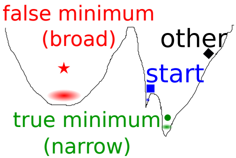
EPSRC
Pioneering research and skills

  - Viv Kendon → Reader coming to end of EPSRC established career fellowship on hybrid quantum classical computing, significant contributions on subject of quantum walks (among other things)
  - Nicholas Chancellor (me) → EPSRC UKRI innovation fellow, three year project to look at hybrid algorithms and early use cases
- One postdoc
  - Jie Chen → Non-quantum background, recruited to help develop use cases
- Four graduate students: Jemma Bennett, Laurentiu Nita, Parth Patel, and Adam Callison (Imperial)

Reverse annealing for quantum subroutines

- Start in candidate solution, search within range defined by $s' \in [0, 1]$ (smaller is longer range)
- Allows classical algorithm to guide local searches on D-Wave quantum annealers
- Figure is experimental data from a D-Wave device*





*For experimental details see my 2018 AQC talk (http://nicholas-chancellor.me/presentations.html) or come talk to me

Reverse annealing in algorithms*

1. Start from one ground state to find other ground states (D-Wave whitpaper 14-1018A-A†)
   - Finding other GS 150x more likely then forward
2. Search locally around classical solution (arχiv:1810.08584†)
   - Start from greedy search solution
   - Speedup of 100x over forward annealing
3. Iterative search (arχiv:1808.08721†)
   - Iteratively increase search range until new solution found
   - Forward annealing could not solve any, reverse solved most
4. Quantum simulation(Nature 560 456–460 (2018)†)
   - Seed next call with result from previous
   - Seeding with previous state makes simulation possible
5. Monte Carlo and Genetic like algorithms (NJP 19, 2, 023024 (2017) and arχiv:1609.05875)
   - Transverse field parameter s' controls tradeoff between exploration and exploitation similar to temperature
   - Quantum analogues of many known classical algorithms
   - Genetic like composes guess from two or more known solutions

*† indicates experimental results

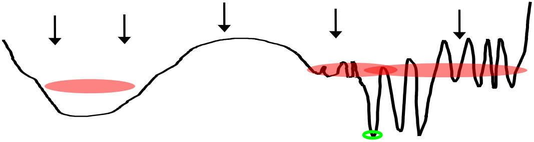
What else can be done

Experiments so far:

- Simple but show major advantages → hint at promise of more complex algorithms
- All use low energy solution to find lower energy solution

Can reverse annealing be used in other ways?

- Forcing exploration of solution space (will be explored as part of NQIT partnership project)
  1. Run traditional quantum annealing
  2. Apply novelty search: objective is to find candidates which are maximally different to known solututions
  3. Seed RA with these candidates, and continually add to list of seen solutions

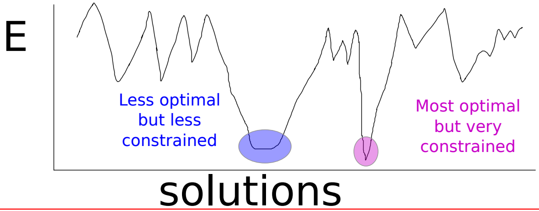


- Finding candidates with other desirable properties: the subject of this talk

Enhancing Robustness of Solutions using reverse annealing

Using quantum annealers to find solutions which are robust in the sense that they can be adjusted to a modified problem definition at little or no energy cost

- Already known that annealers preferentially find good solutions which are ‘near’ other good solutions $\rightarrow$ leverage these effects algorithmically
- If a good solution is already known, can we use an annealer to trade optimality for robustness?



Funded by BP, NQIT, and EPSRC, work with Simon Benjamin group

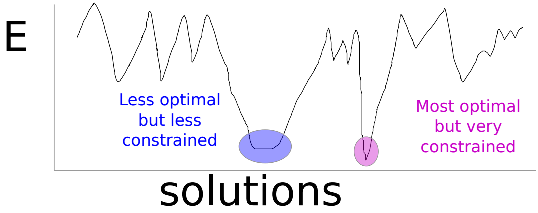
bp

NQIT Networked Quantum Information Technologies

EPSRC Pioneering research and skills

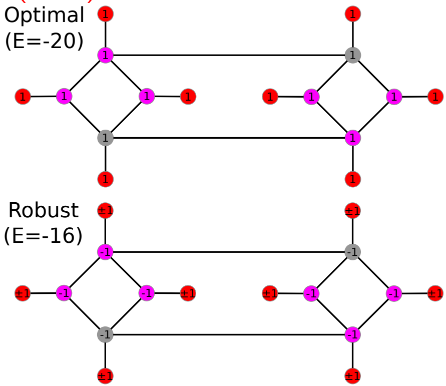
Why might we want this?

- Adjust solution if we later learn that our problem definition was slightly incorrect
- Penalty terms which are too expensive to encode on annealer could be implemented by adjustments in post-processing
  - Global non-linear constraints for instance are expensive to map
- Find ‘template’ solution which can be adjusted to solve many similar but not identical problems



A simple (motivational) example

Consider 16 qubit gadget from N. G. Dickson et. al. Nature Comm. 4, 1903 (2013) :



- a is the ground state but
- A D-Wave 2000Q with $1,280,000$ $5\mu s$ runs finds b $1,277,824$ times and a only 17 times

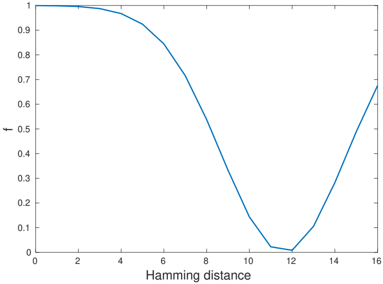
Simple test: add global penalty and do greedy search

Global penalty:

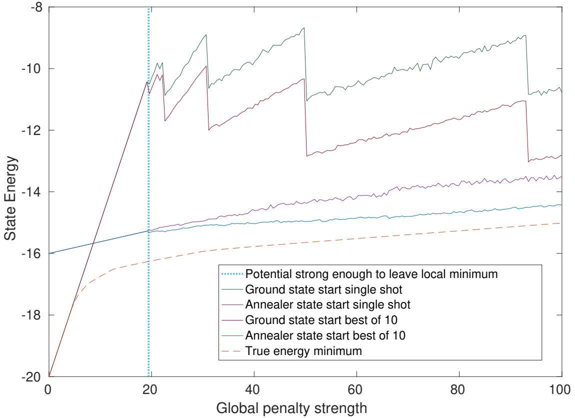
$$E(q) = E_{\text{Ising}}(q) + g\, f[\mathfrak{h}(q, r)]$$

where:

- q is a bitstring representing the state
- g is the strength of the penalty
- $\mathfrak{h}$ is Hamming distance
- r is a random bitstring
- f is a single variable function:



Starting in true ground state vs. state annealer finds



The large degeneracy in the state the annealer finds allows for much more effective adjustment $\rightarrow$ higher energy but more robust

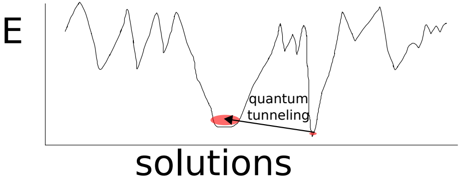
Reverse annealing to trade off optimality and robustness

Hypothetical situation:

- Already know the most optimal (planted) solution
- But we want more flexibility
- Are willing to 'pay' some optimality for a more flexible solution

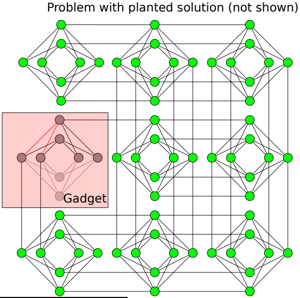
Algorithm:

1. Start reverse annealing in planted solution
2. Search over a set range
3. Repeat many times
4. Keep most optimal solutions with certain robust features



Free variable gadgets (binary version)

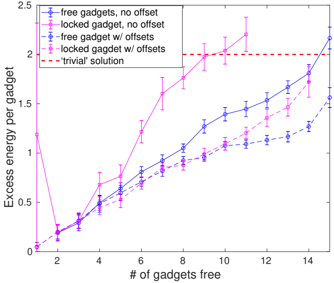
- Use planted solution method from Hen et. al. Phys. Rev. A 92, 042325 (2015) to make 'hard'* problems with all -1 and all $+1$ ground state
- Before constructing replace some unit cells with 'free' variable gadgets
  - All variables fixed if 'outside' varibles agree
  - Become free (same energy for ± 1 values of some variables) if they do not (but energy unchanged)
  - Energy penalty because has to leave planted solution



*Hard for the annealer to solve, may or may not be hard for all algorithms

Testing the mechanism

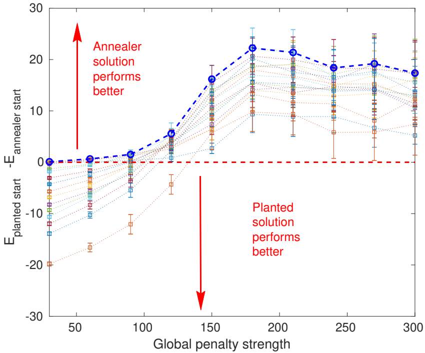
- D-Wave 2000Q, Use a variety of s' to find best solution with a set number of gadgets 'free'
- Compare excess energy per 'free' gadget to version with 'locked' (no fluctuating variables) gadgets
- Bonus: anneal offsets $\rightarrow$ adjust fluctuations in gadgets



Fluctuations help find more robust solutions whether or not offsets are used

Putting solutions to the test: greedy search with global penalty

- Greedy search starting from best found solution with a given number ($0 - 15$) of free gadgets found
- Chip-sized version of global non-linear penalty used in motivational example
- Able to find better solution when penalty is included

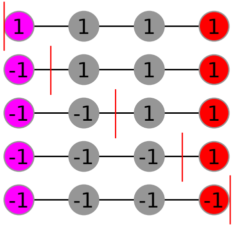


A more realistic version: integer variables

Concept of 'free' variables is a bit artificial much more natural for integer variables (broad versus narrow minima)

- Cumbersome to encode using traditional (one hot) method: N value integer variable $\rightarrow$ N qubit fully connected subgraph
- Better 'domain wall' encoding (see arχiv: 1903.05068*)
  " " $\rightarrow$ $N-1$ qubit linearly connected subgraph

encoded value	qubit configuration
0	1111
1	-1111
2	-1-111
3	-1-1-11
4	-1-1-1-1



*New version appeared Monday!

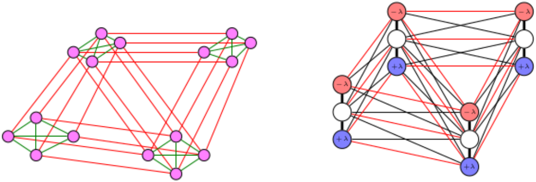
Interactions between domain walls

Ising chains with single domain wall -1 boundary condition to the left, $+1$ boundary to the right

- $\delta_i = \frac{1}{2}(Z_i + Z_{i-1})$, $\delta_i = 1$ iff domain wall between i and $i-1$, 0 otherwise
- Products of δ_i on different chains are quadratic $\rightarrow$ arbitrary interactions between pairs of domain wall variables is qudratic
- 'virtual' Ising variables beyond end of chain $\rightarrow$ binary variable is special $N = 2$ case of domain wall encoding

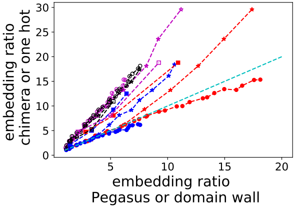
Use natural structure of problem to 'spread out' embedding

Four colouring example, 'layered' structure in Domain wall (right), no structure in one hot, (left)



Domain wall encoding is a powerful tool for problem mapping

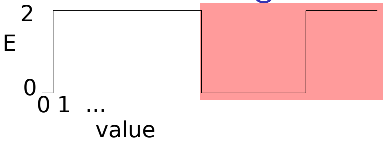
- Reduce number of qubits per variable by one
- Fewer connections within variable
- Structure tends to be better for embedding



- Red and blue $\rightarrow$ comparisons of domain wall versus one hot
- magenta and black $\rightarrow$ effect of more advanced 'pegasus' hardware graph

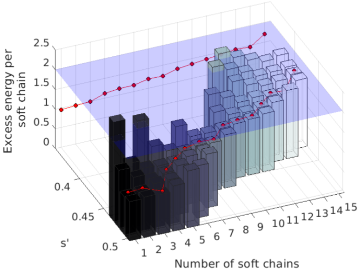
Domain wall encoding can make as much of a difference as re-engineered hardware graph! (see arχiv: 1903.05068)

Finding robust solutions over integer variables



- Mixed integer/binary planted solution problem
- Unique minimum energy where binary part can be in lowest energy state
- Range over which it cannot, but has wider minima in red

Perform same experiment as for integer gadgets, chain is said to be 'soft' if domain wall is in wider minima

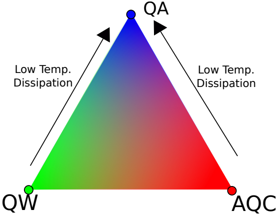


Beyond QA: quantum computing in continuous time

Three known ways in which continuous time quantum systems can solve problems, each has *reverse annealing-like* algorithm:

1. AQC (closed system) *slow transformation* $\rightarrow$ eigenstate maintained through adiabatic theorem of quantum mechanics Quant. Inf. Proc.10(1):33–52, (2011)
2. QA (open system) $\rightarrow$ low temperature dissipation finds low energy states reverse annealing relies on this dissipation
3. Quantum Walk (QW)$\rightarrow$ dynamics with a fixed Hamiltonian Phys. Rev. A **95**, 052309 (2017)*

Is there a method similar to reverse annealing which uses all three?



*Used to match energy, so subtly different than RA

Solving optimisation problems with QW*

Consider the following:

1. Transverse field Ising $H_d = -\sum_{i=1}^{n} \sigma_i^x$,
   $H_{\mathrm{problem}} = \sum_{i=1}^{n} \sum_{j=1}^{n} J_{ij} \sigma_i^z \sigma_j^z$

$$H = \gamma\, H_d + H_{\mathrm{problem}}$$

2. Start in ground state of H_d, $|\psi(t=0)\rangle = |\omega\rangle = \frac{1}{2^n} \sum_{i=1}^{2^n} |i\rangle$
3. By symmetry $\langle \omega \mid H_{\mathrm{problem}} \mid \omega \rangle = 0 \;\therefore$
   $\langle \psi(t=0) \mid H \mid \psi(t=0) \rangle = -\gamma\, n$
4. $\langle \psi(t>0) \mid H_d \mid \psi(t>0) \rangle \geq -\gamma\, n \;\therefore$ by energy conservation $\langle \psi(t>0) \mid H_{\mathrm{problem}} \mid \psi(t>0) \rangle \leq 0$ dynamics preferentially seeks out states with low energy w.r.t. H_{problem}

- Applied to Sherrington-Kirkpatric spin glass: arχiv:1903.05003 (see also: arχiv:1904.13339)
- Like extreme annealing schedule consisting of pause bracketed by instantaneous quenches

*Work with Viv Kendon (see prior talk) and Adam Callison

Interpolating between AQC and QW

The energy conservation argument from the previous slide can be extended to any monotonic (closed system) quench

$$H(t) = A(t)\,H_d + B(t)\,H_{\mathrm{problem}} \quad \frac{A(t)}{B(t)} \geq \frac{A(t+\delta t)}{B(t+\delta t)} \forall_t$$

Sketch of proof:

1. Trotterize time evolution: $A(t) \rightarrow A(t+\delta t)$ and $B(t) \rightarrow B(t+\delta t)$ and apply $|\psi(t+\delta t)\rangle = \exp(-iH(t)\delta t)|\psi(t)\rangle$ in separate steps
2. Rescale time so that Hamiltonian always resembles quantum walk $H_{eff}(\gamma(t)) = \gamma(t)\,H_d + H_{\mathrm{problem}}$
3. In rescaled version $\gamma(t) \geq \gamma(t+\delta t) \therefore$ $\langle H_{eff}(\gamma(t))\rangle_{\psi(t)} - \gamma(t)\,n \geq \langle H_{eff}(\gamma(t+\delta t))\rangle_{\psi(t)} - \gamma(t+\delta t)\,n$
4. Because $\langle H_{eff}(\gamma(t))\rangle_{\psi(t)} \geq -\gamma(t)\,n \ \forall_t$, $\langle H_{\mathrm{problem}}\rangle_{\psi(t)} \leq 0 \ \forall_t$

Biased driver Hamiltonian* See poster 26 for more...

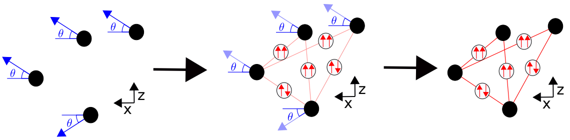
Define driver Hamiltonian using fields which are not (completely) transverse $H_d = \sum_{i=1}^{n} -\cos(\theta)\sigma_i^x - g_i \sin(\theta)\sigma_i^z$

- Start in ground state of H_d: $|\psi(t=0)\rangle = \bigotimes_{i=1}^{n} \frac{1}{\sqrt{2+2\,g_i\cos(\theta)}}[(1+g_i\cos(\theta))|0\rangle + \sin(\theta)|1\rangle]$
- Starting state biased toward classical bitstring g, $g_i \in \{-1, 1\}$
- Closed system with monotonic sweep (including QW), time evolution improves the guess (on average):

$$\langle H_{\mathrm{problem}}\rangle_{\psi(t)} \leq \langle H_{\mathrm{problem}}\rangle_{\psi(0)}$$

- Ground state is optimal solution so adiabatic theorem holds and dissipation can assist as well

  Can use AQC, QW and QA mechanisms simultaneously



*with Laur Nita, Jie Chen, Adam Callison, Viv Kendon and Matthew Walsh.
Note related work: arχiv:1906.02289 and Chinese Physics Letters, 30 1 010302

Take home messages

Reverse annealing

- Promising experimental results based on simple applications
- Find lower energy solution from low energy
- Can be used in other ways, finding more robust solutions is one example

Domain wall encoding

- Can reduce embedding overhead for (some) problems as much as re-engineered problem graph

Multiple mechanisms in continuous time

- Hybrid subroutines which use multiple mechanisms at once
- Can prove advantage on average in closed system case