APPLICATIONS ON QUANTUM ANNEALERS AT FZJ

JUNIQ: Jülich Unified INfrastructure for Quantum Computing

INQA CONFERENCE 2022 I DR. DENNIS WILLSCH

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1. Airline Scheduling
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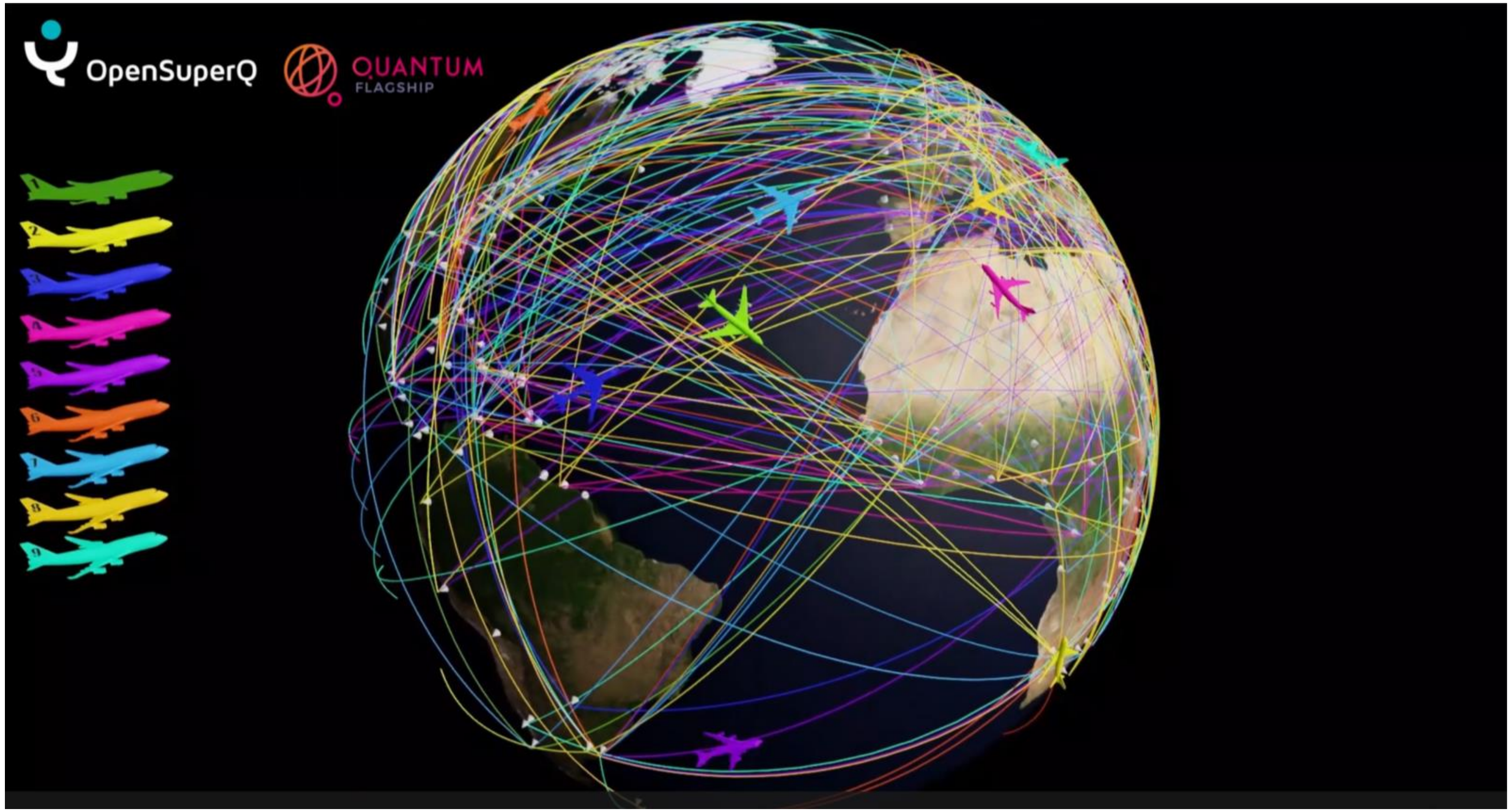
Willsch et al. (2022)
QINP **21**, 141
arXiv:2105.02208

TAIL ASSIGNMENT PROBLEM

Application: Airline scheduling

Find optimal flight schedule such that each flight is covered exactly once



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BOEING
OpenSuperQ
QUANTUM FLAGSHIP

Willsch et al. (2022)
QINP **21**, 141
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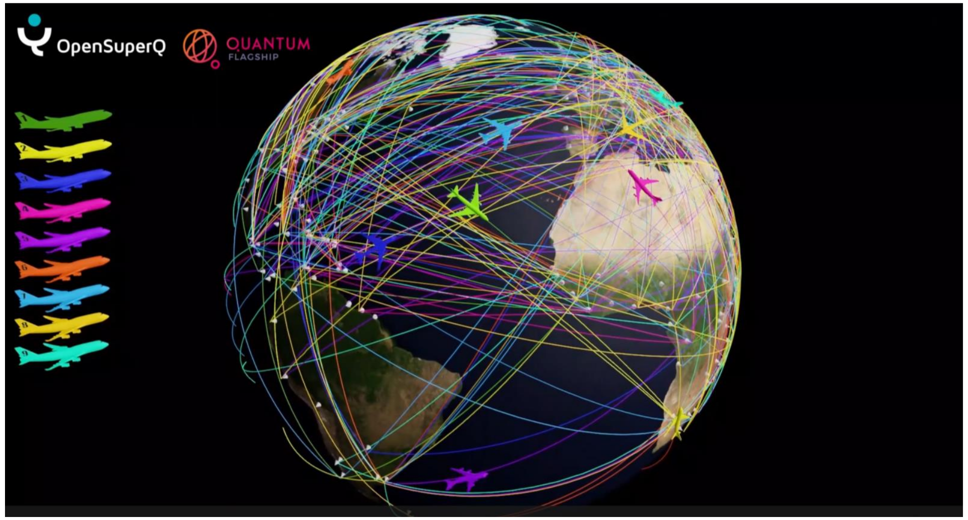
TAIL ASSIGNMENT PROBLEM

Problem specification

Find optimal flight schedule
such that each flight is covered
exactly once



	Flight 0	Flight 1	Flight 2	Flight 3	Flight 4	Flight 5	⋯	Flight 469	Flight 470	Flight 471
Route 0	0	1	0	0	0	0		0	0	0
Route 1	0	0	0	0	1	0		0	0	0
⋮										
Route 10	0	0	0	0	0	1		0	0	1
Route 11	0	0	1	0	0	0		0	0	0
Route 12	0	0	0	1	0	0		1	0	0
Route 13	0	0	1	0	0	0		0	0	0
Route 14	0	0	0	1	0	0		0	0	0
Route 15	0	0	0	0	1	0		0	0	0
Route 16	0	1	0	0	0	0		0	1	0
⋮										
Route 37	0	0	0	0	0	1		0	0	0
Route 38	0	0	0	1	0	0		0	0	0
Route 39	0	0	0	1	0	0		0	0	0

Willsch et al. (2022)
QINP **21**, 141
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TAIL ASSIGNMENT PROBLEM

Mathematical formulation

	Flight 0	Flight 1	Flight 2	Flight 3	Flight 4	Flight 5	⋯	Flight 469	Flight 470	Flight 471
Route 0	0	1	0	0	0	0		0	0	0
Route 1	0	0	0	0	1	0		0	0	0
⋮										
Route 10	0	0	0	0	0	1		0	0	1
Route 11	0	0	1	0	0	0		0	0	0
Route 12	0	0	0	1	0	0		1	0	0
Route 13	0	0	1	0	0	0		0	0	0
Route 14	0	0	0	1	0	0		0	0	0
Route 15	0	0	0	0	1	0		0	0	0
Route 16	0	1	0	0	0	0		0	1	0
⋮										
Route 37	0	0	0	0	0	1		0	0	0
Route 38	0	0	0	1	0	0		0	0	0
Route 39	0	0	0	1	0	0		0	0	0

- Linear assignment problem

$$\begin{aligned} &\text{minimize} && \vec{f}^T\vec{x} \\ &\text{subject to} && A\vec{x} = \vec{b} \end{aligned}$$

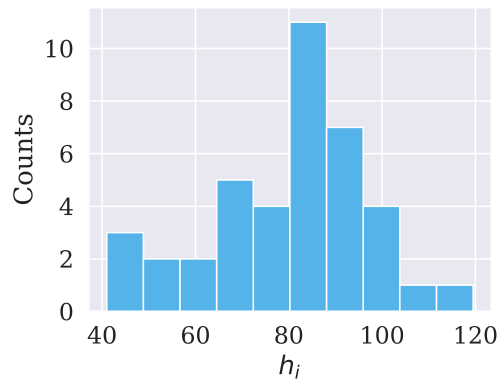
encodes cost of assigning airplanes to routes

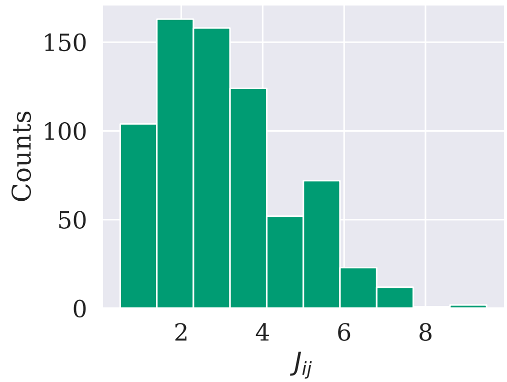
exact cover problem: each flight covered once

- Reformulation as Ising problem

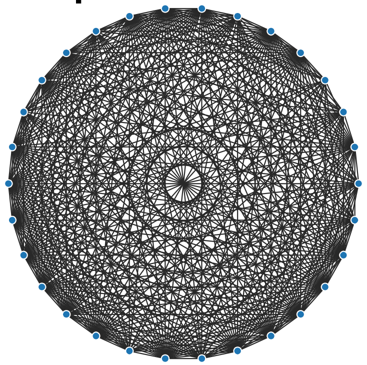
$$\text{QUBO} \leftrightarrow \text{Ising}: \quad x_i = (1+s_i)/2$$

$$\min_{x_i=0,1}\left(\left(A\vec{x}-\vec{b}\right)^2 + \lambda\vec{f}^T\vec{x}\right) = \min_{s_i=\pm1}\left(\sum_i h_i s_i + \sum_{i<j} J_{ij}s_i s_j + \text{const}\right)$$

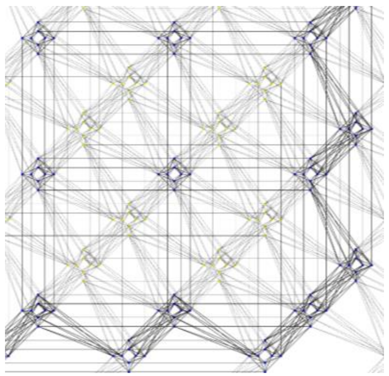




- 25 - 40 qubit almost fully-connected (“clique”) Ising problems



embedding needed



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Willsch et al. (2022)
QINP **21**, 141
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TAIL ASSIGNMENT: RESULTS

30 - 40 qubit problems (90% nonzero couplers)

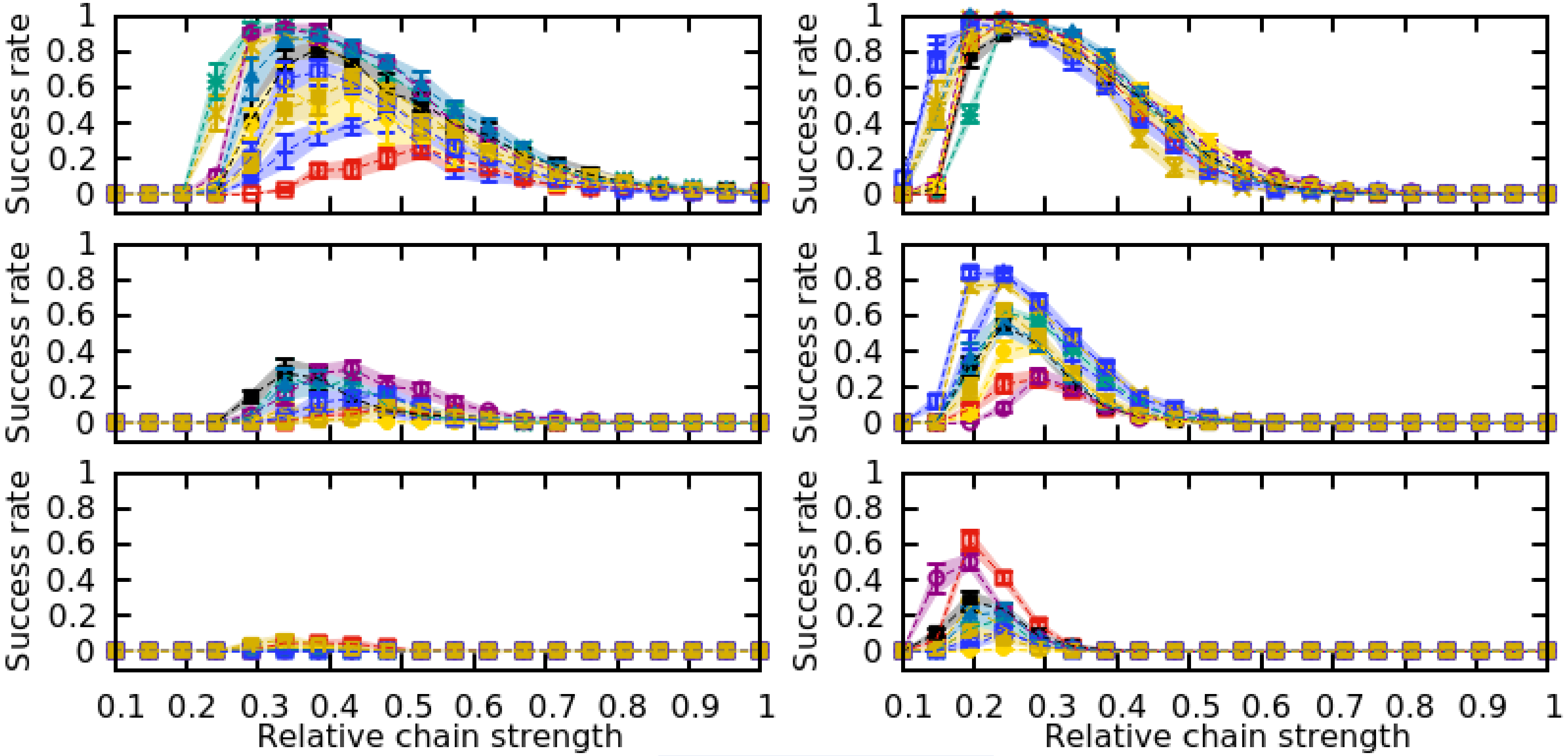
Scan of 10 different embeddings and 20 relative chain strengths:

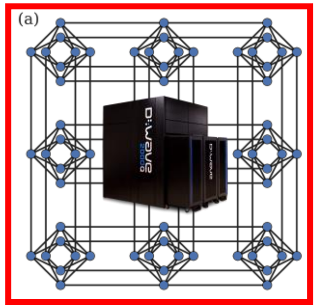
DW2000Q **Advantage**

30 qubits

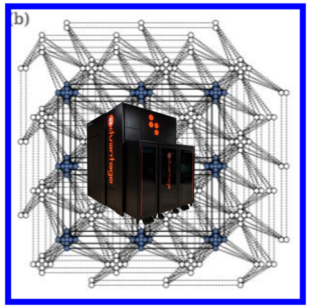
36 qubits

40 qubits





vs.



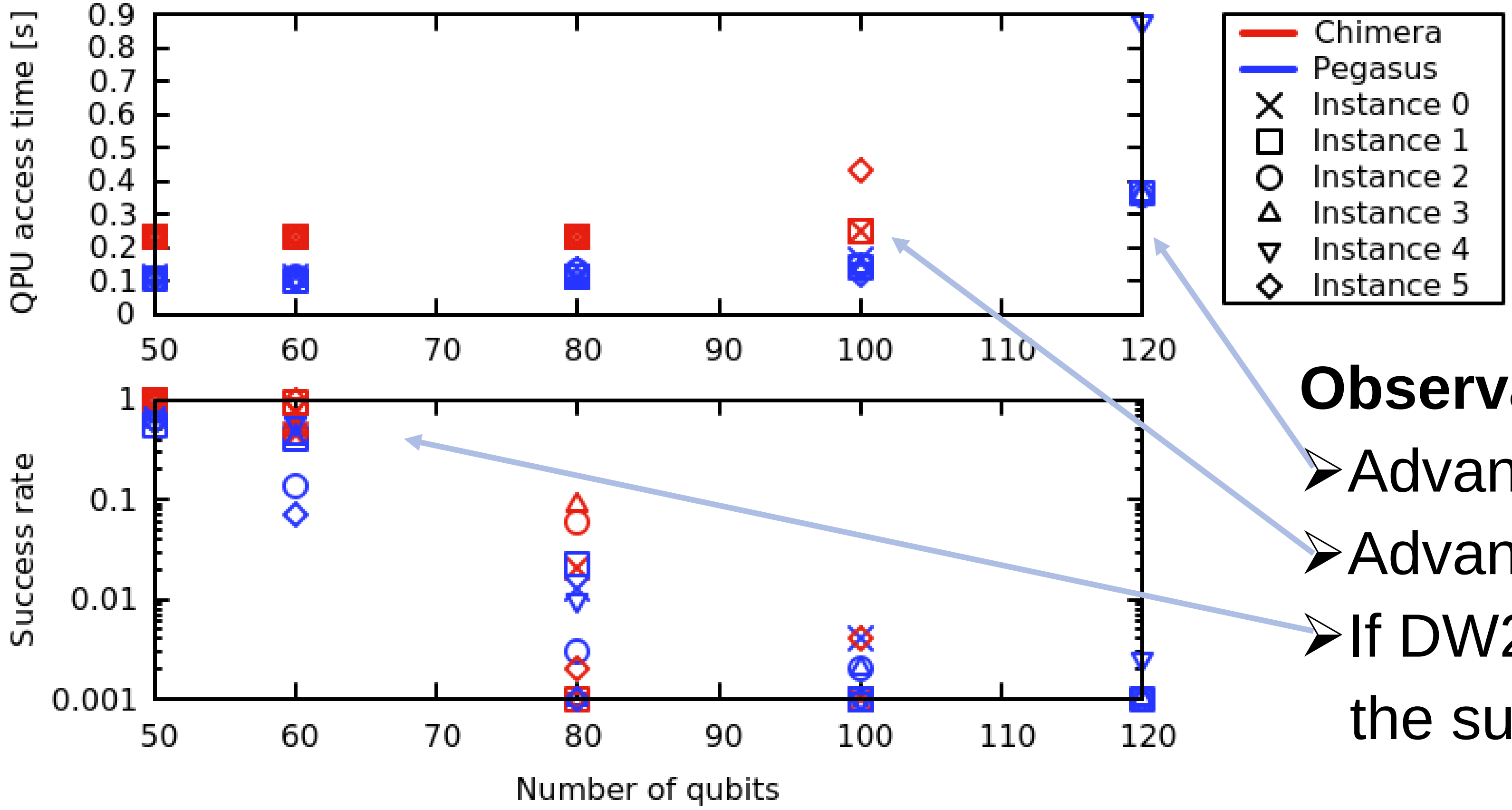
Relative chain strength
= CS / max(|hi|, |Jij|)

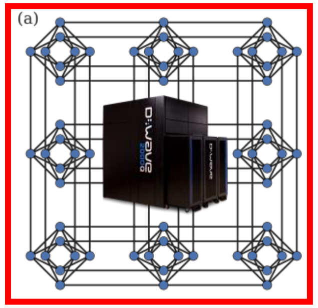
Willsch et al. (2022)
QINP **21**, 141
arXiv:2105.02208

TAIL ASSIGNMENT: RESULTS

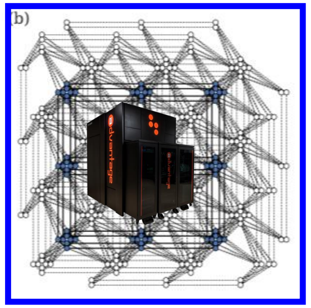
50-120 qubits: larger but sparser problems (20% nonzero couplers)

The fastest successful runs that reproducibly gave a solution:





vs.



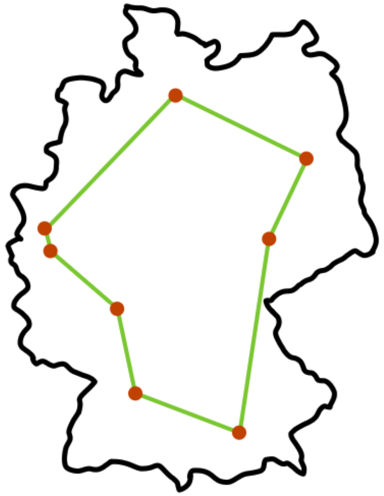
Observations:

- Advantage solves larger problems
- Advantage solves problems faster
- If DW2000Q can solve a problem, the success rate is sometimes higher

Nemes et al. (2022)
https://tsp-quantum.netlify.app/

TRAVELING SALESMAN PROBLEM

QUBO formulation



$$\min_{x_k=0,1} \vec{x}^T Q \vec{x}$$

Cost to travel from city i to city j

$$\min_{x_{it}=0,1}\left\{\lambda\sum_{i=0}^{n-1}\sum_{\substack{j=0\\ j\neq i}}^{n-1}\sum_{t=0}^{n-1} c_{ij}x_{it}x_{j(t+1)} + \sum_{i=0}^{n-1}\left(\sum_{t=0}^{n-1}x_{it}-1\right)^2 + \sum_{t=0}^{n-1}\left(\sum_{i=0}^{n-1}x_{it}-1\right)^2\right\}$$

time steps

cities

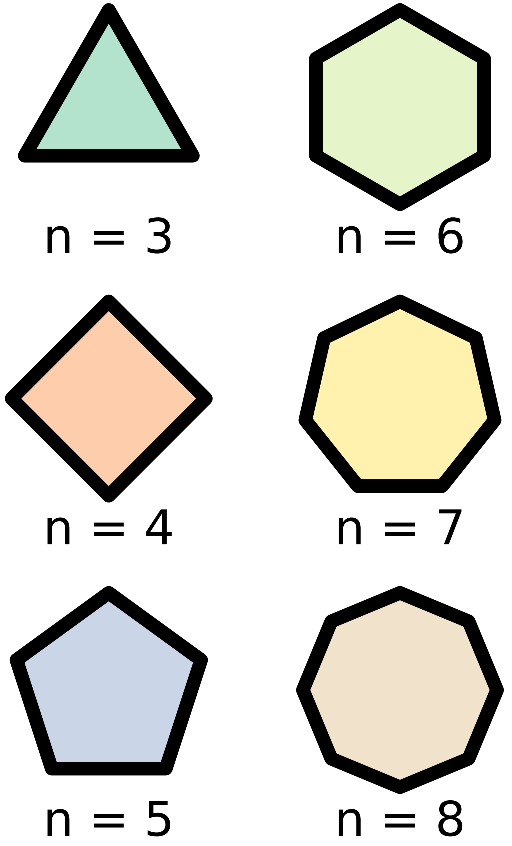
	0	1	2	3
A	1	0	0	0
B	0	0	0	1
C	0	1	0	0
D	0	0	1	0

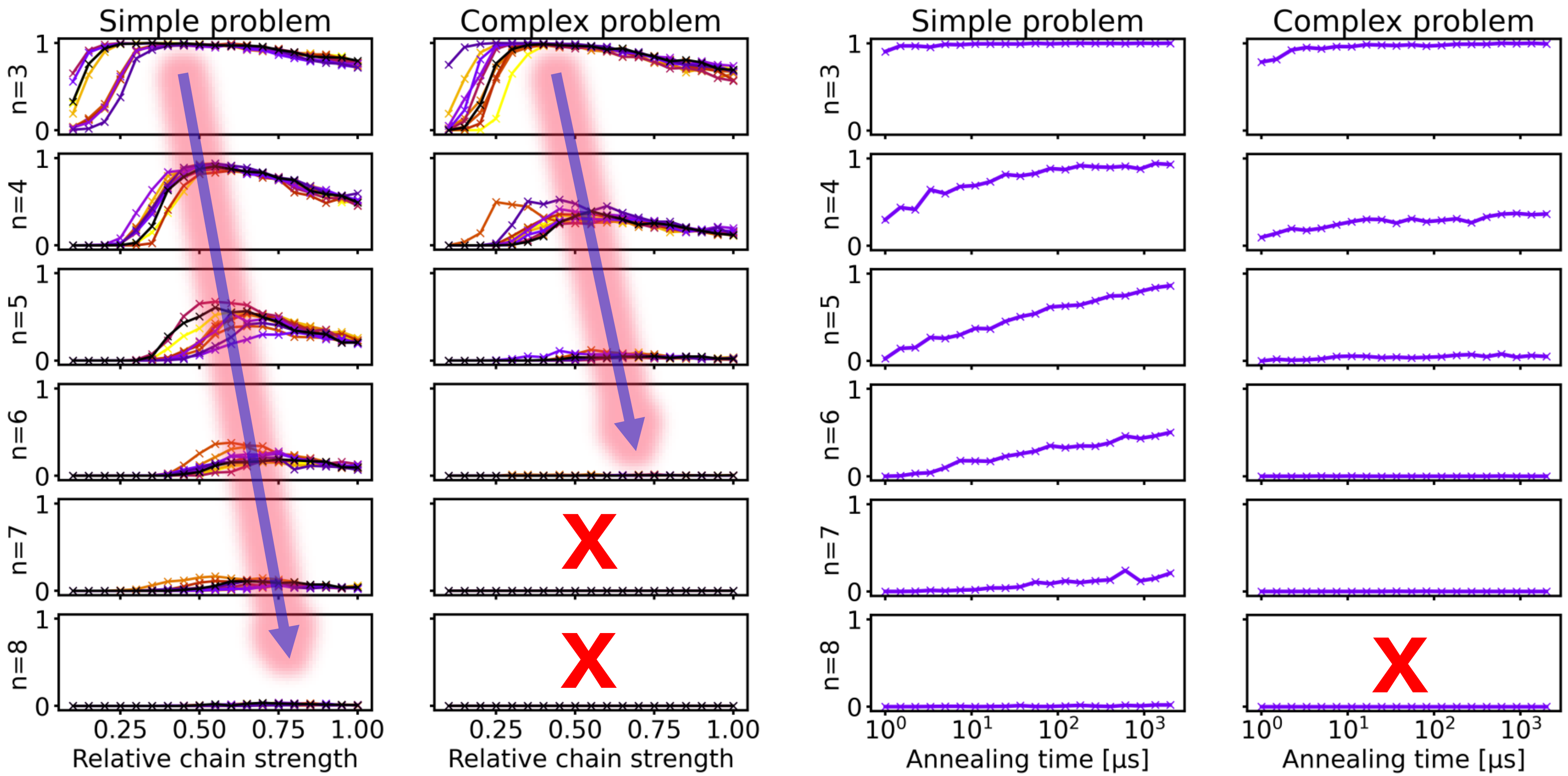
- Assign cities & times to qubits:
  - Qubit $x_{it} = 1$ means the traveler is at city i at time t
  - Count the cost c_{ij} if the traveler goes from i to j at some time step
  - Traveler must pass city i only once
  - Traveler can only be at one city at each time step
- Not the DFJ formulation: linear but exp. many inequality constraints
- Could simplify by fixing starting point → Number of qubits $(n-1)^2$

Nemes et al. (2022)
https://tsp-quantum.netlify.app/

TRAVELING SALESMAN PROBLEM

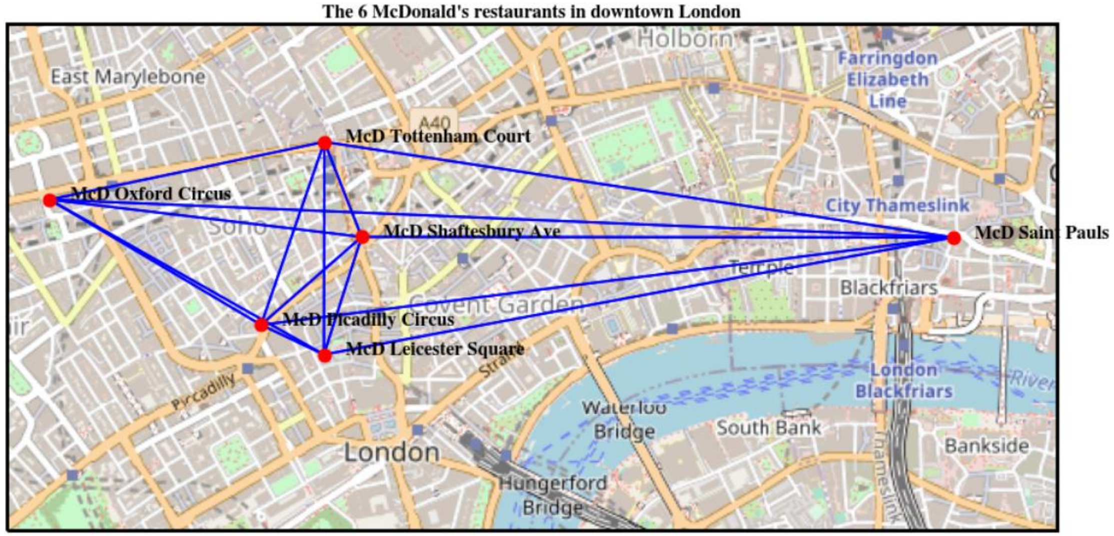
Scaling of chain strength and annealing time

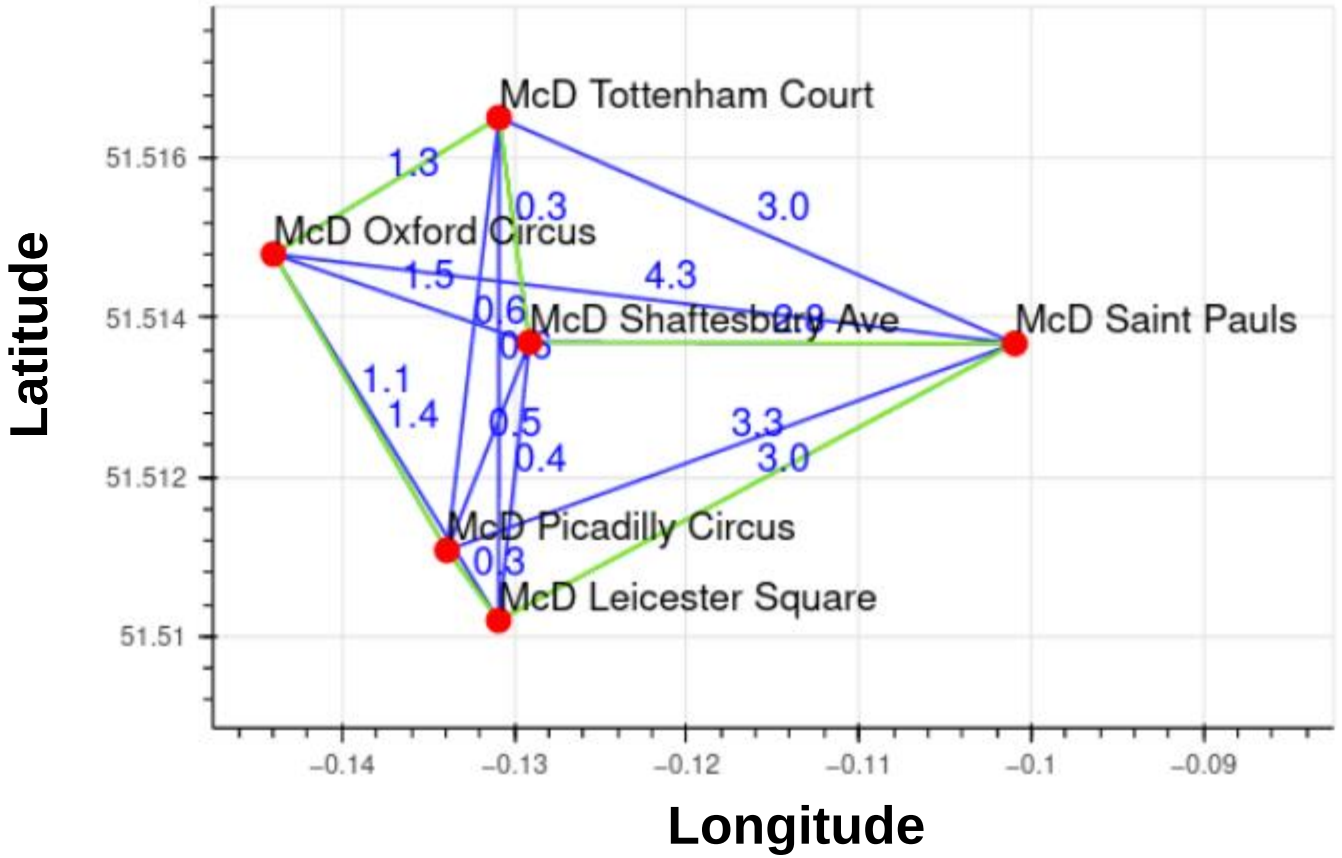




TRAVELING SALESMAN PROBLEM

The 6 McDonald's restaurants in downtown London



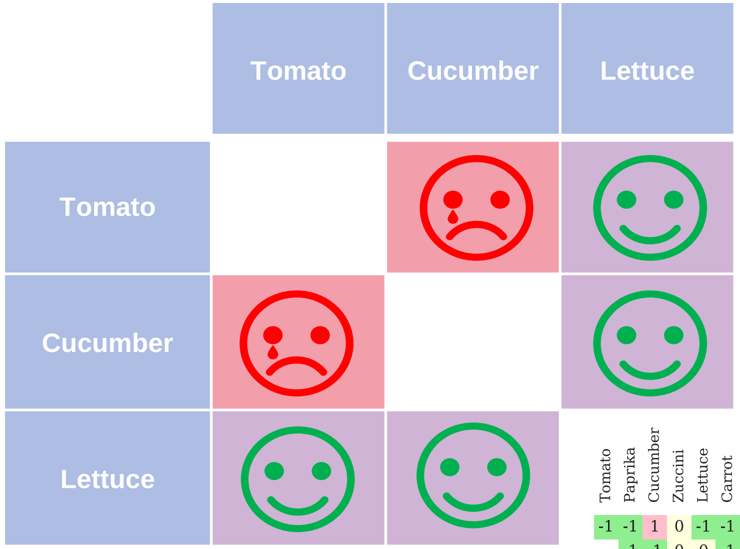


Gonzalez Calaza et al. (2021)
QINP **20**, 305
arXiv:2101.10827
https://jugit.fz-juelich.de/qip/garden-optimization-problem

VEGETABLE GARDEN OPTIMIZATION

Overview

➢ Problem: Companion planting in polyculture vegetable gardens



	Tomato	Paprika	Cucumber	Zuccini	Lettuce	Carrot	Onion	Raddish	Oregano	Basil	Thyme	Parsley	Chives	Rosemary	Sage	Dill	Coriander	Mint
Tomato	-1	-1	1	0	-1	-1	-1	0	-1	-1	0	-1	-1	0	0	0	-1	-1
Paprika		-1	-1	0	0	-1	0	0	-1	-1	0	0	0	0	0	0	0	0
Cucumber			-1	1	-1	0	-1	-1	0	0	0	-1	0	0	0	-1	0	0
Zuccini				-1	0	0	-1	0	0	0	0	-1	0	0	0	0	0	0
Lettuce					-1	-1	-1	-1	0	0	0	1	0	0	-1	-1	-1	-1
Carrot						-1	-1	-1	0	0	0	0	-1	-1	-1	-1	0	-1
Onion							-1	0	0	0	0	-1	0	0	0	-1	0	0
Raddish								-1	0	0	0	-1	0	0	0	0	0	0
Oregano									-1	-1	0	0	0	0	0	0	0	0
Basil										-1	0	0	0	0	0	0	-1	0
Thyme											-1	0	0	0	0	0	0	0
Parsley												-1	-1	0	0	0	-1	0
Chives													-1	0	0	-1	1	0
Rosemary														-1	0	0	0	0
Sage															-1	0	0	0
Dill																-1	-1	0
Coriander																	-1	0
Mint																		-1

➢ Task: Find an optimal placement of plants in the garden considering the characteristics of their nearest neighbours

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VEGETABLE GARDEN OPTIMIZATION

QUBO formulation

$$\min_{x_k=0,1} \vec{x}^T Q \vec{x}$$

Tomato	Paprika	Cucumber	Zuccini	Lettuce	Carrot	Onion	Raddish	Oregano	Basil	Thyme	Parsley	Chives	Rosemary	Sage	Dill	Coriander	Mint	
-1	-1	1	0	-1	-1	-1	0	-1	-1	0	-1	-1	0	0	0	-1	-1	Tomato
	-1	-1	0	0	-1	0	0	-1	-1	0	0	0	0	0	0	0	0	Paprika
		-1	1	-1	0	-1	-1	0	0	0	-1	0	0	0	-1	0	0	Cucumber
			-1	0	0	-1	0	0	0	0	-1	0	0	0	0	0	0	Zuccini
				-1	-1	-1	-1	0	0	0	1	0	0	-1	-1	-1	-1	Lettuce
					-1	-1	-1	0	0	0	0	-1	-1	-1	-1	0	-1	Carrot
						-1	0	0	0	0	-1	0	0	0	-1	0	0	Onion
							-1	0	0	0	-1	0	0	0	0	0	0	Raddish
								-1	-1	0	0	0	0	0	0	0	0	Oregano
									-1	0	0	0	0	0	0	-1	0	Basil
										-1	0	0	0	0	0	0	0	Thyme
											-1	-1	0	0	0	-1	0	Parsley
												-1	0	0	-1	1	0	Chives
													-1	0	0	0	0	Rosemary
														-1	0	0	0	Sage
															-1	-1	0	Dill
																-1	0	Coriander
																	-1	Mint

$$\min_{x_{ij}=0,1} \Bigg\{ \sum_{i,i'=0}^{n-1} J_{ii'} \left(1 + \sum_{j,j'=0}^{t-1} x_{ij} C_{jj'} x_{i'j'}\right)$$
$$+\lambda_1 \sum_{i=0}^{n-1} \left(1 - \sum_{j=0}^{t-1} x_{ij}\right)^2$$
$$+\lambda_2 \sum_{j=0}^{t-1} \left(c_j - \sum_{i=0}^{n-1} x_{ij}\right)^2$$
$$+\lambda_3 \sum_{i=0}^{n-1} \sum_{j=0}^{t-1} \left(i\%2 - s_j\right)^2 x_{ij} \Bigg\}$$

- Assign plants to pots in the garden:
  - Qubit $x_{ij} = 1$ means species j is placed in pot i
  - All plants should have a good relationship with their neighbors
  - Use all available plants and pots
  - Big plants should not shadow small ones

n: nr. of pots in the garden
t: nr. of plant species to place
J: connectivity between pots
C: relationship between species
c_j: nr. of plants of species j
s_j: size of species j

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VEGETABLE GARDEN OPTIMIZATION

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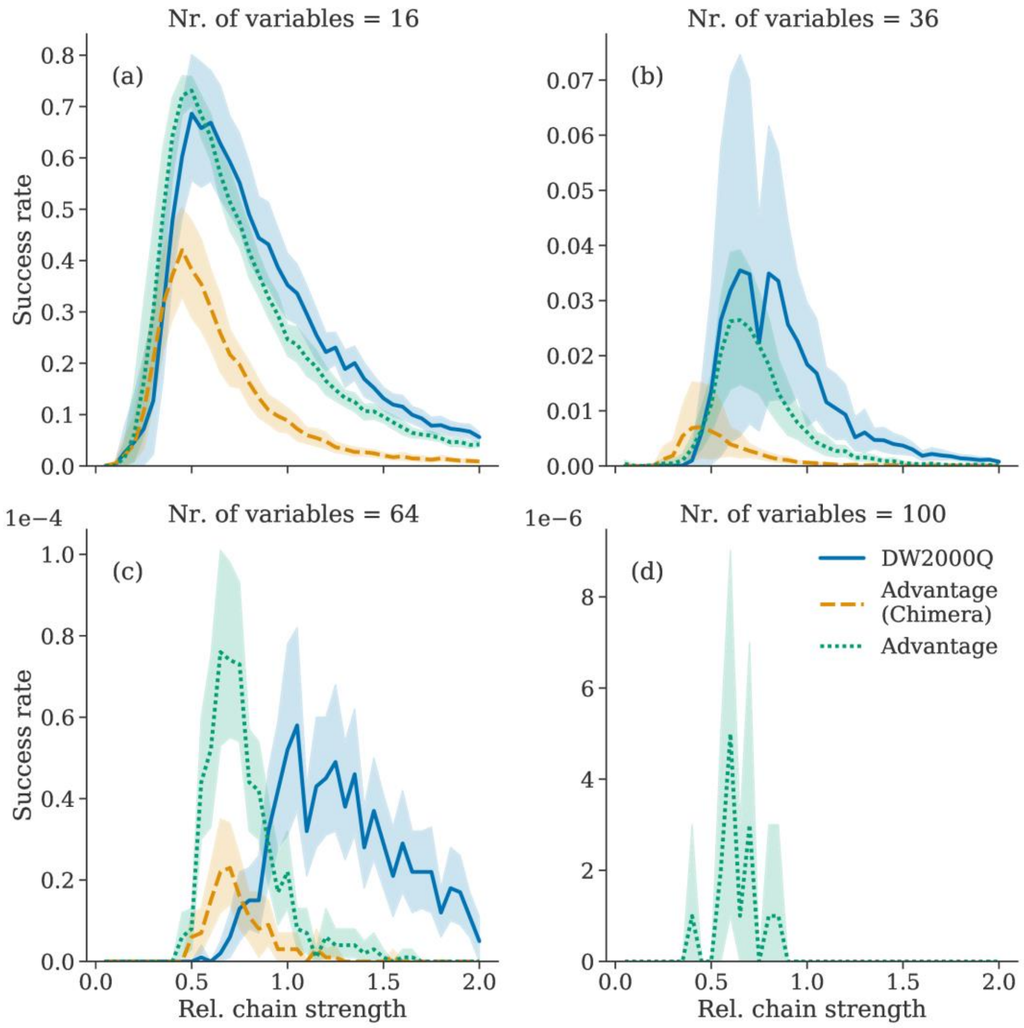
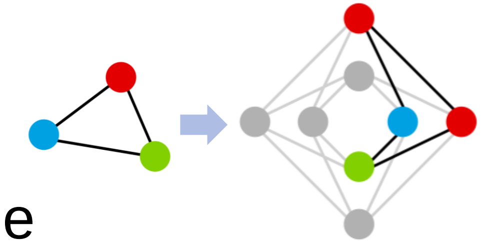
Finding the optimal chain strength: Results





Experiment:

- 4 problems of increasing size
- Success = constraints weren't violated
- 10 different embeddings for each system
- Scanned 40 different values for:

  Rel. chain strength = CS / max(|ai|,|bij|)

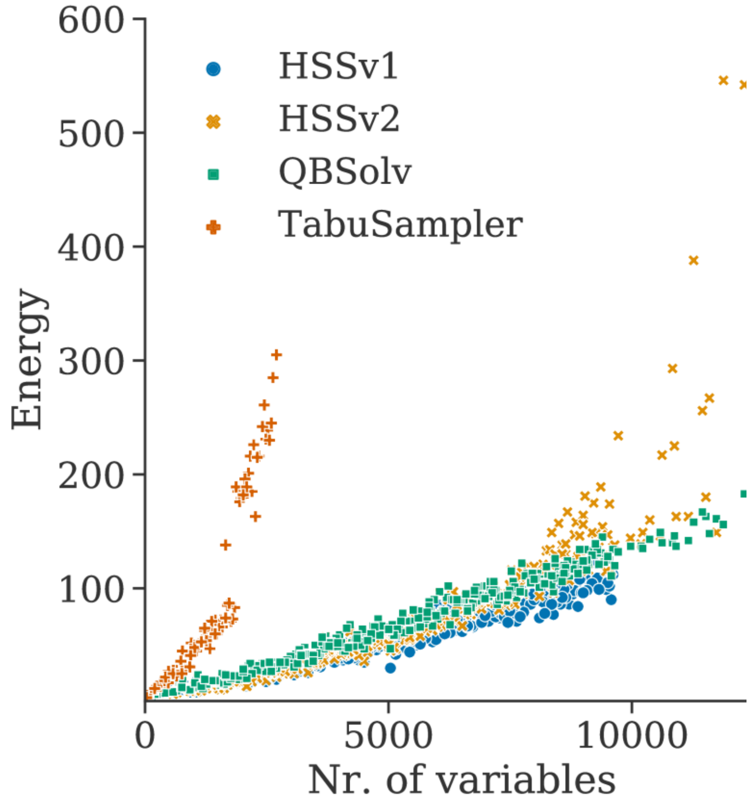
Conclusions:

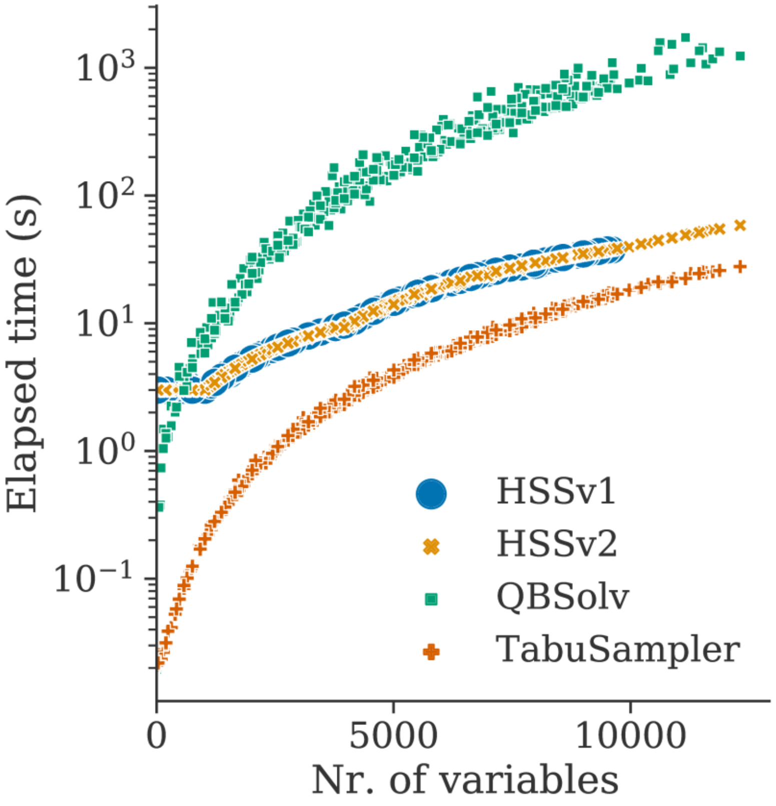
- Trying several embeddings is very important
- Chain strength heavily affects success rate
- Longer chains require higher chain strengths

Gonzalez Calaza et al. (2021)
QINP **20**, 305
arXiv:2101.10827
https://jugit.fz-juelich.de/qip/garden-optimization-problem

CLASSICAL AND HYBRID SOLVERS

Comparing energies and run times



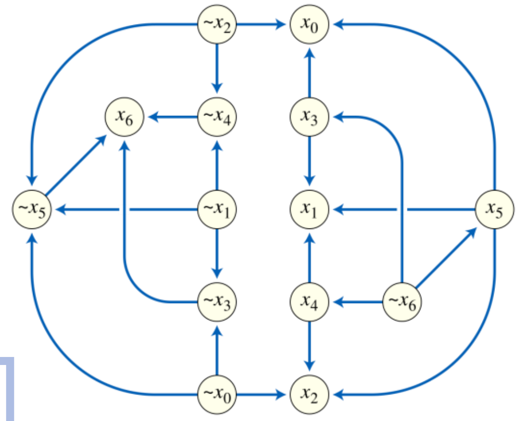


Results:
- HSSv1: best but only up to 10k vars.
- HSSv2: same as v1 up to 2k vars., worse later.
- QBSolv: good but very slow.
- TabuSampler: returns unusable results extremely fast.

Conclusion:
- Hybrid solvers outperform classical solvers.

2-SATISFIABILITY

Mehta et al., PRA **105**, 062406 (2022)
Mehta et al., PRA **104**, 032421 (2021)



Overview

- Mathematical formulation

$$F = (L_{1,1} \vee L_{1,2}) \wedge (L_{2,1} \vee L_{2,2}) \wedge .... \wedge (L_{M,1} \vee L_{M,2})$$

where $L_{j,k} = x_i$ or $\overline{x_i}$ with $x_i = 0, 1$

→ find assignment to x_i that makes F true

Ising: $$\min_{s_i=\pm 1} \left(\sum_i h_i s_i + \sum_{i<j} J_{ij} s_i s_j \right)$$

- Reformulation as Ising Problem

$$H_{2SAT} = \sum_{\alpha=1}^{M} h_{2SAT}(\epsilon_{\alpha,1} s_{i[\alpha,1]}, \epsilon_{\alpha,2} s_{i[\alpha,2]})$$

$x_i = 0 \Leftrightarrow s_i = -1$
$x_i = 1 \Leftrightarrow s_i = +1$

$\epsilon_\alpha = 1$ for x_i
$\epsilon_\alpha = -1$ for $\overline{x_i}$

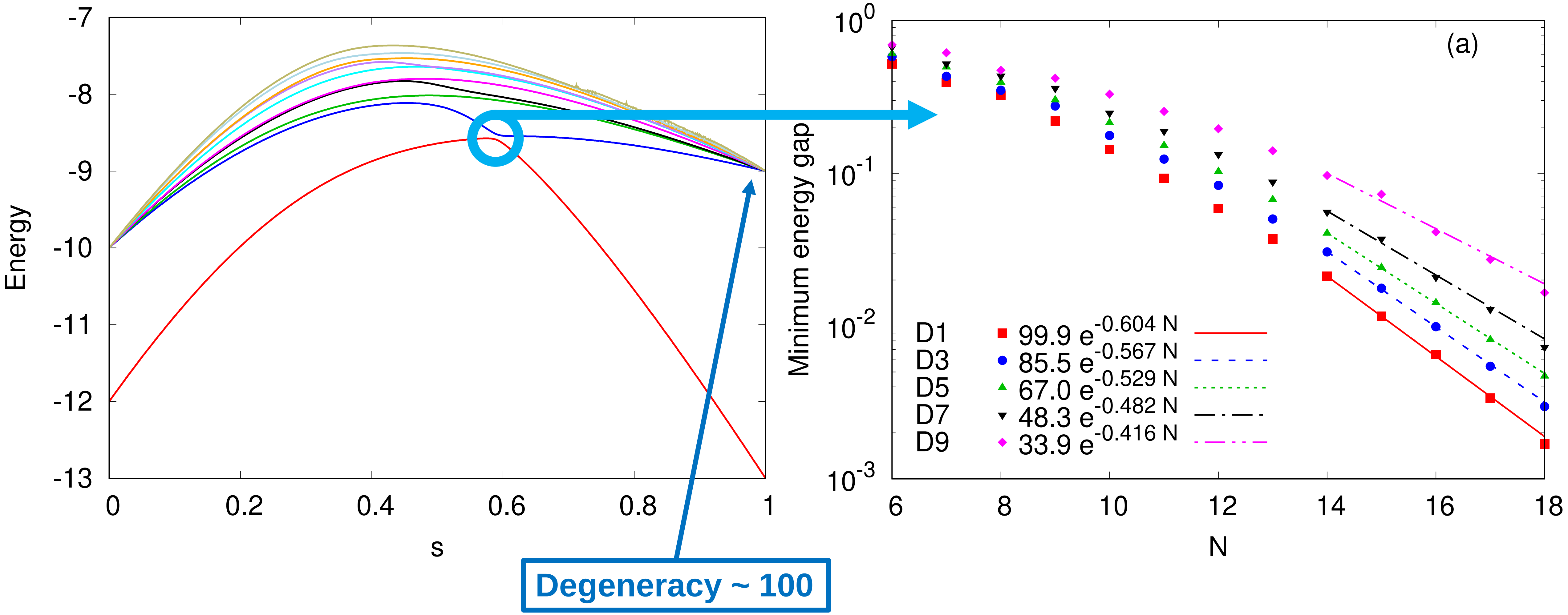
  - Example for clause $x_1 \vee x_2$: $h_{2SAT} = s_1 s_2 - (s_1 + s_2) + 1$

- "Hard 2-SAT problems": The purpose is benchmarking
  - Chosen to be "hard" for quantum annealers (not for digital computers)

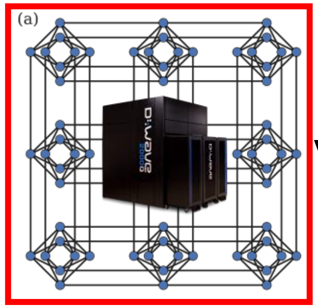
Mehta et al., PRA **105**, 062406 (2022)
Mehta et al., PRA **104**, 032421 (2021)

2-SATISFIABILITY

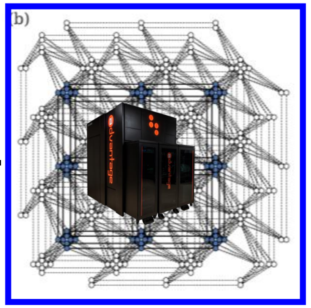
Properties: unique ground state, highly degenerate first excited level, small gaps



2-SATISFIABILITY: RESULTS



vs.

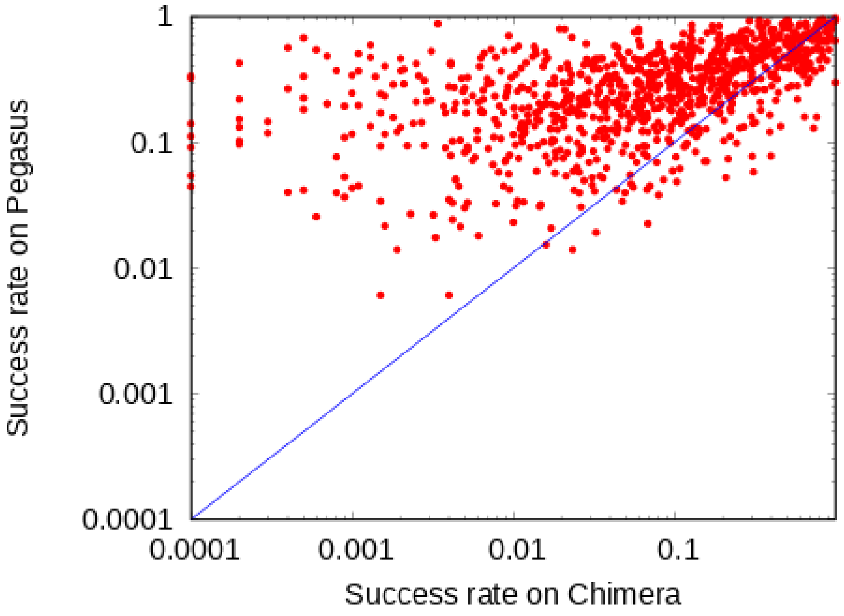


Mehta et al., PRA **105**, 062406 (2022)
Mehta et al., PRA **104**, 032421 (2021)

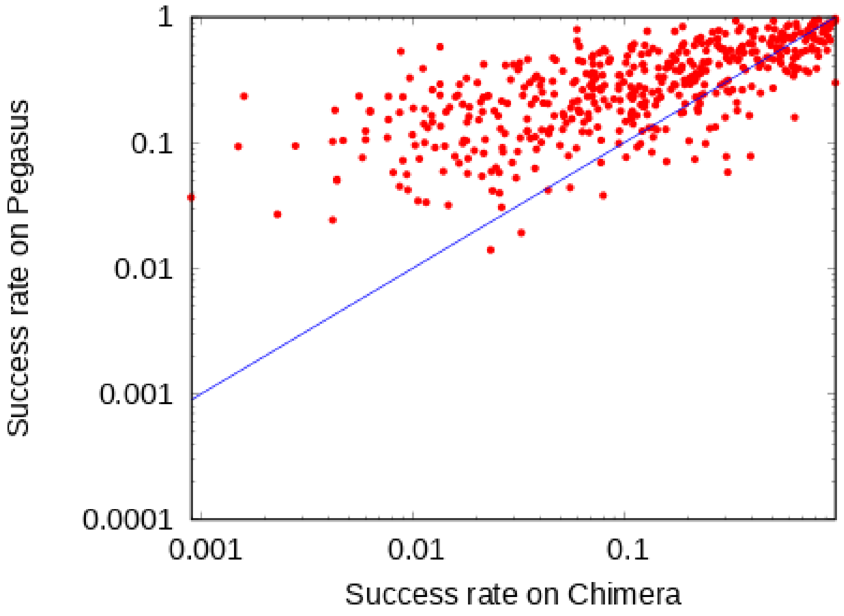
Success rate for 1000 2-SAT problems

- **Direct mapping:**
  ~50% on DW2000Q
  ~90% on Advantage
- Advantage performs better for a majority of the problems, especially the difficult problems

All problems



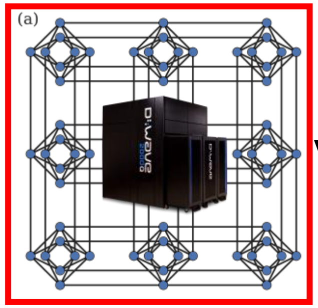
Problems with direct mapping



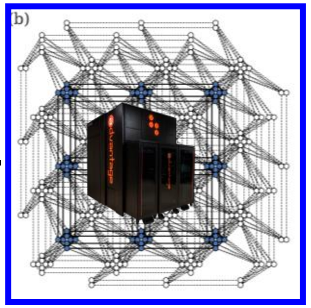
- Largest enhancement for cases that require embedding only on Chimera
  ➔ Improvement due to increased connectivity

2-SATISFIABILITY: RESULTS

Mehta et al., PRA **105**, 062406 (2022)
Mehta et al., PRA **104**, 032421 (2021)

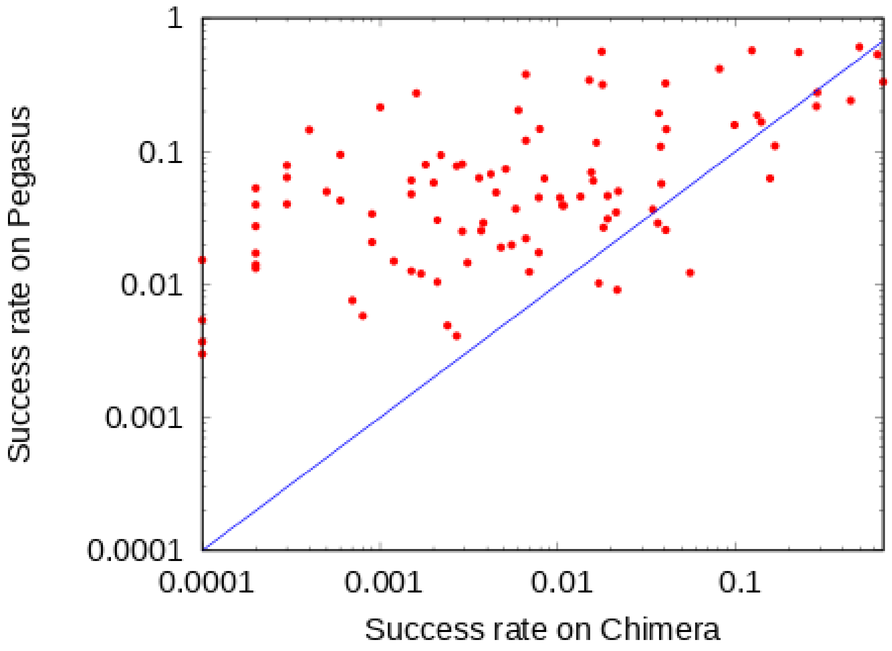


vs.

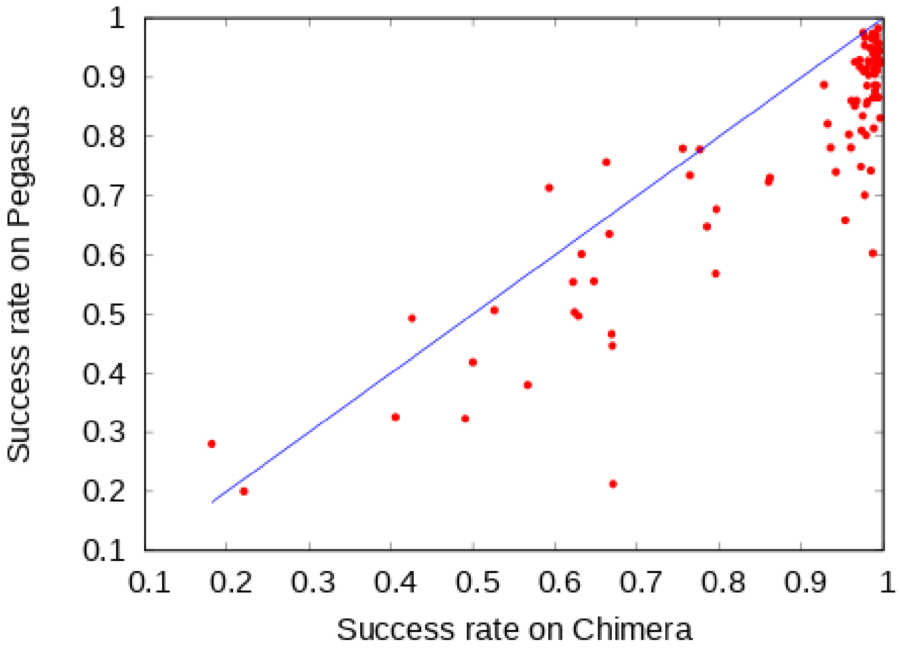


Success rate for 2 particular 2-SAT problems

Hard Problem



Easy problem

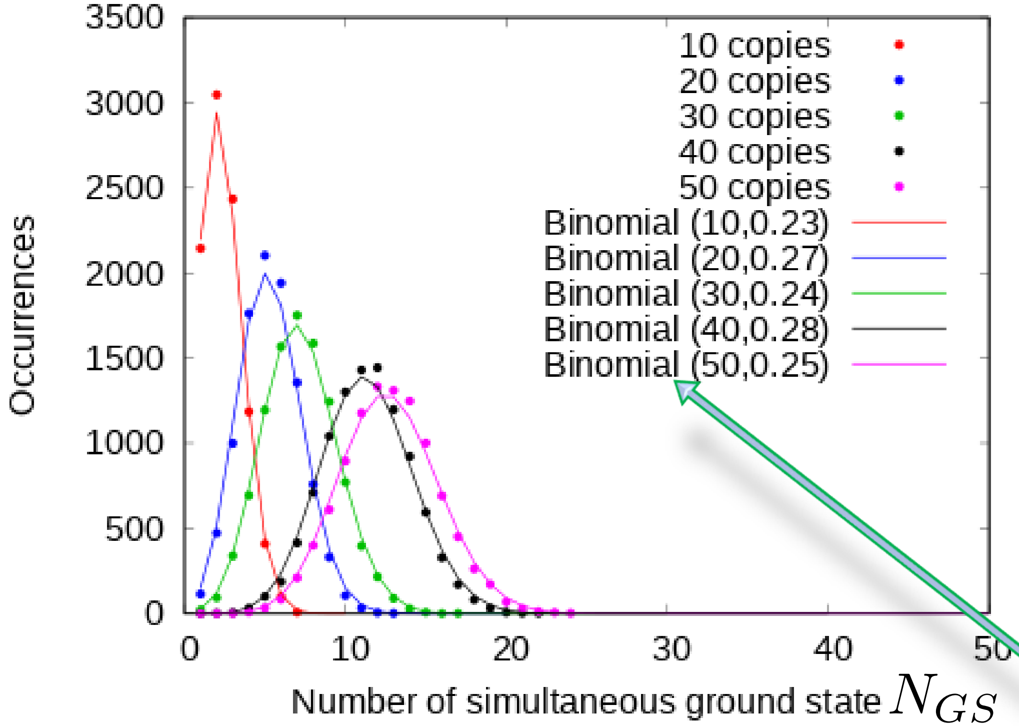


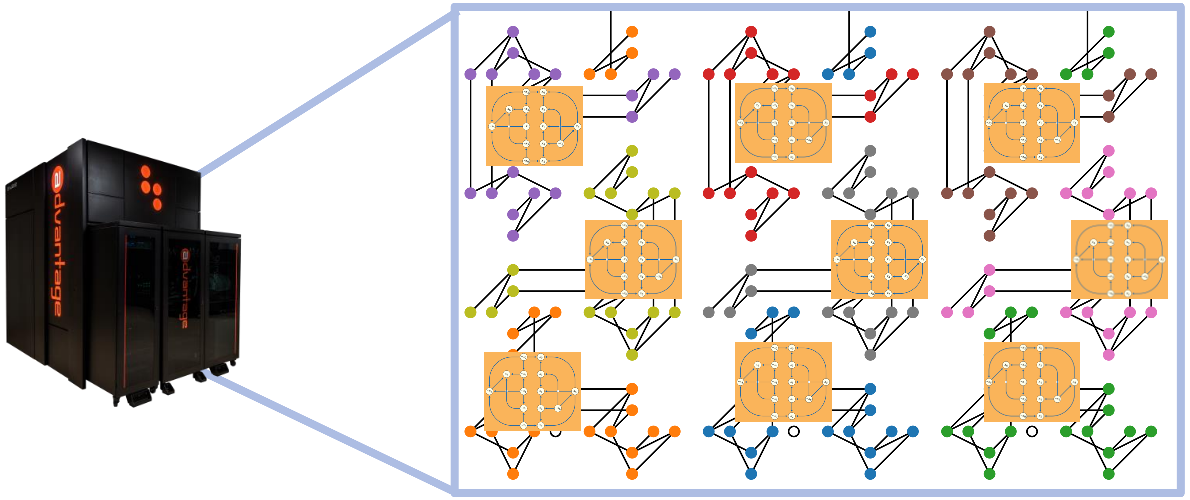
- For a hard problem, Advantage performs better
- However, for an easy problem, DW2000Q performs better

Mehta et al., PRA **105**, 062406 (2022)
Mehta et al., PRA **104**, 032421 (2021)

2-SATISFIABILITY: RESULTS

Embed the same problem multiple times





$$\binom{N_{\text{copies}}}{N_{GS}} p^{N_{GS}} (1-p)^{N_{\text{copies}}-N_{GS}}$$

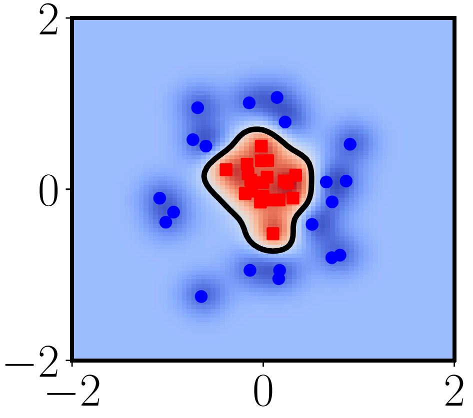
Success rate: probability to find the unique solution (GS)

- The occurrence of optimal solutions follows a binomial distribution
- Parts of the solver corresponding to each copy work almost independently
- Note that in no run could all ground states be found simultaneously

Willsch et al., CPC **248**, 107006 (2021)
Delilbasic et al., IGARSS 2021, 2608 (2021)
Cavallaro et al., IGARSS 2020, 1973 (2020)

QUANTUM SUPPORT VECTOR MACHINES

From classical SVM to quantum SVM



- An SVM is a supervised machine-learning method for binary classification
- Given a training set

Feature vector
Label

$$D = \{(\mathbf{d}_n, t_n) : n = 0, \ldots, N-1\}$$

an SVM is trained by solving the Quadratic Programming problem

$$\text{minimize} \qquad E(\{\alpha_n\}) = \frac{1}{2}\sum_{nm} \alpha_n \alpha_m t_n t_m k(\mathbf{d}_n, \mathbf{d}_m) - \sum_n \alpha_n$$

$$\text{subject to} \qquad 0 \le \alpha_n \le C \quad \text{and} \quad \sum_n \alpha_n t_n = 0$$

Continuous problem variables

Kernel function (nonlinear SVM)

- QUBO problems are also quadratic, but for binary variables

Number of qubits per problem variable

→ Use encoding: $\boxed{\alpha_n = \sum_{k=0}^{K-1} B^{k-P} x_{[n,k]}}$ $\longrightarrow$ $E(\{\alpha_n\})$ $\longrightarrow$ QUBO formulation

Base & Exponent

$$\min_{x_i = 0,1} \left(\sum_{i,j} x_i Q_{ij} x_j \right)$$

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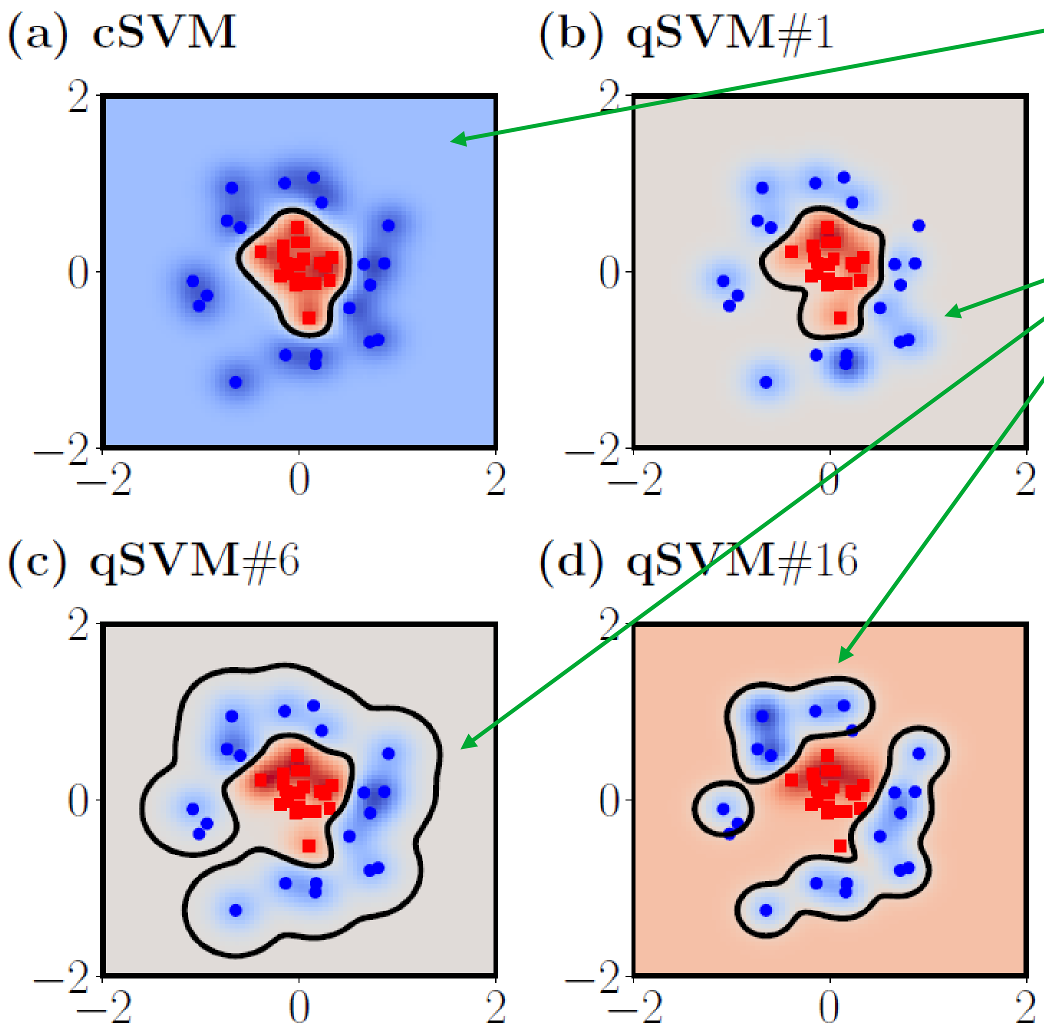
Willsch et al., CPC **248**, 107006 (2021)
Delilbasic et al., IGARSS 2021, 2608 (2021)
Cavallaro et al., IGARSS 2020, 1973 (2020)

Results



- Classical SVM (**cSVM**) yields the global minimum, but only for the training data
- Quantum SVM (**qSVM**) yields additional low-energy classifiers from ensemble of solutions

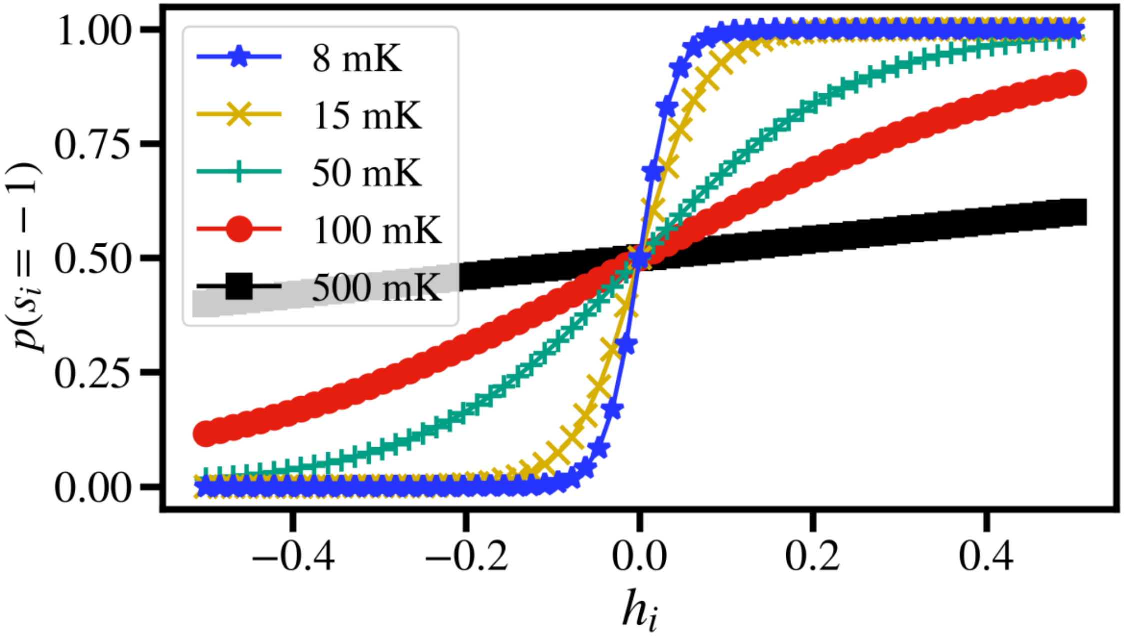
Combination of multiple low-energy qSVM classifiers generalizes better to unseen data

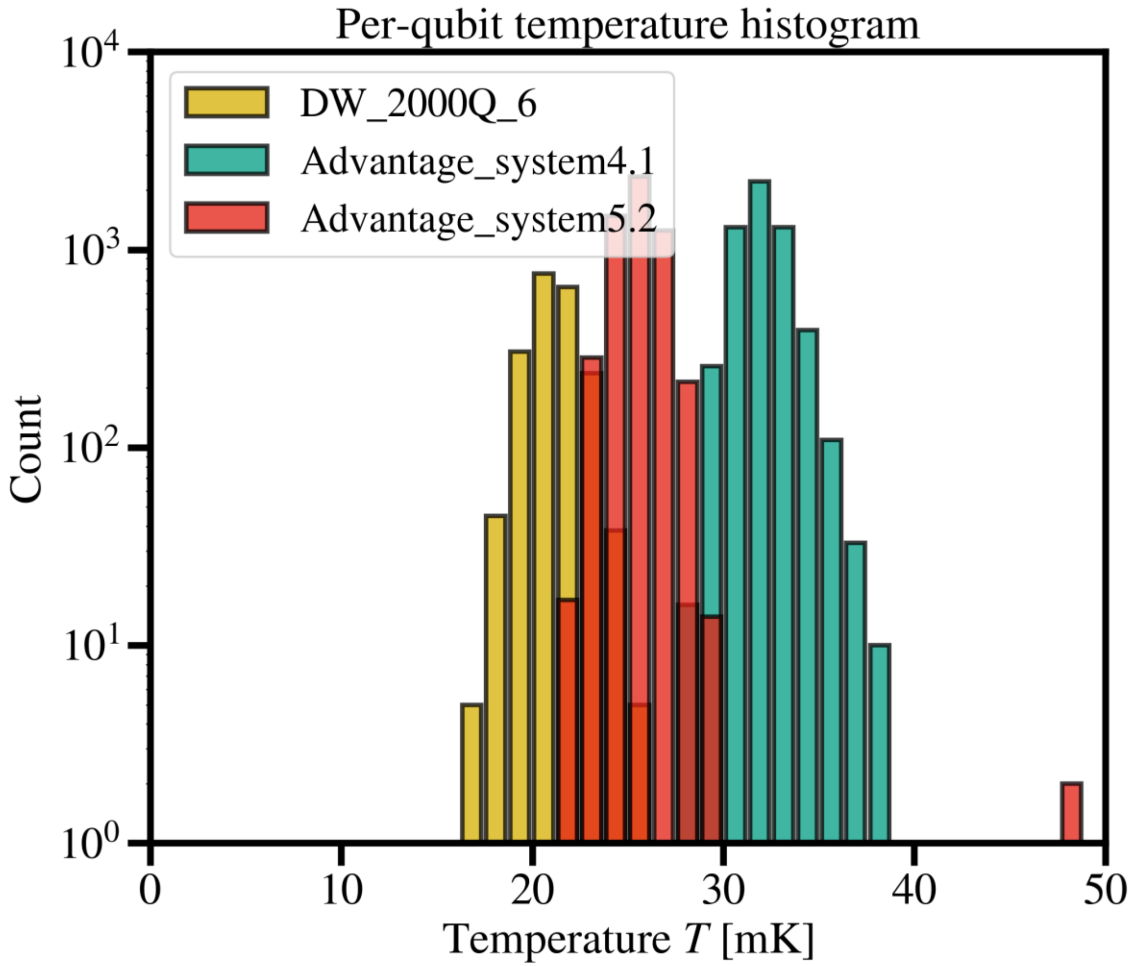
QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

$$H(s) = \frac{A(s)}{2}\left(\sum_i \sigma_i^x\right) + \frac{B(s)}{2}\left(\sum_i \boxed{h_i \sigma_i^z} + \sum_{i<j} \cancel{J_{ij}} \sigma_i^z \sigma_j^z\right)$$

$$\boxed{p(s_i = \pm 1) = \langle s_i | \frac{1}{Z} e^{-\beta H(1)} | s_i \rangle = \frac{1}{2}\left(1 + \tanh\left(-\frac{B(1) h_i}{2 k_B T} s_i\right)\right)}$$

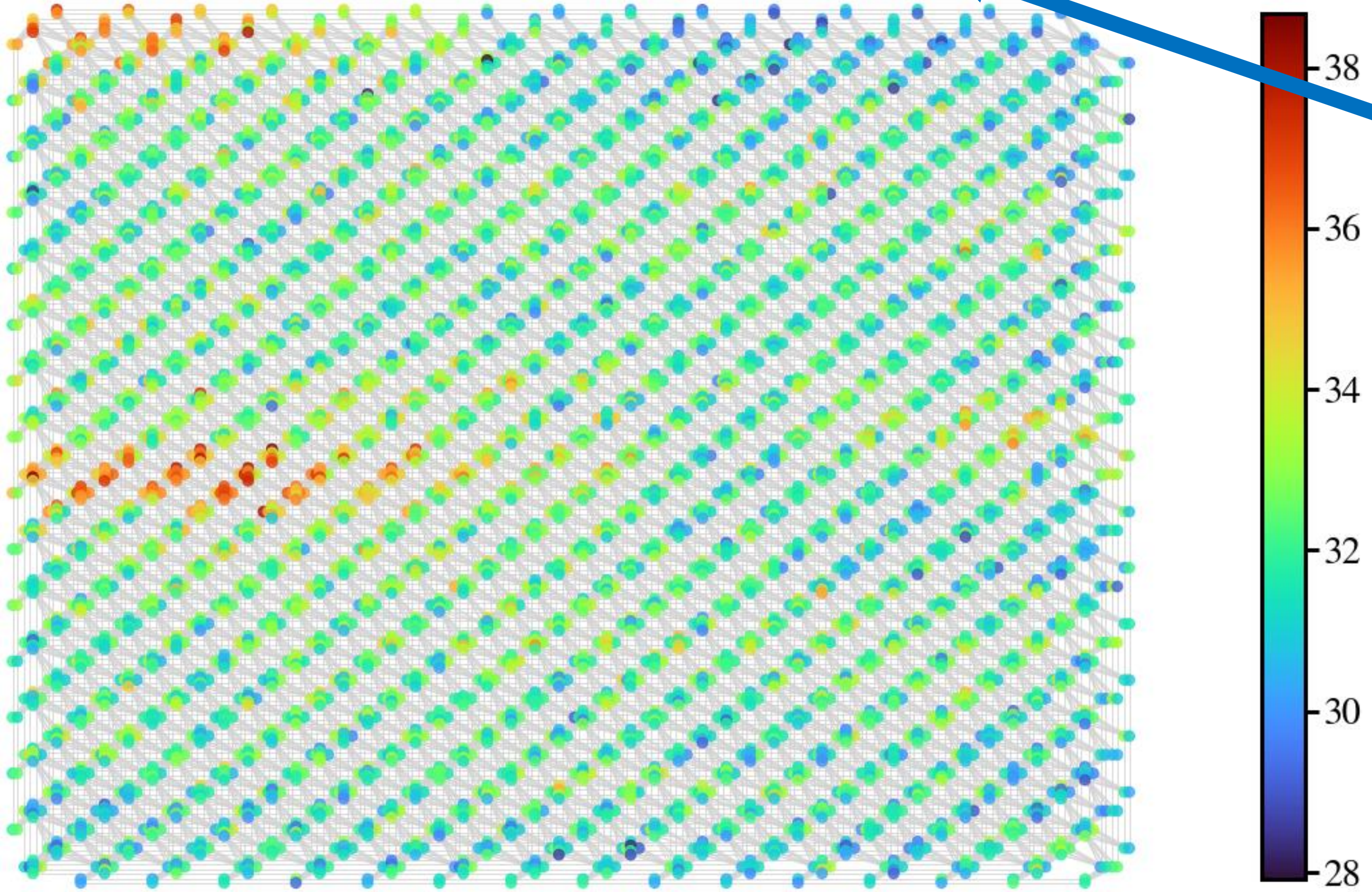


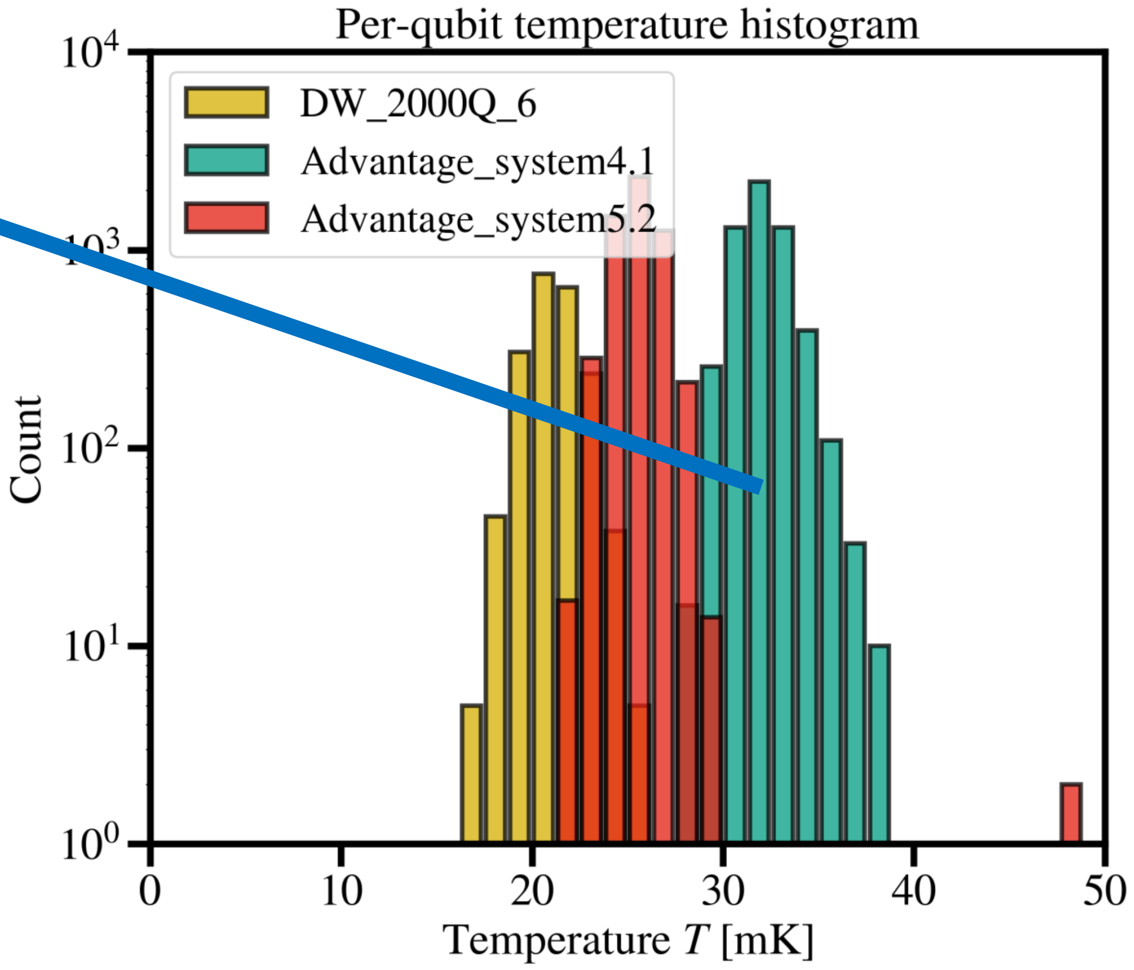


QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

Advantage_system4.1



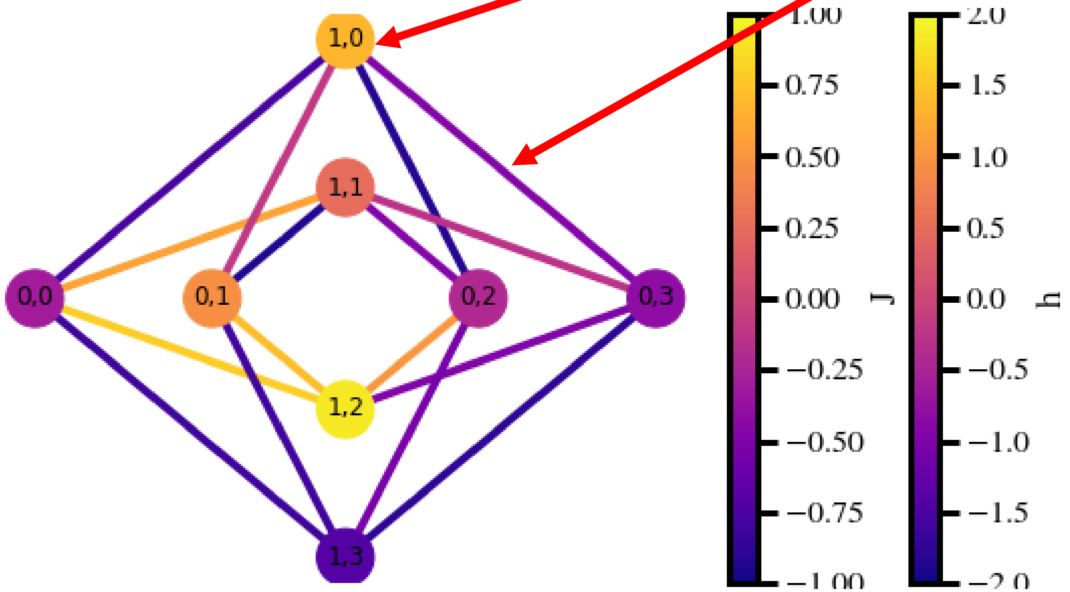


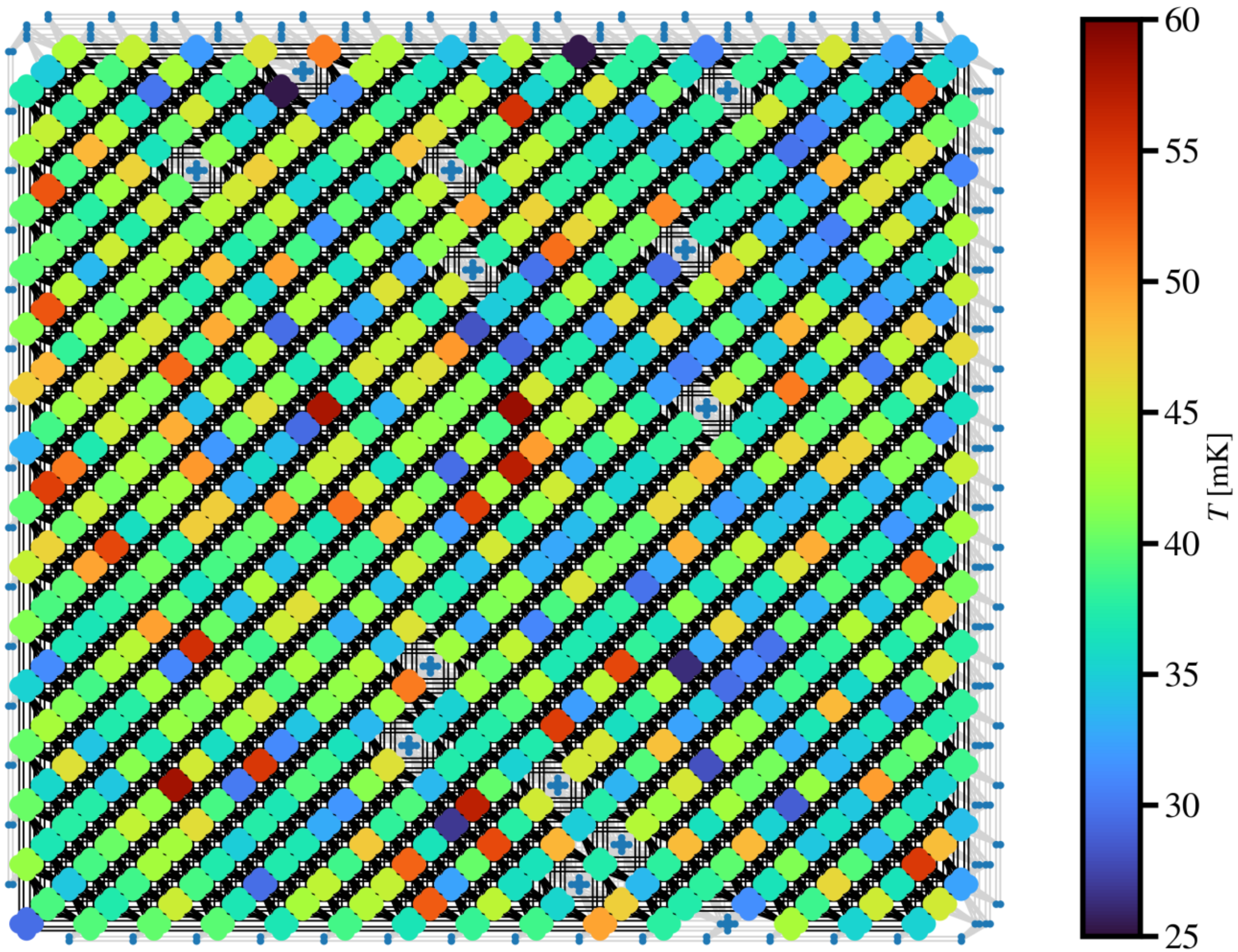
Perot et al. (2022)
https://jugit.fz-juelich.de/qip/qbm-quant-finance

QUANTUM BOLTZMANN MACHINES

Experiment #2: 8-qubit problem on each Chimera cell of the Pegasus graph

$$H(s) = \frac{A(s)}{2}\left(\sum_i \sigma_i^x\right) + \frac{B(s)}{2}\left(\sum_i \boxed{h_i\sigma_i^z} + \sum_{i<j} \boxed{J_{ij}\sigma_i^z\sigma_j^z}\right)$$





Fit Boltzmann distribution to observed samples at $s = 1$ to infer $\beta = 1/k_B T$:

$$p(\{s_i = \pm 1\} \mid \beta, s) = \langle \{s_i = \pm 1\} | \frac{1}{Z} e^{-\beta H(s)} | \{s_i = \pm 1\} \rangle$$

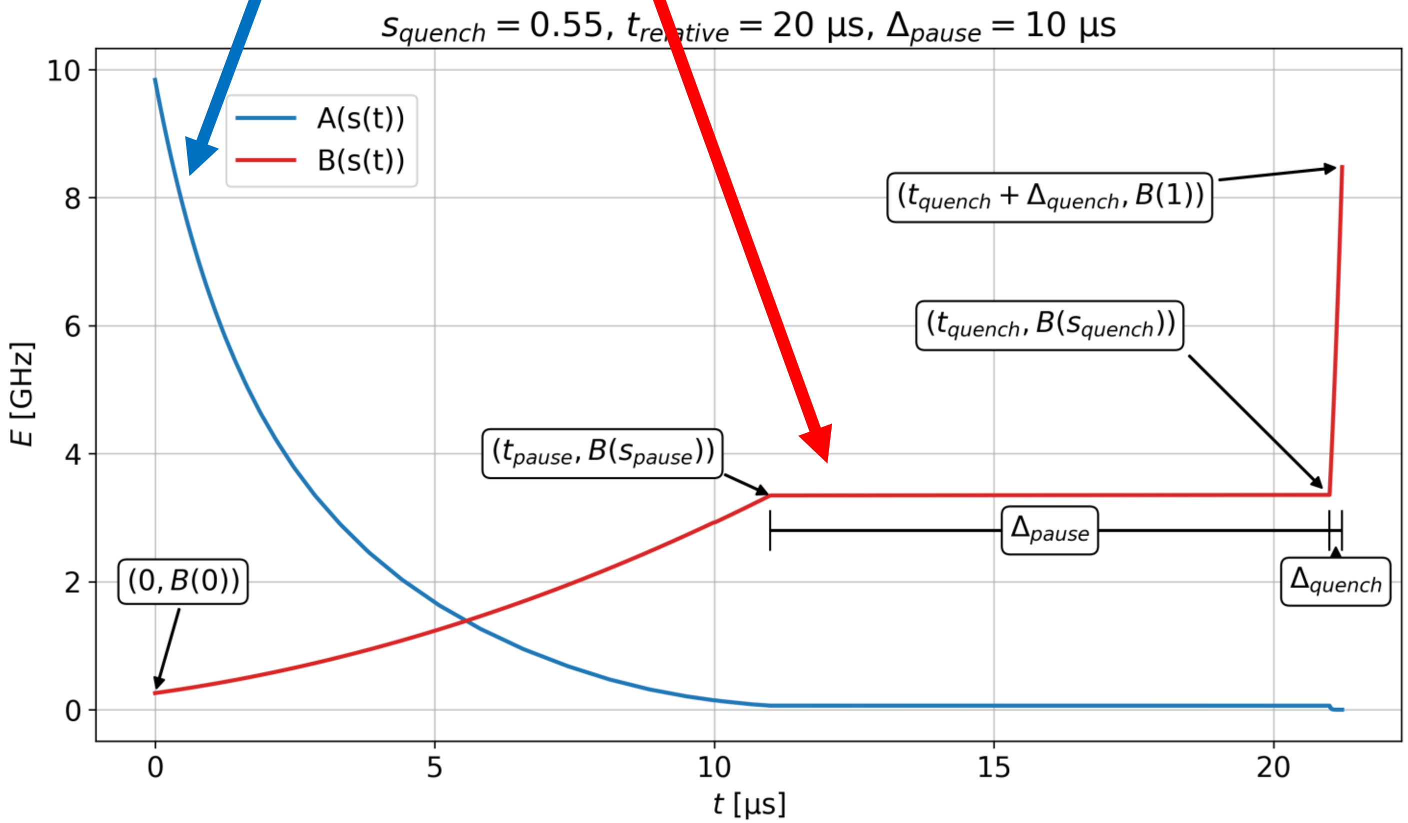
QUANTUM BOLTZMANN MACHINES

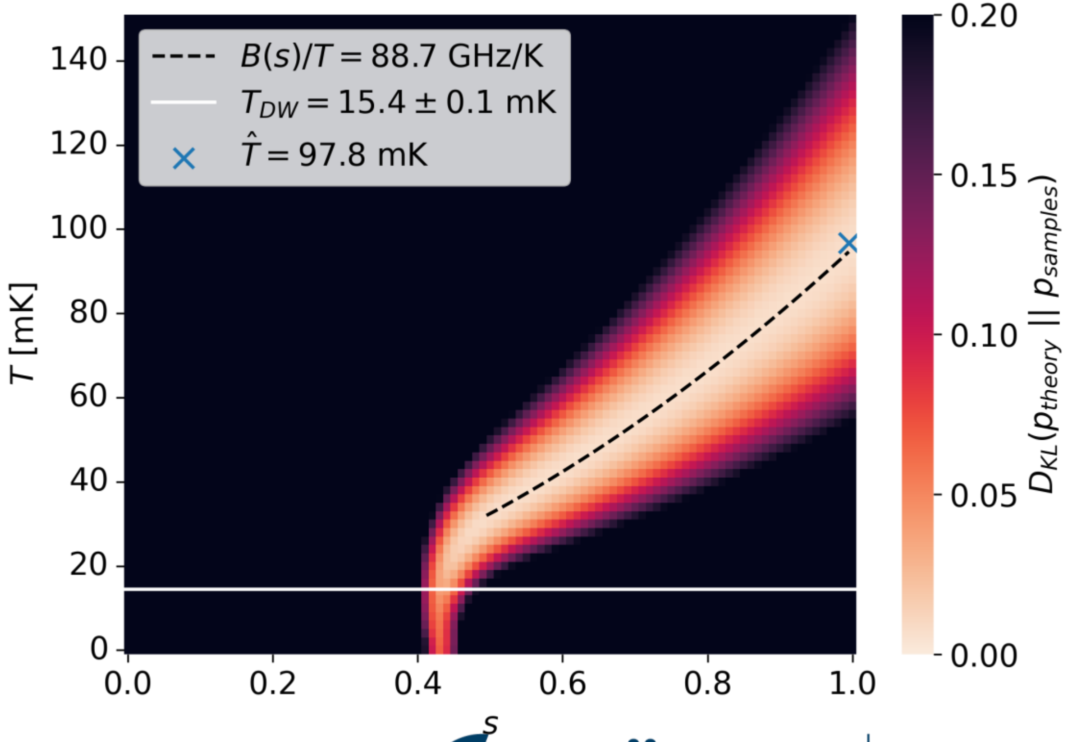
Experiment #3: 12-qubit problem (also for intermediate times s != 1)

$$H(s) = \boxed{\frac{A(s)}{2}} \left(\sum_i \sigma_i^x \right) + \boxed{\frac{B(s)}{2}} \left(\sum_i h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z \right)$$

Quantum Boltzmann distribution
at inverse temperature β and time s:

$$p(\{s_i = \pm 1\} \mid \beta, s) = \langle \{s_i = \pm 1\} | \frac{1}{Z} e^{-\beta H(s)} | \{s_i = \pm 1\} \rangle$$





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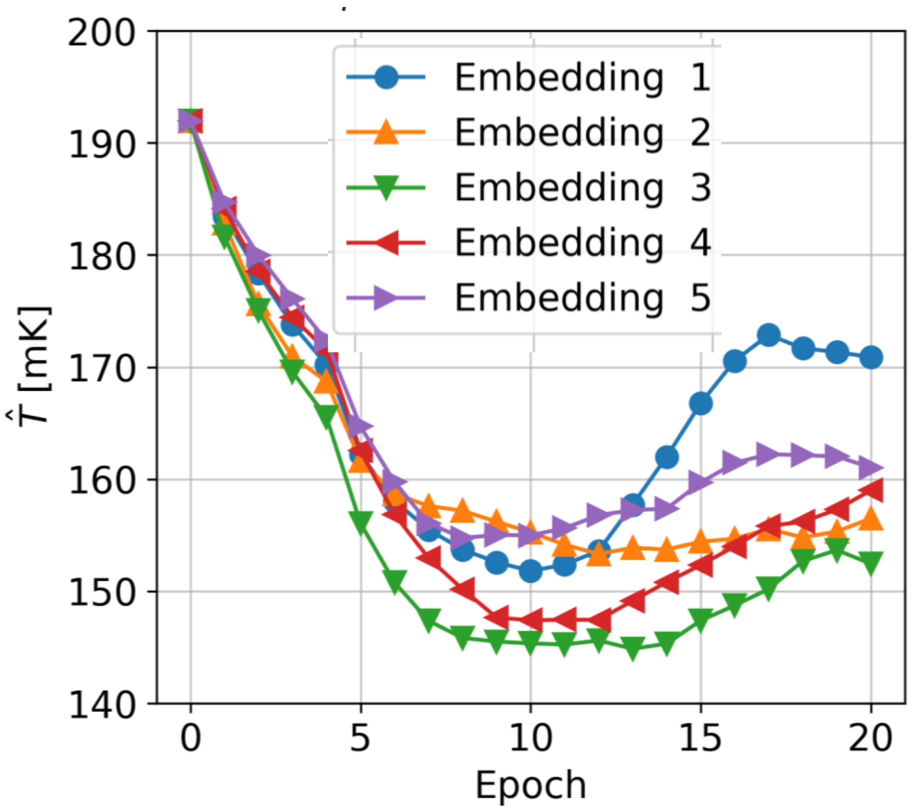
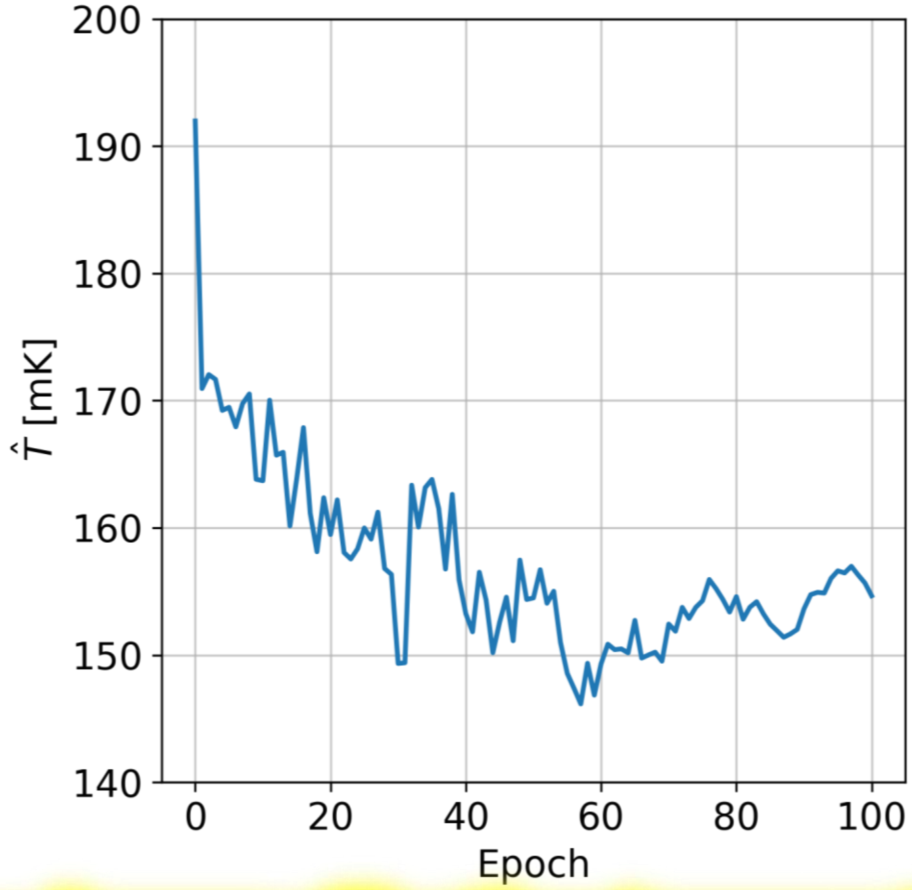
Perot et al. (2022)
https://jugit.fz-juelich.de/qip/qbm-quant-finance

QUANTUM BOLTZMANN MACHINES

Experiment #4: 96-qubit problem (~400 physical qubits, application in quantitative finance)





→ Observation: Larger problems ~ larger effective temperature

SUMMARY

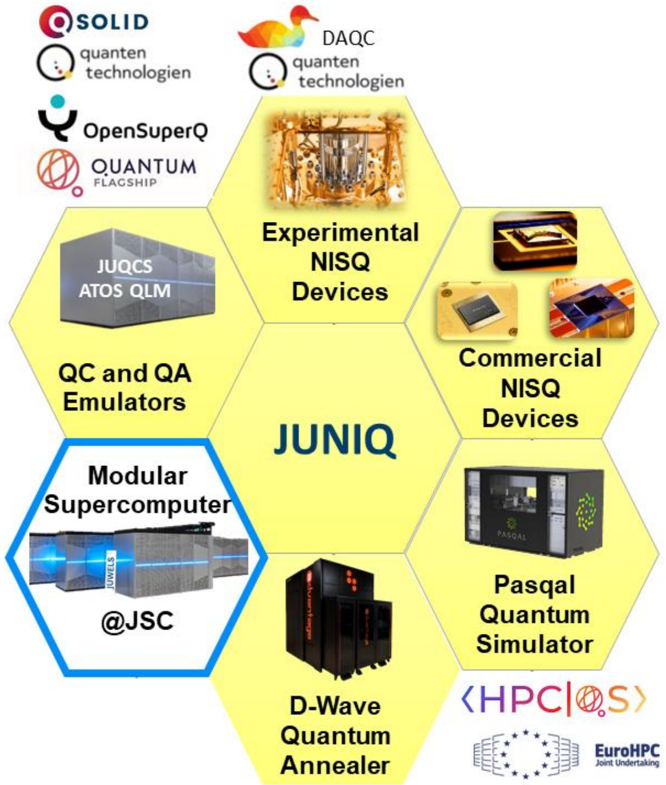
1. **Airline Scheduling**
2. **Traveling Salesman**
3. **Garden Optimization**
4. **2-Satisfiability**
5. **QSVM**
6. **QBM**

optimization problem
with constraints
[increasing complexity]

constraints only

optimization only [basically]

sampling problem



THANK YOU FOR YOUR ATTENTION

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