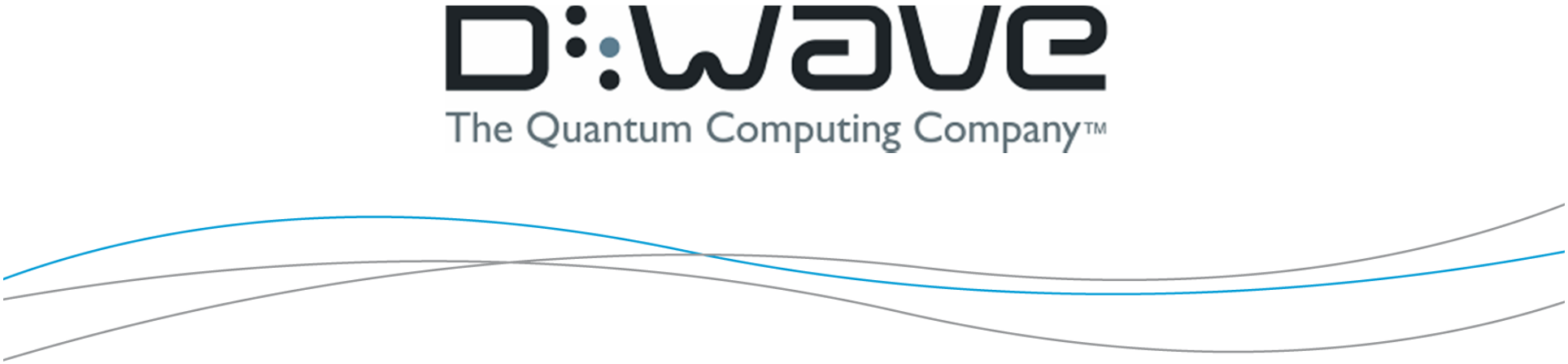

Mapping discrete optimization problems to sparse Ising models

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Joint work with
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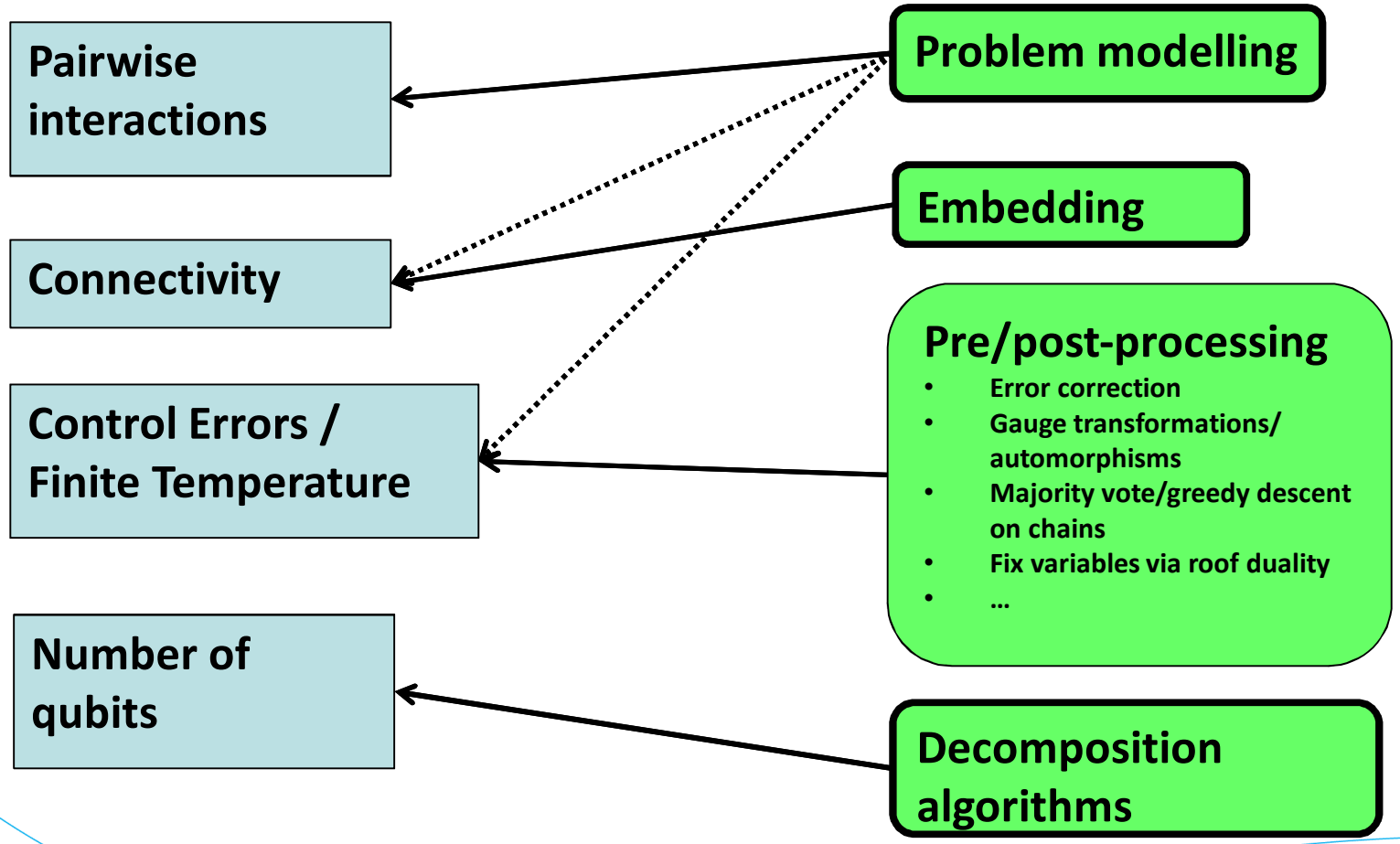
Current D-Wave hardware specs

- **Pairwise interactions**
  - Final Hamiltonian has form $H_P = \Sigma_i h_i {\sigma_i}^z + \Sigma_{i,j} J_{ij} {\sigma_i}^z \otimes {\sigma_i}^z$ with $h,\ J$ and annealing time programmable

    i.e. minimizes Ising model energy $E(s|h,J) = \Sigma_i h_i s_i + \Sigma_{i,j} J_{ij} s_i s_j, \quad s_i \in \{-1,1\}$
- **Connectivity, number of qubits**
  - 512 qubits, maximum degree 6
- **Control Errors**
  - Finite dynamic range $h, J \in [-1,1]$
  - Input misspecification up to 4%
- **Finite Temperature**
  - Current energy scales are about $\frac{E}{T} \sim$ 3-4

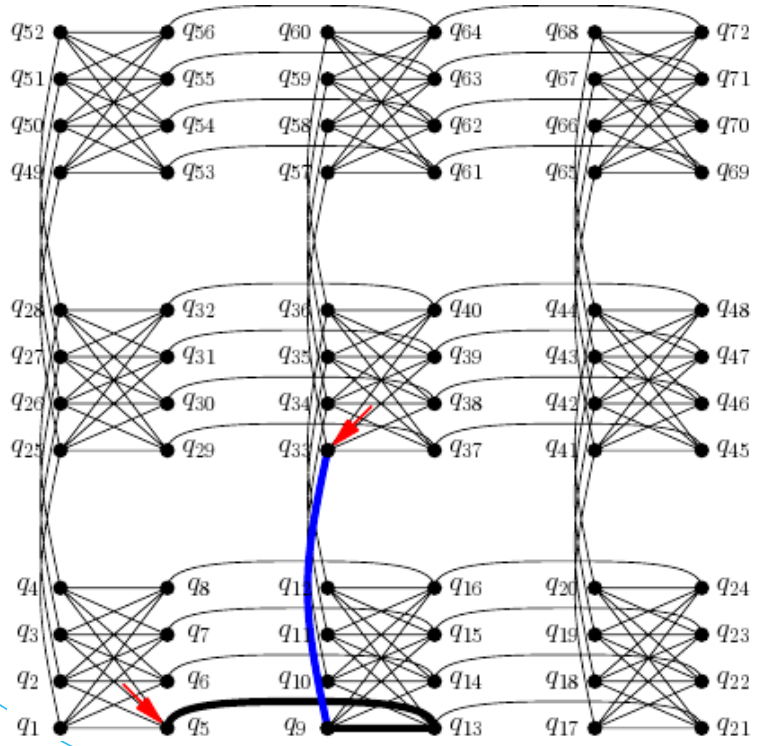
Hardware limitations / Software solutions



Mapping Ising models to the hardware

Embedding

- **In general D-Wave's hardware is too sparse (degree 6) to represent the interactions of a given Ising model**
- **One solution: let multiple qubits represent the same variable**



eg) to model an interaction between qubits q_{33} and q_5:

- Apply strong ferromagnetic couplings to ensure that qubits q_5, q_{13}, and q_9 all take the same value:

$$\boldsymbol{J_{5,13} = J_{13,9} = -1}$$

- Now the required $\boldsymbol{q_{33}q_5}$ term can be implemented on the blue edge

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The minor-embedding problem

- **Every variable is represented by a connected subset of qubits (a *chain*)**
  - If variables x and y share an interaction in the Ising model, there must be an edge between their chains
  - Chains must be disjoint
- **Embedding problem depends only on graph H of problem variable interactions and graph G of qubit interactions**
- **This is the *minor-embedding problem:***

H can be represented in G using chains if and only if H is a minor of G.

Embedding is hard in general

- Graph-minors problem is NP-complete
- Best exact algorithm for embedding H in G, k = branchwidth(G):

$$O(2^{(2k+1)\log k}\,|H|^{2k}\,2^{|H|^2}\,|H|)$$

- For fixed H, determining if G has an H-minor is technically P-time, but algorithm is not known or practical.

But…

- We do not require optimal embedding
- If embedding exists, probably many exist
- Therefore probabilistic algorithms are OK (but not studied!)

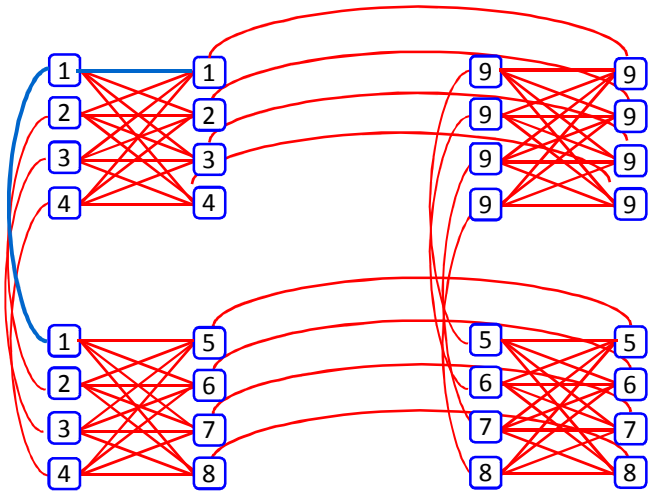
Chimera specific structure can be exploited

- **Complete graph of $4N + 1$ vertices in C_N**

  Any QUBO on N variables maps to a hardware graph of size O(N^2) with chains of size O(N)

- **Tile structure makes the problem easier**
  - Planar-like embeddings may be easier than general embeddings

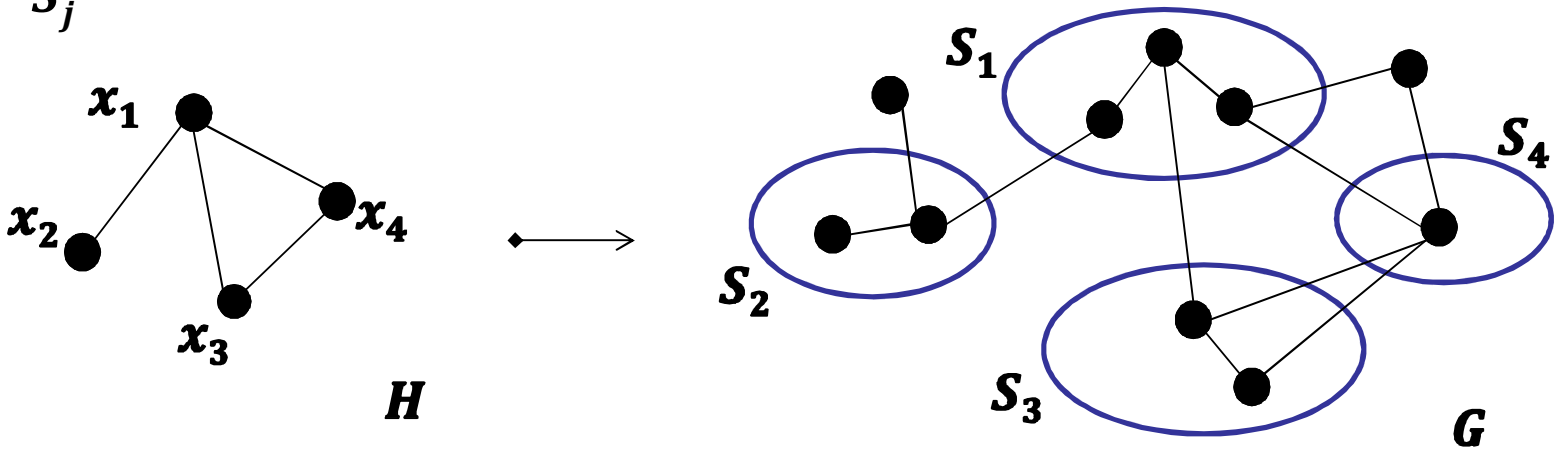
K_9 in C_2



- **Large automorphism group: $|\mathrm{Aut}(C_N)| = 8(4!)^{2N}$**
  - Implies many possible embeddings if an embedding exists
- **Sparsity is conducive to shortest path algorithms**

First greedy heuristic for minor-embedding H into G

- **Represent each variable x_i of H by a connected subgraph (chain) S_i of G such that if $x_i \sim x_j$ then there is an edge between S_i and S_j**



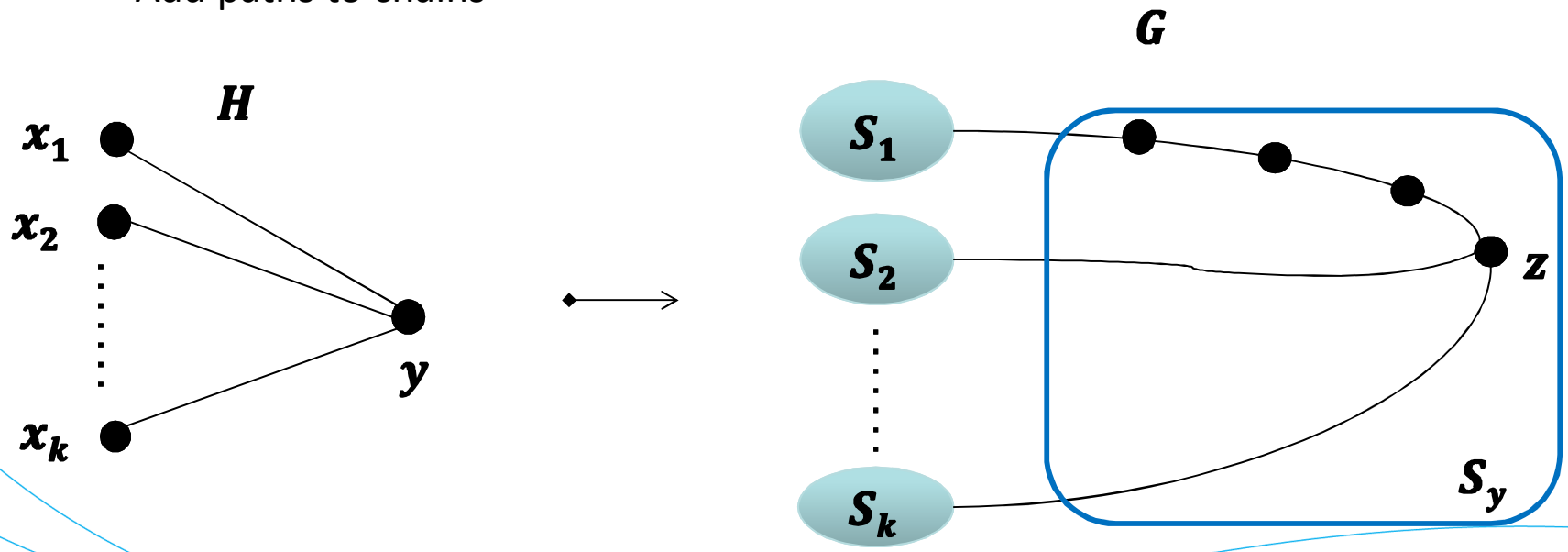
- **Add $x_1, \cdots, x_n$ to an embedding in order, ensuring that a variable is adjacent to all its earlier neighbours and S_i's are disjoint**

- **For each x_i, try to minimize $|S_i|$.**
  - Related to minimal Steiner Tree problem, itself NP-hard.
  - However, polynomial approximations exist.

First greedy heuristic for minor-embedding H into G

To embed variable y of H with neighbours $x_1, \cdots, x_k$ represented by chains $S_1, \cdots, S_k$:

- Find shortest path from S_i to every unused qubit in G (Dijkstra's algorithm)
- Represent y by root qubit z with smallest sum of path lengths
- Add paths to chains



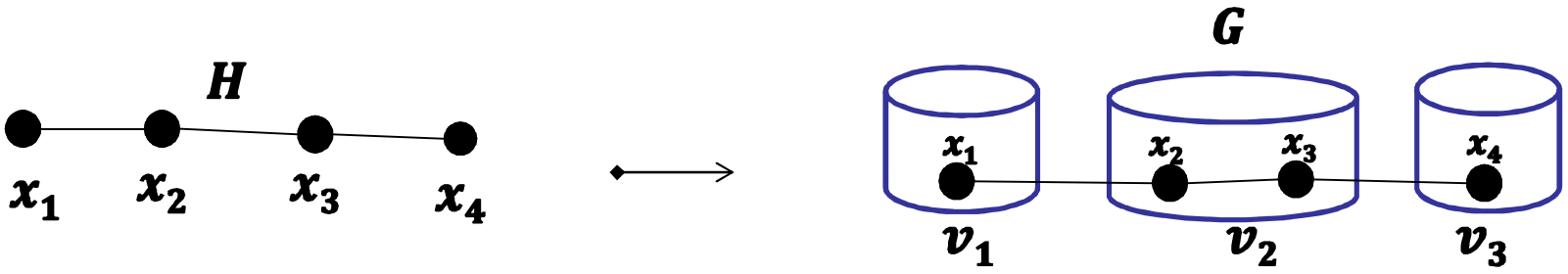
A better heuristic for minor-embedding H into G

- **Simply greedy vertex addition fails quickly**

  Eg) If x_1 has degree 7 but is embedded at a qubit of degree 6

- **So, allow multiple variables of H to be embedded at the same qubit of G**

  "bags": B_v = {variables of H embedded at v in G}



- **After all variables added, remove and try to re-embed x_1, x_2 , …**

- **Repeat until an embedding with bags of size 1 is found or you get stuck.**

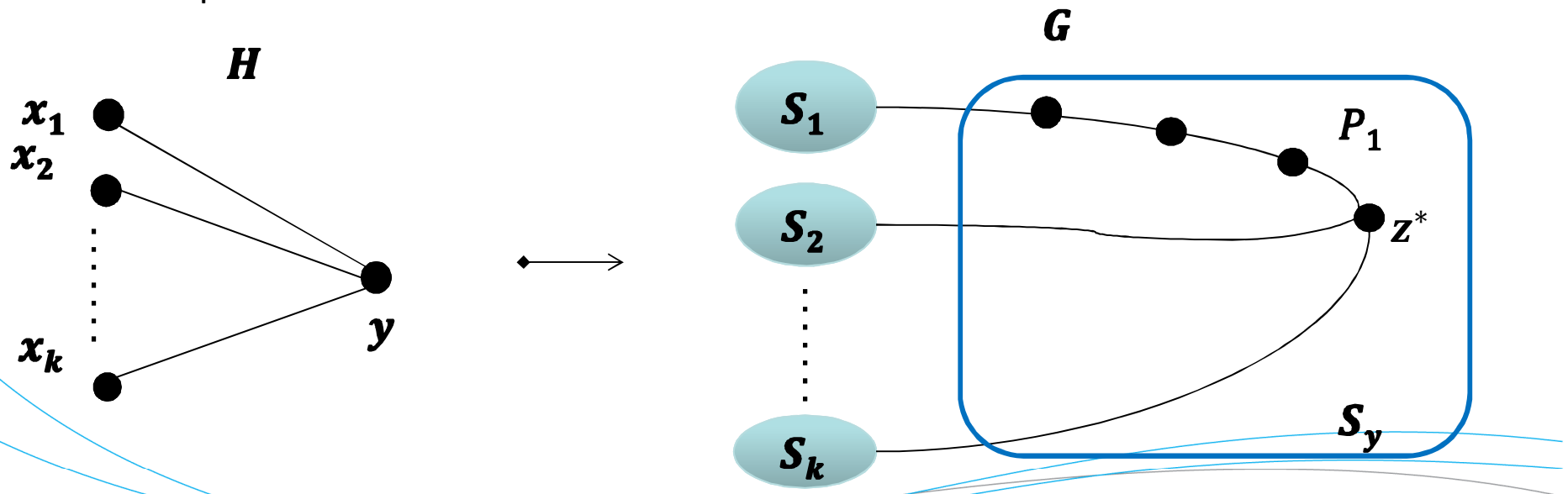
A better heuristic for minor-embedding H into G

To embed variable y of H with neighbours $x_1, \cdots, x_k$ represented by chains $S_1, \cdots, S_k$:

- Find *weighted* shortest path from S_i to every qubit z in G:

$$\text{weight}(P) = \sum_{v \in P} \exp(|\{x_i \neq y : v \in S_i\}|)$$

- Represent y by root vertex z^* with smallest sum of path weights
- Add paths to chains



Demo

Summary

- **Many ways to map to the hardware**
  - **Minor-embedding is the cleanest**
- **Global algorithms are tractable at current scale**
  - **Each iteration costs** $\mathrm{O}(|\mathrm{E}(H)|^*|\mathrm{V}(G)|\log|\mathrm{V}(G)|)$
- **Number of qubits / chain size matter**
  - **Embedding algorithms need to account for this**

Mapping boolean constraints to Ising models

Constraint Satisfaction Problems

- NP problems have simple verification circuits
- If we encode the verification circuit as an optimization objective we can reverse the flow of information from outputs to inputs
  - E.g. factor by representing multiplication circuits
- To carry this out in hardware we need to represent constraints as penalty functions
  - Focus on sparse constraints

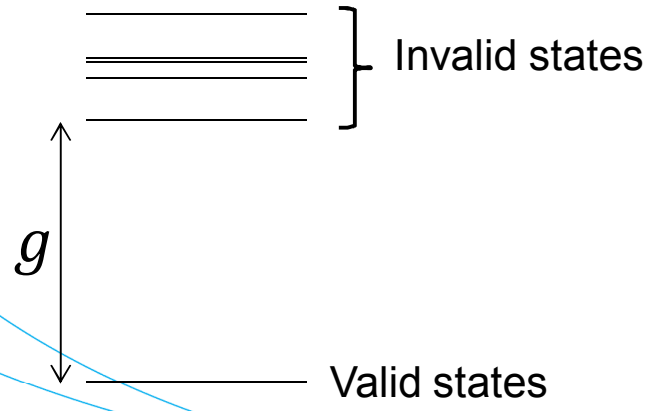
Penalty functions for local constraints

- **A local constraint is a list of feasible configurations F**
  - **For a constriant on K variables, $F \subseteq \{0,1\}^K$**

- **Represent F by a penalty Ising model $E(x)$ defined so that**

$$E(x) = \begin{cases} 0 & \text{if } x \in F \\ \geq g & \text{if } x \notin F \end{cases}$$

where $g > 0$ is a gap



- **Large g mitigates the effects of control errors and finite temperature**
- **May also increase the quantum gap**

Ancillary variables

- **Typically we will require additional ancillary variables which are minimized over:**

$$\boldsymbol{E}(\boldsymbol{x}) = \min_{\boldsymbol{a}} \boldsymbol{P}(\boldsymbol{x}, \boldsymbol{a})$$

  - Introducing more ancilla than necessary can increase g
- **Ancillary variables can also accommodate hardware connectivity:**
  - **Impose hardware connectivity constraints on z = [x,a]**

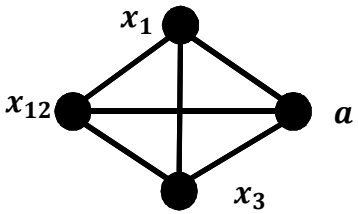
Example: Parity check

$$x_1 + x_2 + x_3 = 0 \bmod 2, \quad x_i \in \{0, 1\}$$

- **Feasible states:** $F = \{000, 011, 101, 110\}$

- **"Obvious" representation:**

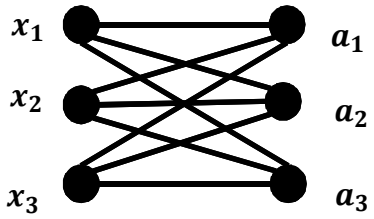
$$P(x, a) = (x_1 + x_2 + x_3 - 2a)^2$$



Energy gap = 1

- **Better representation:**

$$P(x, a) = -a_1 + a_2 - a_3 + x_1(a_1 + a_2 + a_3) + x_2(-a_1 + a_2 + a_3) + x_3(a_1 + a_2 - a_3)$$



Energy gap = 2

Finding penalties: problem formulation

- **Let $\boldsymbol{\theta} = \boldsymbol{c} \cup \{\boldsymbol{h_v}\} \cup \{\boldsymbol{J_{v,v'}}\}$ (c constant offset)**
- **Identify $\boldsymbol{\theta}$ by solving:**

$$\max_{\boldsymbol{\theta},\boldsymbol{g}} \quad \boldsymbol{g}$$

$$\begin{aligned} \text{subject to:} \quad & \boldsymbol{P(x,a|\theta)} \geq \boldsymbol{0} && \forall \boldsymbol{x} \in \boldsymbol{F}, \forall \boldsymbol{a} \\ & \boldsymbol{P(x,a|\theta)} \geq \boldsymbol{g} && \forall \boldsymbol{x} \notin \boldsymbol{F}, \forall \boldsymbol{a} \\ & \exists \boldsymbol{a}\ \boldsymbol{P(x,a|\theta)} \leq \boldsymbol{0} && \forall \boldsymbol{x} \in \boldsymbol{F} \\ & \boldsymbol{-1 \leq \theta \leq 1} \end{aligned}$$

- **Note: we need to determine the state of the ancillary**

$$\boldsymbol{a_*(x)} = \arg\min_{\boldsymbol{a}} \boldsymbol{P(x,a)} \qquad \forall \boldsymbol{x} \in \boldsymbol{F}$$

- **This is a hard problem**
  - **Optimizing for $\boldsymbol{a_*(x)}$ for any given problem defined by $\boldsymbol{\theta}$, and then optimizing over all problems**

Observations

- **Energy function is linear in θ for fixed $z = [x, a]$:**

$$P(x, a|\theta) = c + \Sigma_i h_i z_i + \Sigma_{i,j} J_{ij} z_i z_j$$

- ***If* we knew the ancillae settings $a_*(x)$ then finding θ reduces to linear program:**

$$\max_{\theta, g} g$$

subject to:

$$\begin{aligned} P(x, a|\theta) &\geq 0 && \forall x \in F, \forall a \\ P(x, a|\theta) &\geq g && \forall x \notin F, \forall a \\ P(x, a_*(x)|\theta) &\leq 0 && \forall x \in F \\ -1 \leq \theta &\leq 1 \end{aligned}$$

- **This LP is solvable at scales of interest**

Strategies for finding ancilla values

- **MILP approach:**
  - **solve with additional variables** $a_*(x) = \arg\min_a P(x, a|\theta)$:

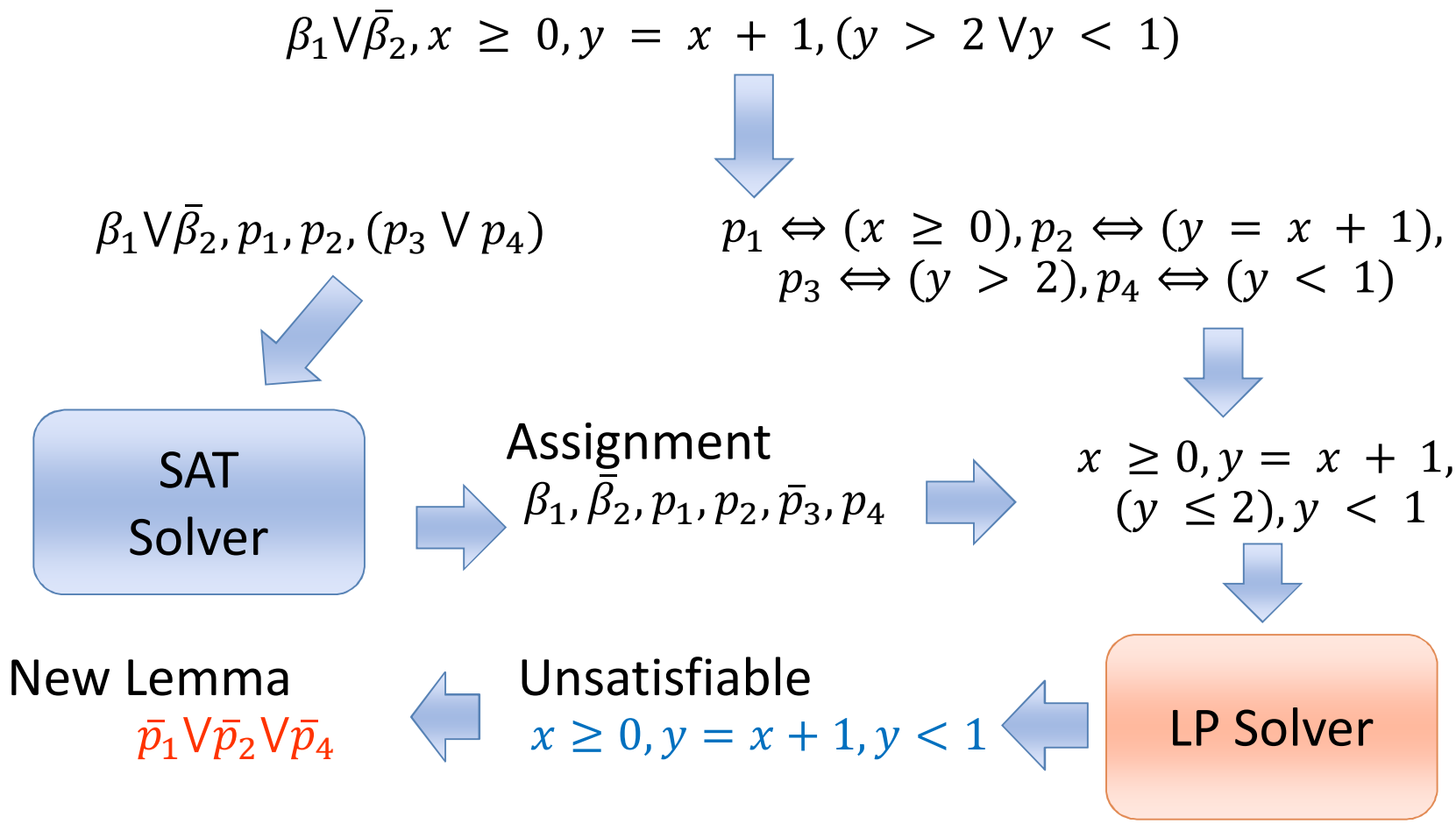
$$P(x, a\,|\theta) \leq 100 \parallel a - a_*(x) \parallel^2 \qquad \forall x \in F, a$$

- **Probabilistic approach:**
  - **Replace min over a with a softmin lower bound**

$$\min_a P(x, a|\theta) \longrightarrow F(x|\theta) = -\frac{1}{\beta} \ln \sum_a exp[-\beta P(x, a|\theta)]$$

  - **Tends to get stuck in local optima with no energy gap**
- **SMT solvers (best so far)**

Satisfiability Modulo Theory (SMT) solvers



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Using SMT solvers to find penalty functions

- **Introduce predicate variables indicating settings of ancillary variables:**

$$\beta(x, i) = \text{true} \qquad \text{iff} \qquad [a_*(x)]_i = 1$$

- **Check if penalty function can be realized for $g = 1, 2, \ldots$**
- **We have found SMT to be faster than CPLEX MILP, and easier to model in**
  - **Can incorporate symmetries and low tree-width**

Summary

- **Methods works well at small scales**
  - **constraints embeddable in up to 50 qubits often solved in less than an hour**
  - **SMT solver effective at searching the entire space**
- **Methods can encapsulate both Ising model *and* embedding**
  - **by imposing Chimera structured constraints on ancillary variables**
- **Better models of the same problem give different classical energy gaps**
  - **resulting in different hardware performance**

Decomposition techniques and real-world problems

Decomposition Techniques

- Used to solve problems that are larger than the hardware
- Split the problem into regions, then communicate between regions to coordinate solutions
- Test application: LDPC decoding
- Test algorithms:
  - Belief propagation
  - Dual decomposition

LDPC Decoding

- **Classical channel error decoding:**

Input: parity check matrix $H \in \{0,1\}^{m \times n}$,

received message $y \in \{0,1\}^{n \times 1}$

Output: codeword x **closest to** y

$$\min_{x \in \{0,1\}^{n \times 1}} ||y - x||^2 \quad \text{s.t.} \quad Hx = 0 \pmod 2$$

- **LDPC:** H **is *low density parity check***
  - **Each check has at most 5 bits**
  - **Each bit in at most 4 checks**
  - **Checks generated randomly**
  - **Can get close to Shannon limit of channel capacity**
  - **Has an effecitve classical decoding scheme (BP)**

LDPC as an Ising model

- **Write each check as a quadratic boolean function:**

$$F_C(x_C) = (x_1 + x_2 + x_3 - 2a_1)^2$$

$$= \begin{cases} 0, & x_1 + x_2 + x_3 = 0 \pmod 2 \\ > 0, & x_1 + x_2 + x_3 = 1 \pmod 2 \end{cases}$$

- **Each variable also has a linear term:**

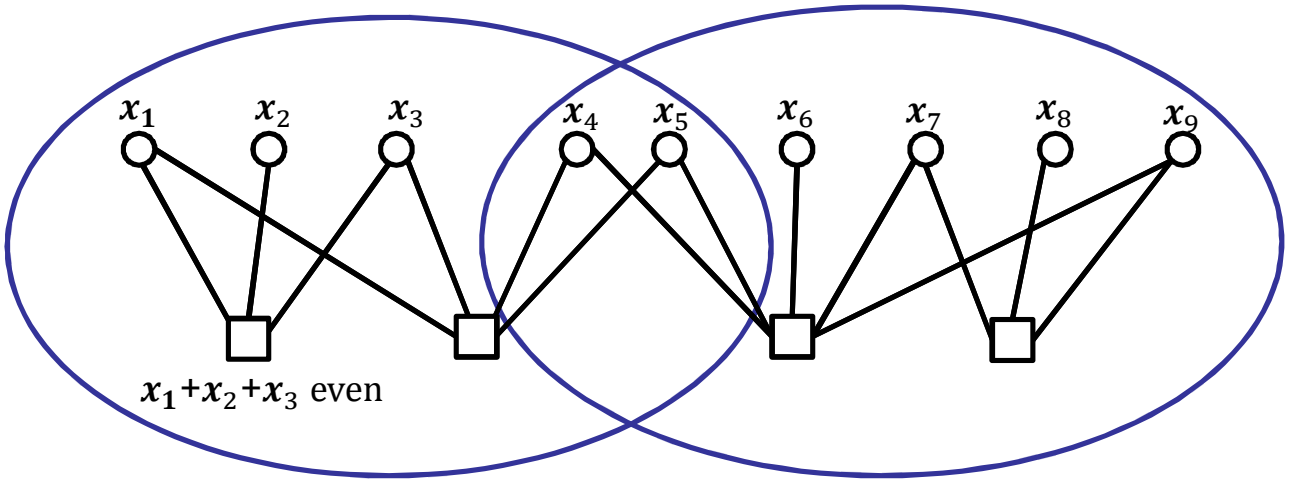
$$F_i(x_i) = (y_i - x_i)^2, \qquad y_i \text{ received value for bit } i$$

- **Overall decoding:**

$$\min_{x} \; F(x) = \sum_i (x_i - y_i)^2 + M \sum_C F_C(x_C)$$

(for some fixed M)

Region-based solutions



Regions should…

- **Be as large as possible while still embeddable in hardware**
  - **Optimize many variables simultaneously, avoid local optima**
- **Have overlap of variables between regions as small as possible**
  - **Minimize communication between regions**

Region-based Belief Propagation

- **Objective function:** $F(x) = \sum_{\alpha} F_{\alpha}(x_{\alpha})$ **where** α **labels the regions which depend on a subset of the variables**
- **Each message is a belief of a "score" (lower score = better) for value** x_i **at variable** i
- **Messages from region to variable nodes:**

$$\mu_{\alpha \to i}(x_i) = \min_{x_\alpha \setminus x_i} \left\{ F_{\alpha}(x_{\alpha}) + \sum_{j \in N(\alpha) \setminus x_i} \mu_{j \to \alpha}(x_j) \right\}$$

- **Messages from variable to region nodes:**

$$\mu_{i \to \alpha}(x_i) = \sum_{\beta \epsilon N(i) \setminus \alpha} \mu_{\beta \to i}(x_i)$$

Dual decomposition

- **To minimize $F(x) = \sum_\alpha F_\alpha(x_\alpha)$ (each α labels a region):**

$$\min_x \; F(x) = \min_{x,\, x^{(\alpha)}} \; \sum_\alpha \; F_\alpha(x^{(\alpha)})$$

$$\text{s.t.} \quad x^{(\alpha)} = x \quad \text{for all } \alpha$$

- **Add Lagrange multipliers:**

$$L(\lambda) = \min_{x,\, x^{(\alpha)}} \; \sum_\alpha \; F_\alpha(x^{(\alpha)}) + \sum_\alpha \; \lambda^{(\alpha)}(x^{(\alpha)} - x)$$

and solve the dual $\max_\lambda L(\lambda)$

- **Subgradient optimization: solving** $\min_{x^{(\alpha)}} F_\alpha\left(x^{(\alpha)}\right)$ **in hardware gives descent moves for** $L(\lambda)$

Region-based algorithms

- **Both Belief Propagation and Dual Decomposition are general algorithms**
  - **can be applied to any QUBO problem**
- **We have tried other algorithms, but BP and DD were the most effective for LDPC decoding**
  - **Correct choice of region–based algorithm is very problem specific**
  - **Both algorithms have their weaknesses**
- **Both BP and DD re-use regions embedded in the hardware**
  - **No need to re-embed at each iteration**

LDPC problems studied

- LDPC instances: 100, 200, 400, 600, 800 and 1000 bits, randomly generated checks
  - # of checks = 70% of # of bits
  - variables in 2-4 checks,
  - checks have 3-5 variables
- Pick a random code word x, and flip 8%, 10%, 12%, 14% of its bits
- Make sure:
  - code word x is the unique solution to decoding problem
  - Standard decoding algorithm fails after 1000 iterations
- Then generate 4-25 regions (20 checks each) and embed each region
  - 150 – 200 variables per region
  - 300 – 350 qubits after embedding
  - 30 – 50 boundary variables in each region

Results: LDPC decoding

Problem			Belief propagation			Dual decomposition		
Bits	Regions	Error rate	Solved?	Iterations	Minimizations	Solved?	Iterations	Minimizations
100	**4**	**8%**	✓	2	296	✓	4	16
		10%	✓	4	452	✓	4	16
		12%	✓	4	561	✓	11	52
200	**7**	**8%**	✓	17	6419	✓	13	105
		10%	✓	7	1975	✓	41	385
		12%	✓	6	1891	✓	81	777
400	**14**	**8%**	✓	6	3057	✓	55	1050
		10%	✓	12	8047	✓	4	56
		12%	✓	8	5724	✓	170	3304
600	**21**	**8%**	✓	7	5386	✓	61	1743
		10%	✓	9	8663	✓	56	1596
		12%	✓	9	9200	×	200	5838
800	**28**	**8%**	✓	6	7417	✓	133	5124
		10%	✓	11	7915	✓	115	4452
		12%	✓	13	13070	×	200	7784
1000	**35**	**8%**	✓	10	10272	✓	139	6685
		10%	✓	9	12935	×	200	9730
		12%	✓	29	18410	×	200	9730
--------	----------	----------						
100		**14%**	✓	19	2413			
200			✓	8	2105			
400			×	20	13421			
600			×	4	4914			
800			×	8	10002			
1000			×	15	61493			

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References

- Z. Bian, F. Chudak, P. Hagerty, R. Israel, B. Lackey, W. G. Macready and A. Roy. "*Discrete optimization using Quantum Annealing on sparse Ising models*", to be submitted to "Frontiers in Physics", 2014.
- J. Cai, W. G. Macready, A. Roy. "*A practical heuristic for graph minors*", 2014. arxiv.org/1406.2741.

V6 vs. V7

Vesuvius 7 online in Burnaby since January:

- **New coupler design to boost maximum coupling strength**
- **Removed several key crosstalks to improve h ICE**
- **New coupler design reduces J ICE from DAC round-off**
- **Added passivation layer to the top of fabrication stack to reduce 1/f noise**
- **481 qubits (low yield typical for new version)**

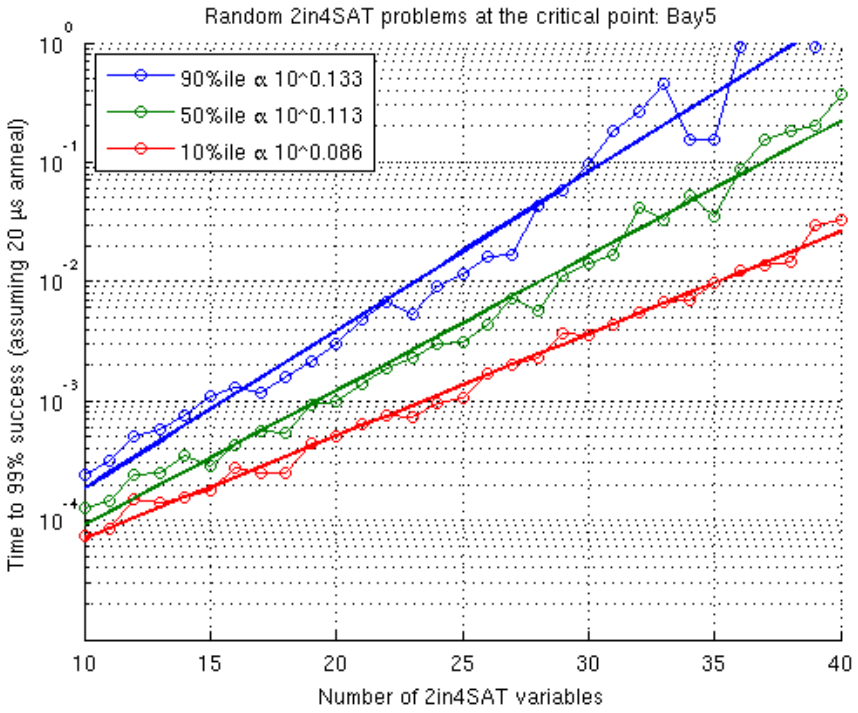
V6 vs. V7 performance on chains: 2in4-SAT tests

- **2in4-SAT: exactly 2 out of 4 literals in every clause are satisfied**
- **Tested at critical clause/variable ratio of 0.7 (phase transition from satisfiable to not satisfiable)**
- **Tested problems: 50 instances of each size with 10-40 variables, embedding with maximum chain length 4-16**
- **Problems embedded on the intersection of working graphs, chain strength 3.5, majority vote post-processing**
- **20 gauge transforms, 1000 samples each**

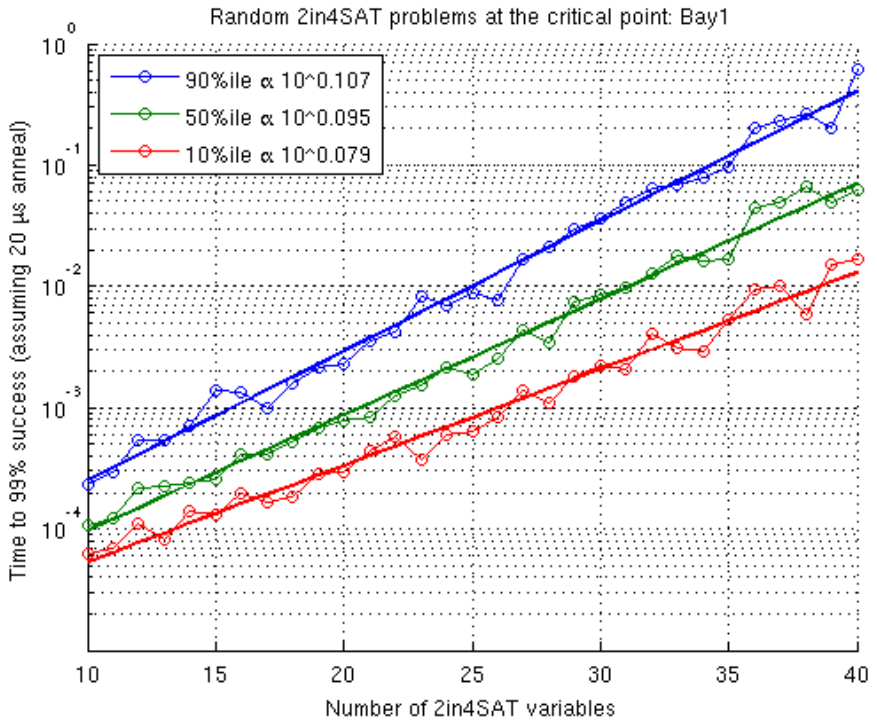
V6 vs. V7 performance on chains

- **2-in-4-SAT: exactly 2 out of 4 literals are true in every clause.**

V6



V7



- **Scaling performance is dominated by ICE, not annealing gap**

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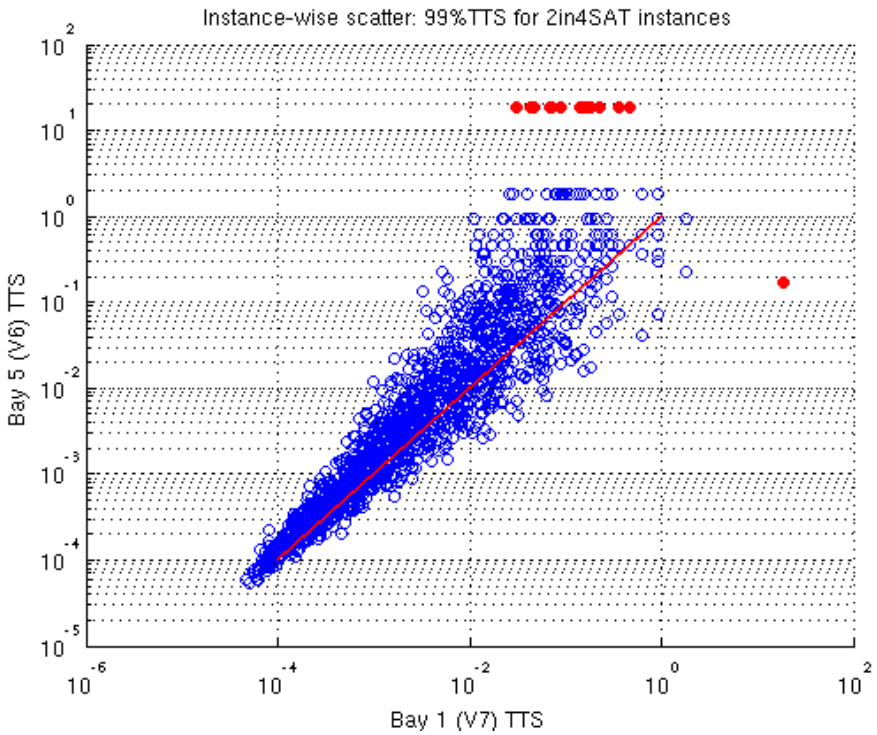
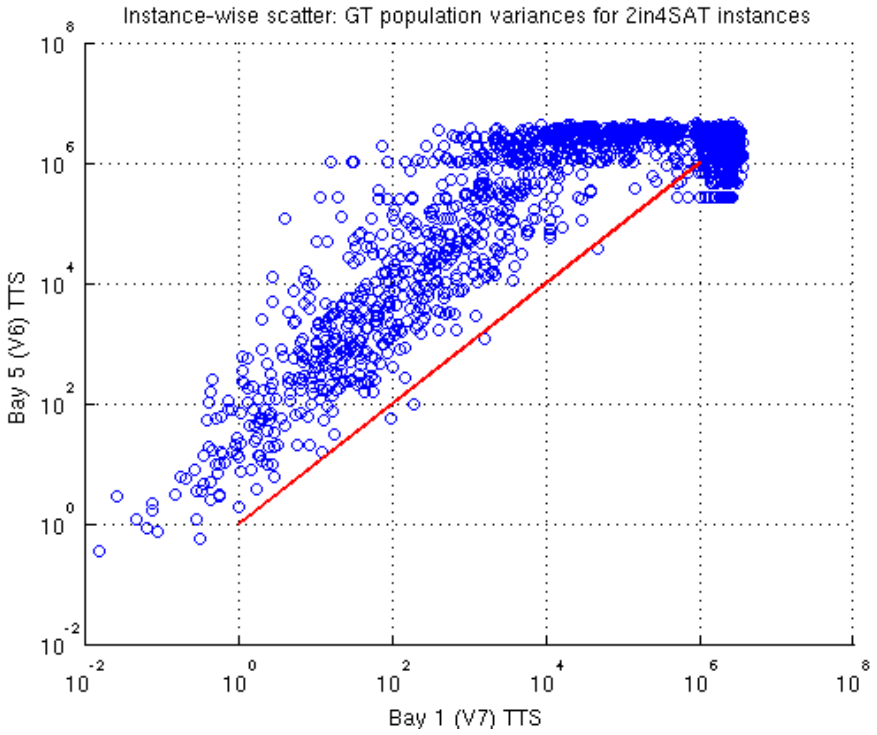
V6 vs. V7 performance on chains





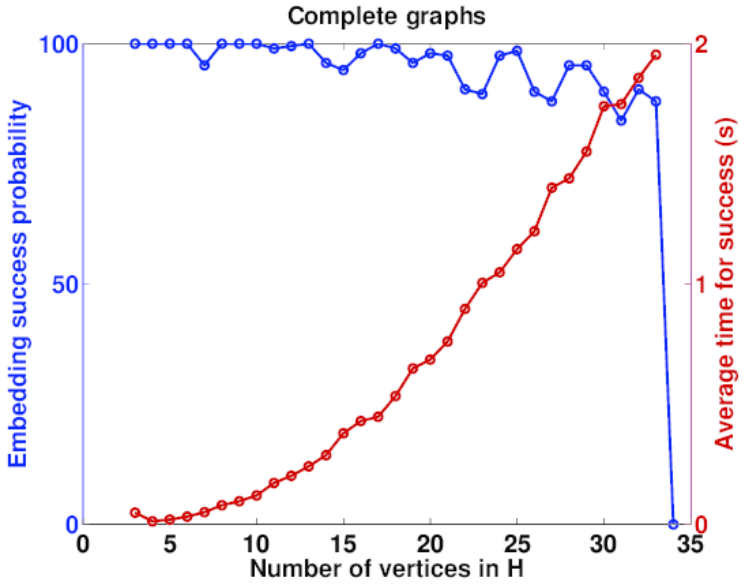
- **Without gauge transformations, performance difference is even more pronounced**

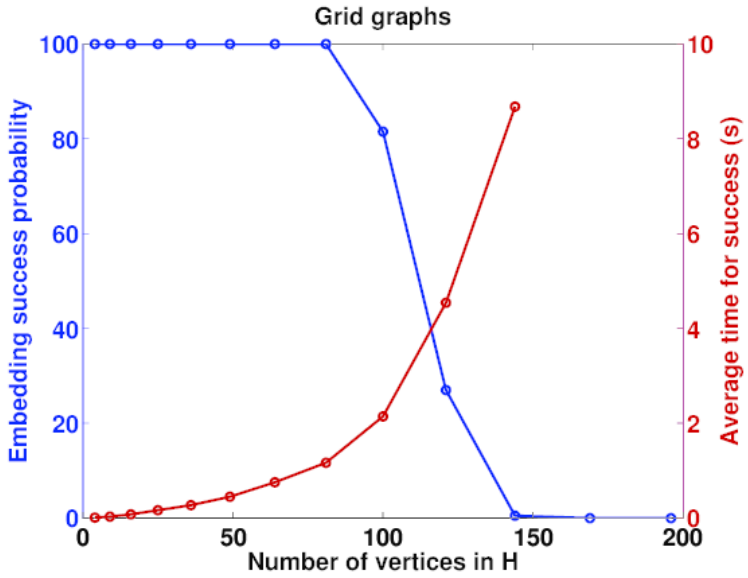
Analysis of run time

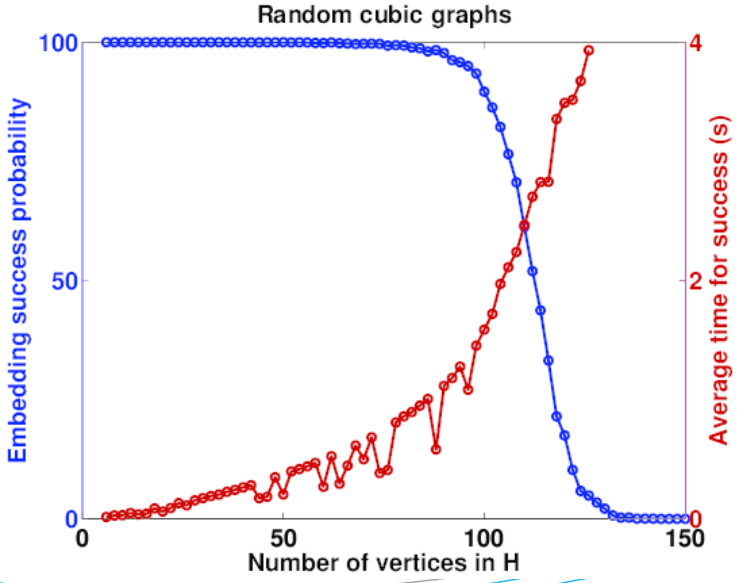
- For $H \to G$: each iteration takes $O(|E(Q)| * |V(G)| \log |V(G)|)$
- Algorithm terminates after $\leq |E(Q)| * |V(G)|$ iterations

- Measured number of iterations/success rate empirically
- "Easy" problem: embed K_N in C_8 for N = 1...33
  - provably largest embeddable complete graph
- "Hard" problem: embed $N \times N$ grid graph in C_8 for N = 1…16
  - again provably largest possible
- Random problem 2: random cubic graphs up to 40 variables
- Ran each problem 100 times (algorithm has several sources of randomness)

Embedding performance







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