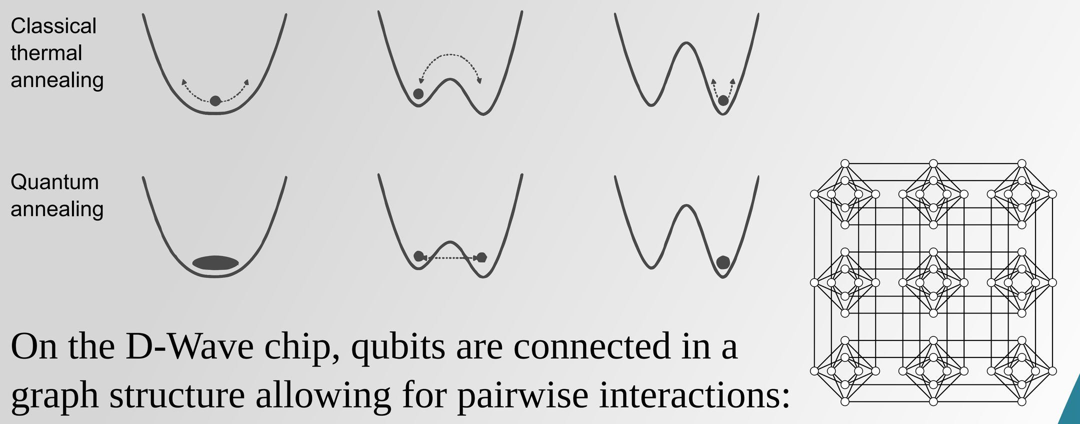
Finding Maximum Cliques on a Quantum Annealer

Background on D-Wave

The D-Wave quantum annealer is a hardware realization of classical (thermal) simulated annealing, a wide-spread optimization technique which minimizes a function by proposing random moves to escape local minima:



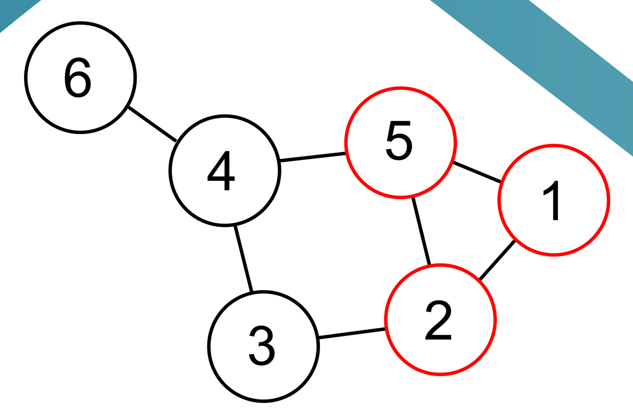
On the D-Wave chip, qubits are connected in a graph structure allowing for pairwise interactions:

D-Wave minimizes a sum of linear and quadratic contributions weighted by given constants a_i, $a_{ij} \in \mathbb{R}$, called **Hamiltonian**:

$$f(q) = \sum_{i \in V} a_i q_i + \sum_{(i,j) \in E} a_{ij} q_i q_j$$

Ising: $q_i \in \{-1,+1\}$ Qubo: $q_i \in \{0,+1\}$

The Maximum Clique Problem



We consider *maximum clique (*MC), a classical NP-hard graph problem.

Applications: network analysis, bioinformatics, computational chemistry.

Let $G = (V,E)$ be an undirected graph. A clique is a subset $S \subseteq V$ forming a complete subgraph (any two vertices of S are connected by an edge in G). A maximal clique is a clique of maximal size.

Qubo for Maximum Clique

We use the equivalence of MC to maximum independent set problem:
For a graph H, S is independent set if any two vertices $v,w \in S$ are not connected in H.

An independent set of $H = (V, \bar{E})$ is a clique in $G = (V, E)$. Constrained minimization:

$$\text{maximize}_{x_i \in \{0,1\}} \sum_{i=1}^{N} x_i \qquad \text{subject to} \sum_{(i,j) \in \bar{E}} x_i x_j = 0$$

The equivalent formulation as unconstrained minimization (Qubo):

$$H = -A \sum_{i=1}^{N} x_i + B \sum_{(i,j) \in \bar{E}} x_i x_j$$

with A = 1 and B = 2 (Lucas, 2014).
Disadvantage: $O(N^2)$ quad. terms, limited D-Wave solubility.

D-Wave Solvers

D-Wave Inc. provide tools to submit Qubo/Ising problems to the annealer, to perform the annealing and to post-process the output:

- ► *Sapi*: "Solver API", highest level control, set annealing cycles or post-processing, load pre-computed embeddings for complete 45 vertex graphs
- ► *QBsolv*: heuristic for instances ≥ 1000 qubits, identifies signif. rows/columns of Hamiltonian, solves subproblem on D-Wave
- ► *QSage*: black-box solver for bitstrings of arbitrary size, tabu search enhanced with DW-generated samples

Experiments: Small graphs with no special structure

Graph	Max. clique size	Runtime [s]						
		Sapi	PPHa	QBsolv	fmc	pmc	SA	Gurobi
p= 0.3	5	0.15	0.15	0.05	$8 \cdot 10^{-6}$	$3 \cdot 10^{-5}$	0.15	102
p= 0.5	8	0.15	0.15	0.06	$3 \cdot 10^{-4}$	$5 \cdot 10^{-5}$	0.37	38
p= 0.7	13	0.15	0.15	0.04	0.002	8.10^{-5}	0.19	33
p= 0.9	20	0.15	0.15	0.04	0.135	8.10^{-5}	0.28	2

Set-up: 45 vertex graphs, random edges with probability p

Results: Every software solver returns correct solution on small random graphs fitting D-Wave's architecture.

Gurobi solves the dual problem (maximum independent set) thus leading to reversed graph densities and timings.

Main observations: *pmc* is an order of magnitude faster than all other methods, D-Wave yields constant time solutions but no quantum speed-up detectable.

Classical Solvers

We benchmark against the following classical approaches:

- ► *SA-Ising*: All-purpose simulated annealing.
- ► *SA-clique*: Simulated annealing specifically for cliques of size m (Geng et al., 2007).
- ► *Fast Max-Clique Finder (fmc, pmc)*: Exact and heuristic efficient search algorithms for max. cliques in sparse graphs.
- ► *Post-processing heuristics alone (PPHa)*: D-Wave's server-side post-processing step applied to random initial solution.
- ► *Gurobi*: Mathematical programming solver for linear, mixed-integer and quadratic programs (Gurobi Optimization Inc., 2015). Applied to the dual of maximum clique (maximum independent set) on the complement graph.

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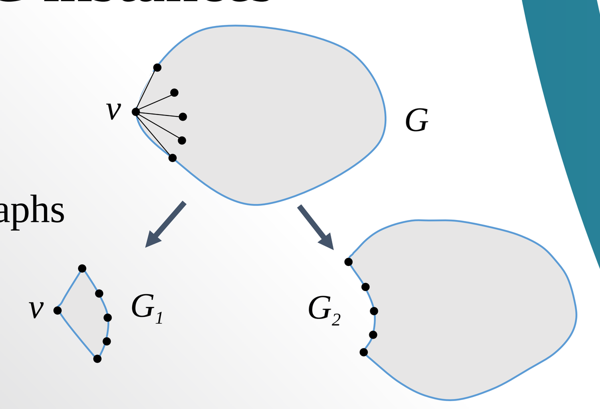
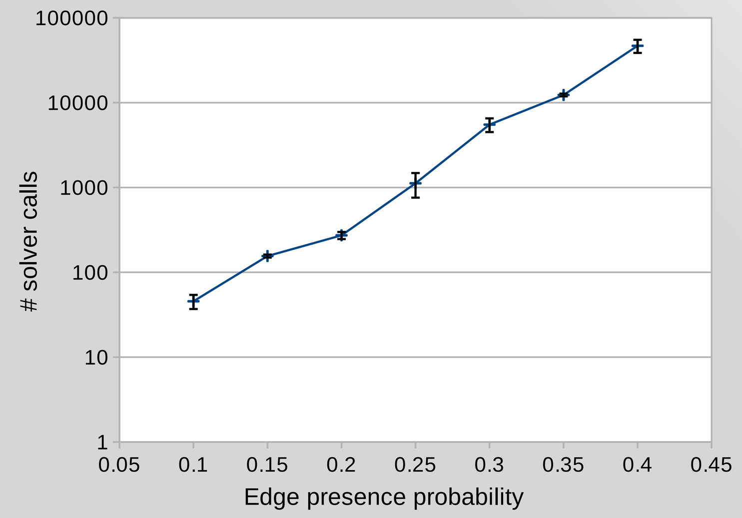
Solving large MC instances

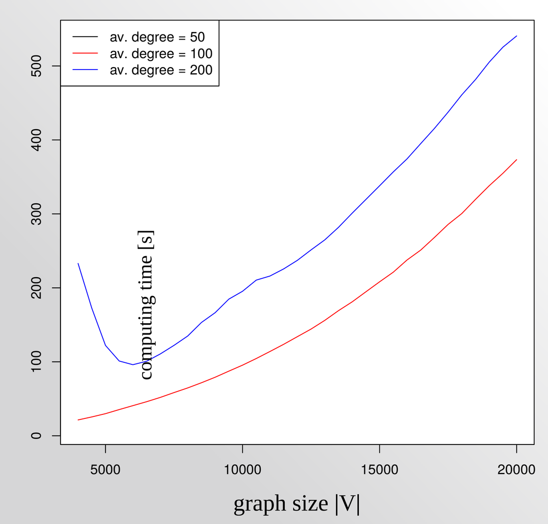


Idea: Remove edges not belonging to a maximum clique and split into subgraphs of at most 45 vertices.

Algorithm: Start with list $L=\{G\}$ and iterate until subgraphs fit DW:

- ► *Extract k-core*: maximal subgraph whose vertices have degree ≥ k; any clique C of size $k+1$ of G is also a clique of the k-core
- ► *Graph partitioning*: divide G into cores C_i and distance one neighbors H_i (halo); maximal clique is equal to the max clique in one of the partitions
- ► *Vertex splitting*: like partitioning but with $C_1=\{v\}$ for $v \in V$ and $C_2 = V \setminus \{v\}$





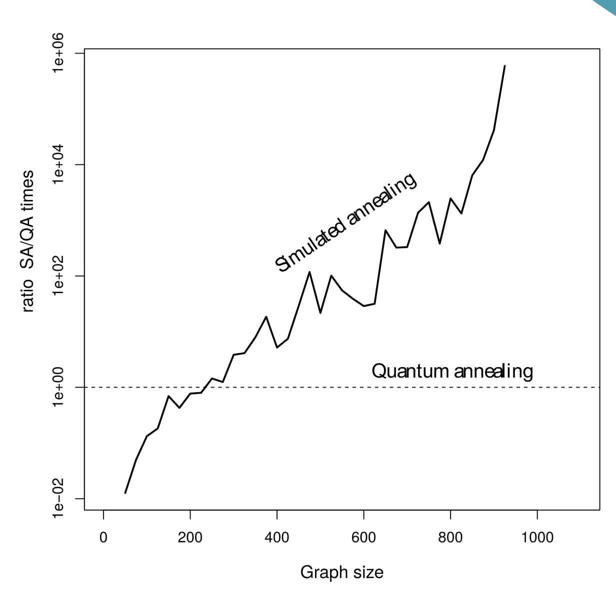
Set-up (left): 500 vertices, edge probability p from 0.1 to 0.4 in steps of 0.05

Set-up (right): graph sizes 3000 to 20000, fixed degree d, edge probability $p = d/(|V|-1)$

Experiments: D-Wave vs SA-clique

Why SA-clique? SA-clique is considered the classical analogue of quantum annealing and thus the closest competitor to D-Wave.

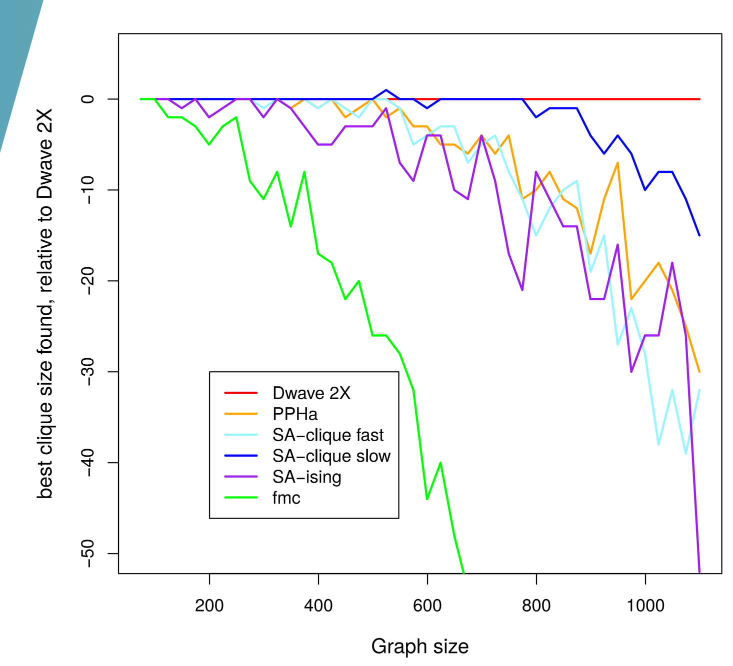
Set-up: 500 anneals on D-Wave on (contracted) chimera graphs, record best solution, then lower cooling schedule of SA-clique until same solution is found.



Conclusions:

- ► Random graphs: too small, optimized classical solvers faster, DW solutions of comparable quality
- ► **No quantum advantage for general instances embeddable on DW**
- ► Special instances designed to fit DW can be magnitudes faster (closer to DW chimera topology=faster)

Experiments: Chimera-like graphs



Motivation: So far no quantum advantage on small graphs. Need comparison on graphs larger than 45 vertices.

Set-up: Use chimera subgraphs generated by contracting edges which always fit the D-Wave topology.

Results: Up to size 400, PPHa finds same result as D-Wave. For size larger than 800, D-Wave is best.

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