Trading off optimality and robustness using a quantum annealer

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April 16, 2019

Talk structure

1. Background
   - Quantum computing: comparison between quantum annealing and 'gate' based QC
   - Quick overview on D-Wave quantum annealers
   - Mapping real problems to Ising models
2. Reverse annealing overview:
   - Powerful new tool enabling hybrid quantum/classical algorithms
   - Experimental results showing reverse annealing searches solution space locally
3. Finding robust solutions with reverse annealing
   - Motivational example
   - Chip scale results with binary and integer variables

Quantum computing

Big idea: harness the fundamental physics of discrete systems (quantum mechanics) to solve important problems

- We know it works in theory: quantum search of unstructured database with N entries in a time proportional to $\sqrt{N}$
- This is not possible without using quantum mechanics (only option without QM is random guess or exhaustive search)

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- ... but how do we use real, imperfect, quantum machines to solve problems people care about

Optimization and sampling

Solution space can roughly be thought of as a structured database with complex and unknown structure

- Finding optimal solutions to many real problems is important and difficult
- Similar to 'toy' database example, may be able to get the same kind of advantages
- Distributions of states which are some how 'optimal' may be used in machine learning

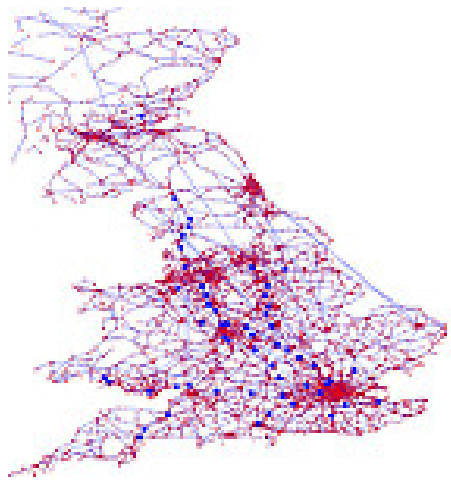


Image: public domain taken from wikimedia commons

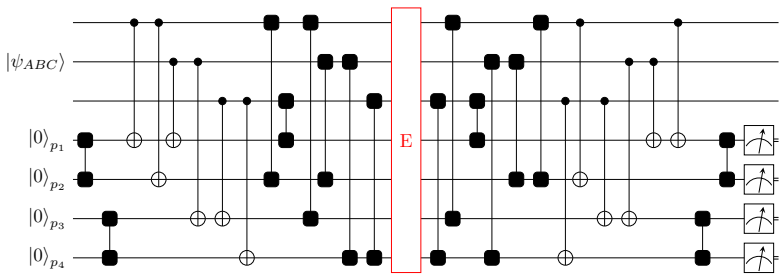
Two different approaches to quantum computing

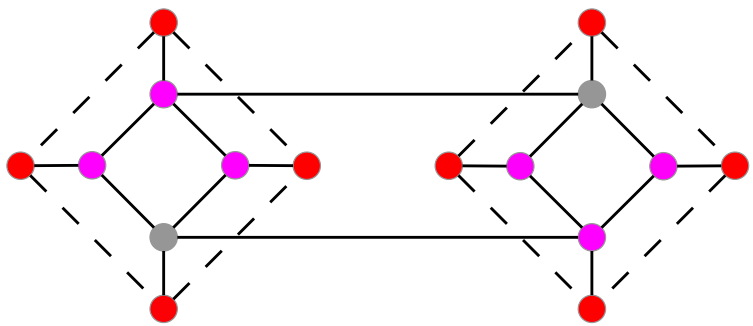
'Gate' based quantum computing

- Discrete quantum operations on qubits
- Construct 'circuits' out of these gates
- Detect and correct errors to reduce effect of noise

Quantum annealing

- Map optimization problem directly to energies of different states
- Allow quantum physics to help search solution space
- Low temperature environment helps solve problems





(some) Advantages and disadvantages of each

'Gate' based quantum computing

- Can simulate arbitrary quantum systems
- Error correction can get rid of all noise *in principle*
- Could simulate quantum annealing *in principle*

- Harder to build, largest device is tens of qubits
- All noise likely to be harmful rather than beneficial

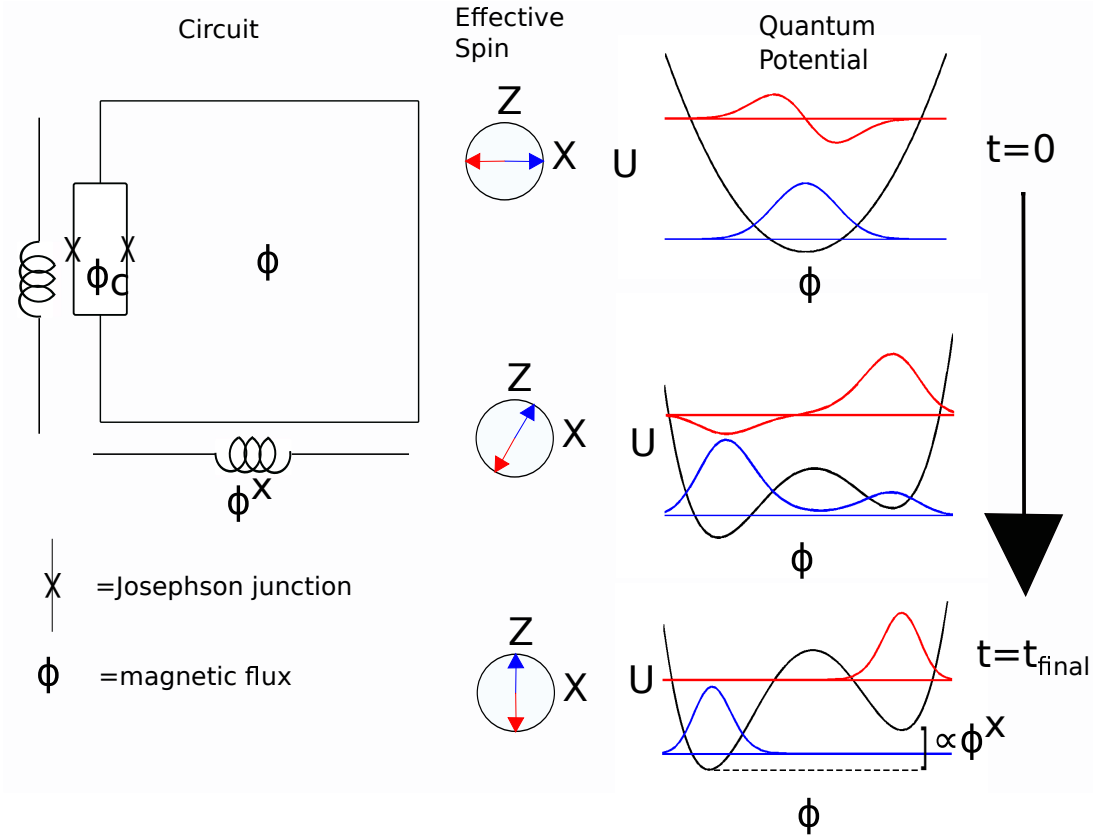
Quantum annealing

- Easier to build, largest device is thousands of qubits
- Tolerant to noise, in fact noise helps solve problems
- Naturally produces thermal distributions

- Unclear if error correction is feasible
- Cannot be used for some quantum algorithms as implemented

D-Wave Quantum annealing hardware

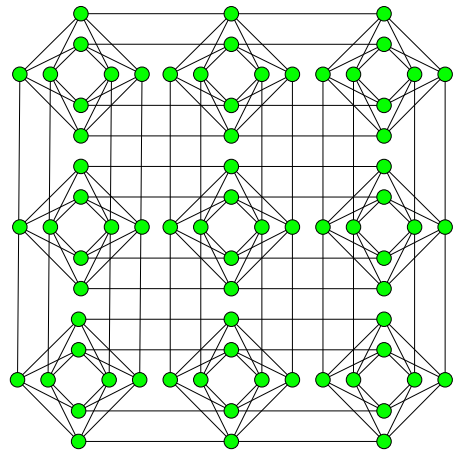
- Superconducting circuit devices with up to 2,048 qubits in 16x16 'chimera' configuration
- Operates in a cryostat at ≈ 0.015 K (200x colder than interstellar space: 3K)



Thermal and quantum fluctuations work together to solve problems

How to actually solve problems with these devices: Optimization (traditional approach)

1. Map problem to one and two body terms of the appropriate form (Ising model) Optimality of solution $\rightarrow$ energy
2. Embed in hardware graph by strongly linking qubits together to form 'logical' qubits (3x3 chimera shown below)



3. Quantum dynamics finds low energy states, run many times and take lowest energy solution

Each run is independent and starts from equal superposition 'state of maximal ignorance' could do better by using information from previous runs (more on this later)

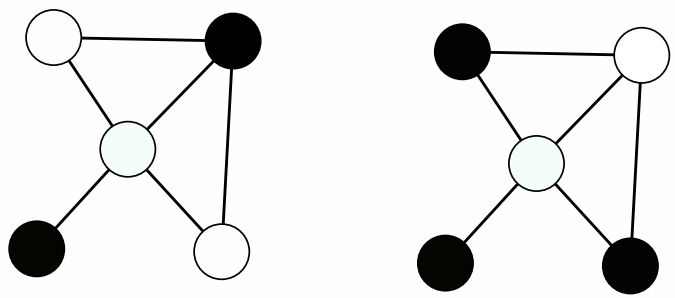
Problem mapping example: maximum independent set

Have:

- Binary variables $Z_i \in \{-1, 1\}$
- Minimisation over Hamiltonian made of single and pairwise terms $\mathrm{H_{Ising}} = \sum_i h_i Z_i + \sum_{j>i} J_{i,j} Z_i Z_j$

Want:

- Maximum* independent set: how many vertexes on a graph can we colour so none touch? $\rightarrow$ NP hard



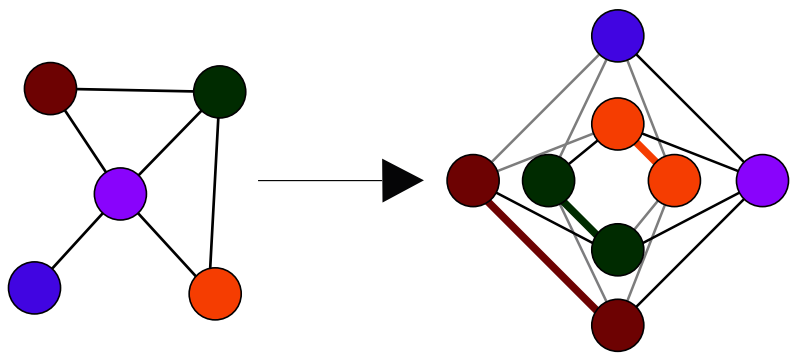
Method:

1. For an edge between vertex i and j add $Z_i + Z_j + Z_i Z_j \rightarrow$ penalizes colouring ($Z = 1$) adacent vertexes
2. Add $-\lambda Z_i$ to reward coloured vertexes ($0 < \lambda < 1$)

*Not to be confused with *maximal* independent set, which is not a hard problem

Minor embedding

- Strong 'ferromagnetic' $(-Z_i Z_j)$ coupling energetically penalizes variables disagreeing
- If strong enough than entire 'chain' acts as a single variable
- Mathematically corresponds to mapping one graph to graph minors of another



Can embed arbitrary graphs into the hardware graph with polynomial (n^2 for fully connected) overhead $\rightarrow$ Ising model restricted to hardware graph is also NP-hard

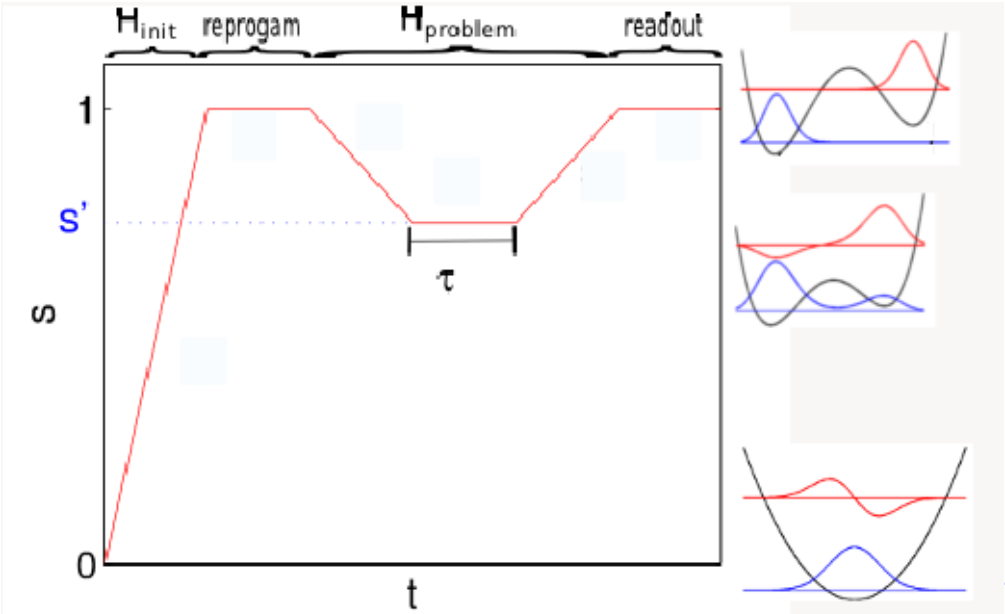
Hybrid quantum/classical algorithms with reverse annealing

Why hybrid (quantum/classical)?

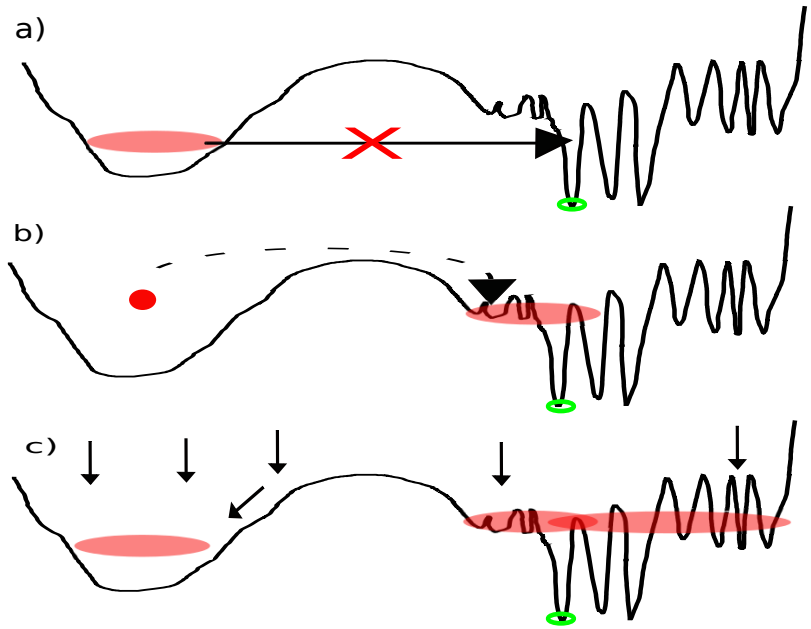
- Many good classical optimization algorithms already exist
- Need every advantage we can get to take advantage of early quantum hardware

Why reverse annealing?

- Easy inclusion of previously found solutions in algorithm calls (search range controlled by parameter s': $s' = 1 \rightarrow$ no search, $s' = 0 \rightarrow$ traditional annealing)
- Flexible: can be used with most existing techniques
- Now available on D-Wave devices



Cartoon example: energy landscape with rough and smooth features (see: NJP 19, 2, 023024 (2017))



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

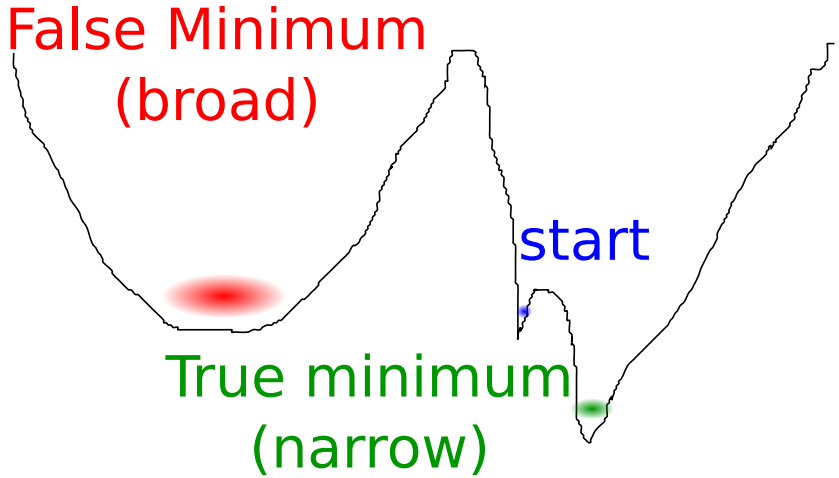
b) Classical algorithms can easily explore the broad features, while the annealer can explore the rough ones

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

Proof-of-principle experiments

Construct a problem Hamiltonian with the following properties:

1. Wide false energy minimum which 'tricks' traditional quantum annealing algorithm
2. Relatively narrow true minimum energy
3. Local minimum near true minimum for start state

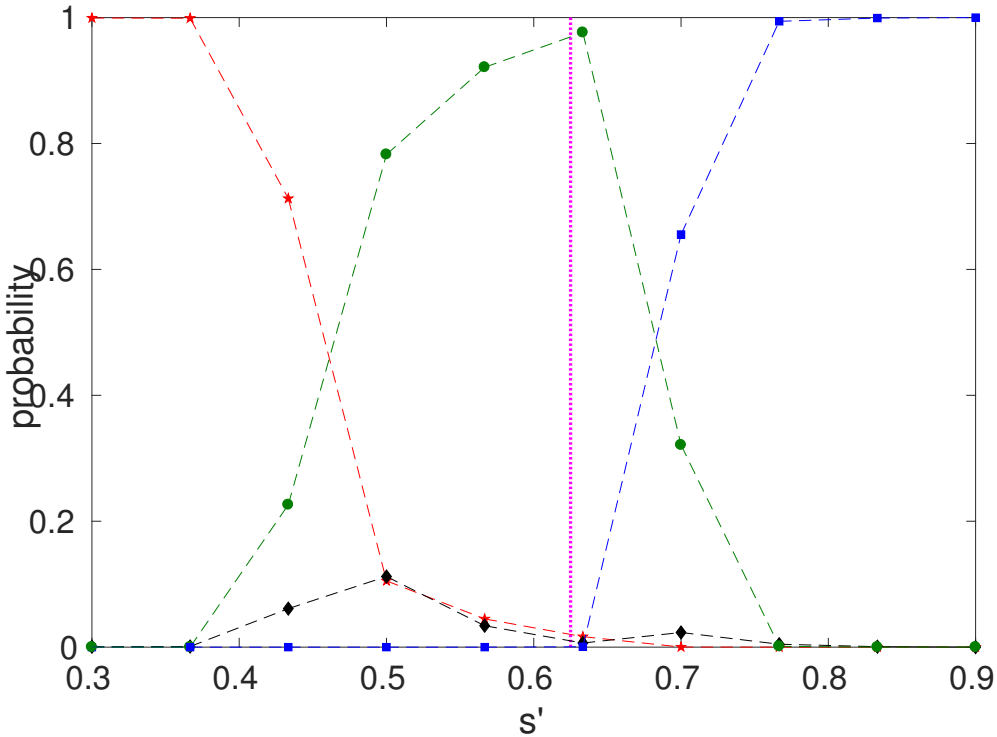


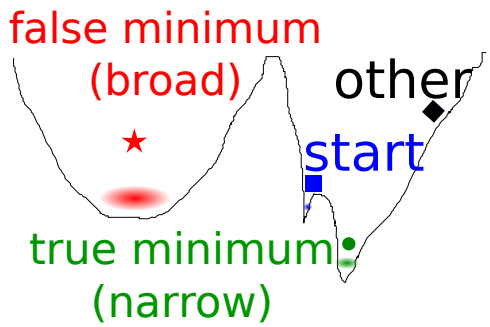
Joint work with Viv Kendon, funded by NQIT and EPSRC

NQIT Networked Quantum Information Technologies

EPSRC Pioneering research and skills

Experimental results ⋆





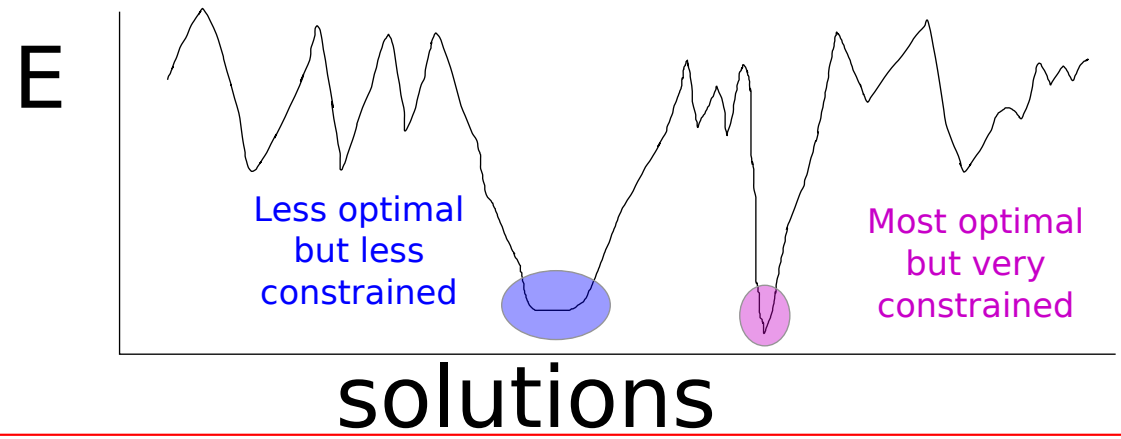
- Level crossing between true ground state and false minima at magenta line → energetically preferable to be in narrow minimum to right of line and broad to the left
- Anneal at maximum allowed rate, wait time (τ) of $20\mu S$
- Frozen in starting state for small s', find true minimum at moderate s', trapped for large s'

⋆For different proof-of-principle results, see: D-Wave white paper on Reverse Quantum Annealing for Local Refinement of Solutions

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

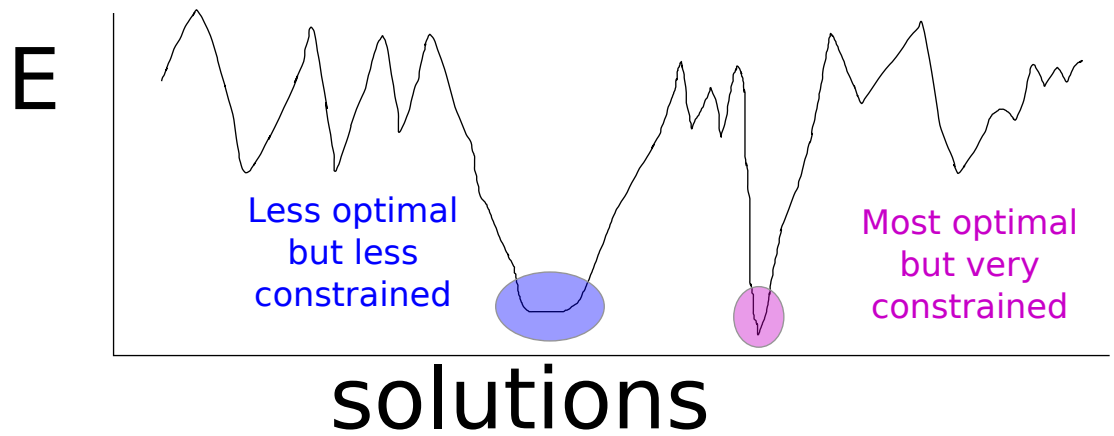
- Already known that annealers preferentially find good solutions which are 'near' other good solutions $\rightarrow$ leverage these effects algorithmically
- If a good solution is already known, can we use an annealer to trade optimality for robustness?



Joint work with Simon Benjamin, funded by BP, NQIT, and EPSRC

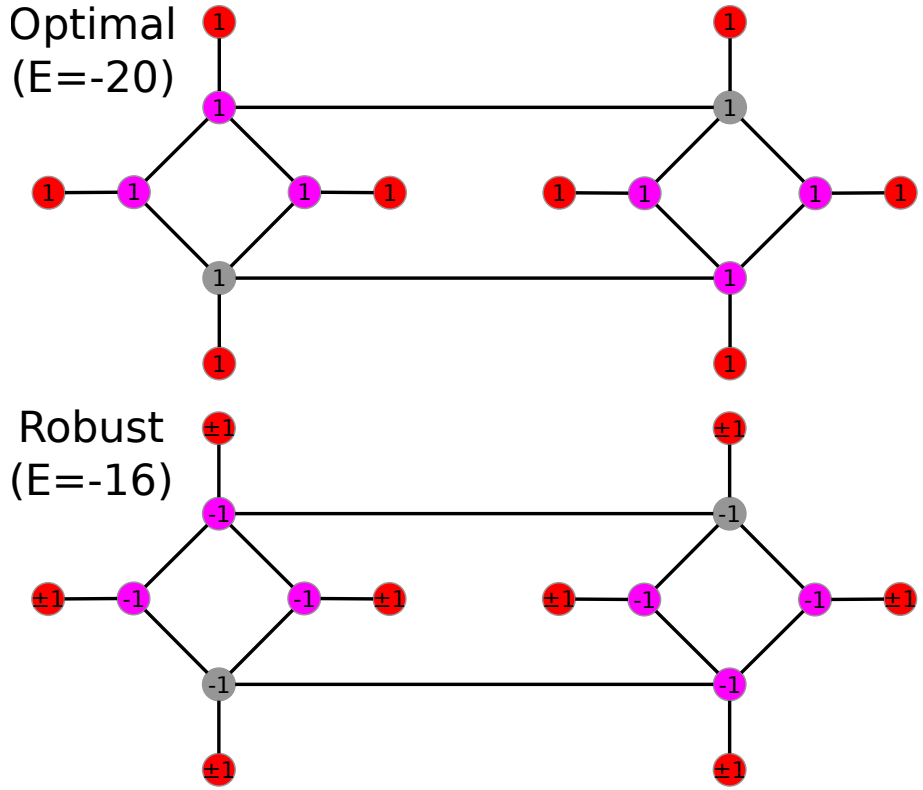
Why might we want this?

- 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

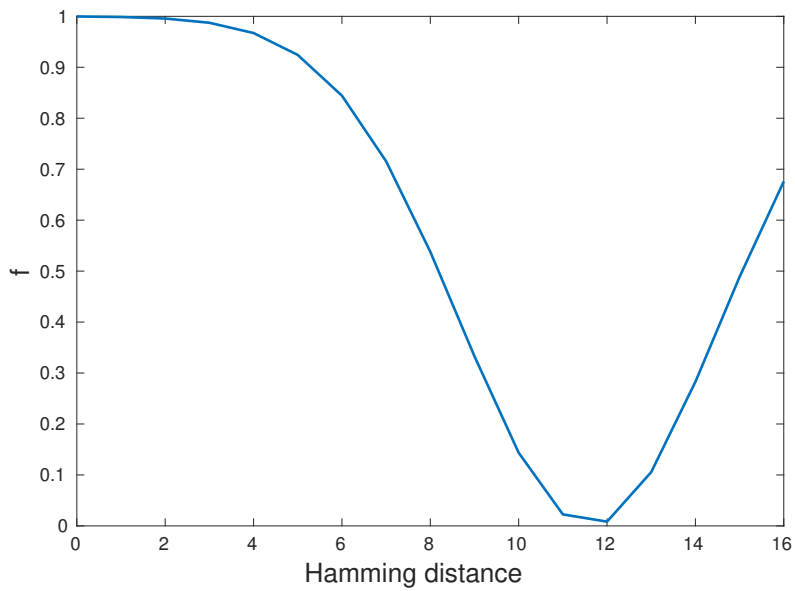
Simple test: add global penalty and do greedy search

Global penalty:

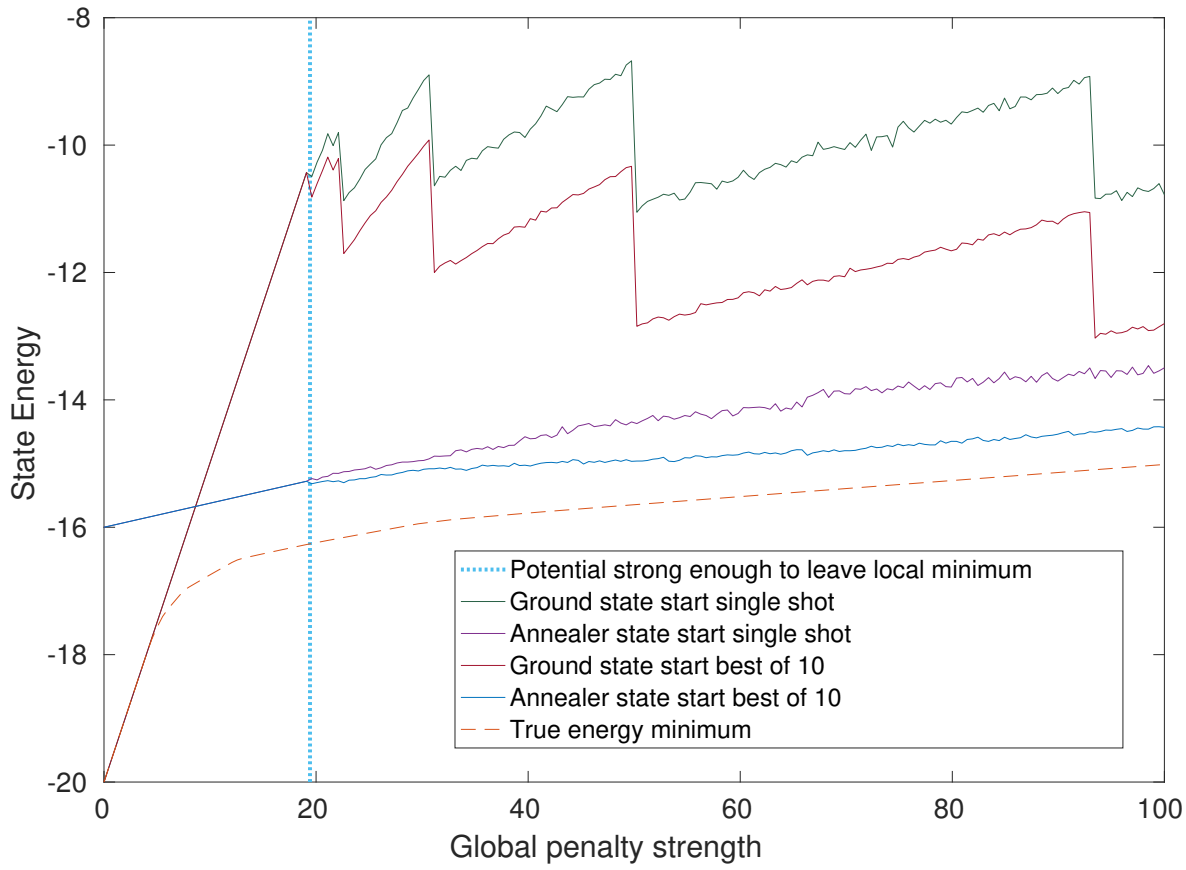
$$E(q) = E_{\mathrm{Ising}}(q) + g\, f[\mathfrak{h}(q, r)]$$

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

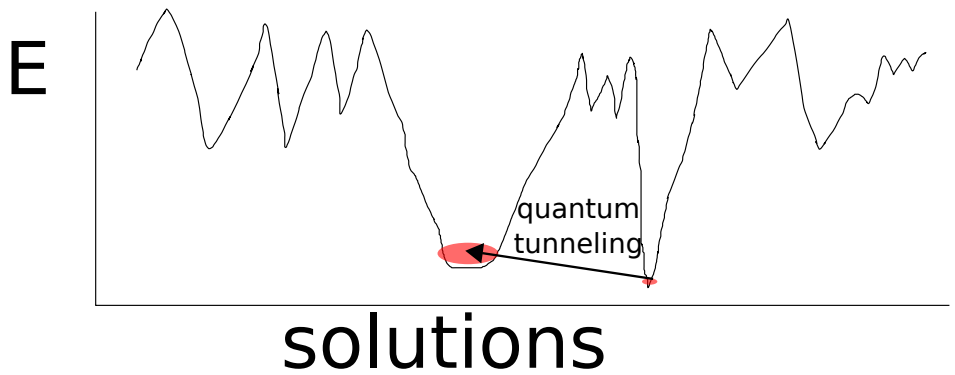
Reverse annealing to trade off optimality and robustness

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

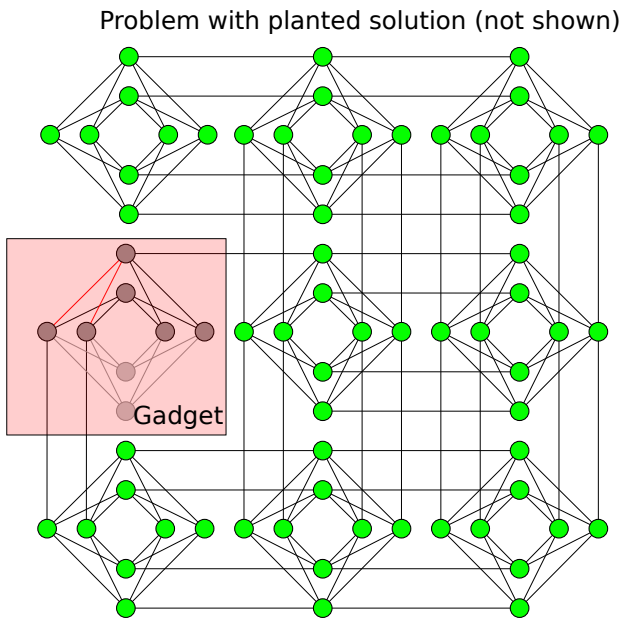
Algorithm:

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



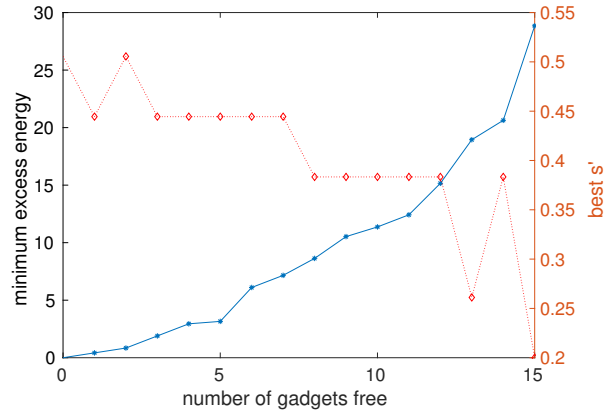
Free variable gadgets (binary version)

- 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

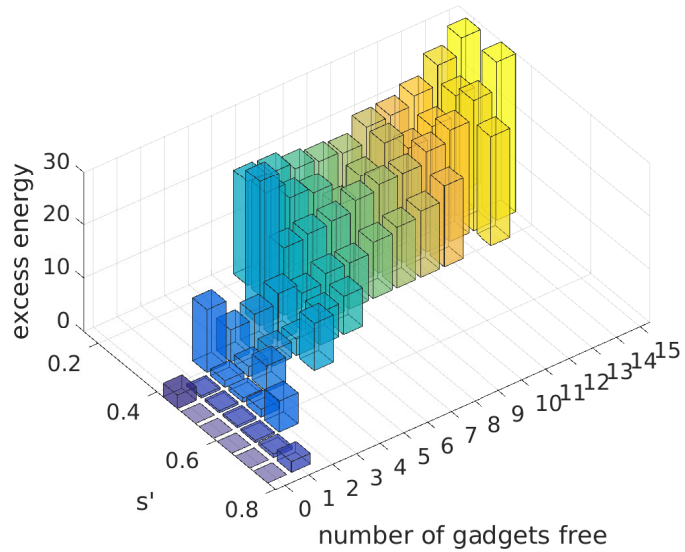


The tradeoff

What is the best excess energy we can find with a given number of gadgets free?

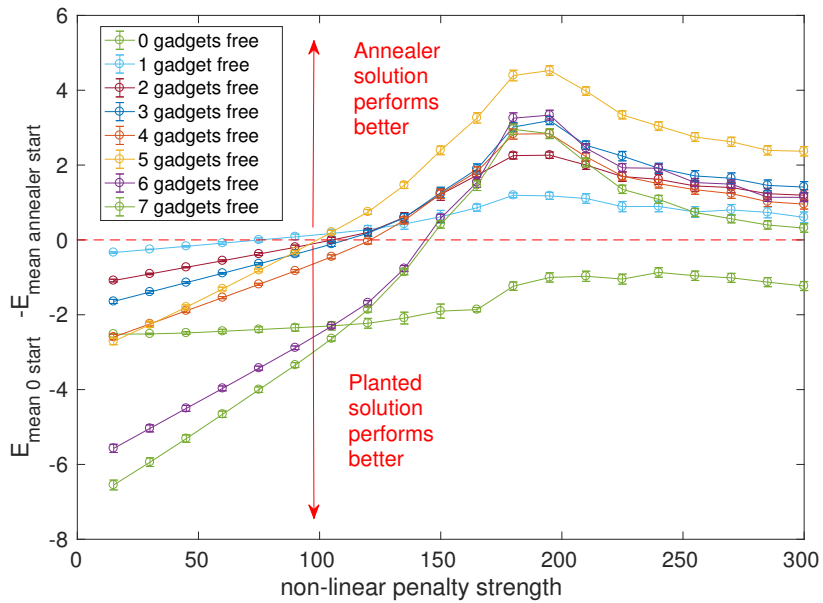


(smallest s' value taken in the event of a tie)



Putting new solutions to the test

- Choose $s' = 0.4444$ dataset $\rightarrow$ contains some of the best solutions
- Choose $10,000$ different instances of non-linear penalties
- Perform greedy search in each case and compare with planted solution
- Compare for different penalty strengths



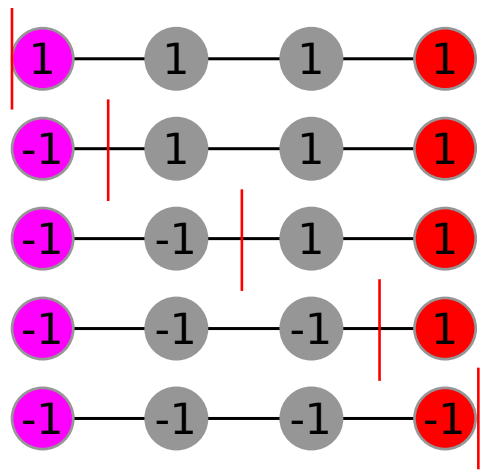
Crossover where annealer solution becomes the better choice

A more realistic version: integer variables

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

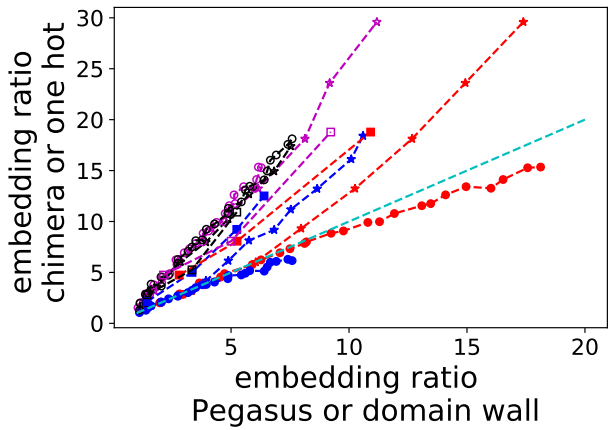
- Cumbersome to encode using traditional (one hot) method: N value integer variable $\rightarrow$ N qubit fully connected subgraph
- Better 'domain wall' encoding (see arχiv: 1903.05068)
  " " $\rightarrow$ $N-1$ qubit linearly connected subgraph

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



One slide aside: Domain wall encoding is a powerful tool for problem mapping

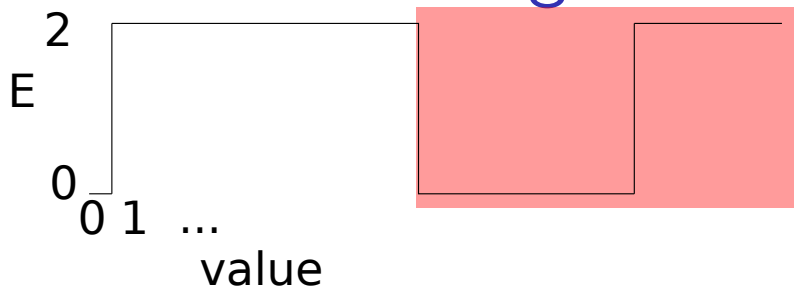
- Reduce number of qubits per variable by one
- Fewer connections within variable
- Structure tends to be better for embedding $\rightarrow$ technical reasons I won't discuss here see arχiv: 1903.05068



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

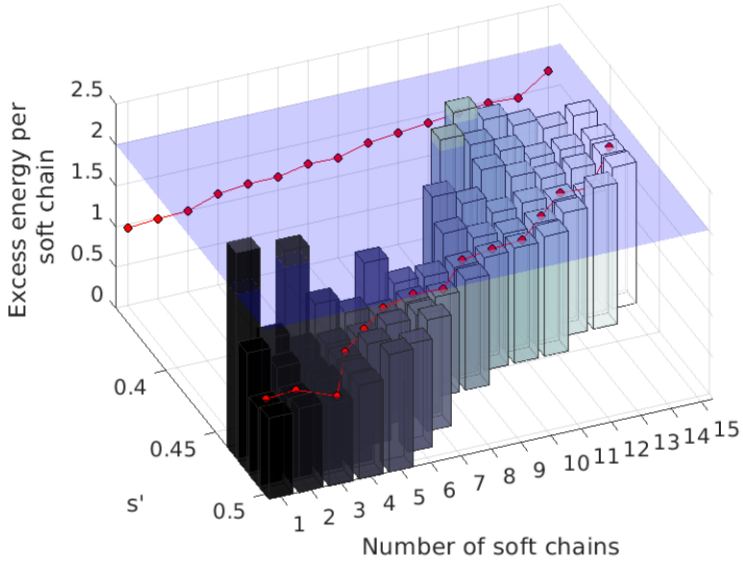
Domain wall encoding can make as much of a difference as rengineered hardware graph!

Finding robust solutions over integer variables



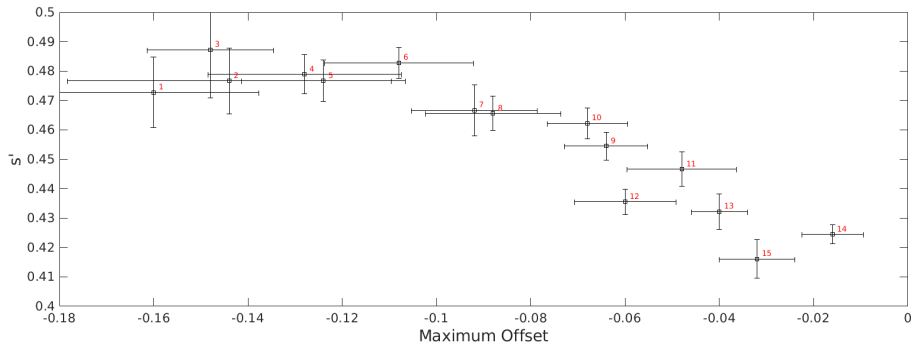
- Mixed integer/binary planted solution problem
- Unique minimum energy where binary part can be in lowest energy state
- Range over which it cannot, but has wider minima in red

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

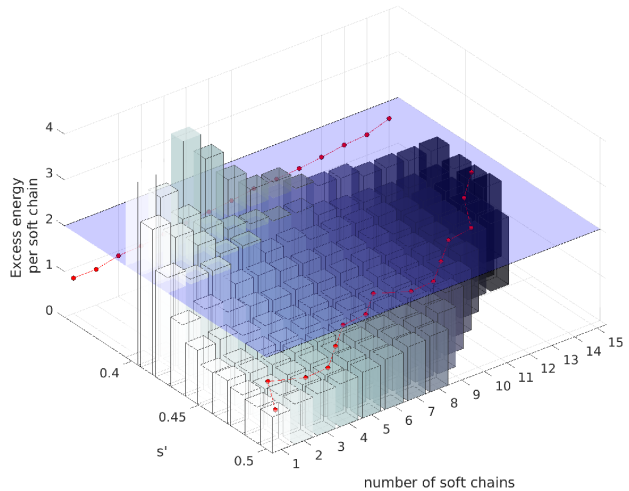


One more trick: anneal offsets

- Anneal different qubits by different amounts $\rightarrow$ more quantum fluctuations on the chains versus the other parts of the problem



Annealing less with smaller offsets useful if fewer soft chains desired



Take away messages

Quantum annealing and gate base quantum computing

- Advantages and disadvantages to each
- Quantum annealing technology more mature

Solution robustness

- Optimality isn't the only concern in the real world
- Natural dynamics of quantum annealers mean they can be used to trade off optimality for robustness

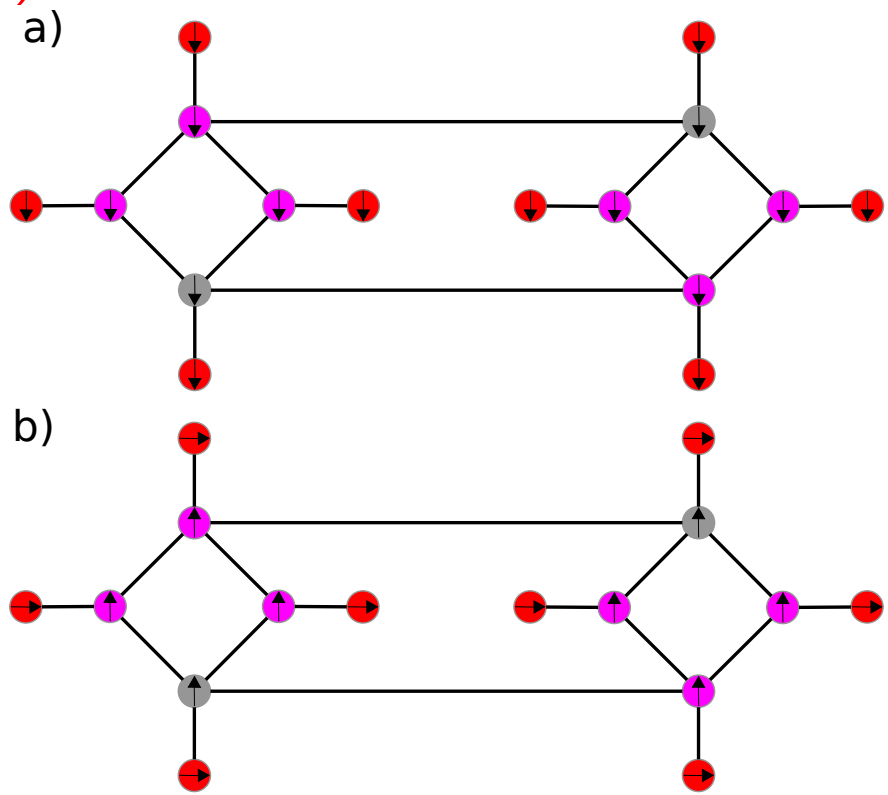
Domain wall encoding

- Powerful new tool to encode integer variables into quantum annealers

Supplementary slides

Constructing proof-of-principle Hamiltonian

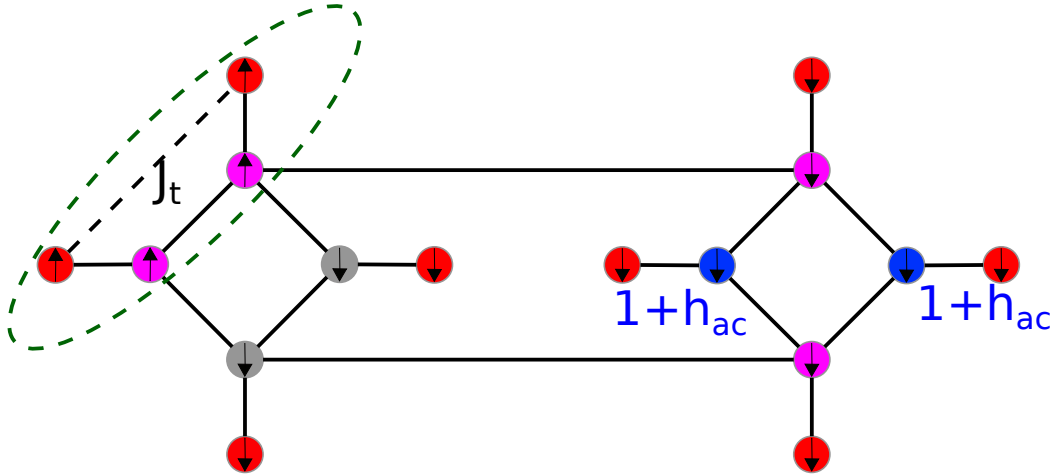
- Hamiltonians with features 1 and 2 are already known: free spin gadgets*
- Start with gadget from N. G. Dickson et. al. Nature Comm. 4, 1903 (2013)



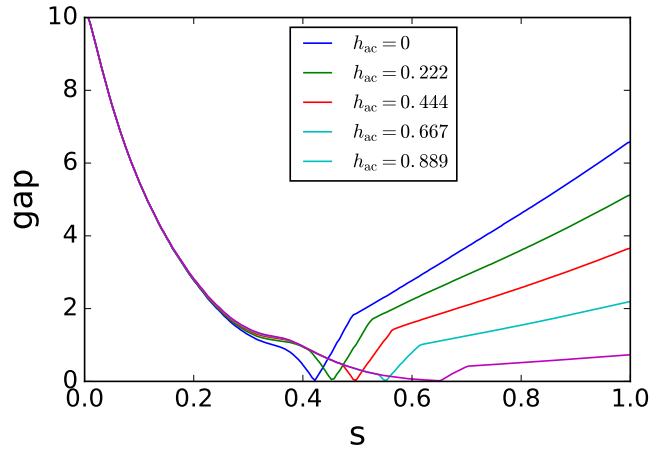
- a: unique ground state (red, h=+1 violet h=-1)
- b: 256-fold degenerate excited state → false minimum

*See for instance: S. Boixo et. al. Nature Comm. 4, 3067 (2013)

Add local minimum and make tunable

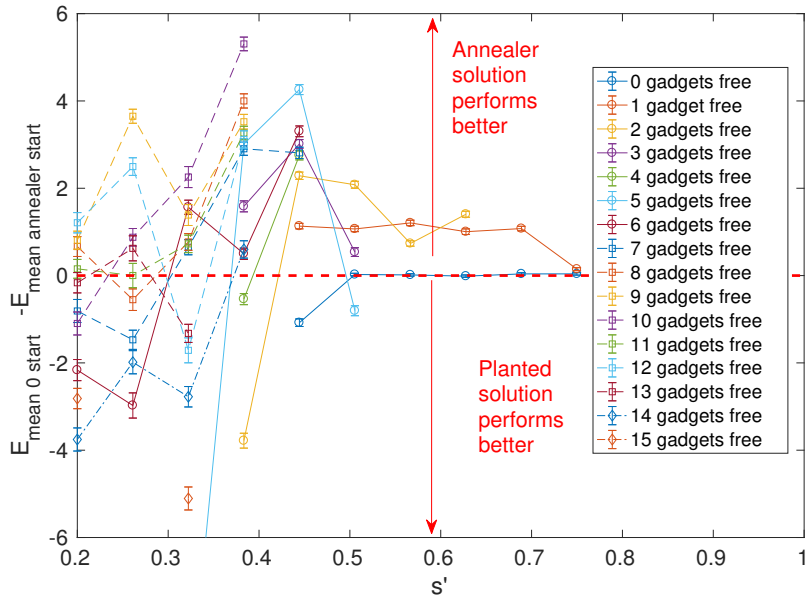


- Starting state shown by arrows, ground state except for circled spins flipped blue field is in - direction
- J_t controls barrier between start state and ground state.
- h_{ac} controls the value of s_{cross}



Comparing performance at different s' values

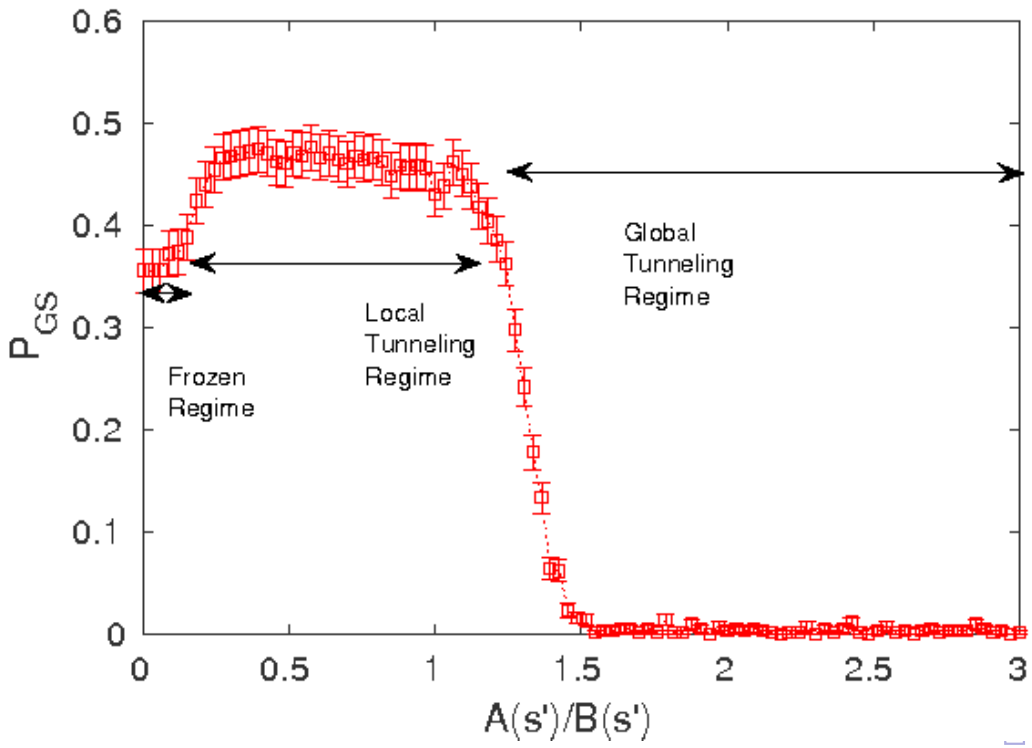
- Choose non-linear penalty strength of 195
- Examine performance of solutions found at different values of s'



- Best performance at intermediate values of s'
- Smaller values of s' better for finding solutions with smaller number of 'free' gadgets

Simple quantum Monte Carlo example

- Toy problem with broad false minima which stymies traditional quantum annealing
- Reverse annealing starting in a random state can find true ground state for large s'via local search
- Behaves like traditional annealing for too small s' values
- see NJP 19, 2, 023024 (2017) for details

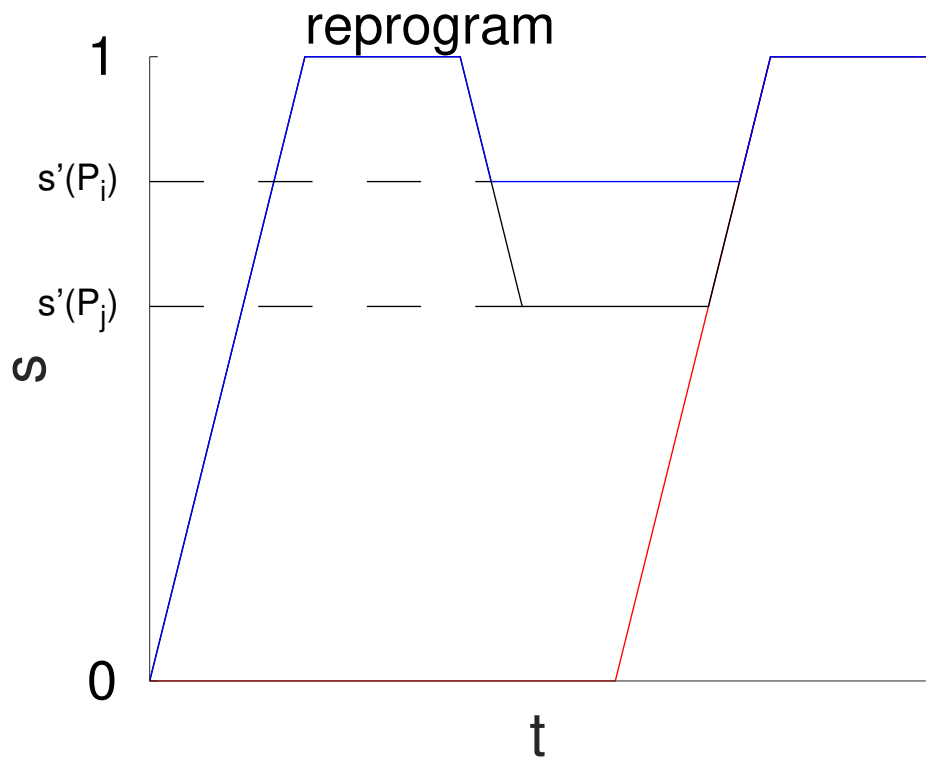


A huge number of possible reverse annealing algorithms

1. Simple version 1: search locally around best classical solution
   - Any improvement is an immediate win
   - But only likely to find solutions 'near' best classical
2. Simple version 2: search locally around randomly chosen state
   - May avoid a broad false minima
3. Monte Carlo like algorithms (see NJP 19, 2, 023024 (2017))
   - Transverse field parameter s' controls tradeoff between exploration and exploitation similar to temperature in Monte Carlo
   - Quantum analogues of many known classical algorithms
4. Genetic algorithms (see arχiv:1609.05875)
   - Compose guess from two or more known solutions
   - Most general version requires more controls than currently available

Extension: anneal qubits differently $\rightarrow$ local uncertainty

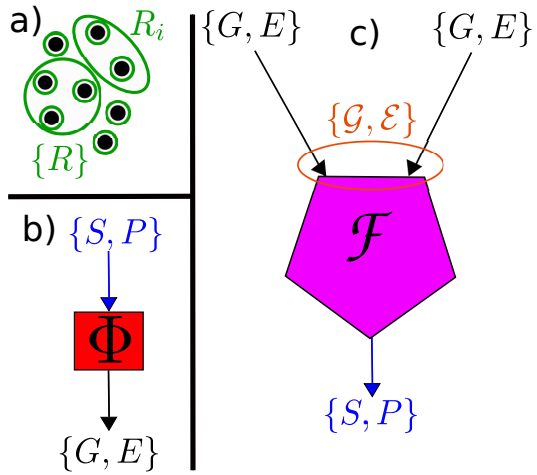
What if we are more sure about some parts of our guess then others? $\rightarrow$ anneal different qubits back to different points



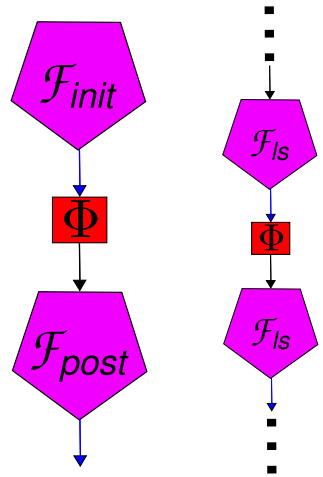
An extreme version of this, which excluded qubits where a value was expected with high certainty has already been done H. Karimi and G. Rosenberg Quantum Inf. Proc. 16(7):166 (2017) and H. Karimi and G. Rosenberg Phys. Rev. E, 96:043312

Representing this graphically: Inference Primitive Formalism

- Represent quantum annealing call as an inference primitive Φ, takes state guess $S \in \{-1, 1\}$ and uncertianty values $P \in [0, 0.5]$, outputs list of states G and energies E
- Processing function $\mathcal{F}$ represents classical processing $\rightarrow$ takes any number (including zero) of annealer outputs (found states G and energies E) and finds new guess S and uncertainty values P
- Easily generalized to multi-body drivers representing uncertainty on clusters of qubits



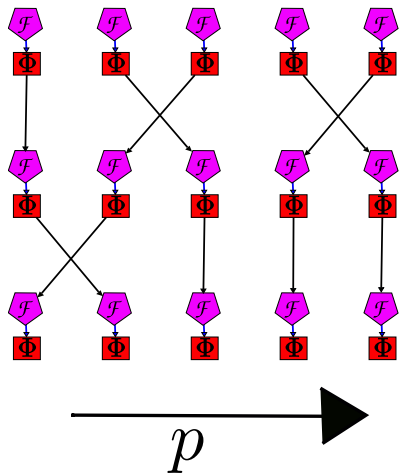
Basic Examples: traditional QA, and repeated local search in this formalism

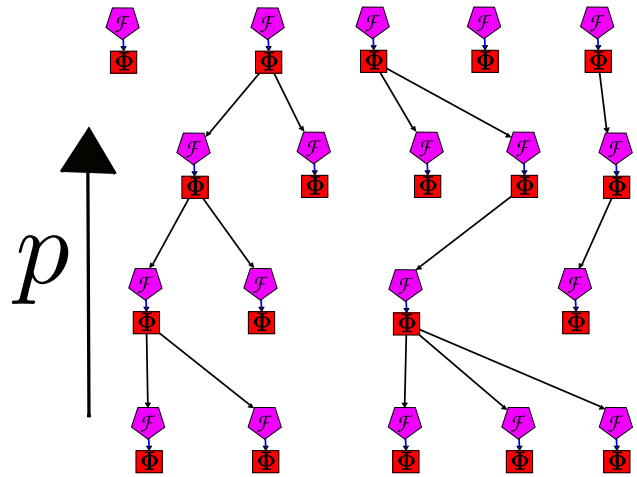


- Traditional QA (left) represented by initialization processing function which takes no inputs and gives complete uncertainty ($P_i = 0.5 \forall i$) on all qubits, followed by post processing function
- Repeated local search (right) from running annealer many times and using the output as an input to the next processing function

More advanced algorithms: Parallel tempering and Population annealing analogues

- Processing function $\mathcal{F}$ returns lowest energy state as guess and gives all qubits the same uncertainty $P_i = p \forall i$
- Assign effective temperature T to each p value and either:
  1. exchange using Parallel tempering rules (left)
     $P_{swap}(i,j) = \min\left[1, \exp\left(\left(\frac{1}{T(i)} - \frac{1}{T(j)}\right)(E_i - E_j)\right)\right]$
  2. kill or replicate states using population annealing rules (right)
     $\bar{N}(E) = \frac{1}{Q}\exp\left(\left(\frac{1}{T_{old}} - \frac{1}{T_{new}}\right)E\right)$





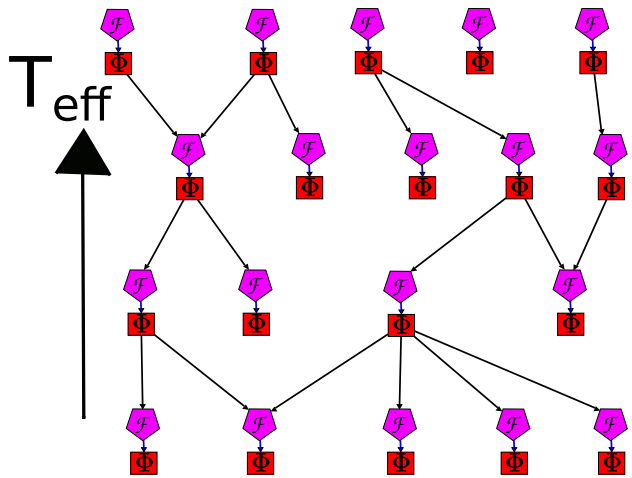
Even more advanced algorithms: Genetic algorithms

- A processing function which takes more than one input is a 'breeding' step of a genetic algorithm
- For instance could be thermally reweighted sum* (u indicates sum over unique states found)

$$S_i = \mathrm{sgn}(\sum_{j=1}^{N_u} G_j^{(u)} \exp(-\frac{E_j^{(u)}}{T_{eff}})),$$

$$P_i = \frac{1}{Z}(\sum_{j=1}^{N_u} \delta_{G_j^{(u)},-S_i} \exp(-\frac{E_j^{(u)}}{T_{eff}}))$$

- Could be used to add crossbreeding to Population annealing analogue, as shown below



*see: arχiv:1609.05875 for details