



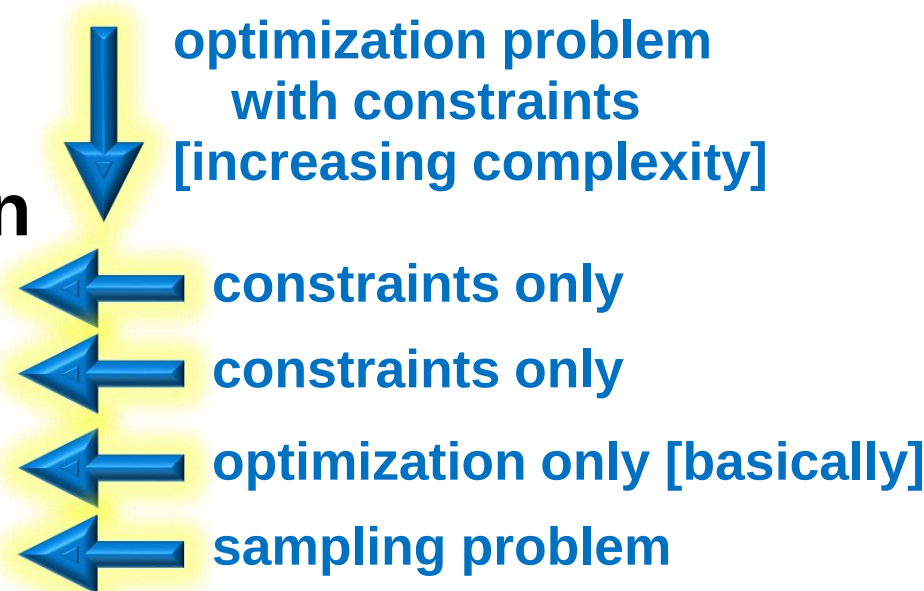
APPLICATIONS ON QUANTUM ANNEALERS AT FZJ

JUNIQ: Jülich Unified INfrastructure for Quantum Computing

DR. DENNIS WILLSCH

CONTENTS

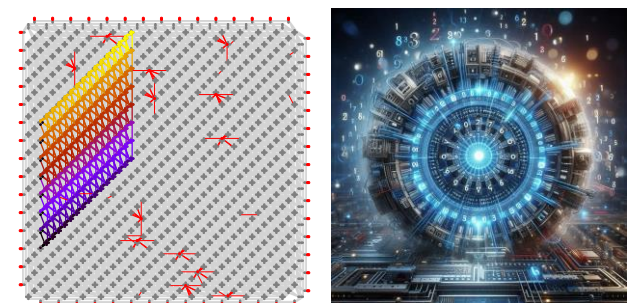
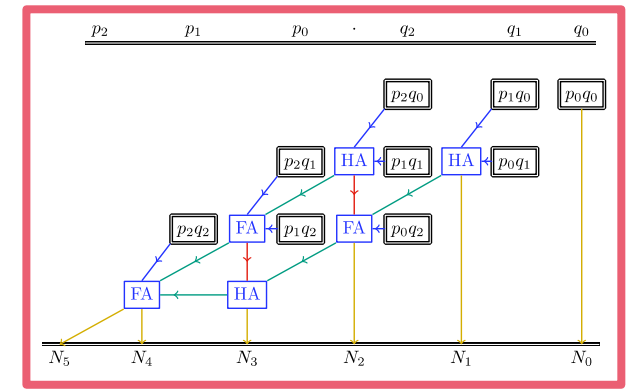
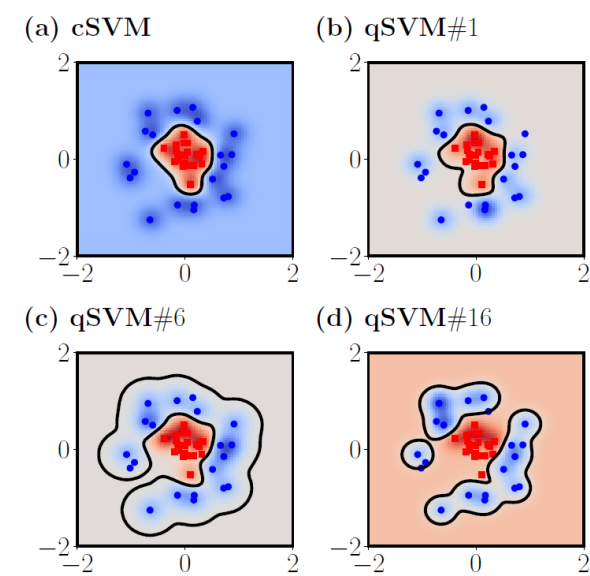
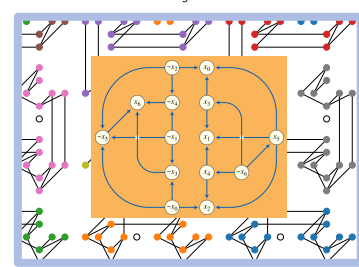
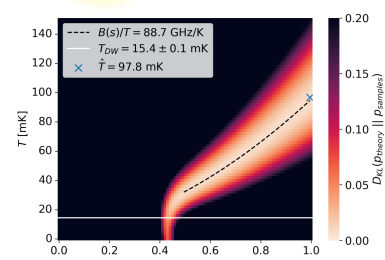
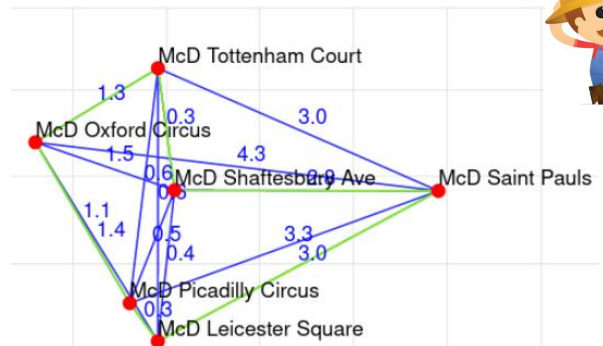
- 1. Airline Scheduling
- 2. Traveling Salesman
- 3. Garden Optimization
- 4. Factorization
- 5. 2-Satisfiability
- 6. QSVM
- 7. QBM



JUNIQ Rolling Call:



or search for
“FZJ JUNIQ ACCESS”



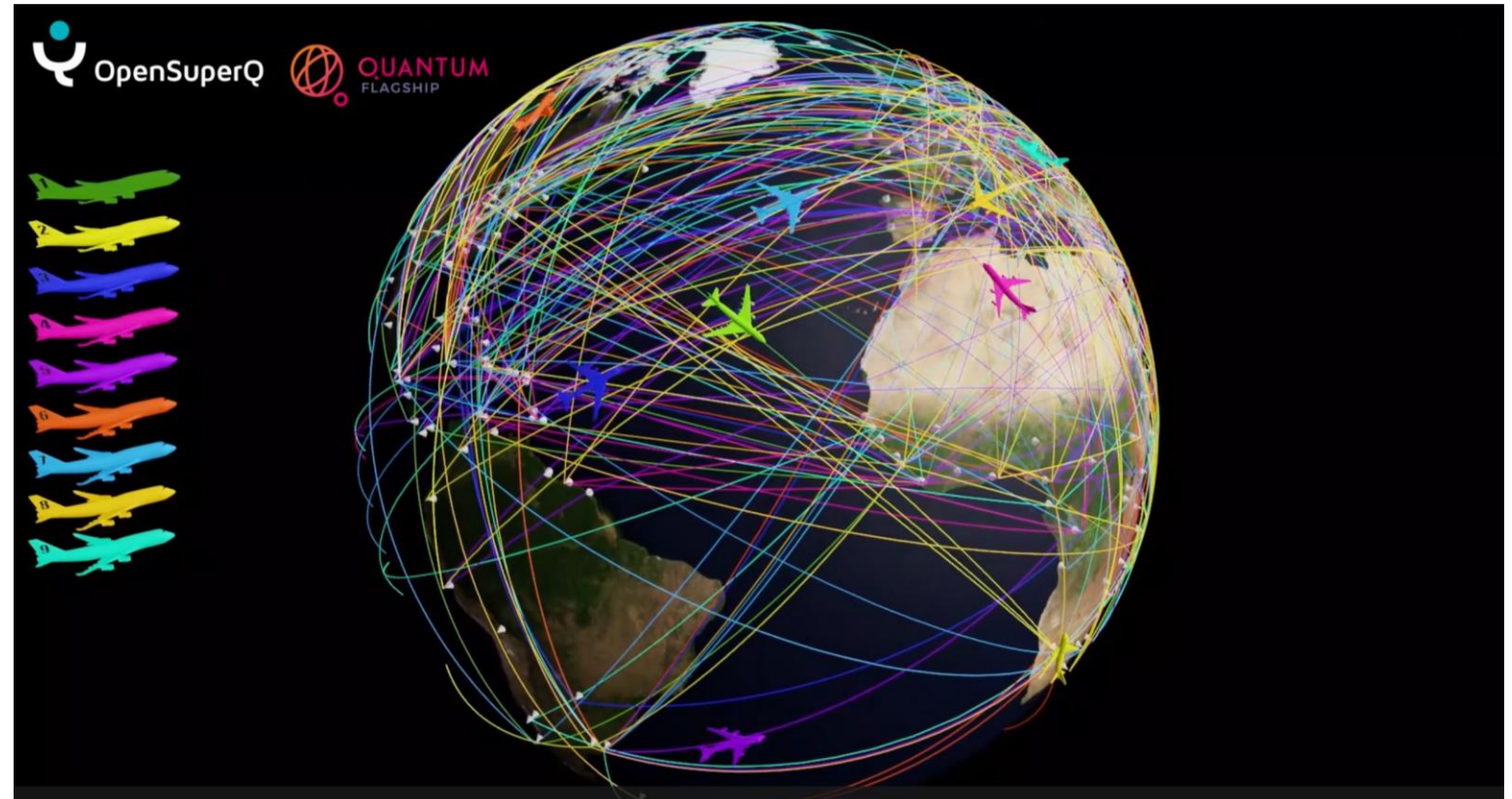
TAIL ASSIGNMENT PROBLEM

Application: Airline scheduling

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

In collaboration with:

Marika Svensson
Jeppesen and
Chalmers University of Technology



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

TAIL ASSIGNMENT PROBLEM

Mathematical formulation

➤ 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

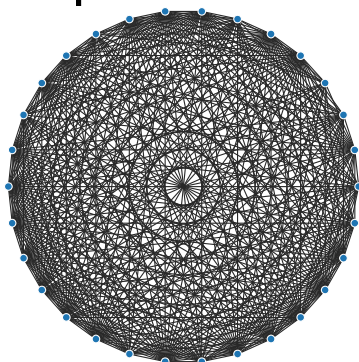
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Route 0	0	1	0	0	0	0		0	0	0
Route 1	0	0	0	0	1	0		0	0	0
...										
Route 10	0	0	0	0	0	1		0	0	1
Route 11	0	0	1	0	0	0		0	0	0
Route 12	0	0	0	1	0	0		1	0	0
Route 13	0	0	1	0	0	0		0	0	0
Route 14	0	0	0	1	0	0		0	0	0
Route 15	0	0	0	0	1	0		0	0	0
Route 16	0	1	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

➤ Reformulation as Ising problem

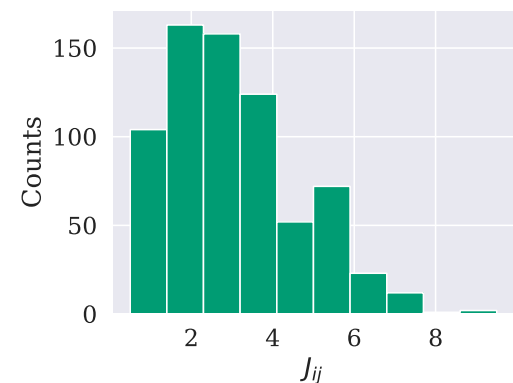
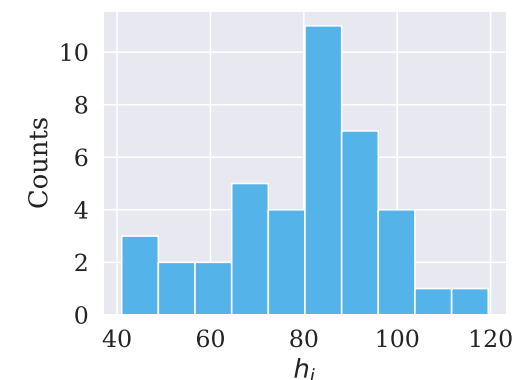
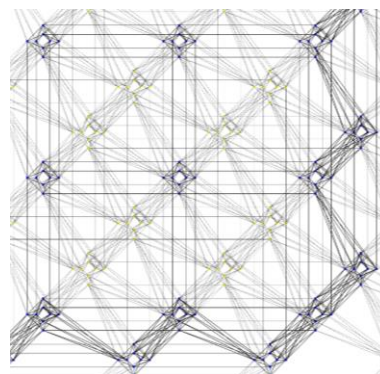
$$\text{QUBO} \leftrightarrow \text{Ising} : x_i = (1 + s_i)/2$$

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

➤ 25 - 40 qubit almost fully-connected ("clique") Ising problems



embedding needed



TAIL ASSIGNMENT: RESULTS

30 - 40 qubit problems (90% nonzero couplers)

Scan of 10 different embeddings and 20 relative chain strengths:

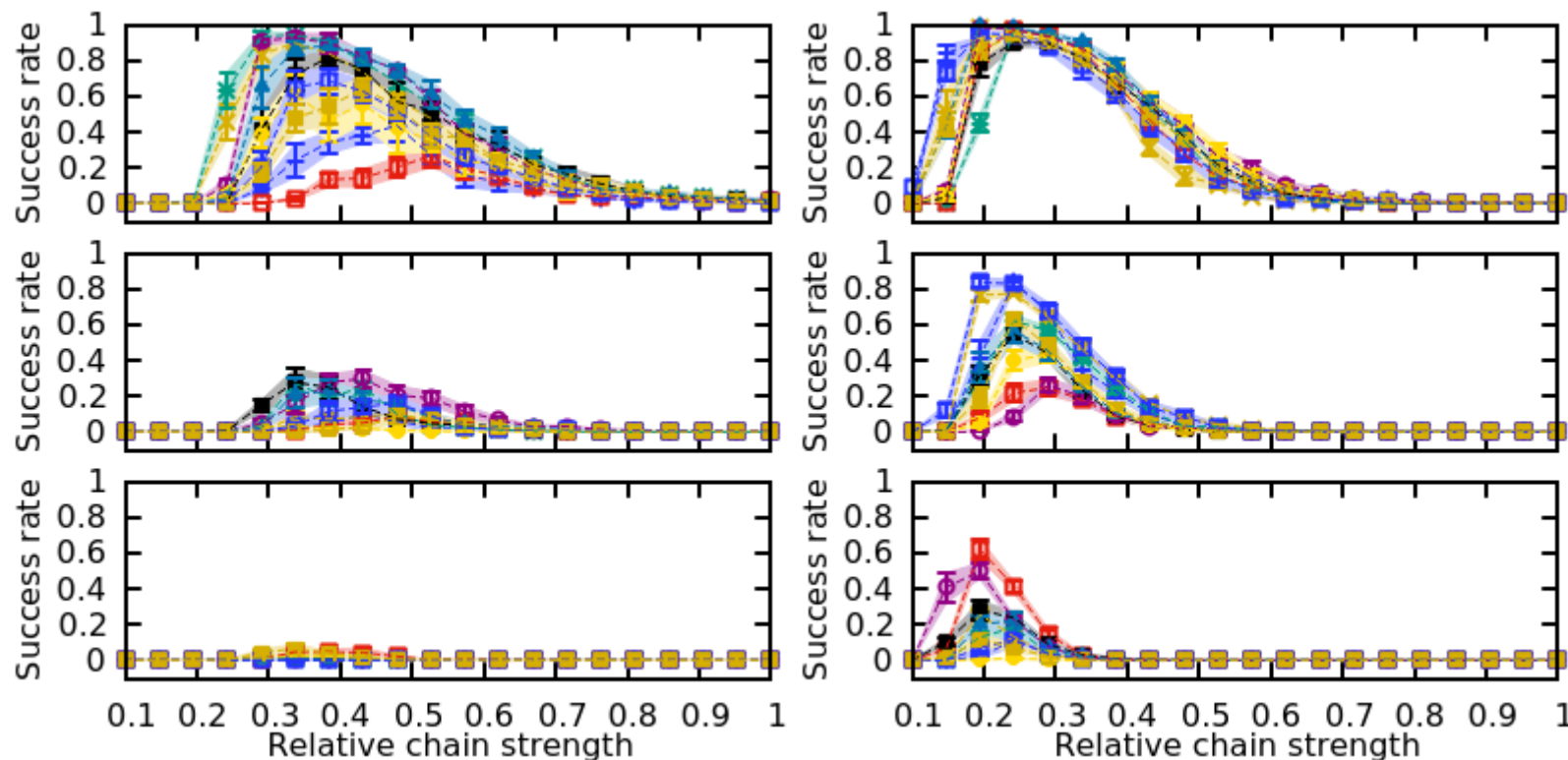
DW2000Q

Advantage

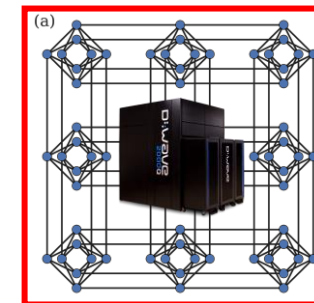
30 qubits

36 qubits

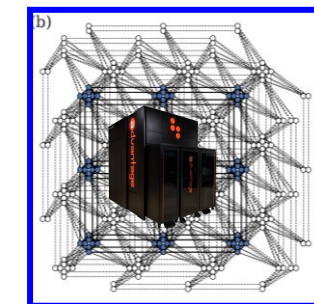
40 qubits



Relative chain strength
= $CS / \max(|h_i|, |J_{ij}|)$



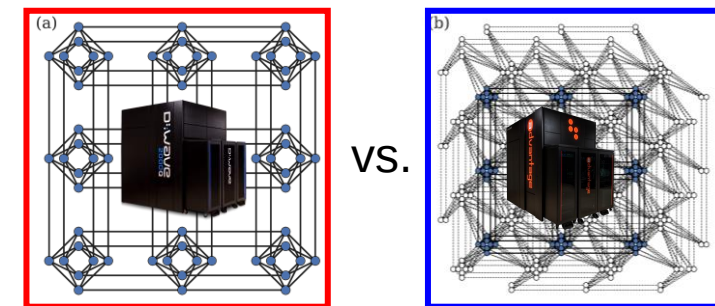
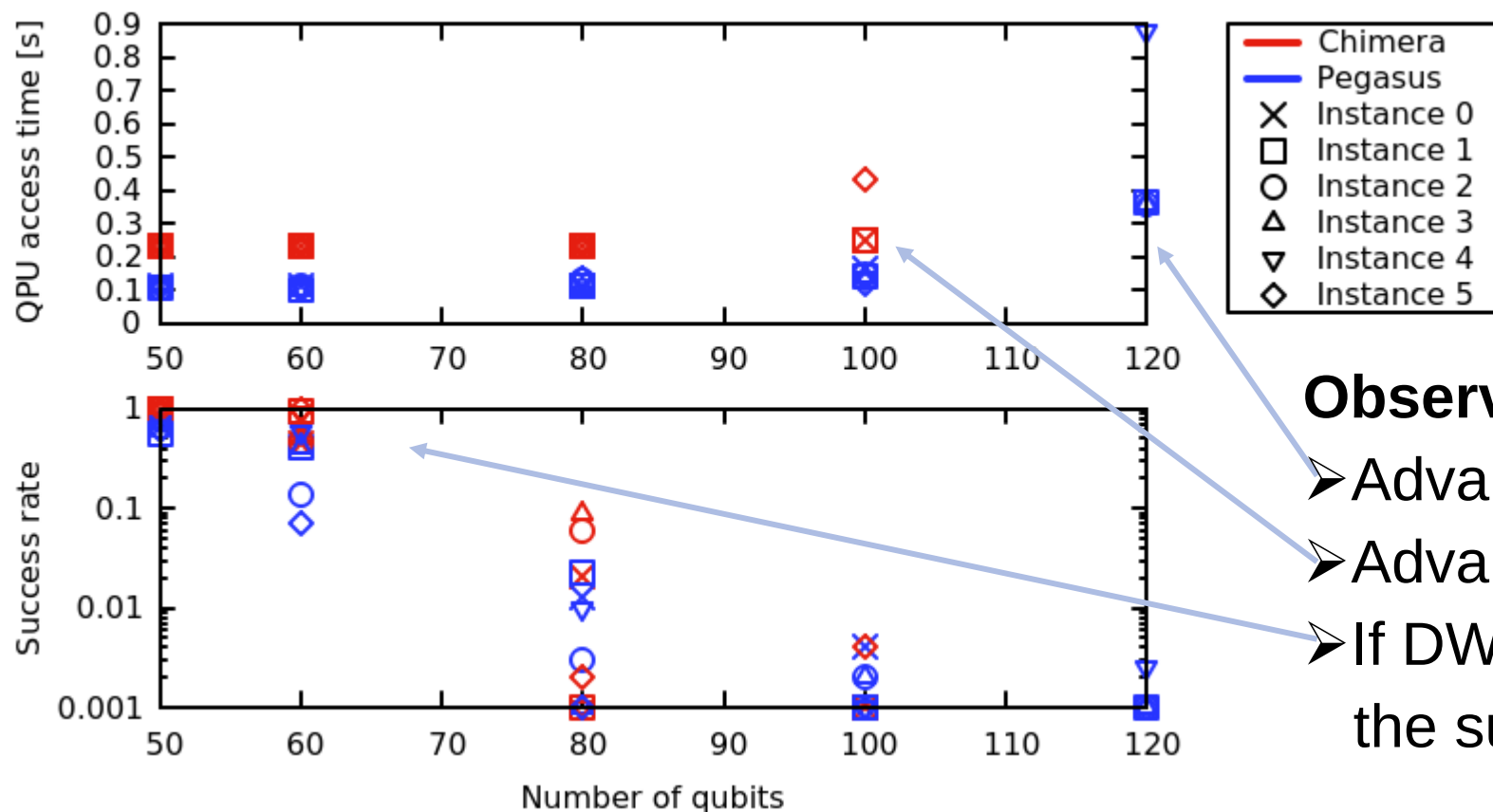
VS.



TAIL ASSIGNMENT: RESULTS

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

The fastest successful runs that reproducibly gave a solution:



Observations:

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

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

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

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

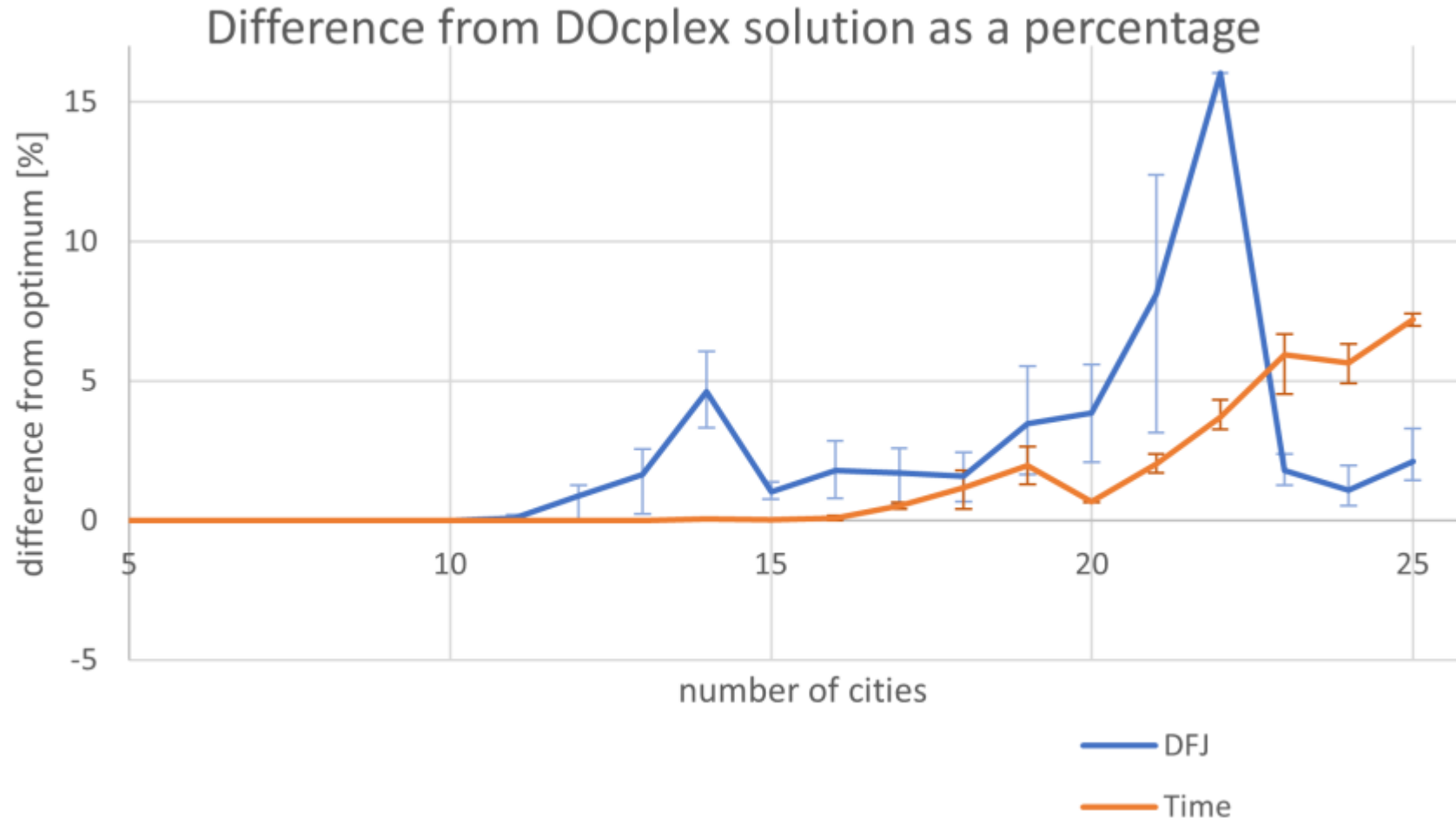
$$+ \sum_{i=0}^{n-1} \left(\sum_{t=0}^{n-1} x_{it} - 1 \right)^2$$

$$\left. + \sum_{t=0}^{n-1} \left(\sum_{i=0}^{n-1} x_{it} - 1 \right)^2 \right\}$$

- 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
- Could simplify by fixing starting point
 → Number of qubits $(n-1)^2$
- Not the DFJ formulation = linear but exp. many inequality constraints

TRAVELING SALESMAN PROBLEM

Results: 25 cities in Europe

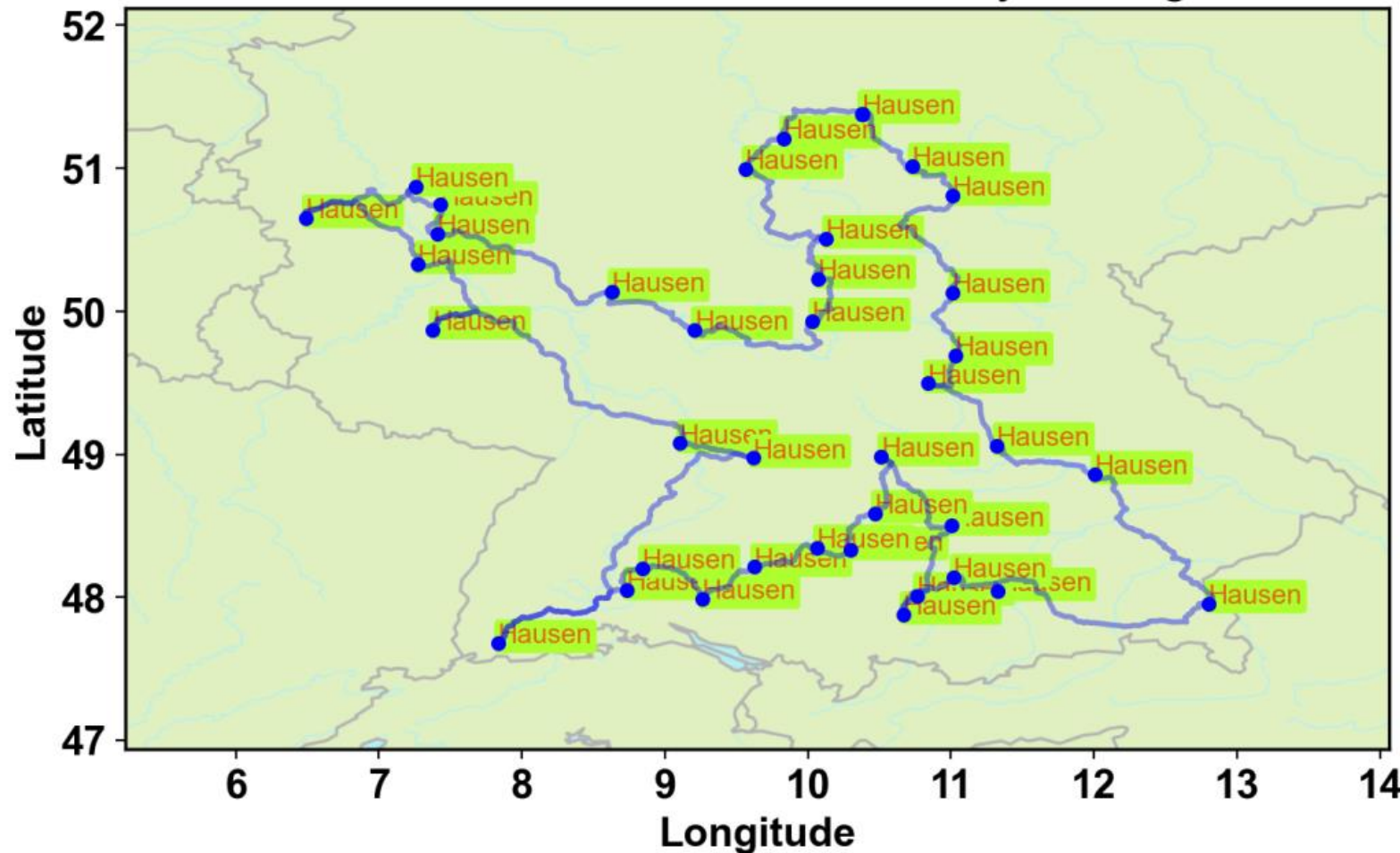


➤ Additional result: D-Wave performance comparable to human performance!

TRAVELING SALESMAN PROBLEM

More results: 45 cities in Germany

45 cities tour of Places Called Hausen In Germany, driving time: 40hrs 50min



VEGETABLE GARDEN OPTIMIZATION

Overview

- Problem: Companion planting in polyculture vegetable gardens



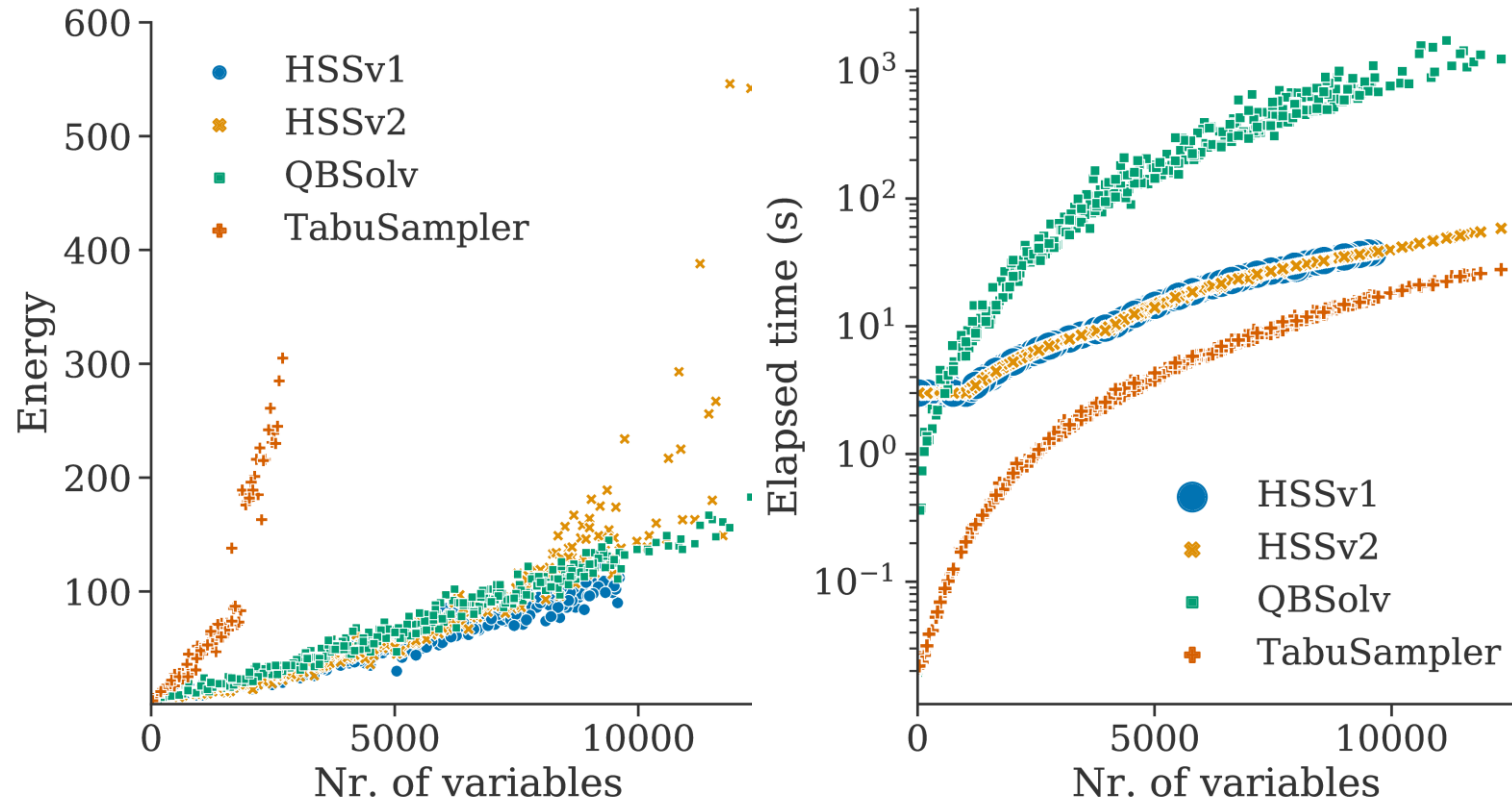
	Tomato	Cucumber	Lettuce
Tomato		☹️	😊
Cucumber	☹️		😊
Lettuce	😊	😊	

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

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

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.

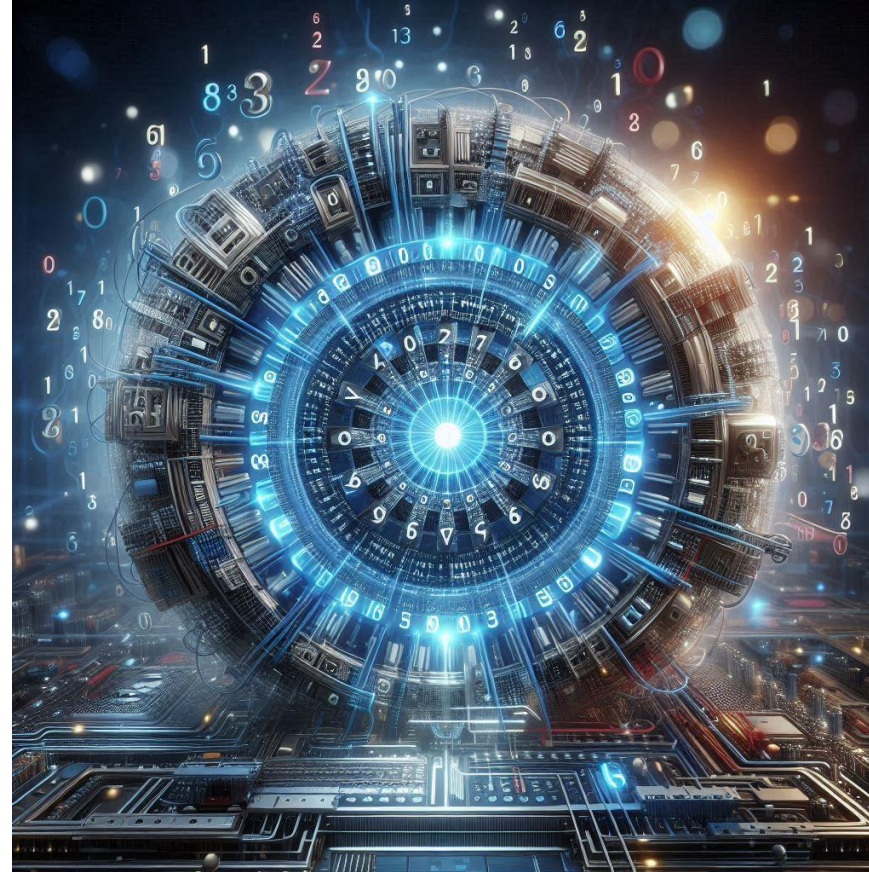
Conclusion:

- Hybrid solvers outperform classical solvers.

THE FACTORING PROBLEM

Willsch et al., Mathematics 11, 4222 (2023)
P. Hanussek, DOI:10.34734/FZJ-2024-05254 (2024)
Willsch et al., arXiv:2410.14397 (2024)

$$N = p \times q$$



FACTORING RECORDS

Willsch et al., Mathematics 11, 4222 (2023)
P. Hanussek, DOI:10.34734/FZJ-2024-05254 (2024)
Willsch et al., arXiv:2410.14397 (2024)

Digital QCs

Shor's Algorithm

$$N = 15, 21, (35) \sim 2^6$$

Martín-López et al., Nat. Photonics 6, 773 (2012)
Monz et al., Science 351, 1068 (2016)
Amico et al., Phys. Rev. A 100, 012305 (2019)

Careful: Oversimplified Shor's Algorithm

$$N \sim 2^{20000}$$

Smolin et al., Nature 499, 7457 (2013)
Gidney, algassert.com/post/2000 (2020)

Variational Quantum Factoring

$$N = 1099551473989 \sim 2^{41}$$

Anschiez et al., arXiv:1808.08927 (2018)
Karamlou et al., npj Quantum Inf. 7, 156 (2021)

Schnorr's Algorithm

$$N = 261980999226229 \sim 2^{48}$$

Schnorr, cryptoeprint:2021/933 (2021)
Hegade and Solano, arXiv:2301.1105 (2023)

← Careful:
preprocessed
down to 3 qubits!

← seems not scalable? →

Ducas, github.com/lducas/SchnorrGate (2021)
Grebnev et al., IEEE Access 11, 134760 (2023)
Khattar and Yosri, arXiv:2307.09651 (2023)
Tesoro et al., arXiv:2410.16355 (2024)

Analog QCs

Direct Method

$$N = 1042441 \sim 2^{20}$$

Peng et al., Phys. Rev. Lett. 101, 220405 (2008)
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Multiplier Circuit

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Andriyash et al., Tech. Rep. 14-1002A-B (2016)
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Simulated Digital QCs

Shor's Algorithm

$$N = 549755813701 \sim 2^{39}$$

Willsch et al., Mathematics 11, 4222 (2023)



Classical (Super)Computers

Number Field Sieve

$$N = \text{RSA-250} \sim 10^{250} \sim 2^{829}$$

Boudot et al., CRYPTO 2020, 62 (2020)

Schnorr's Algorithm

$$N \sim 2^{100}$$

Tesoro et al., arXiv:2410.16355 (2024)

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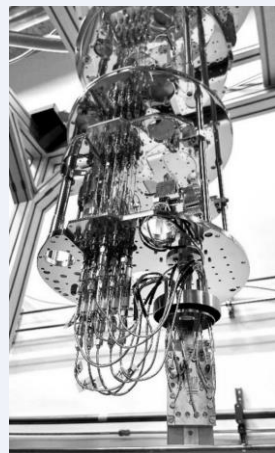
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Boudot et al., CRYPTO 2020, 62 (2020)

Schnorr's Algorithm

$$N \sim 2^{100}$$

Tesoro et al., arXiv:2410.16355 (2024)

FACTORING ON ANALOG QCS

Mehtods

- Problem needs to be expressed as QUBO / Ising
- We investigated **3 approaches**:

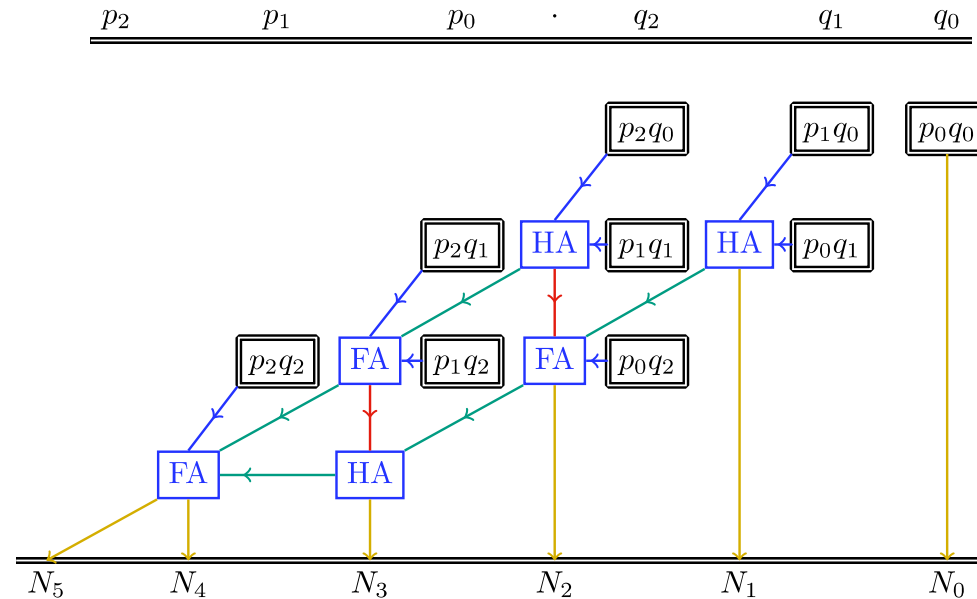
Direct Method

Peng et al., Phys. Rev. Lett. 101, 220405 (2008)

$$\min_{p,q} (N - pq)^2$$

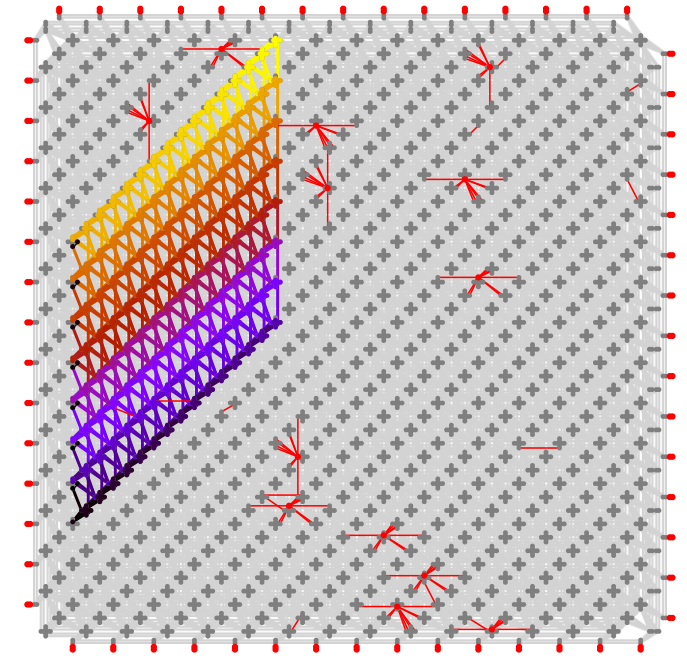
Multiplication Circuit Method

Andriyash et al, D-Wave TR 14-1002A-B (2016)



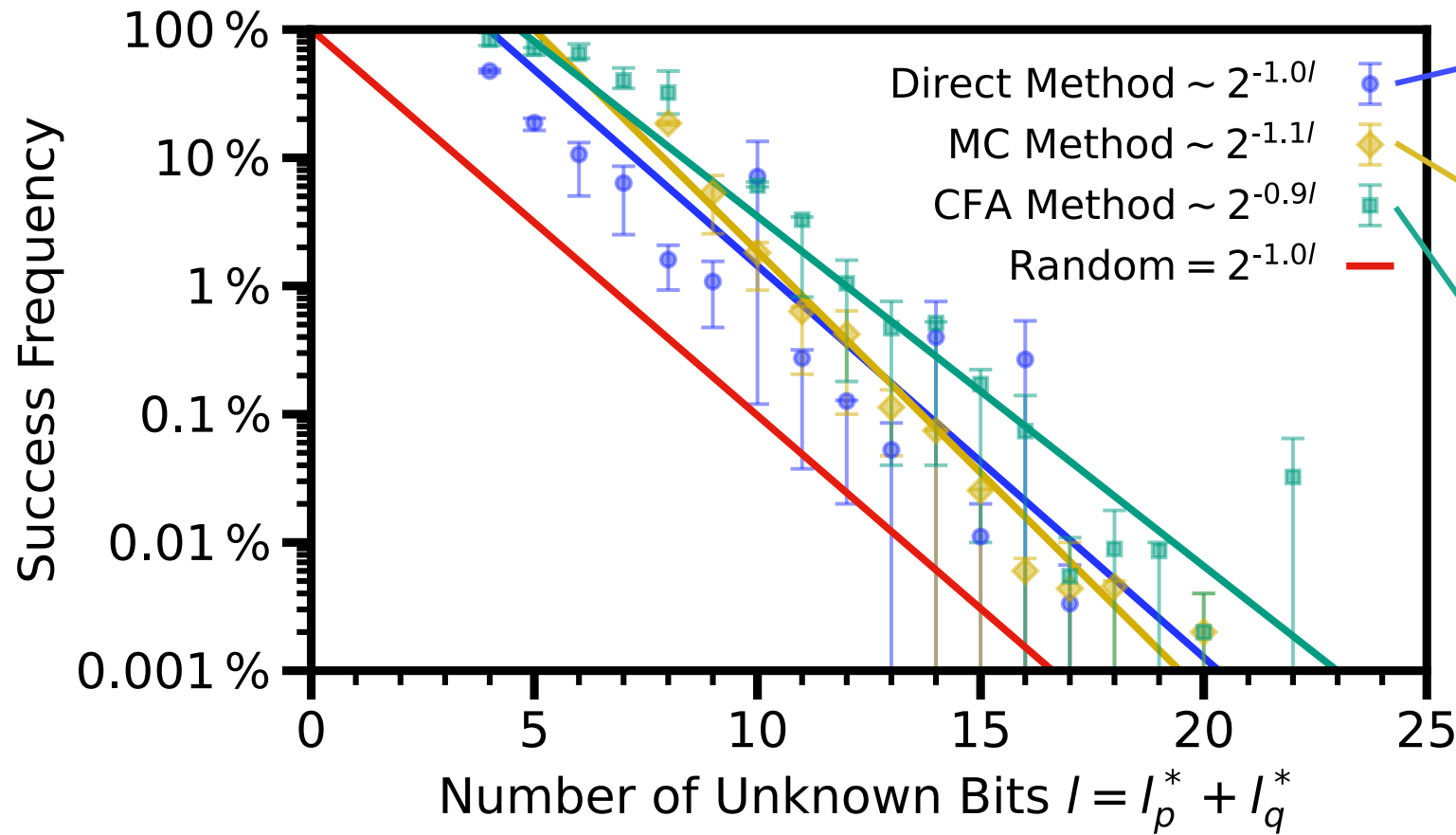
Controlled Full-Adder Method

Ding et al., Sci. Rep. 14, 1 (2024)

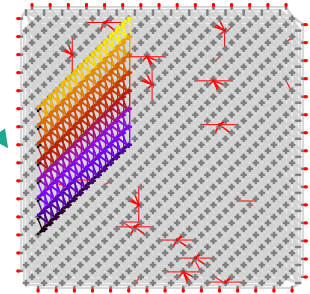
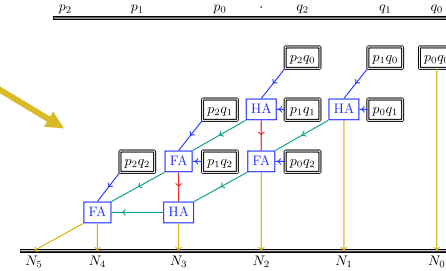


FACTORING ON ANALOG QCS

Results



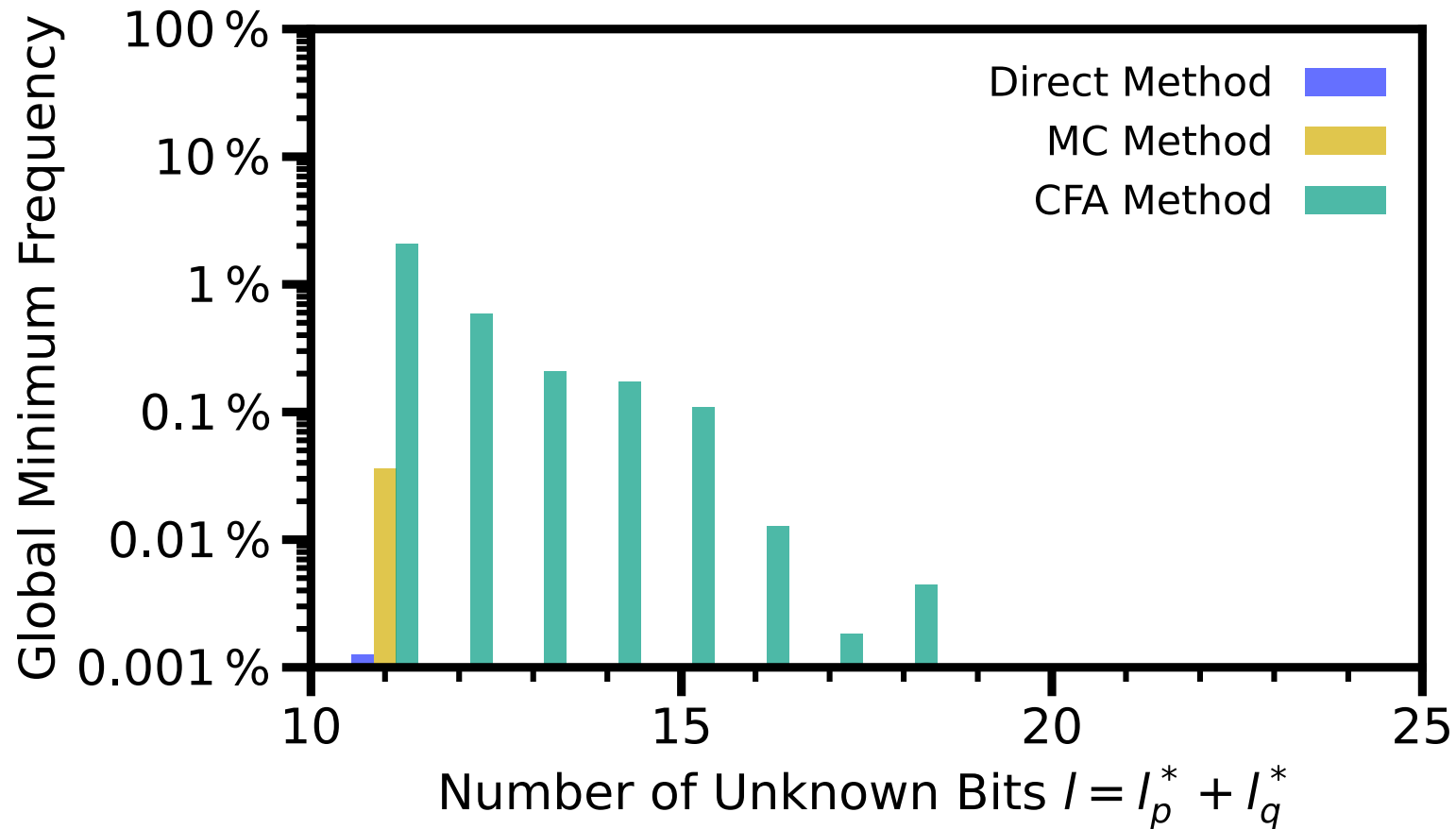
$$\min_{p,q} (N - pq)^2$$



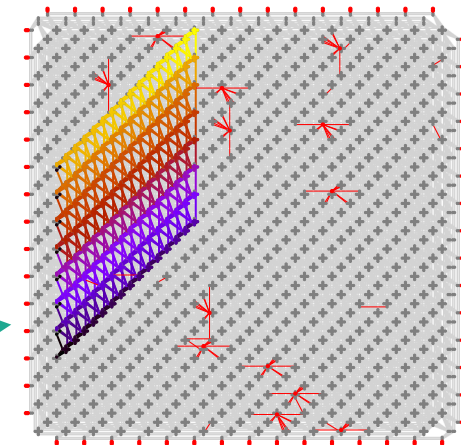
- All methods are absolutely better than random guessing
- CFA method also scales better
- **BUT:** All methods scale exponentially!

FACTORING ON ANALOG QCS

Results



- CFA method finds true ground state much more often!
- **Reason:** Custom embedding on the hardware



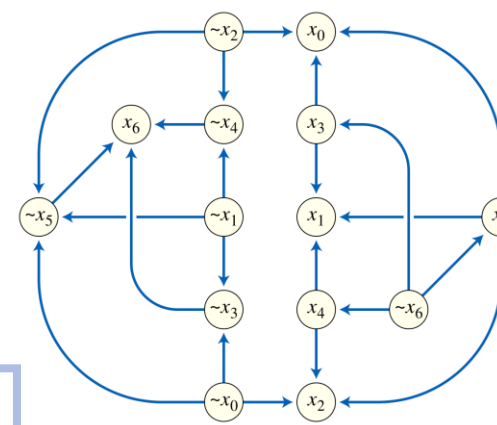
2-SATISFIABILITY

Overview

➤ Mathematical formulation

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

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



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

find assignment to x_i that makes F true

➤ Reformulation as Ising Problem

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

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

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

$$\begin{aligned} x_i = 0 &\Leftrightarrow s_i = -1 \\ x_i = 1 &\Leftrightarrow s_i = +1 \end{aligned}$$

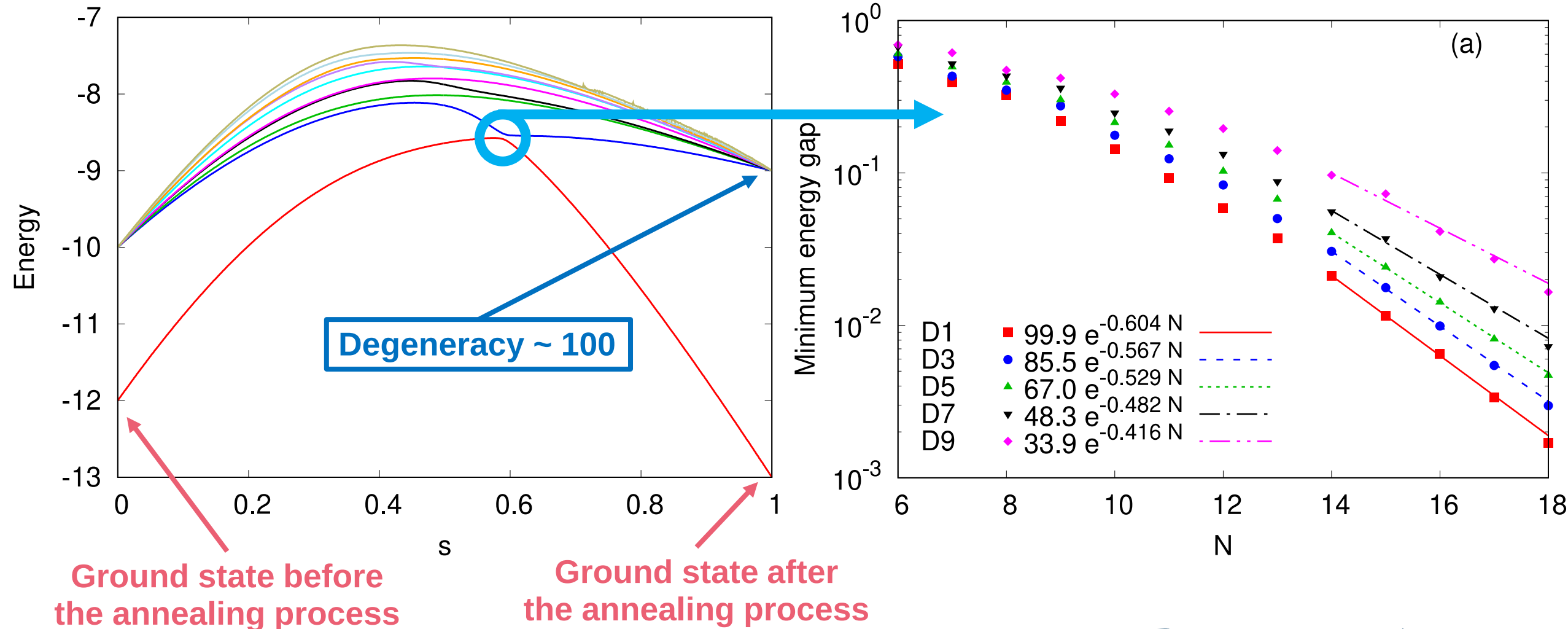
$$\begin{aligned} \epsilon_{\alpha} &= 1 \text{ for } x_i \\ \epsilon_{\alpha} &= -1 \text{ for } \overline{x_i} \end{aligned}$$

➤ “Hard 2-SAT problems”: The purpose is benchmarking

➤ Chosen to be “hard” for quantum annealers (not for digital computers)

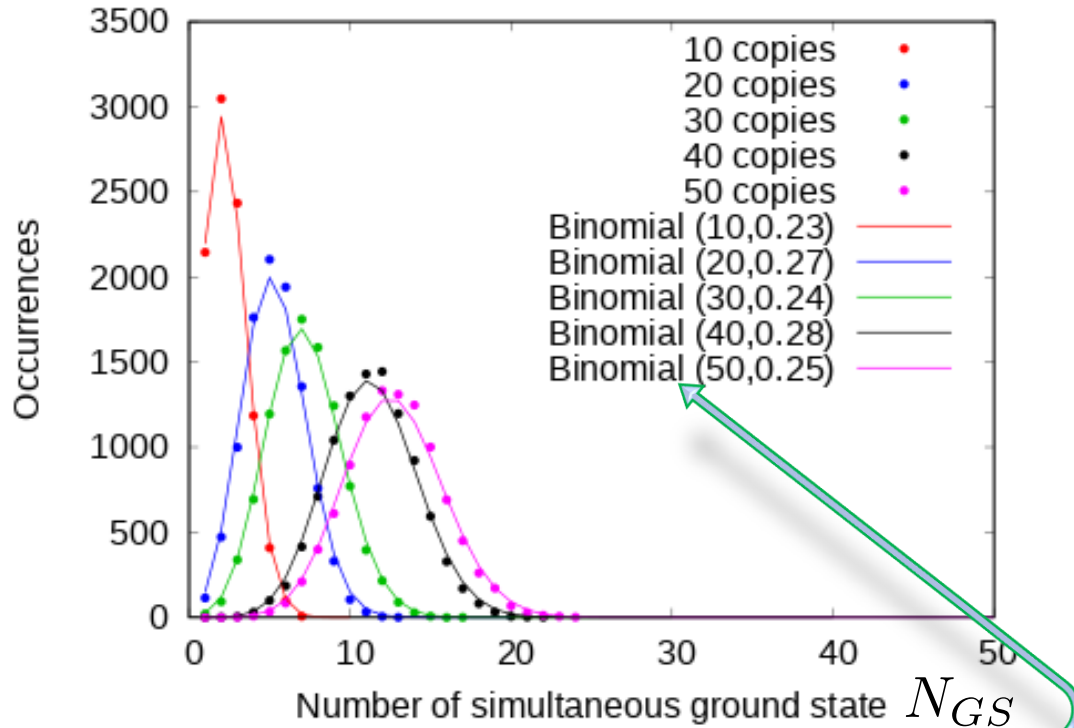
2-SATISFIABILITY

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



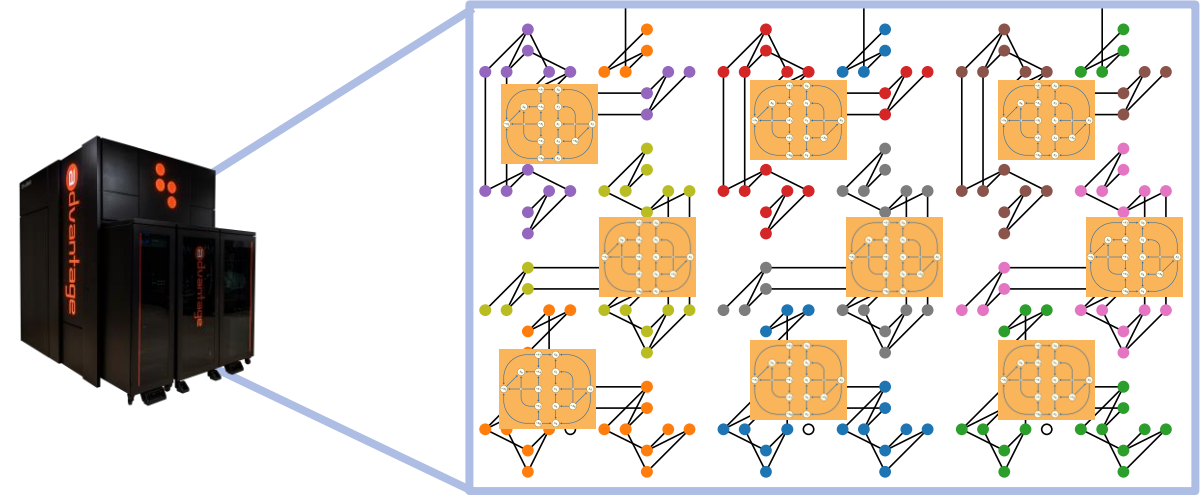
2-SATISFIABILITY: RESULTS

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
- In no run could all ground states be found simultaneously
- Different parts of the QPU work almost independently

QUANTUM SUPPORT VECTOR MACHINES

From classical SVM to quantum SVM

➤ An SVM is a supervised machine-learning method for binary classification

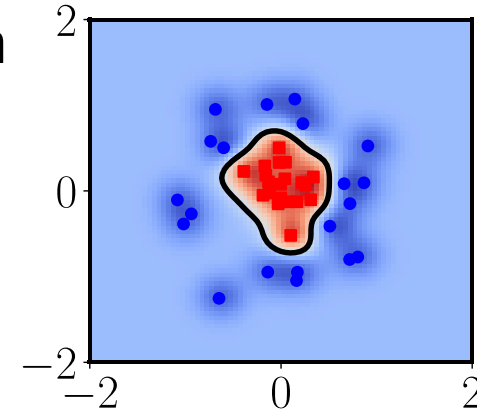
➤ Given a training set

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

an SVM is trained by solving the Quadratic Programming problem

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

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



Continuous problem variables

Kernel function (nonlinear SVM)

➤ QUBO problems are also quadratic, but for **binary variables**

Number of qubits per problem variable

→ Use encoding:

$$\alpha_n = \sum_{k=0}^{K-1} B^{k-P} x_{[n,k]}$$

Base & Exponent

$$E(\{\alpha_n\})$$

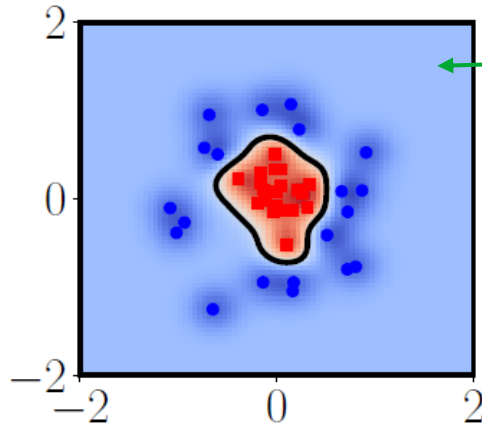
QUBO formulation

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

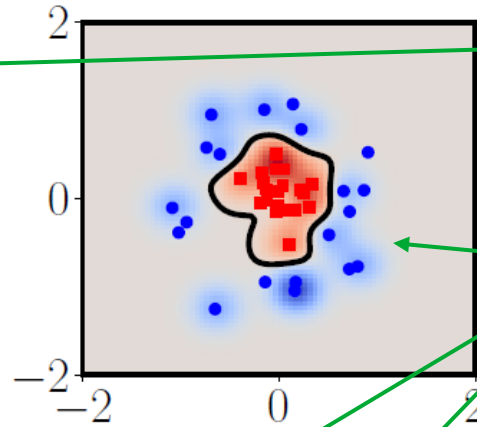
QUANTUM SUPPORT VECTOR MACHINES

Results

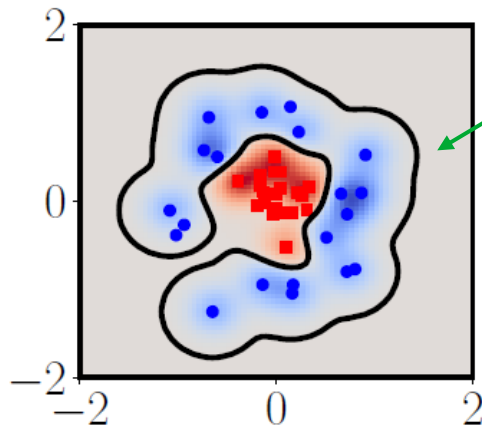
(a) cSVM



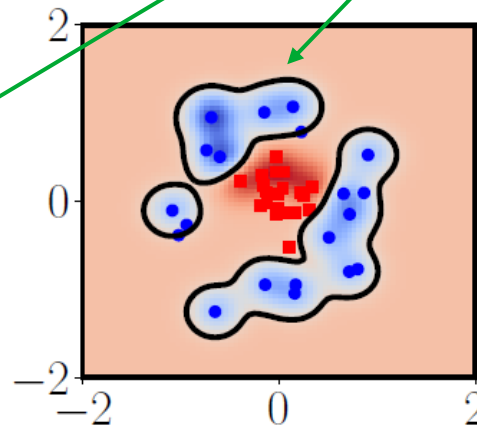
(b) qSVM#1



(c) qSVM#6



(d) qSVM#16



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 SUPPORT VECTOR MACHINES

Application to remote sensing

Willsch et al., CPC 248, 107006 (2020)
Cavallaro et al., IGARSS 2020, 1973 (2020)
Delilbasic et al., IGARSS 2021, 2608 (2021)
Pasetto et al., GRSL 1505705 (2023)
Delilbasic et al., JSTARS 17, 1434 (2023)
Pasetto et al., JSTARS 17, 3263 (2024)



QUANTUM SUPPORT VECTOR MACHINES

Application to remote sensing: Results

Willsch et al., CPC 248, 107006 (2020)
Cavallaro et al., IGARSS 2020, 1973 (2020)
Delilbasic et al., IGARSS 2021, 2608 (2021)
Pasetto et al., LGRS 19, 1505705 (2022)
Delilbasic et al., JSTARS 17, 1434 (2023)
Pasetto et al., JSTARS 17, 3263 (2024)
Zardini et al., TQE 5, 3103512 (2024)

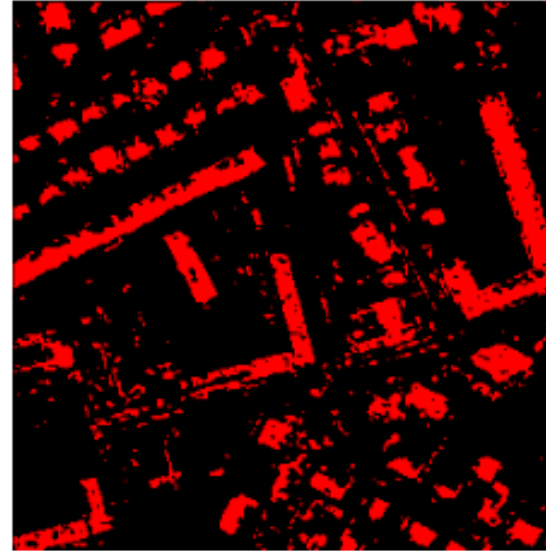
Original



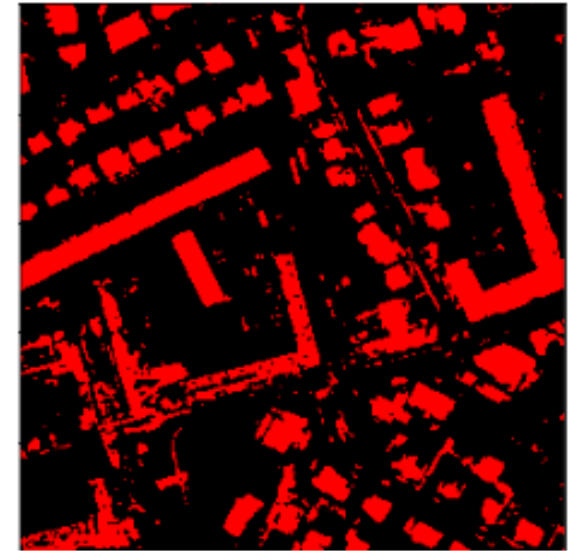
Ground truth



Classical SVM



Quantum SVM



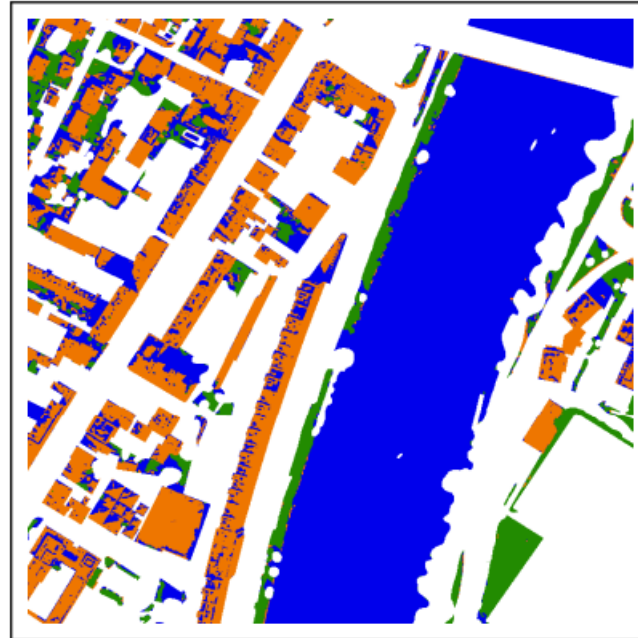
QUANTUM SUPPORT VECTOR MACHINES

Extension to multiple classes

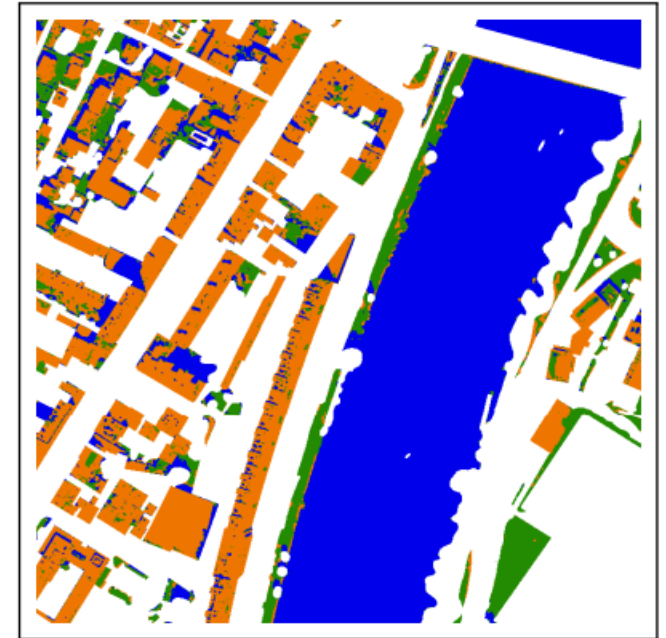
Willsch et al., CPC 248, 107006 (2020)
Cavallaro et al., IGARSS 2020, 1973 (2020)
Delilbasic et al., IGARSS 2021, 2608 (2021)
Pasetto et al., LGRS 19, 1505705 (2022)
Delilbasic et al., JSTARS 17, 1434 (2023)
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Zardini et al., TQE 5, 3103512 (2024)



Ground truth



Classical SVM



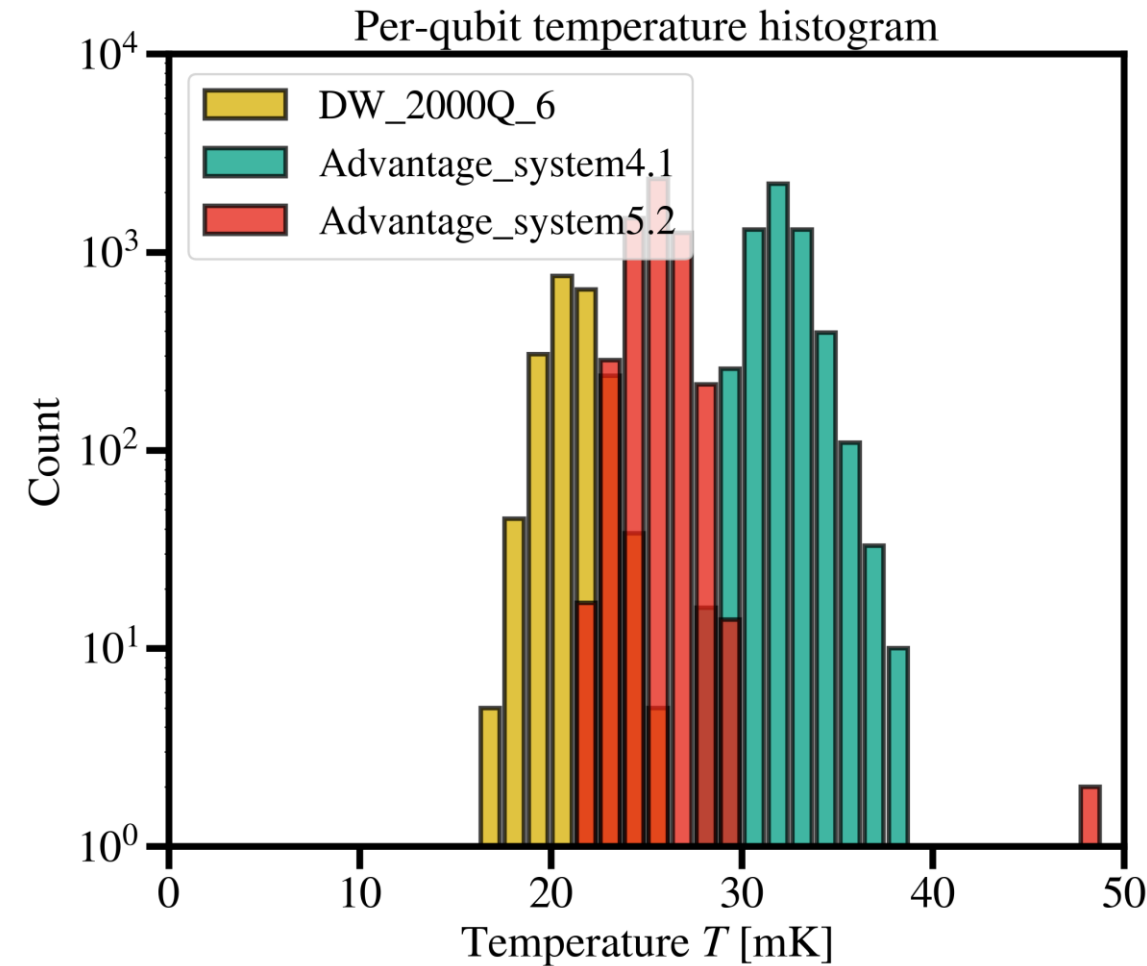
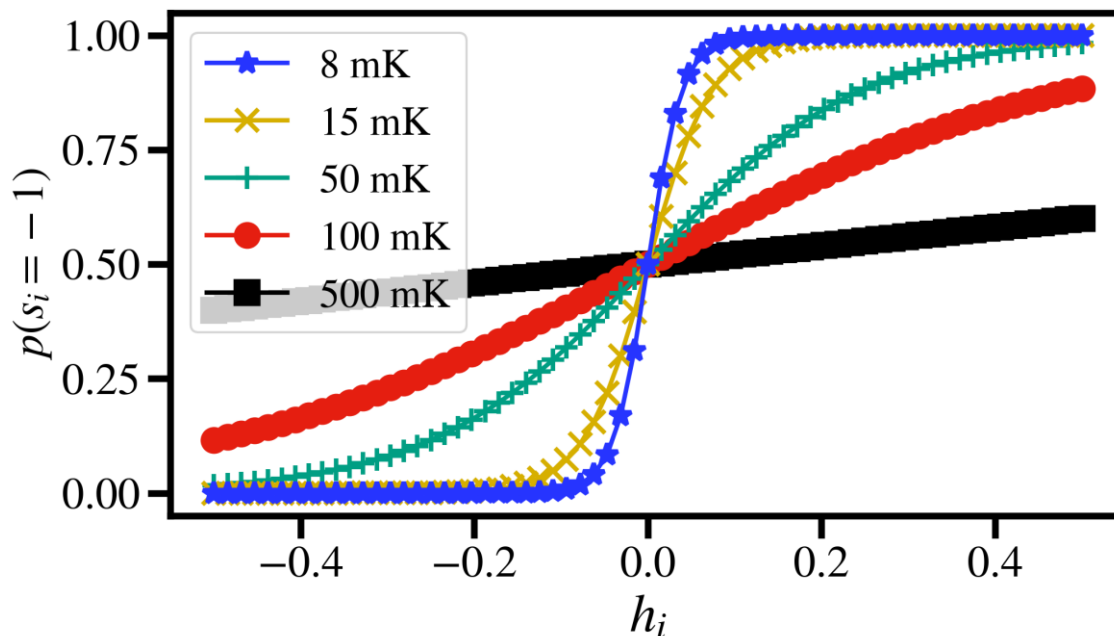
Quantum SVM

QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

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

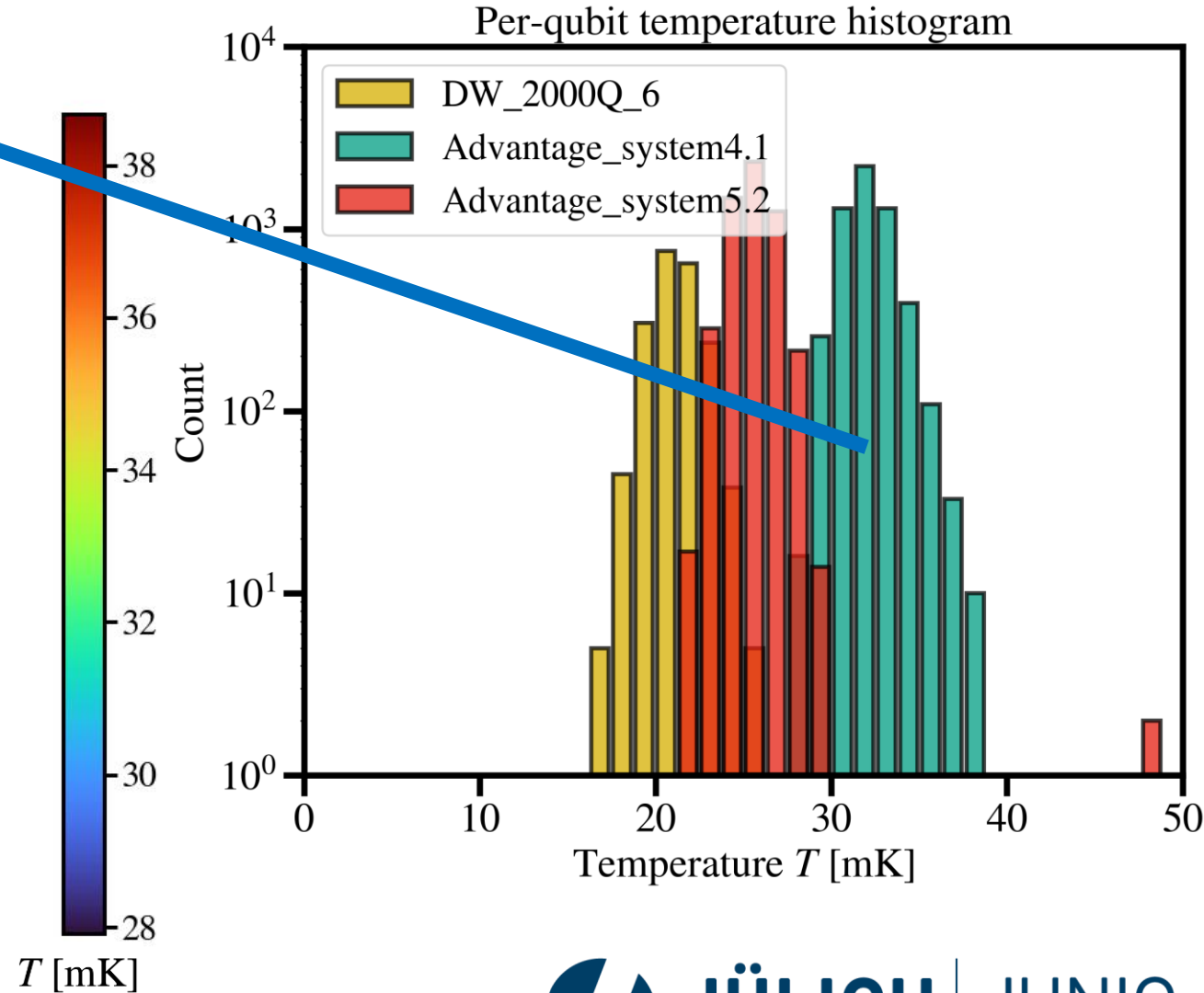
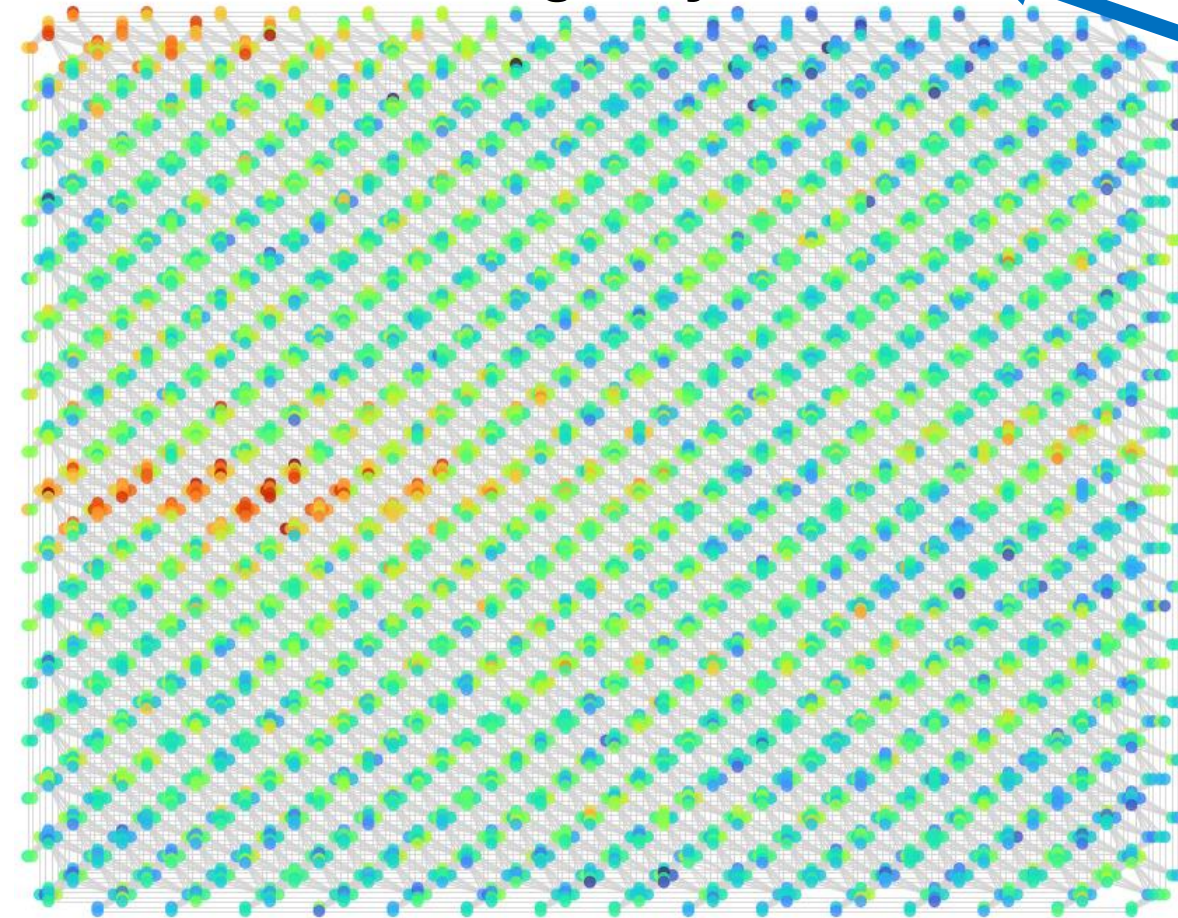
$$p(s_i = \pm 1) = \langle s_i | \frac{1}{Z} e^{-\beta H(1)} | s_i \rangle = \frac{1}{2} \left(1 + \tanh \left(-\frac{B(1)h_i}{2k_B T} s_i \right) \right)$$



QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

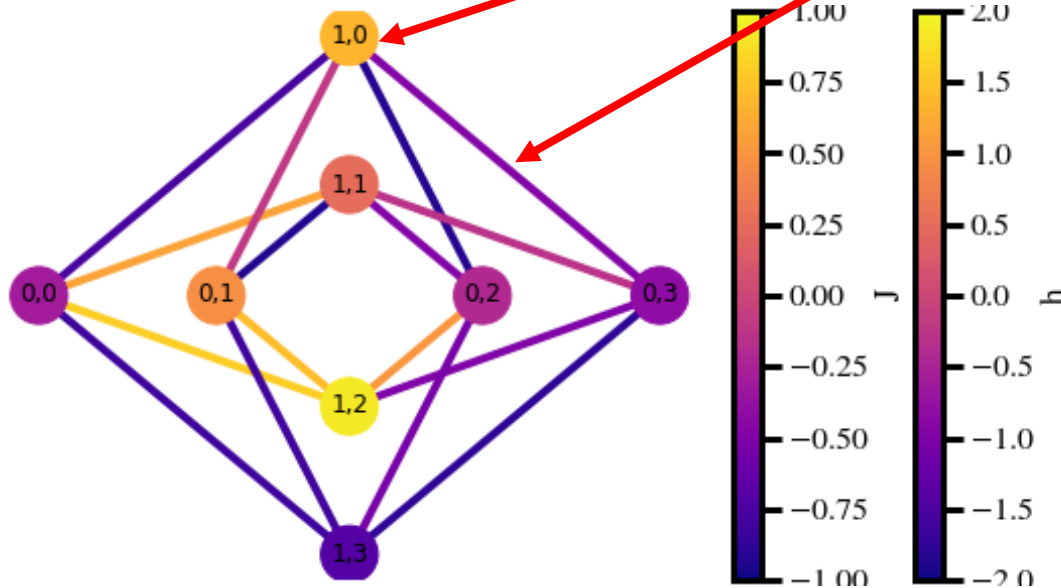
Advantage_system4.1



QUANTUM BOLTZMANN MACHINES

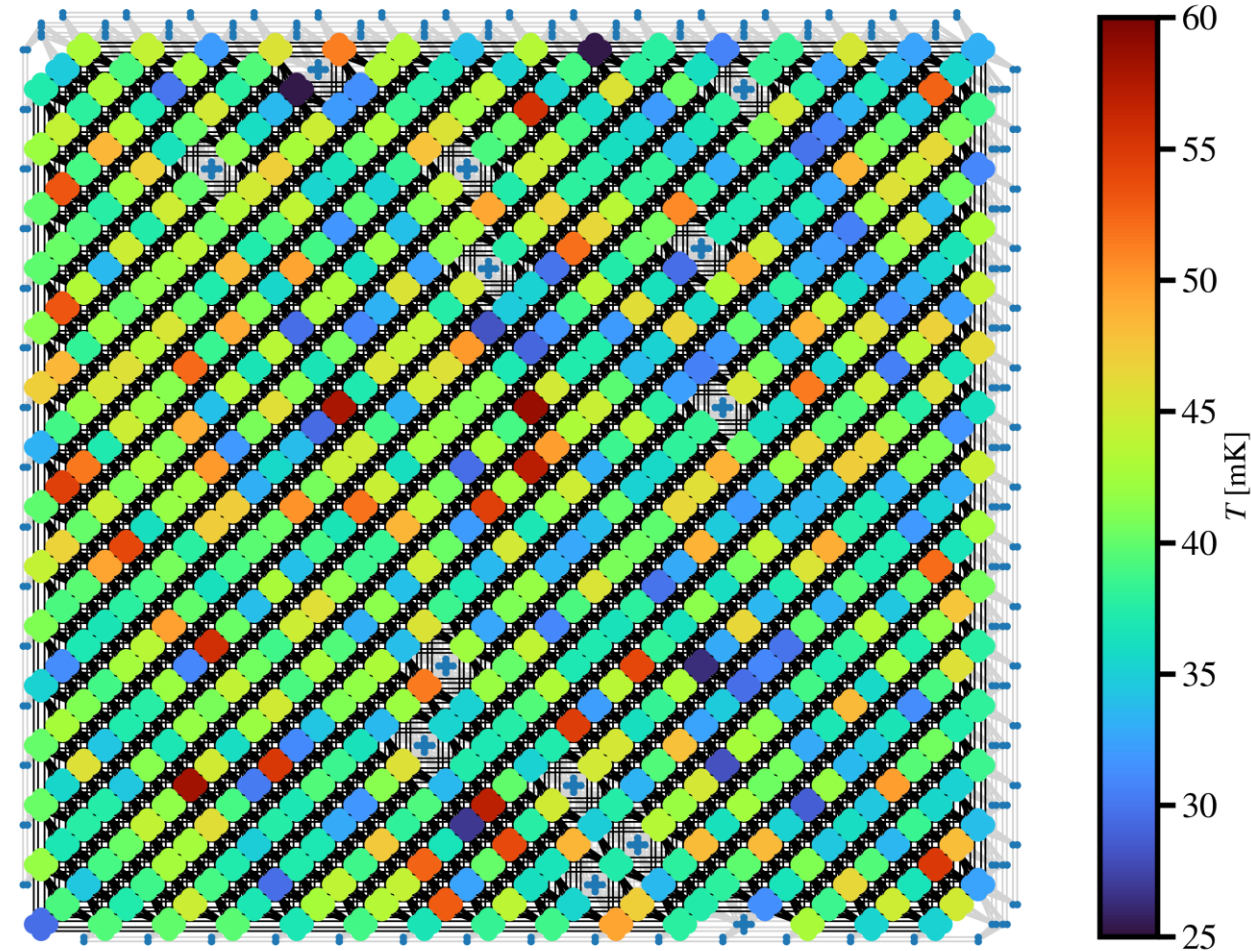
Experiment #2: 8-qubit problem on each Chimera cell of the Pegasus graph

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



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

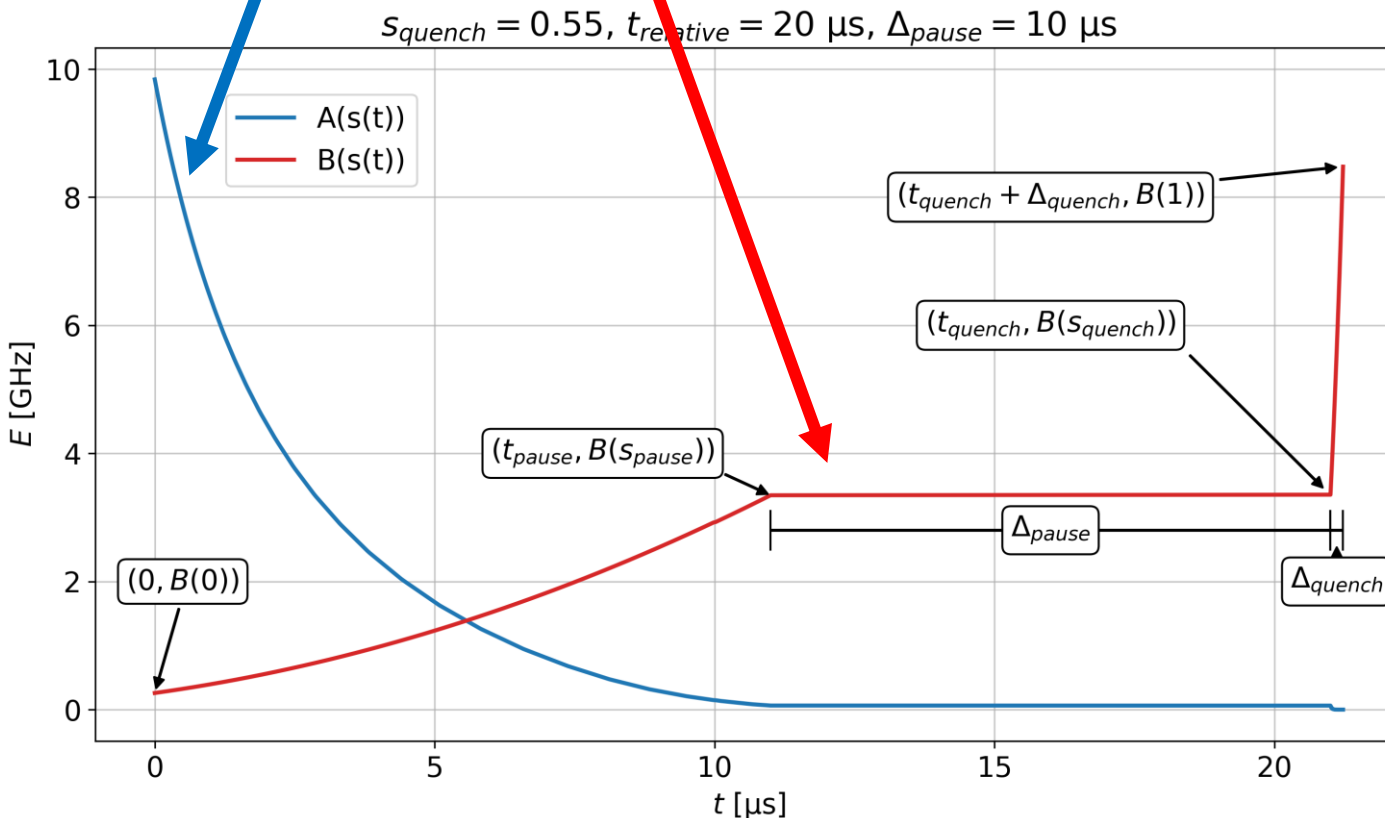
$$p(\{s_i = \pm 1\} \mid \beta, s) = \langle \{s_i = \pm 1\} \mid \frac{1}{Z} e^{-\beta H(s)} \mid \{s_i = \pm 1\} \rangle$$



QUANTUM BOLTZMANN MACHINES

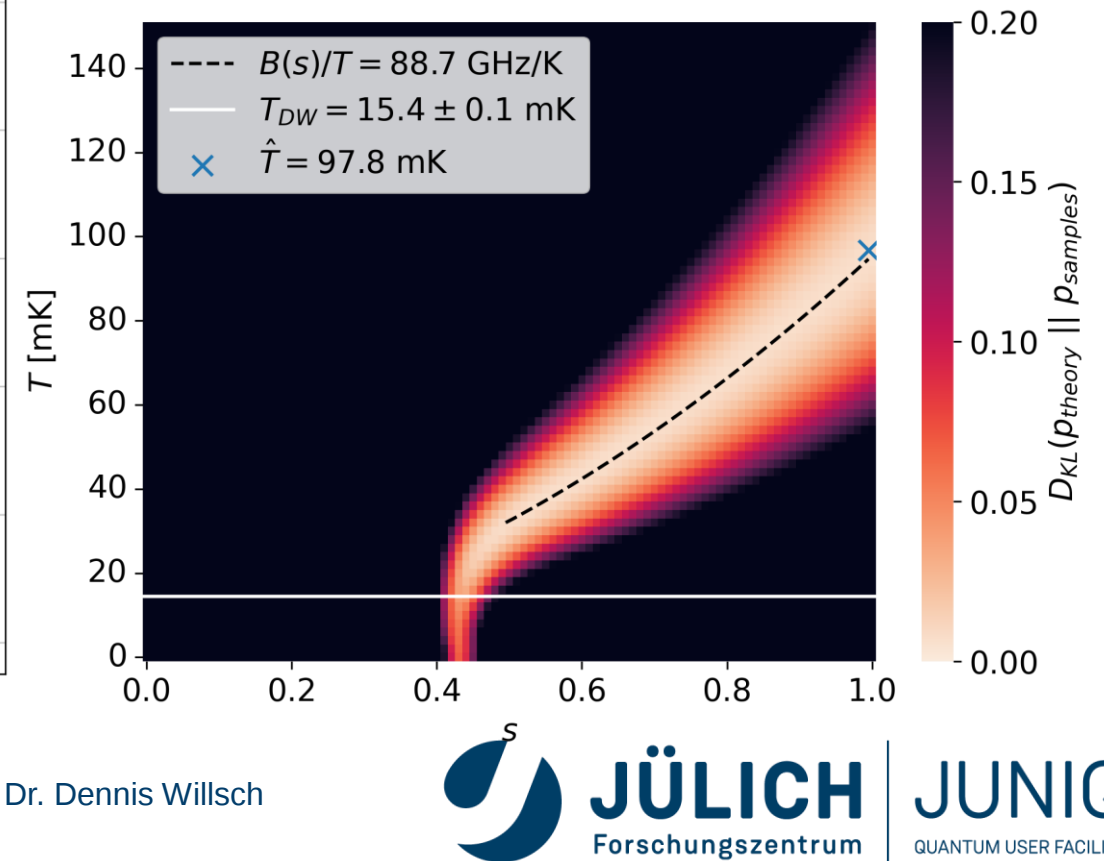
Experiment #3: 12-qubit problem (also for intermediate times $s \neq 1$)

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



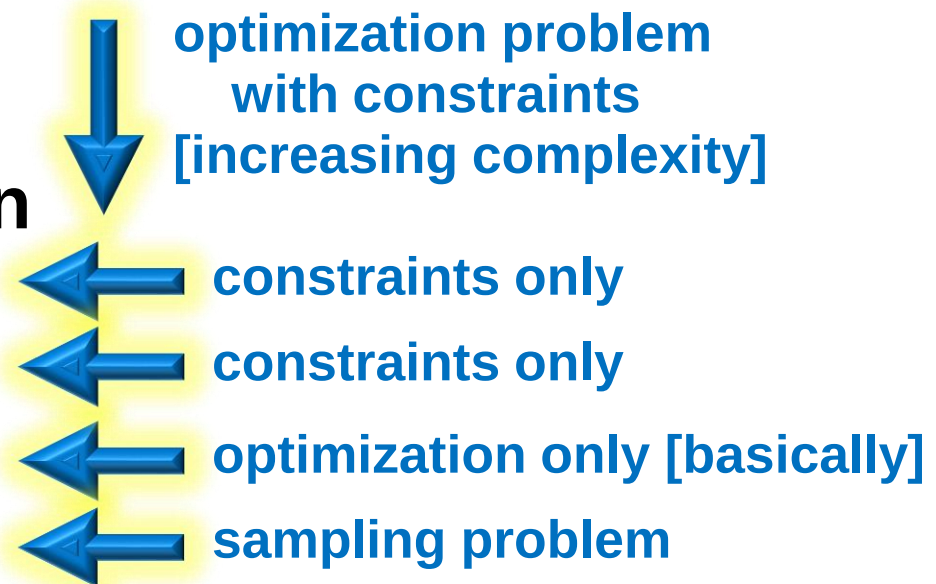
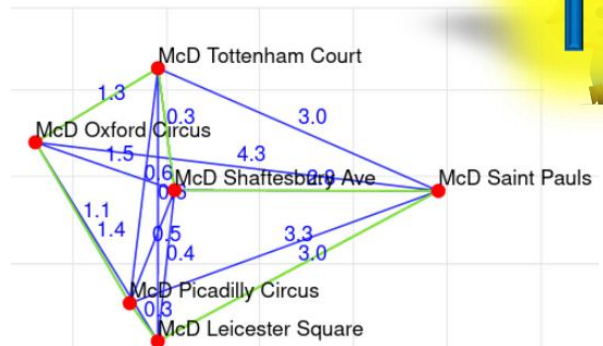
Quantum Boltzmann distribution
at inverse temperature β and time s :

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



CONTENTS

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

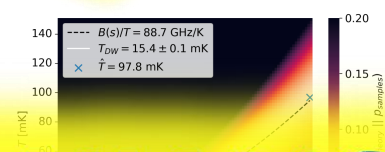


JUNIQ Rolling Call:

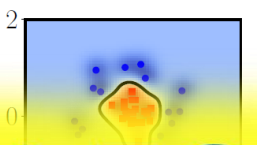


or search for
“FZJ JUNIQ ACCESS”

THANK YOU FOR YOUR ATTENTION



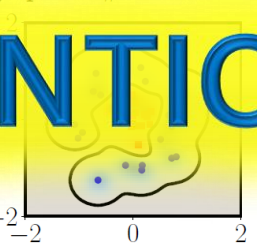
(a) cSVM



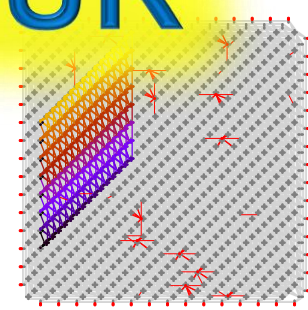
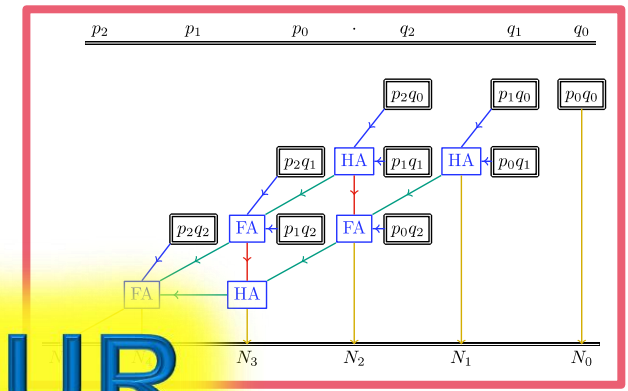
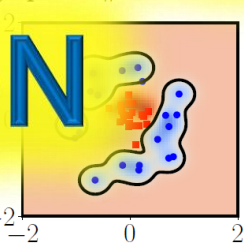
(b) qSVM#1



(c) qSVM#6

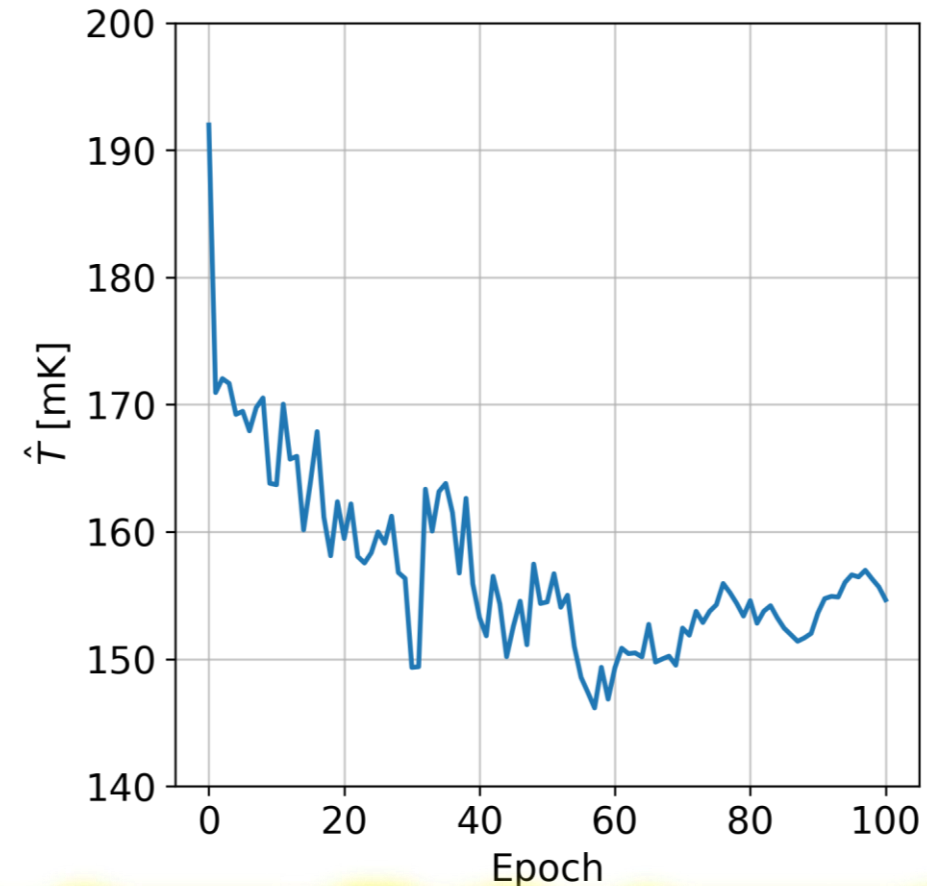
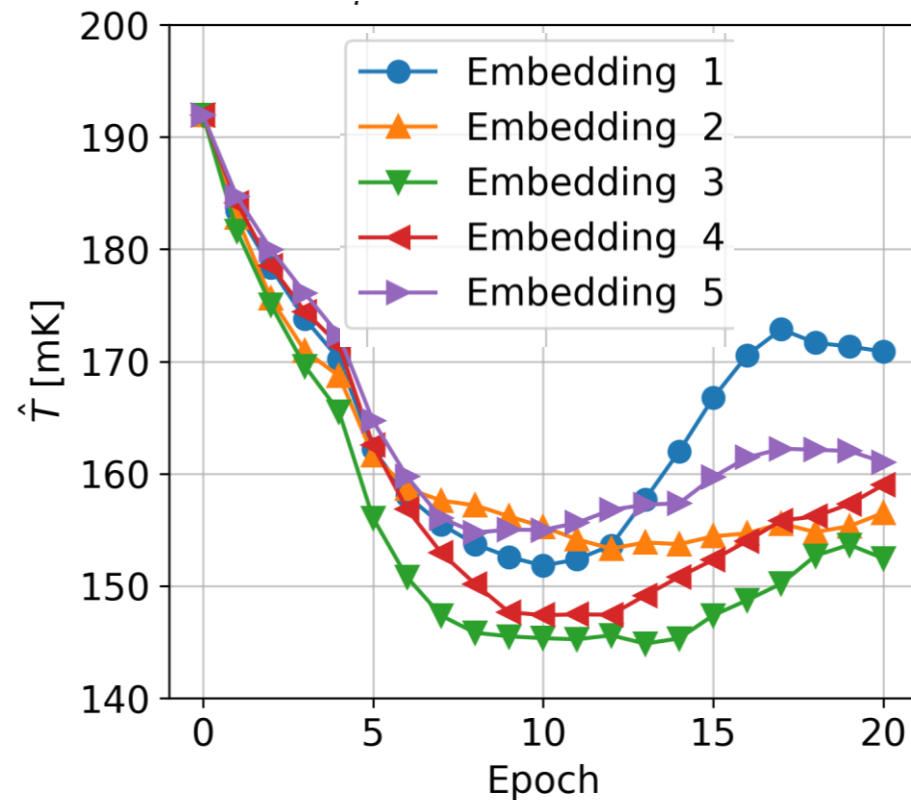


(d) qSVM#16



QUANTUM BOLTZMANN MACHINES

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



→ **Observation: Larger problems ~ larger effective temperature**