APPLICATIONS ON QUANTUM ANNEALERS AT FZJ

JUNIQ: Jülich Unified INfrastructure for Quantum Computing

DR. DENNIS WILLSCH

WE COMPUTE WITH QUANTUM COMPUTERS
supported by
Bundesministerium für Bildung und Forschung
Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen

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Prof. Dr. Kristel Michielsen

Prof. Dr. Hans De Raedt

Dr. Dennis Willsch

Dr. Madita Willsch

Vrinda Mehta

Carlos Gonzalez Calaza

Manpreet Jattana

Tamás Nemes

Cameron Perot

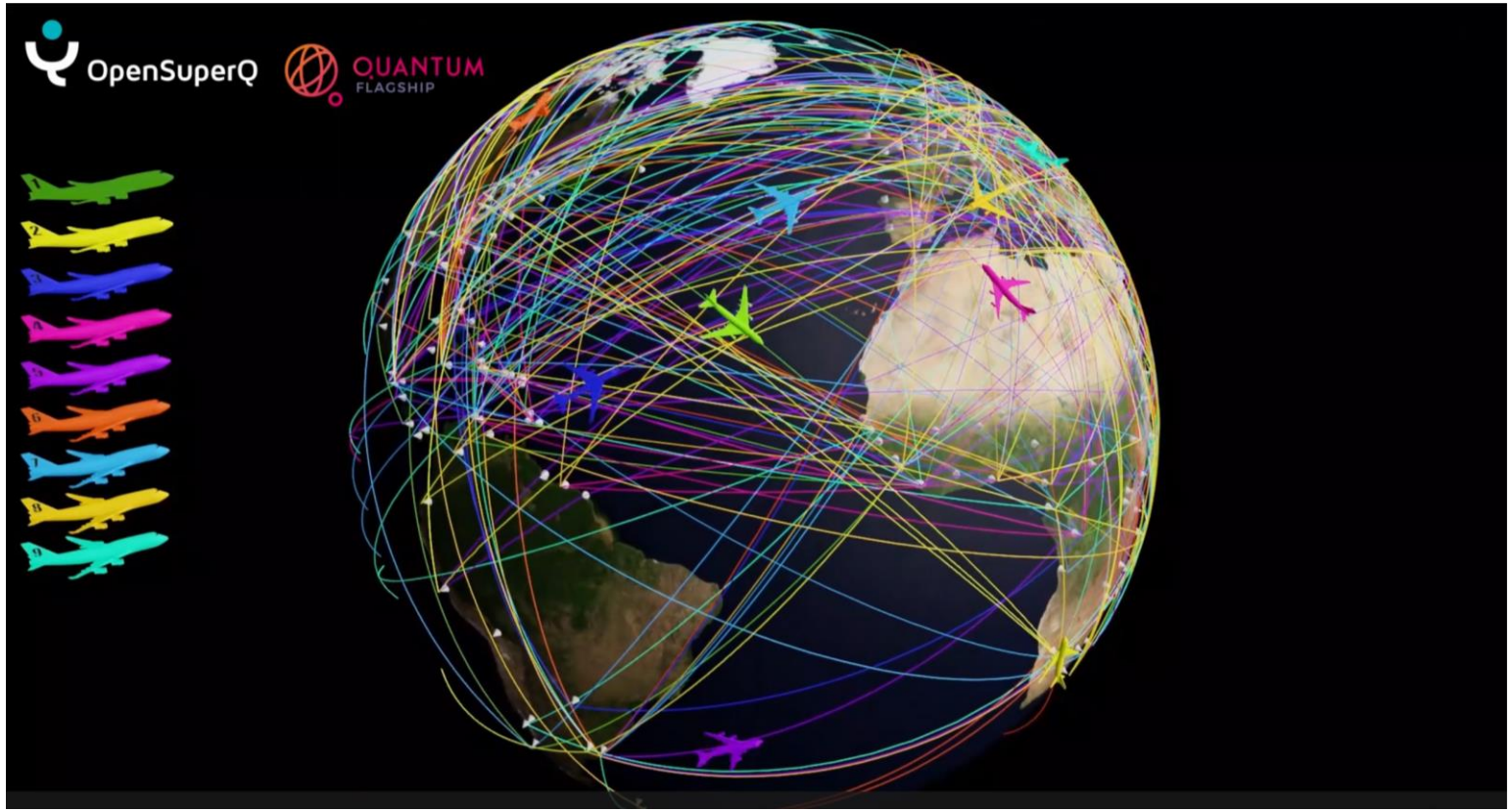
Dr. Fengping Jin

TAIL ASSIGNMENT PROBLEM

Application: Airline scheduling

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

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



In collaboration with:
Marika Svensson
Jeppesen and
Chalmers University of Technology

BOEING

OpenSuperQ QUANTUM FLAGSHIP

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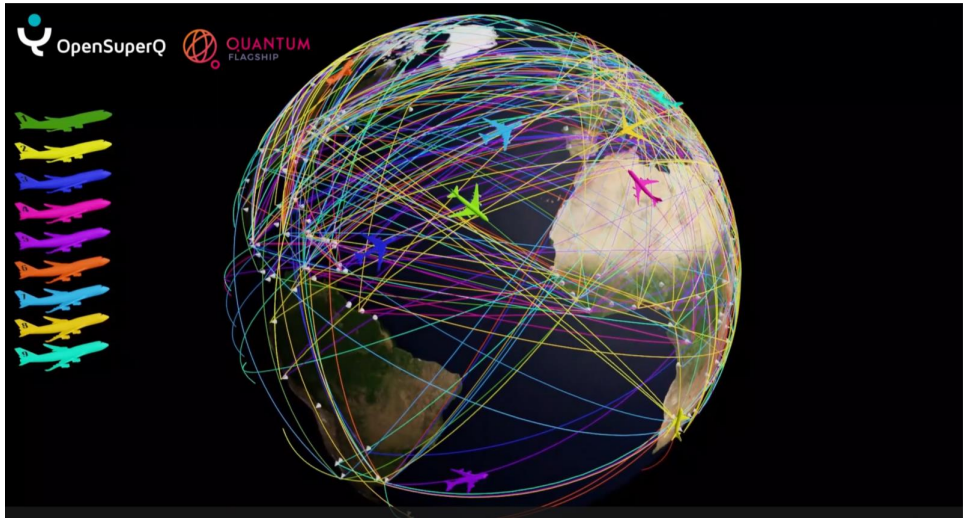
Problem specification

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

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TAIL ASSIGNMENT PROBLEM

Mathematical formulation

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- Linear assignment problem

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

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encodes cost of assigning airplanes to routes

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exact cover problem: each flight covered once

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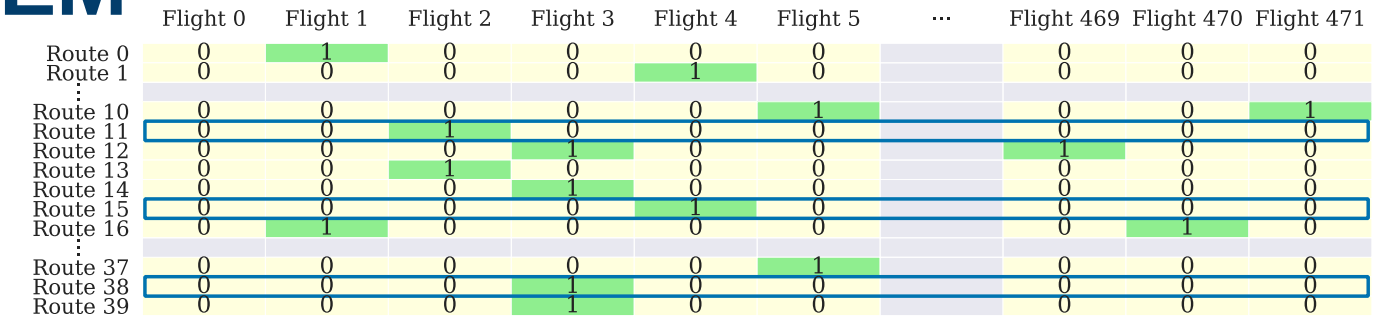

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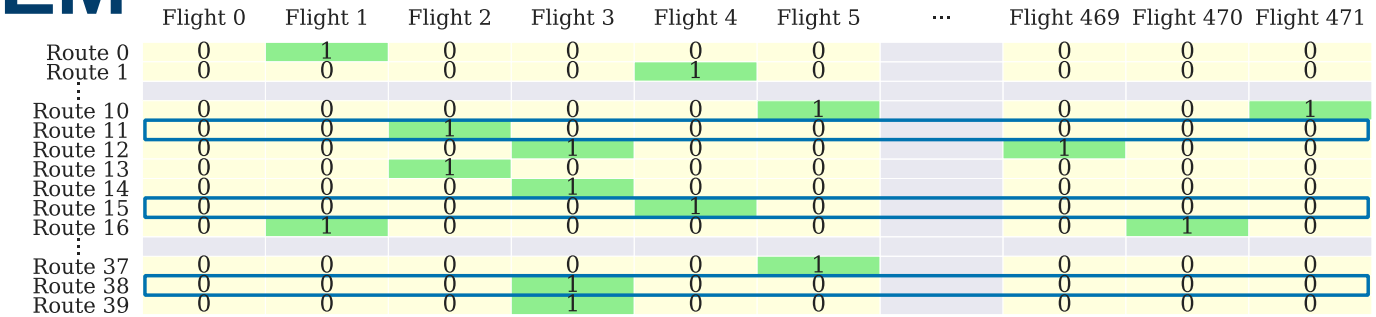

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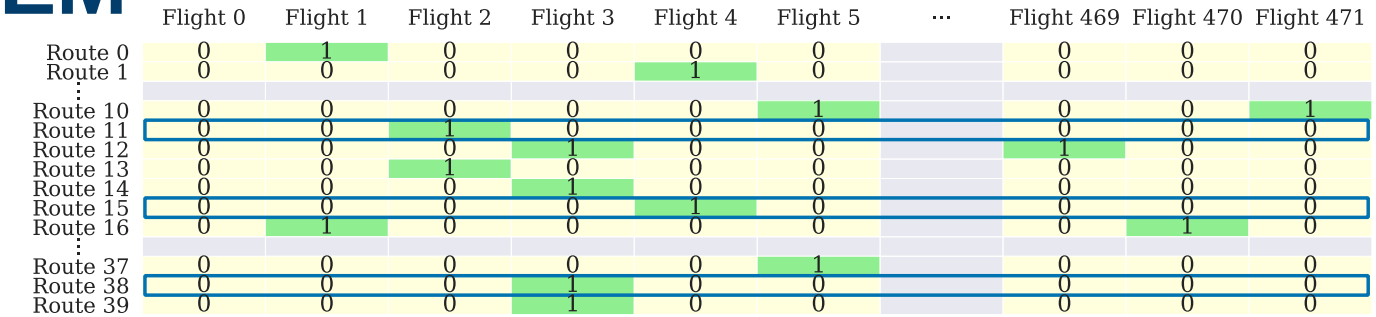

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$$\min_{x_i=0,1} \left(\left(A\vec{x} - \vec{b} \right)^2 + \lambda \vec{f}^T \vec{x} \right)$$

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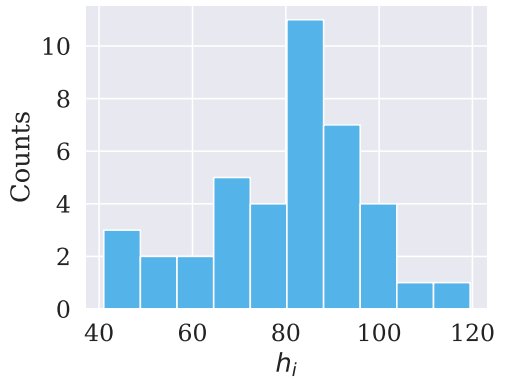
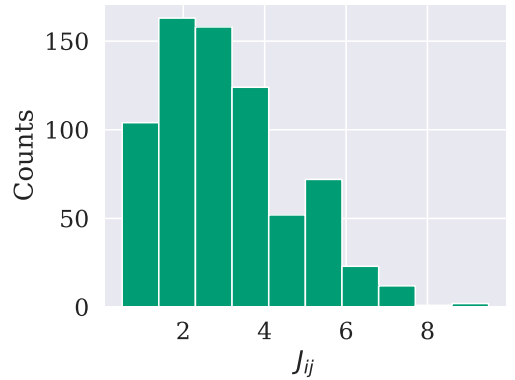
$$\text{QUBO} \leftrightarrow \text{Ising}: \quad x_i = (1 + s_i)/2$$

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





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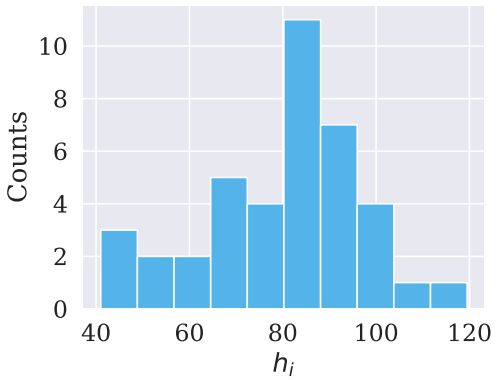
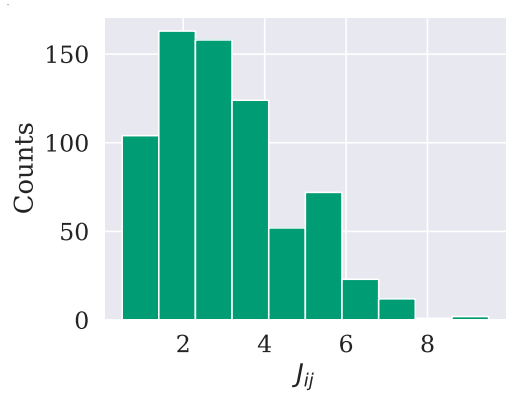
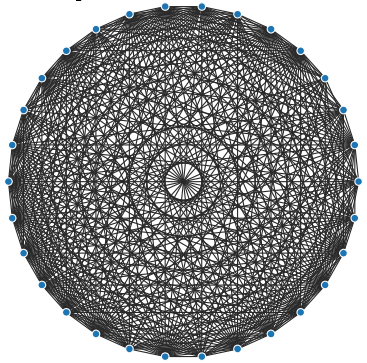




- 25 - 40 qubit almost fully-connected (“clique”) Ising problems



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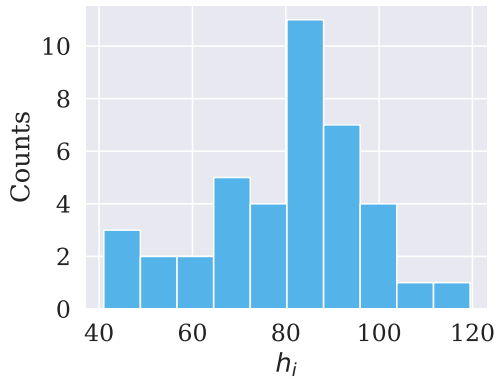

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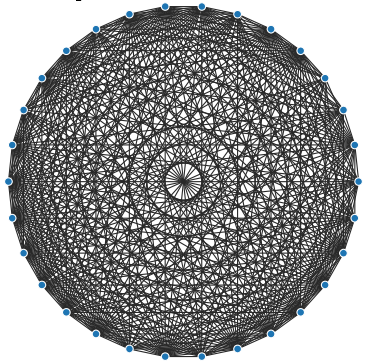
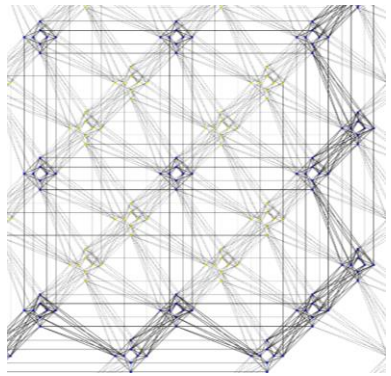
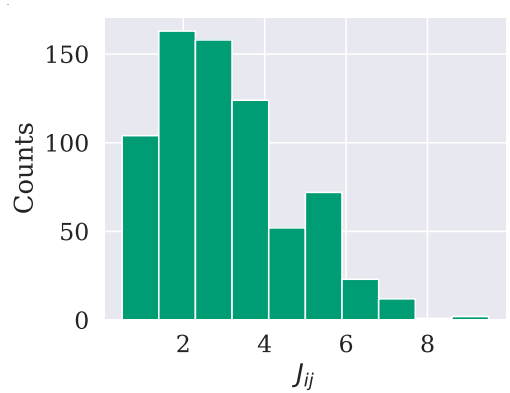


embedding needed





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TAIL ASSIGNMENT: RESULTS

30 - 40 qubit problems (90% nonzero couplers)

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Scan of 10 different embeddings and 20 relative chain strengths:

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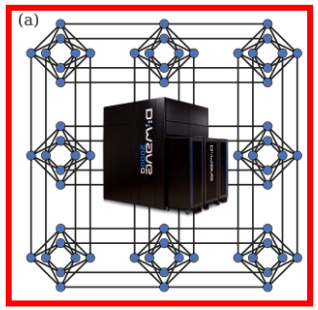
DW2000Q **Advantage**



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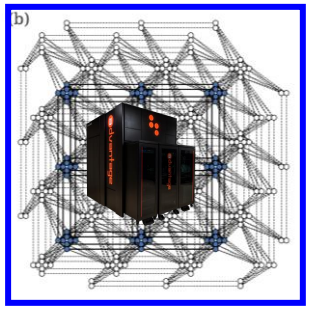

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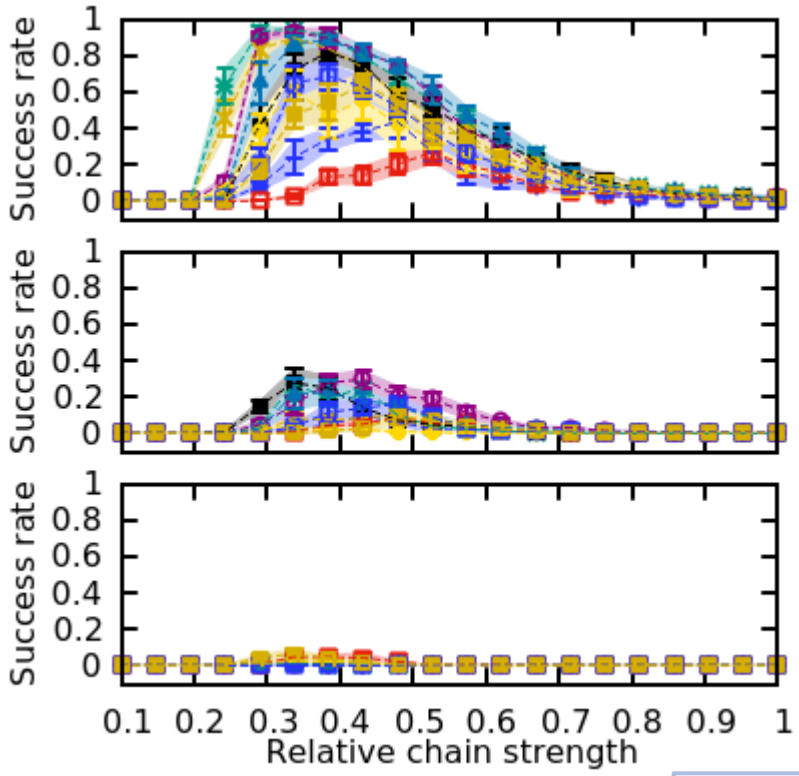
DW2000Q **Advantage**

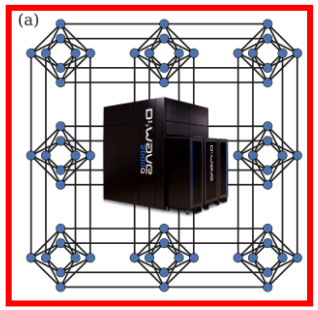
30 qubits

36 qubits

40 qubits



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



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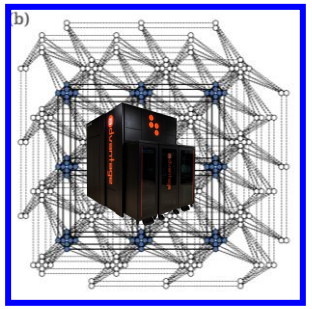

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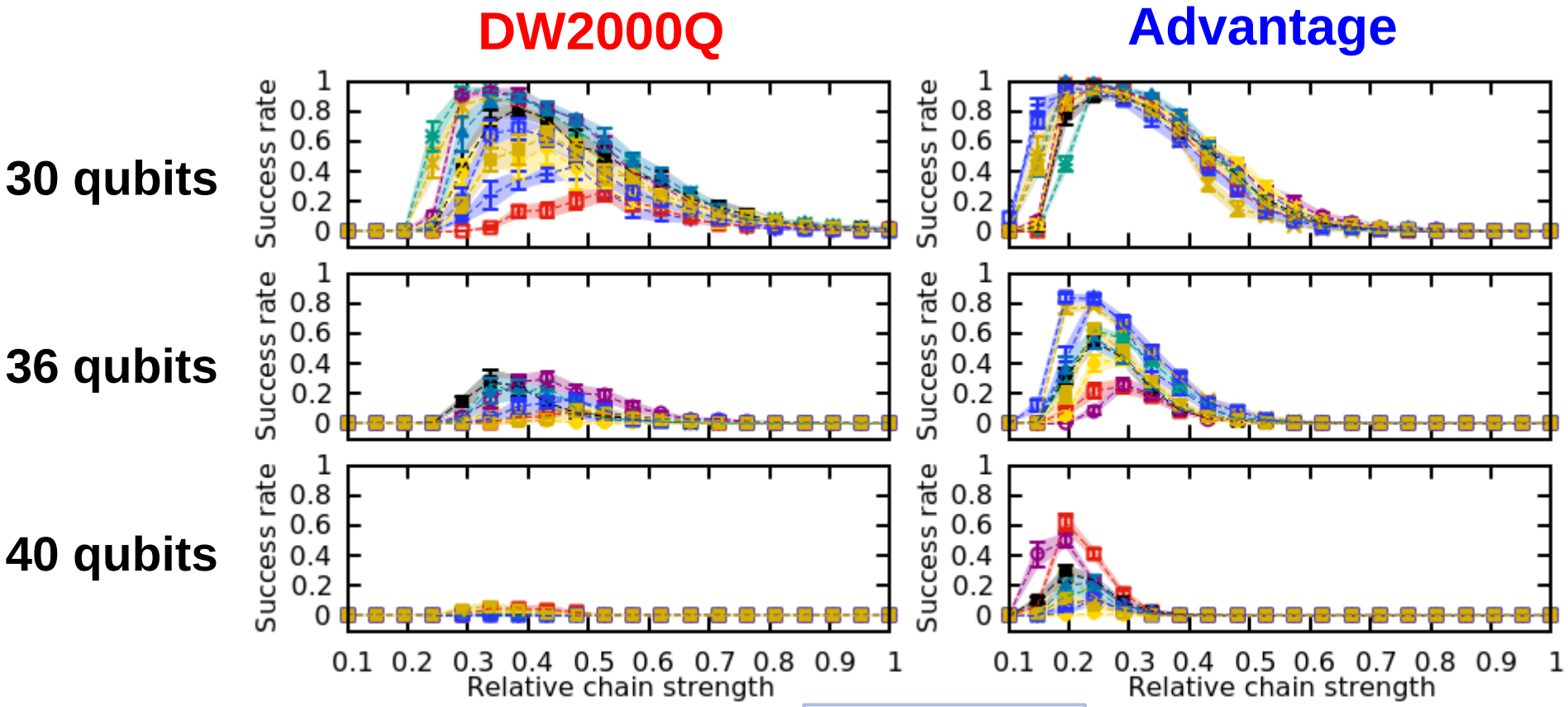

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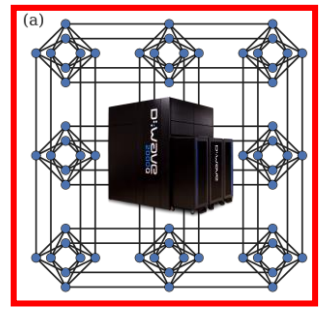

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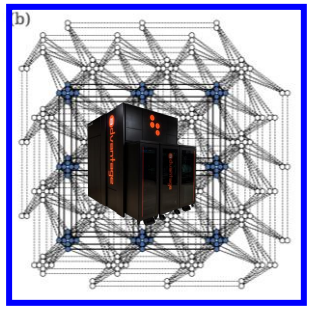

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TAIL ASSIGNMENT: RESULTS

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

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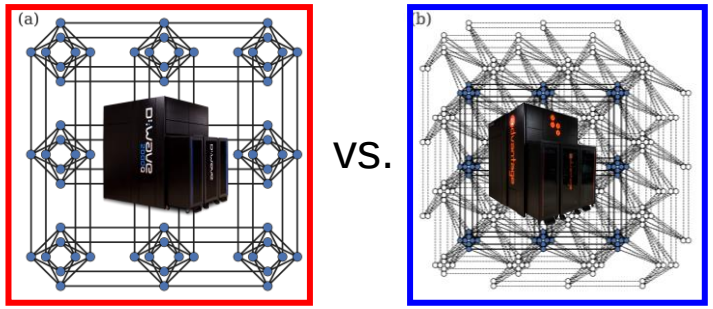
The fastest successful runs that reproducibly gave a solution:



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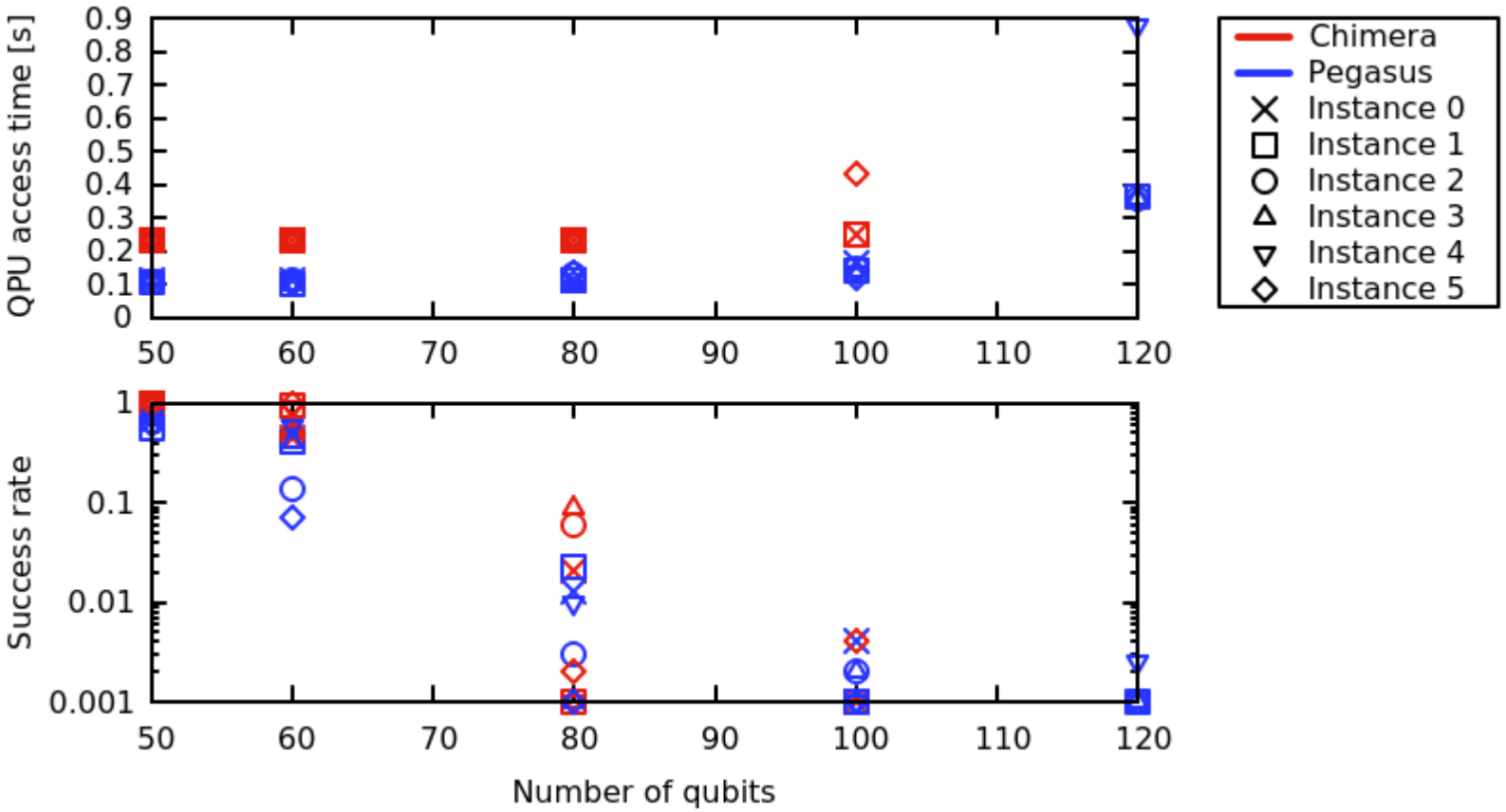

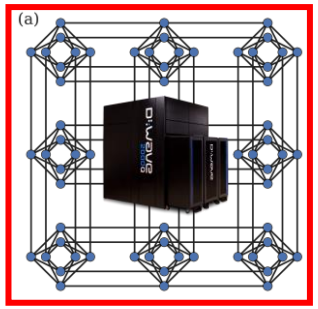

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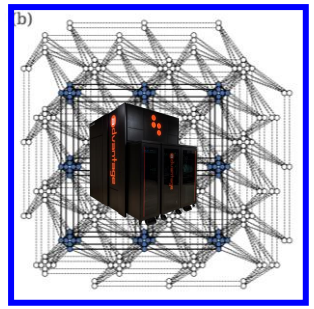

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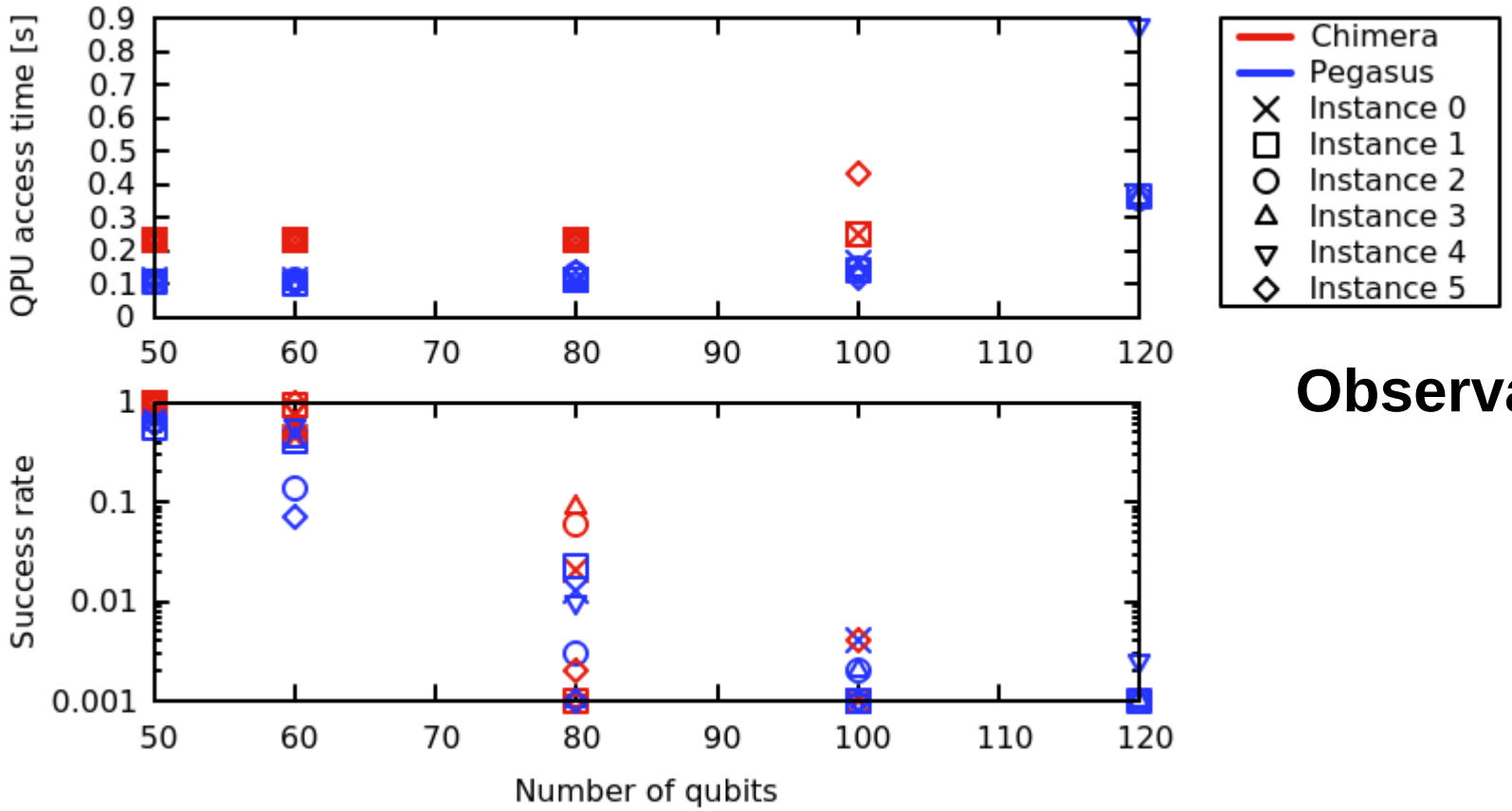

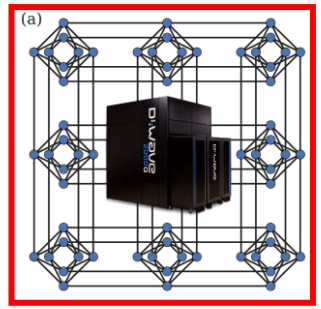

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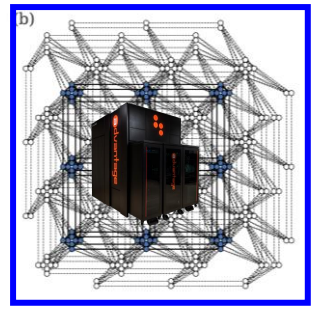

Observations:

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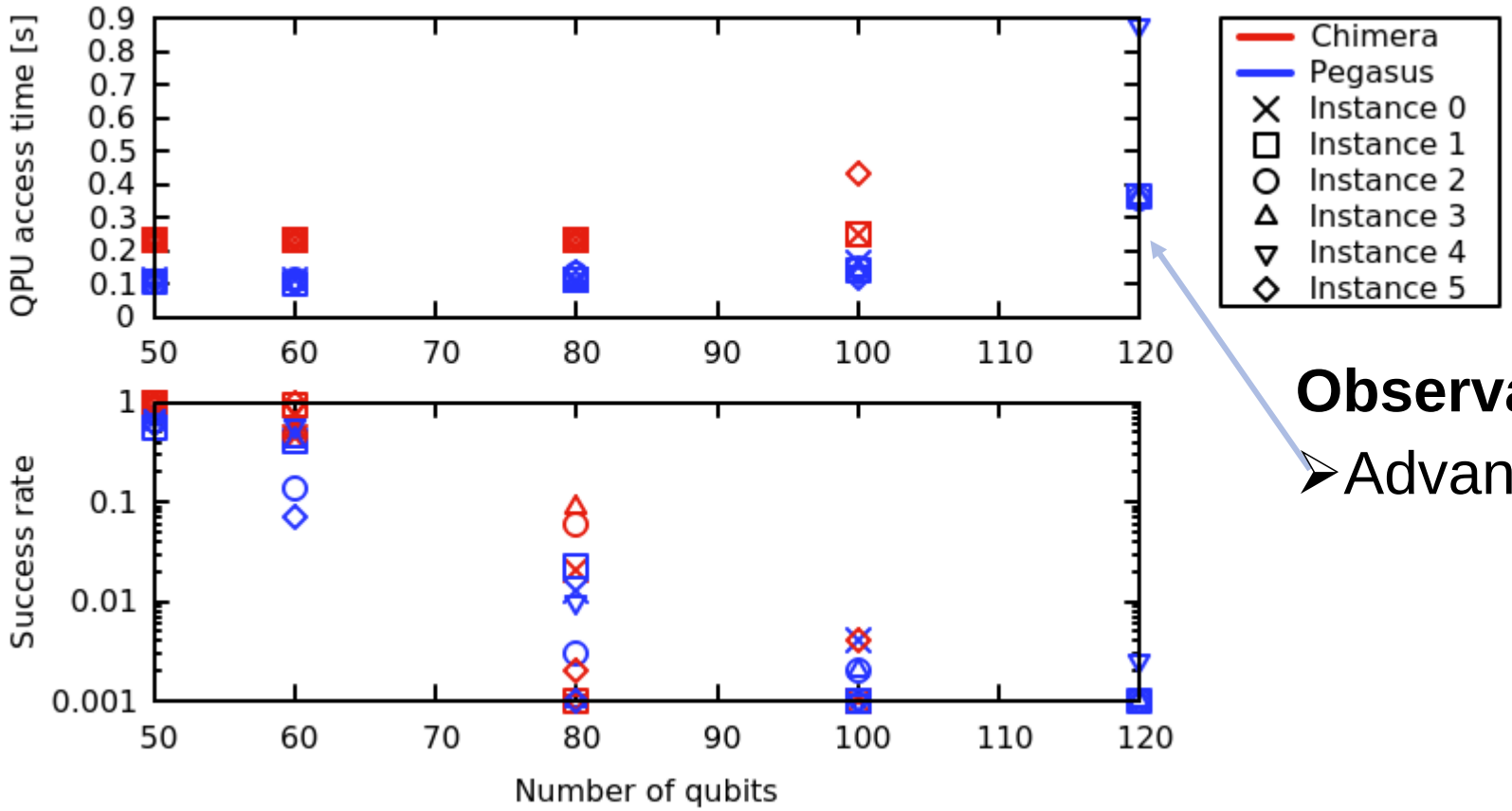

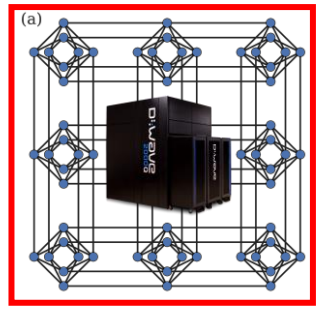

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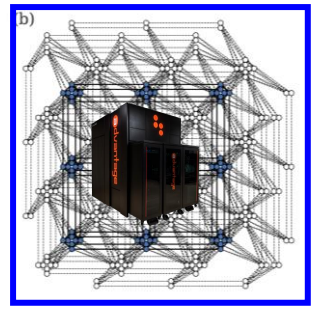

Observations:

- Advantage solves larger problems

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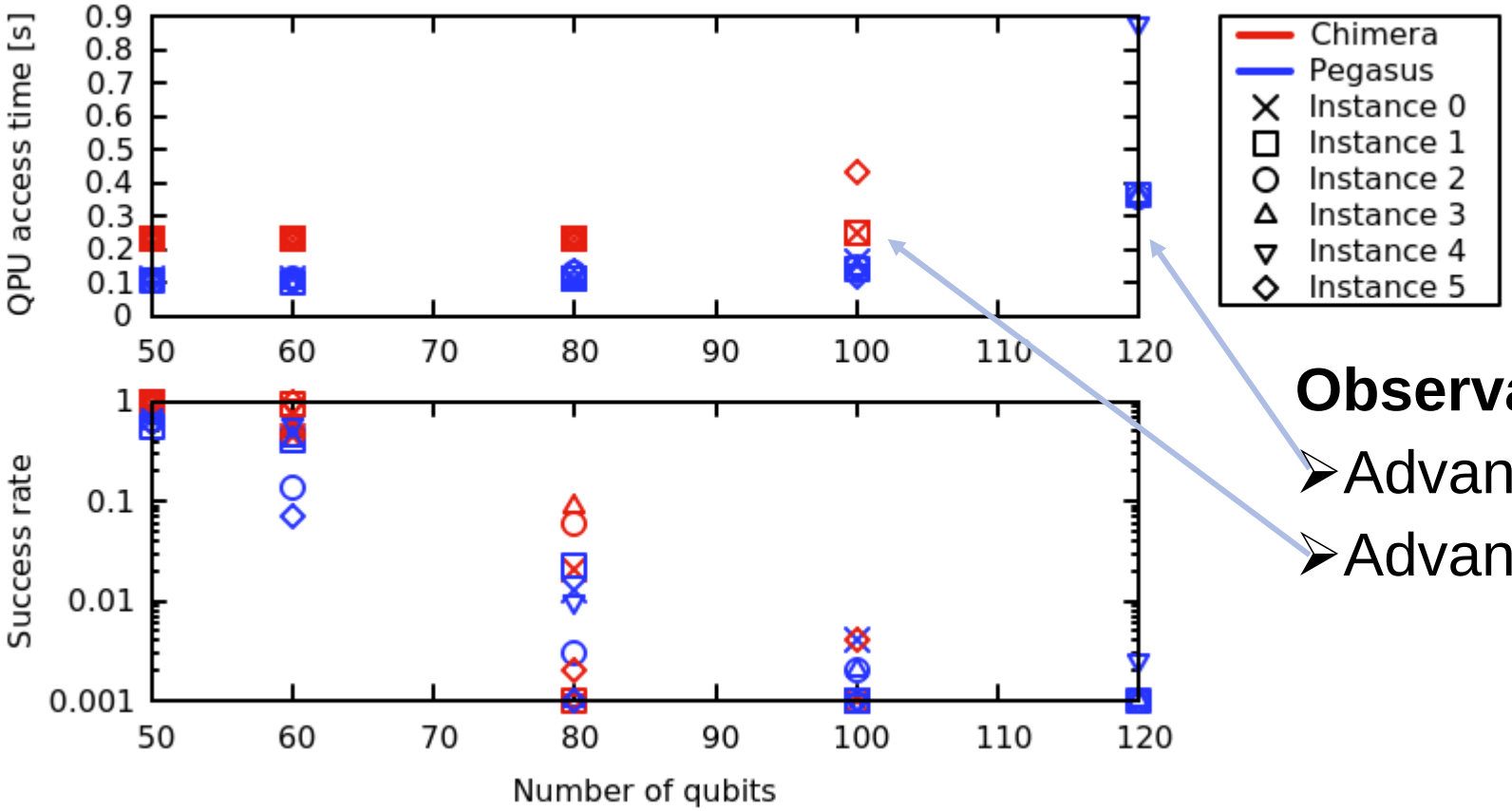

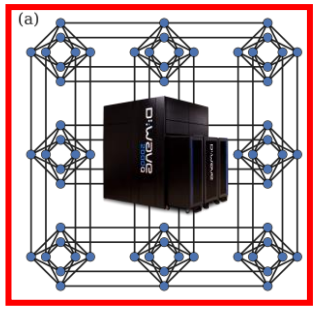

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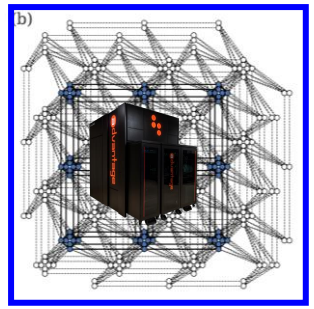

Observations:

- Advantage solves larger problems
- Advantage solves problems faster

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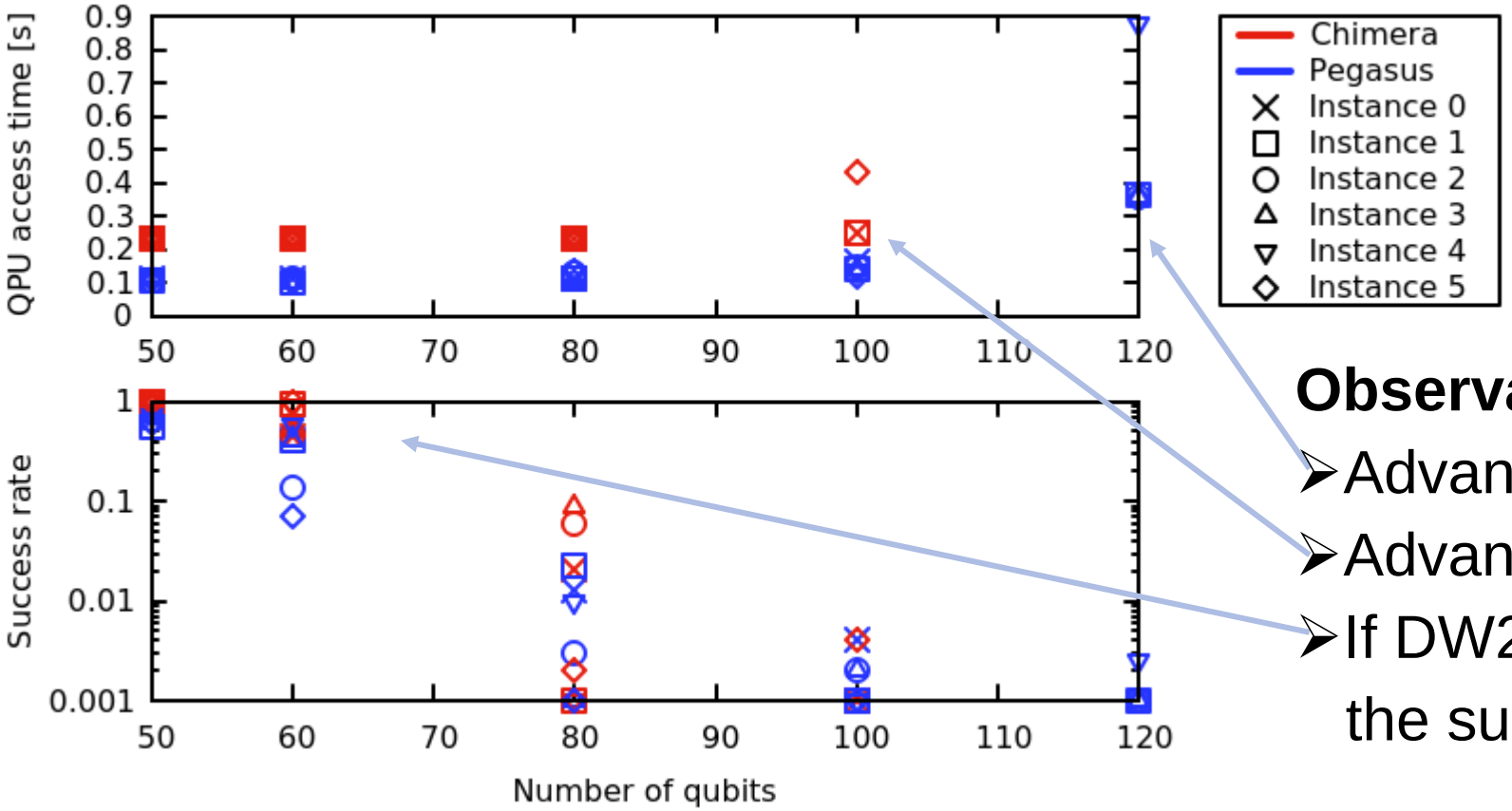

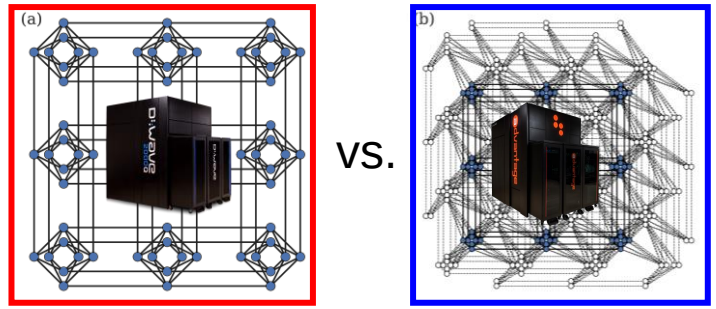

vs.

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)
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TRAVELING SALESMAN PROBLEM

QUBO formulation

Nemes et al. (2022)
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$$\min_{x_k=0,1} \vec{x}^T Q \vec{x}$$

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- Assign cities & times to qubits:
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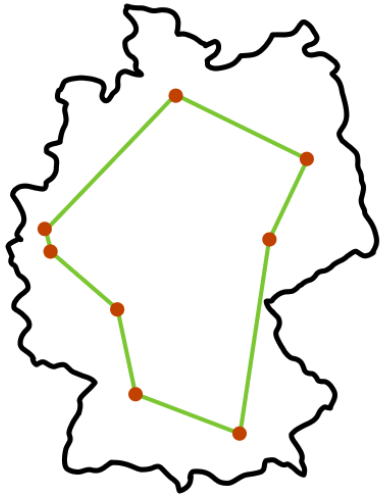

$$\min_{x_k=0,1} \vec{x}^T Q \vec{x}$$

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

- 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

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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

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

time steps

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time steps

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- 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

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  - 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 $(n-1)^2$

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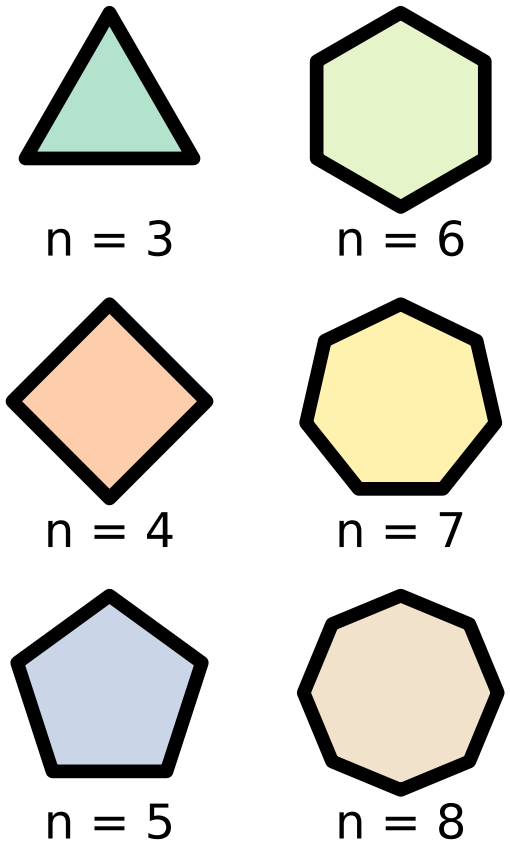
TRAVELING SALESMAN PROBLEM

Scaling of chain strength and annealing time



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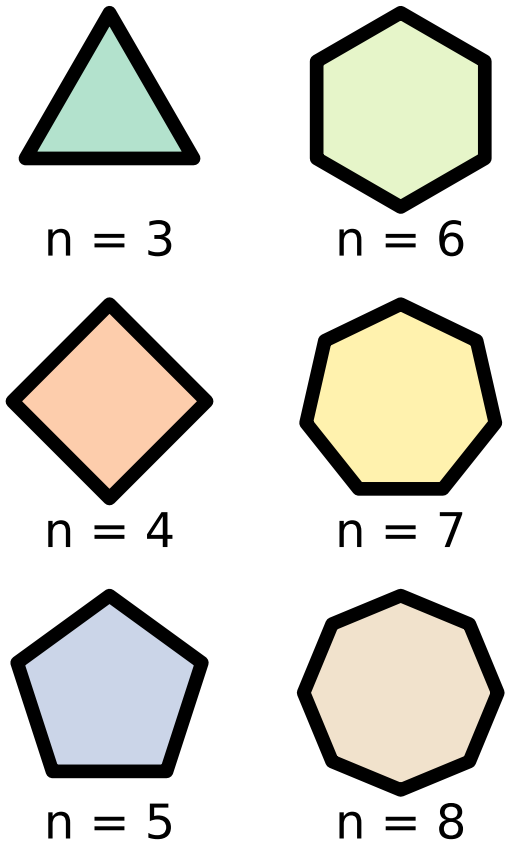

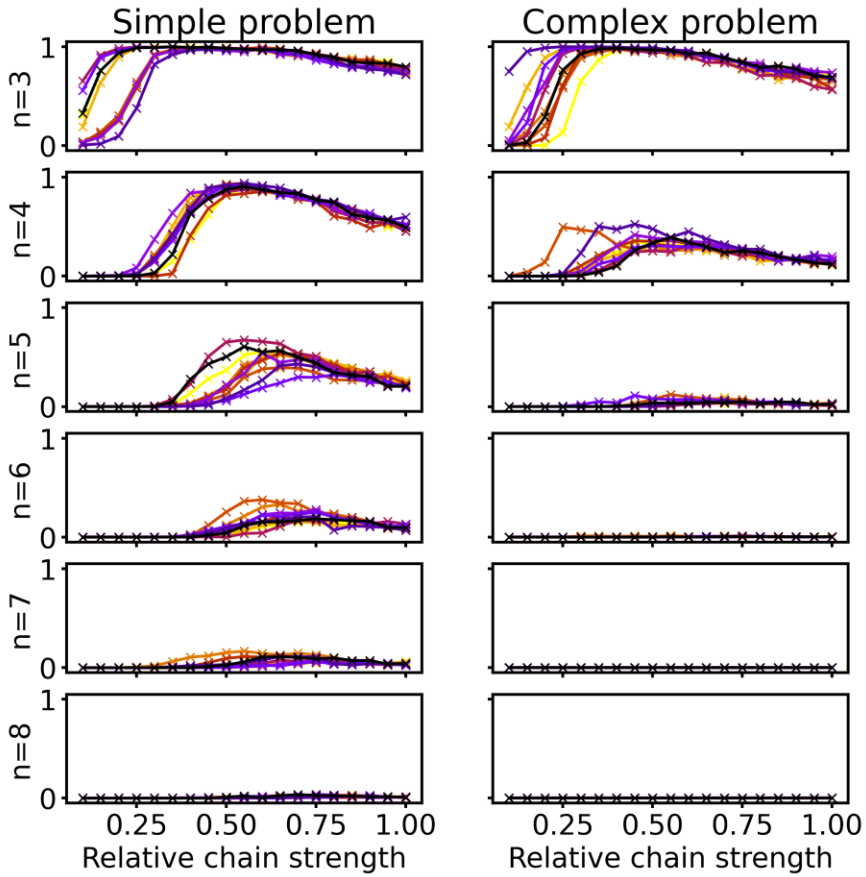

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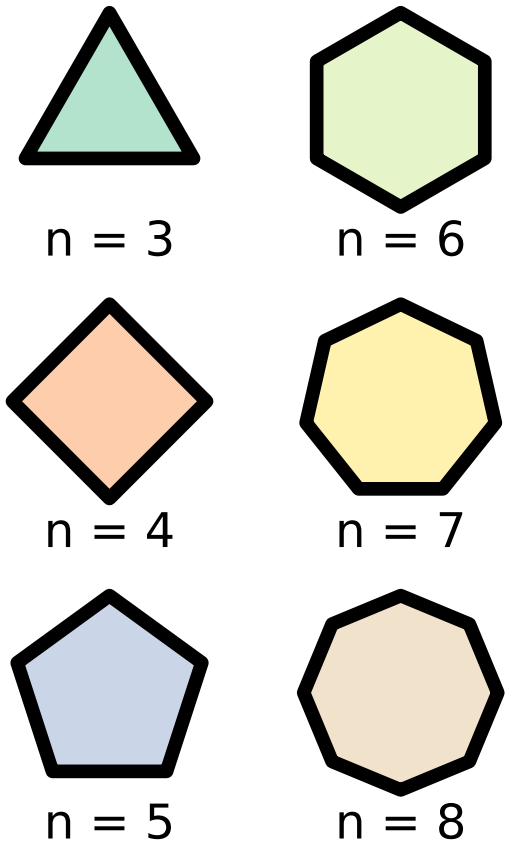

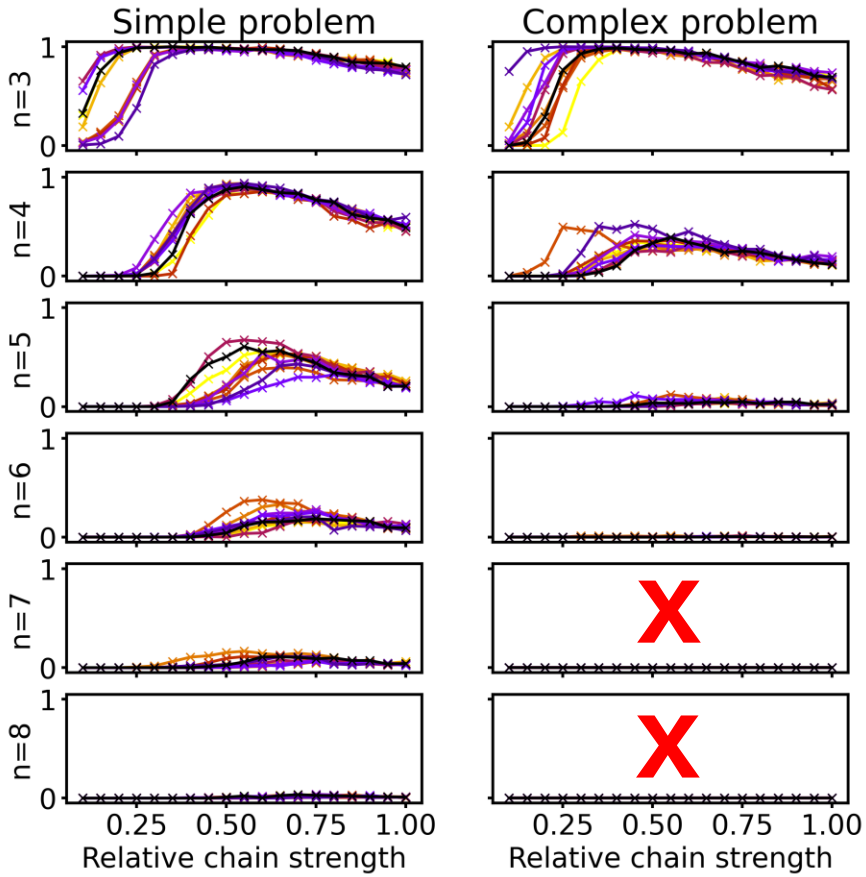

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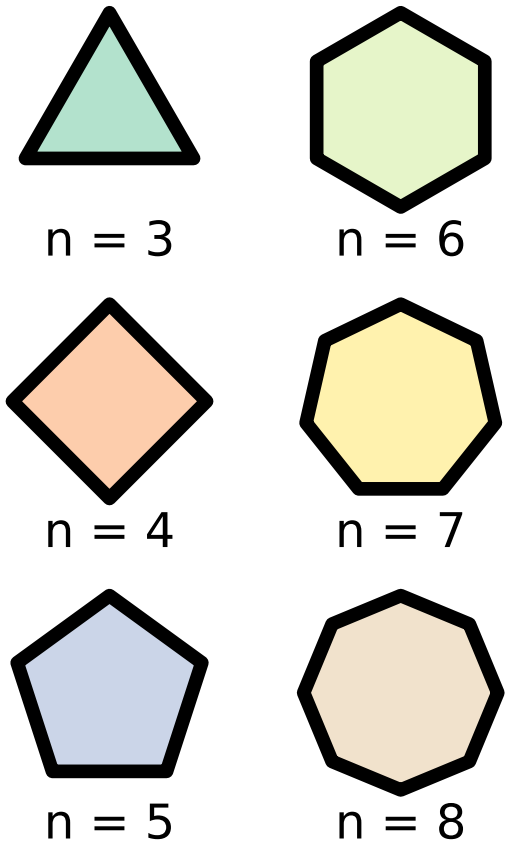

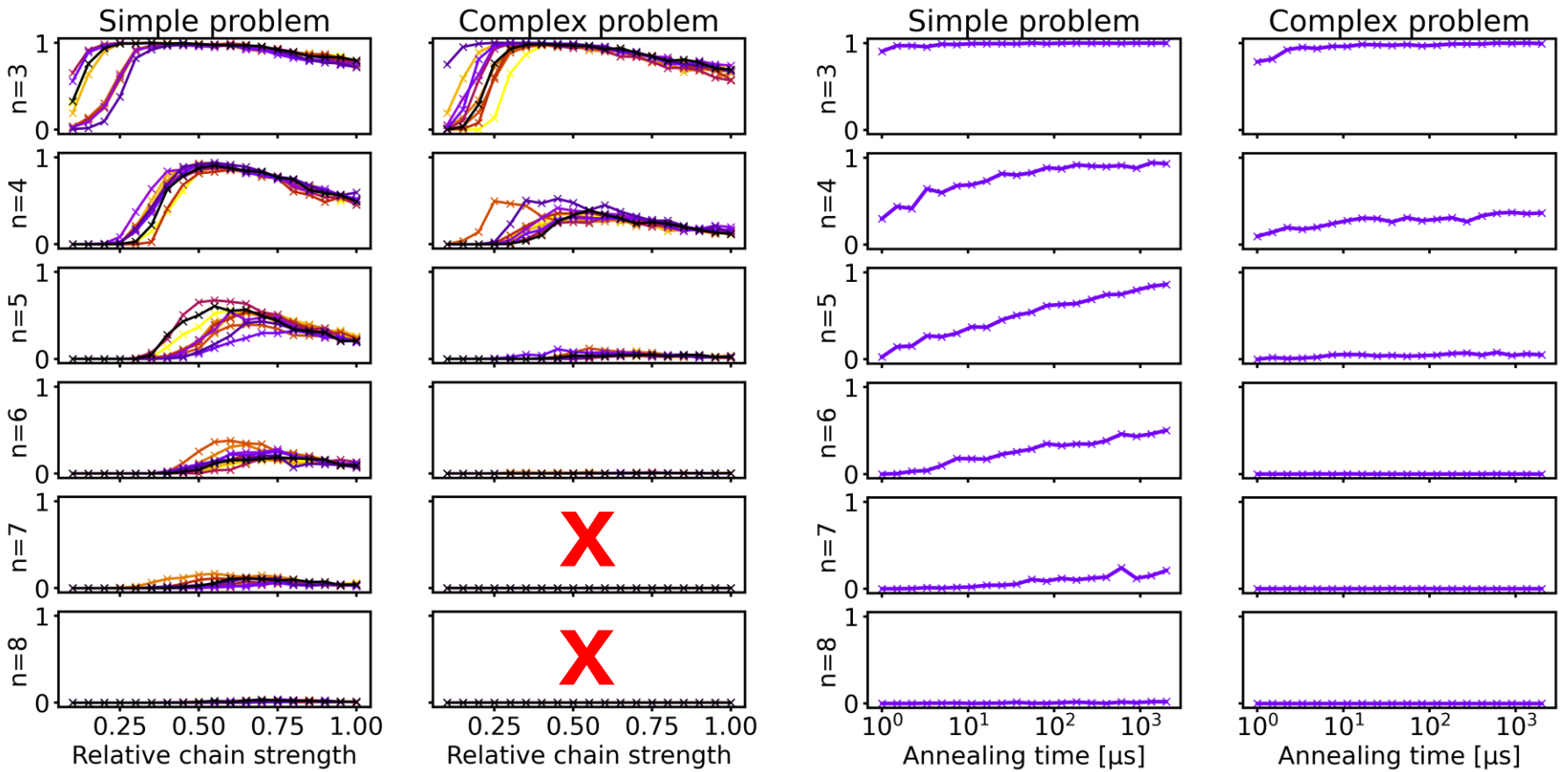

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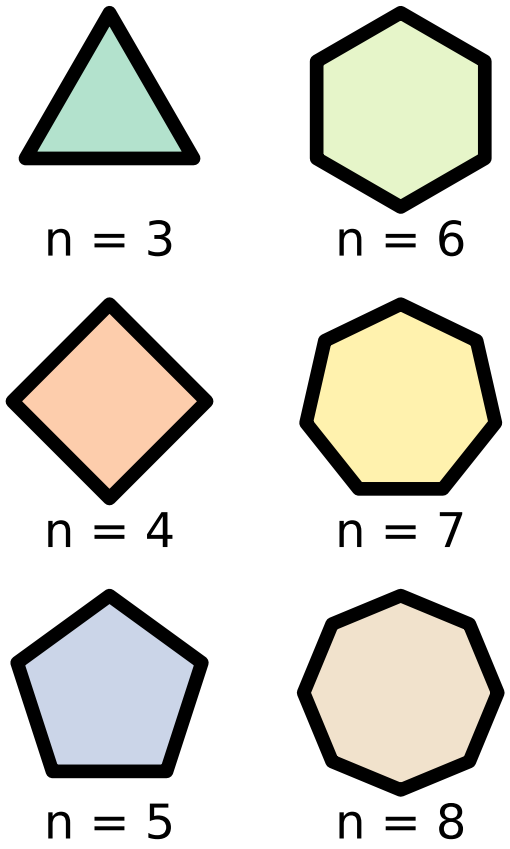

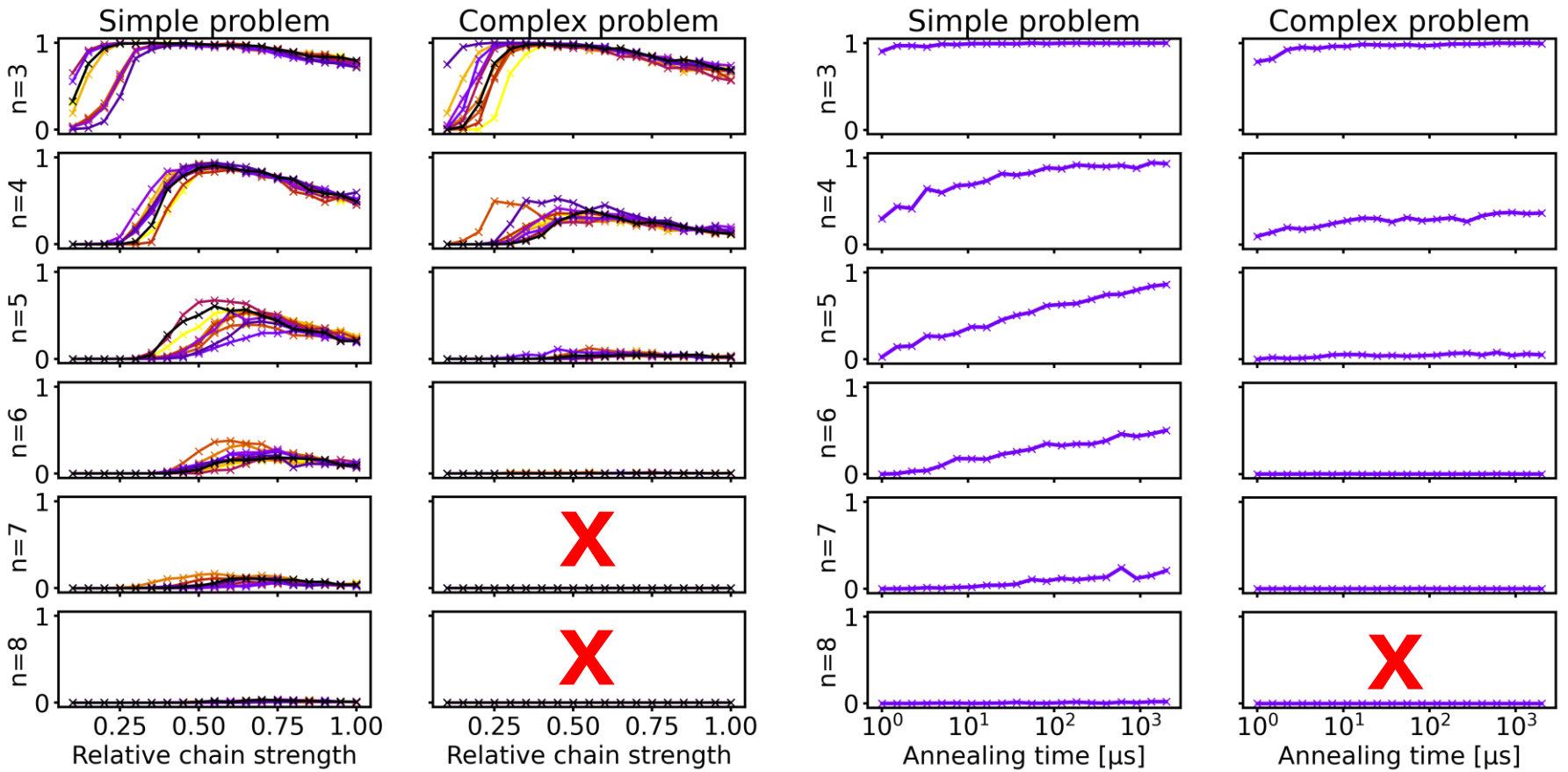

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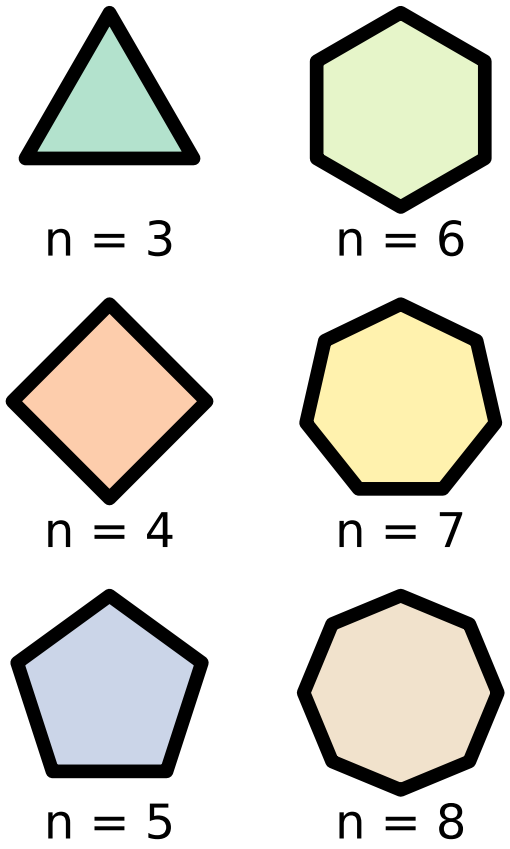

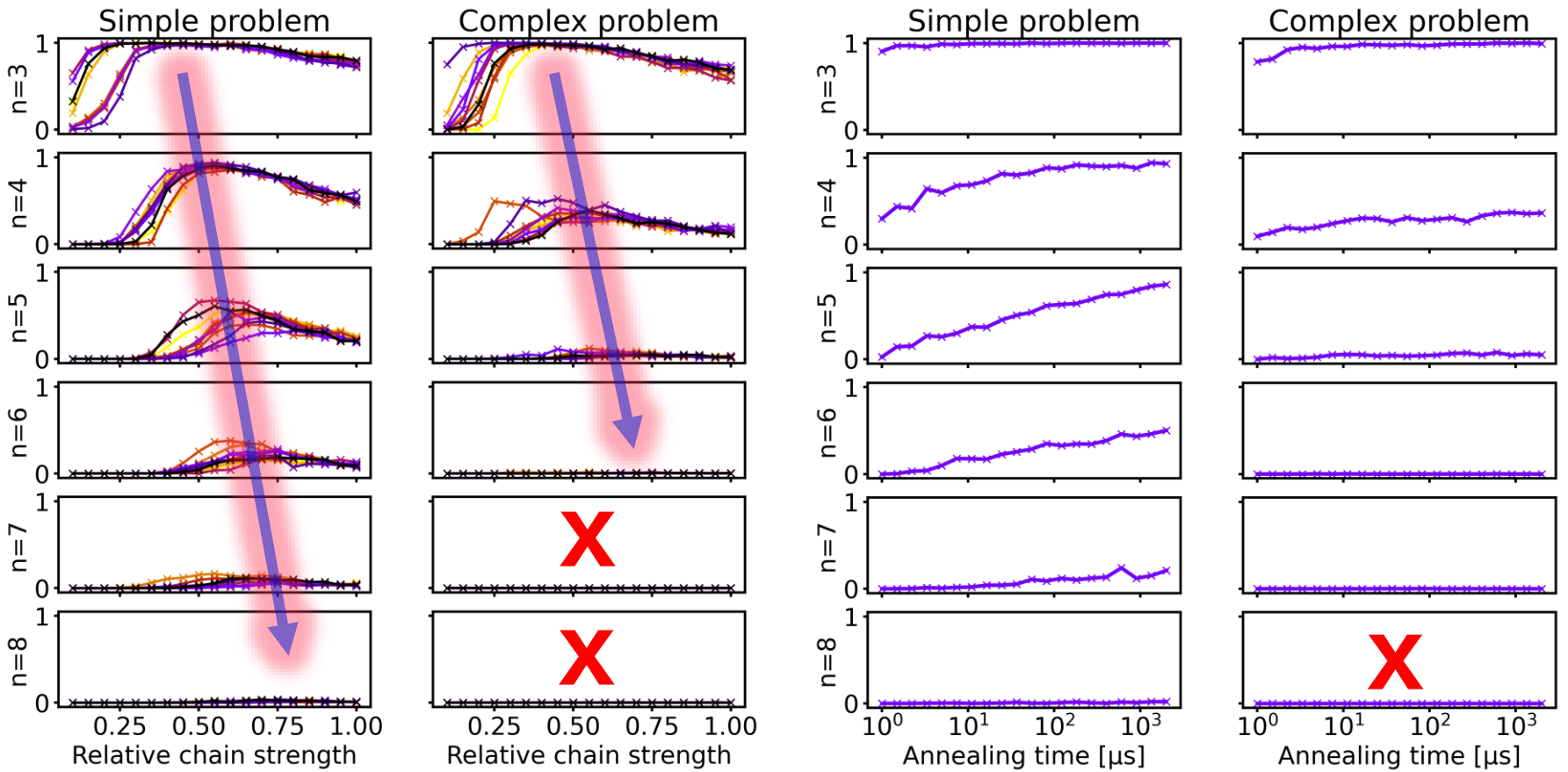

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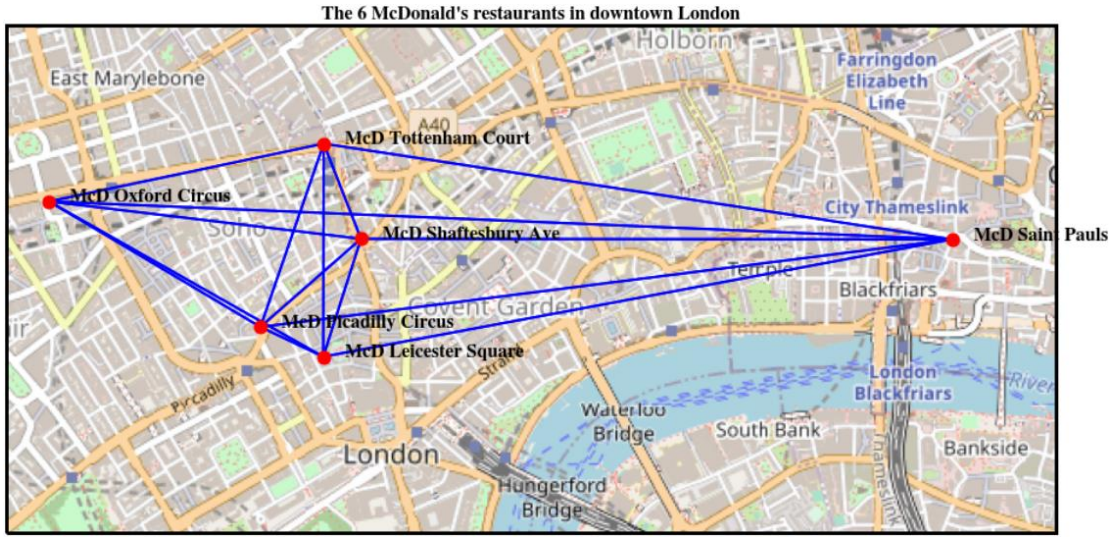
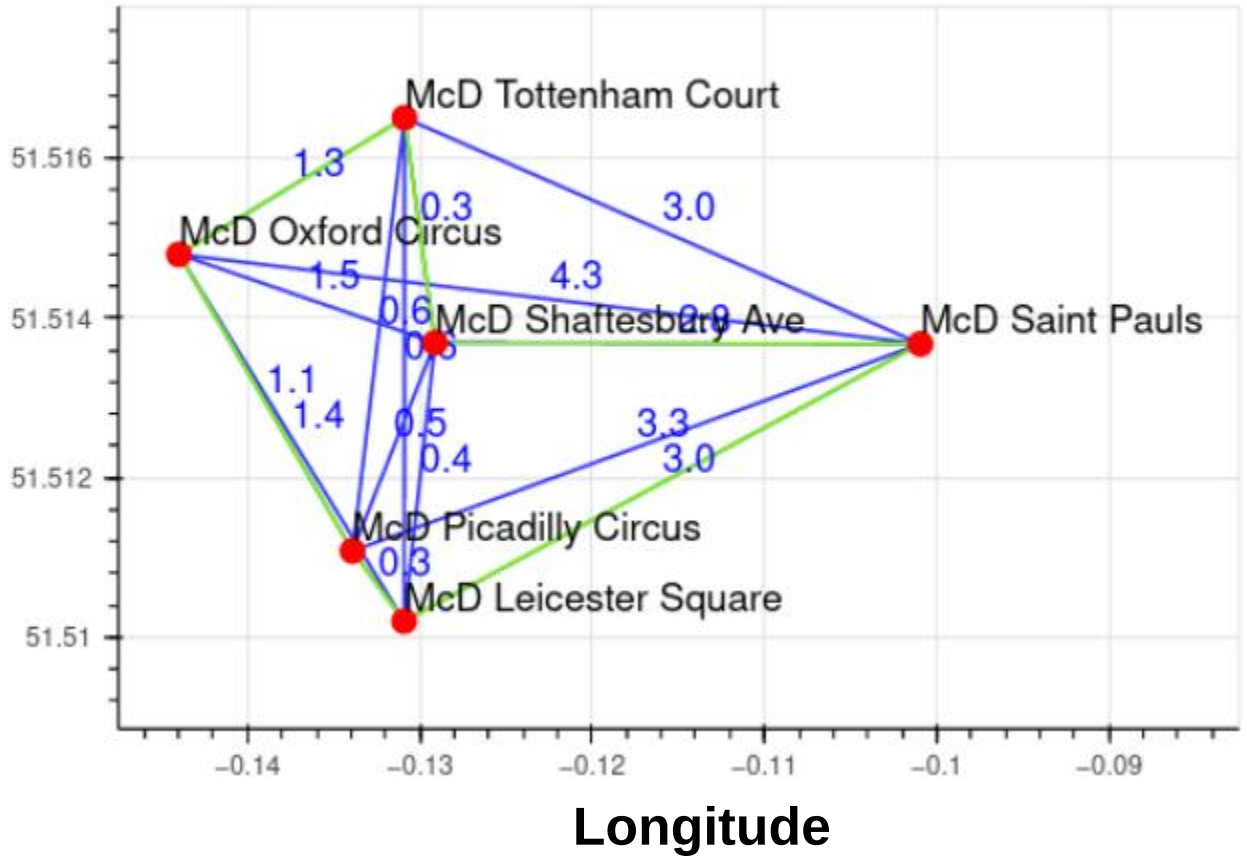
TRAVELING SALESMAN PROBLEM

The 6 McDonald's restaurants in downtown London





VEGETABLE GARDEN OPTIMIZATION

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

Overview

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Overview

- Problem: Companion planting in polyculture vegetable gardens

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Overview

➢Problem: Companion planting in polyculture vegetable gardens

	Tomato	Cucumber	Lettuce
Tomato		☹	☺
Cucumber	☹		☺
Lettuce	☺	☺	

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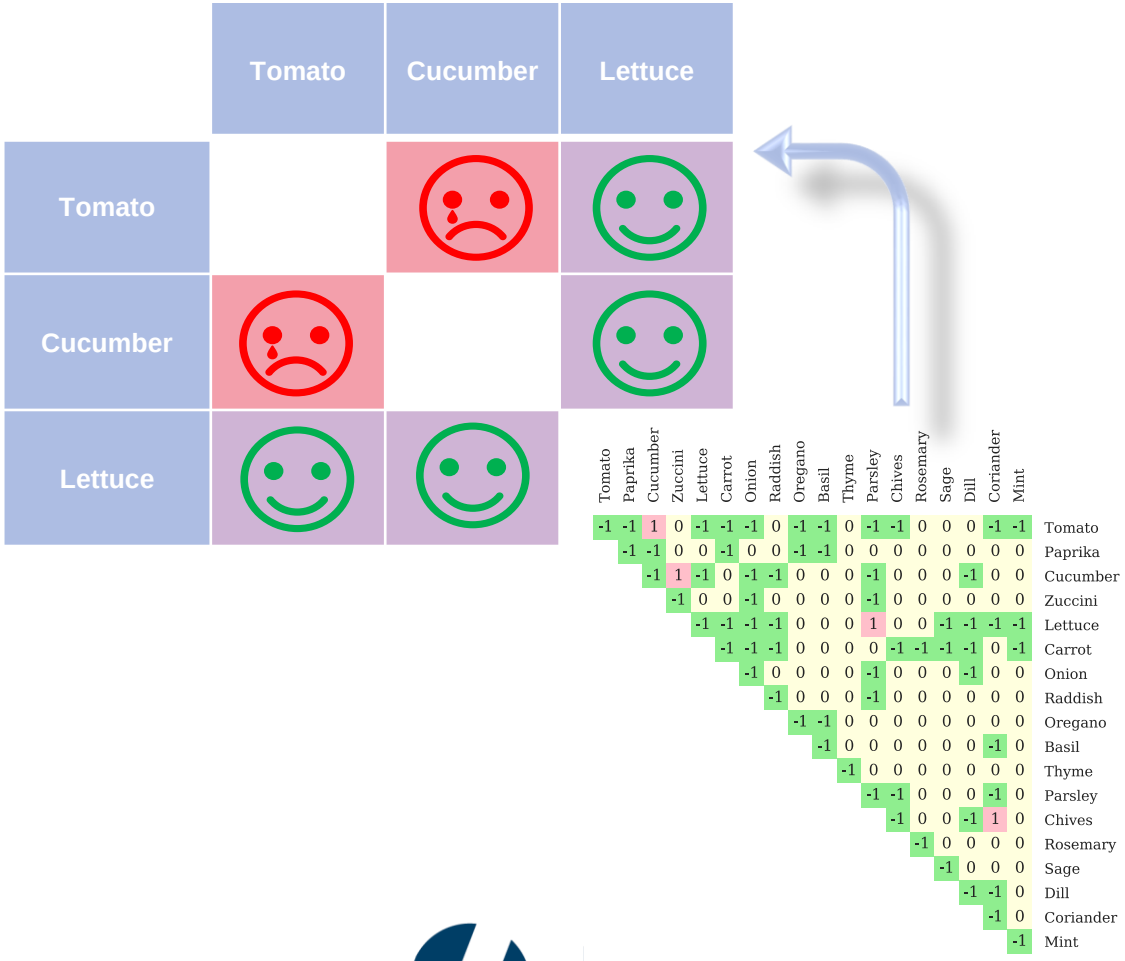

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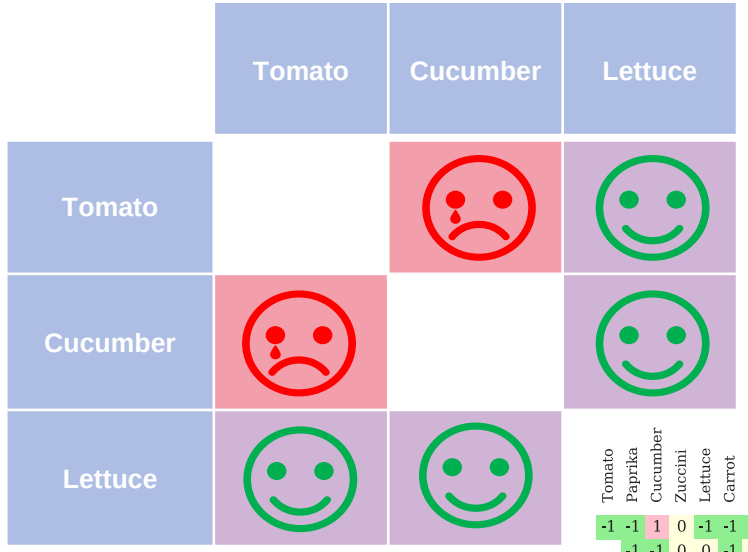

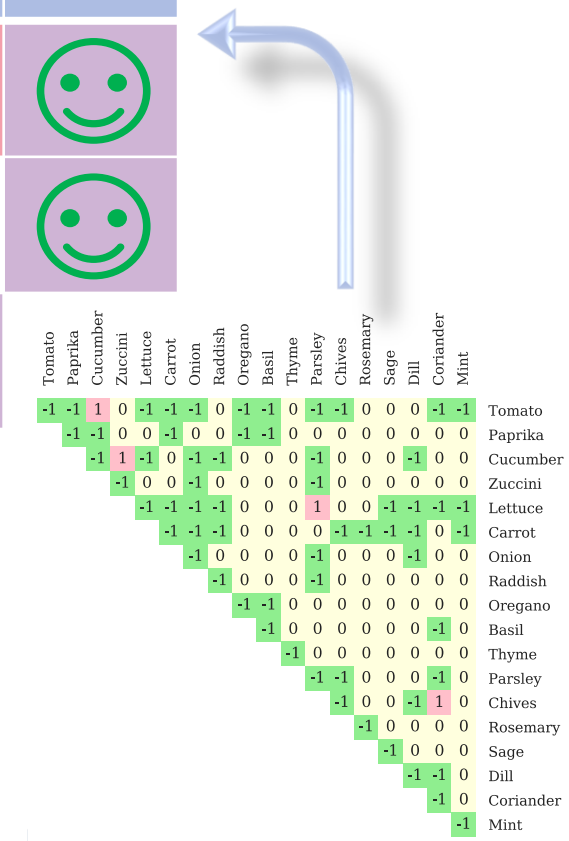

- Task: Find an optimal placement of plants in the garden considering the characteristics of their nearest neighbours

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- Assign plants to pots in the garden:
  - Qubit $x_{ij} = 1$ means species j is placed in pot i

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- 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

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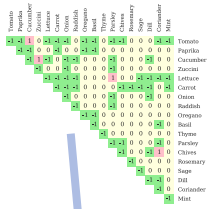

- Assign plants to pots in the garden:
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  - All plants should have a good relationship with their neighbors

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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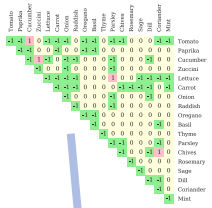

- Assign plants to pots in the garden:
  - Qubit $x_{ij} = 1$ means species j is placed in pot i
  - All plants should have a good relationship with their neighbors
  - Use all available plants and pots

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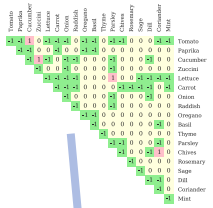

- Assign plants to pots in the garden:
  - Qubit $x_{ij} = 1$ means species j is placed in pot i
  - All plants should have a good relationship with their neighbors
  - Use all available plants and pots
  - Big plants should not shadow small ones

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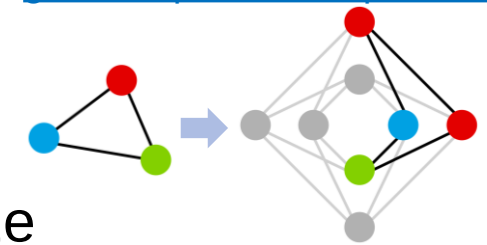
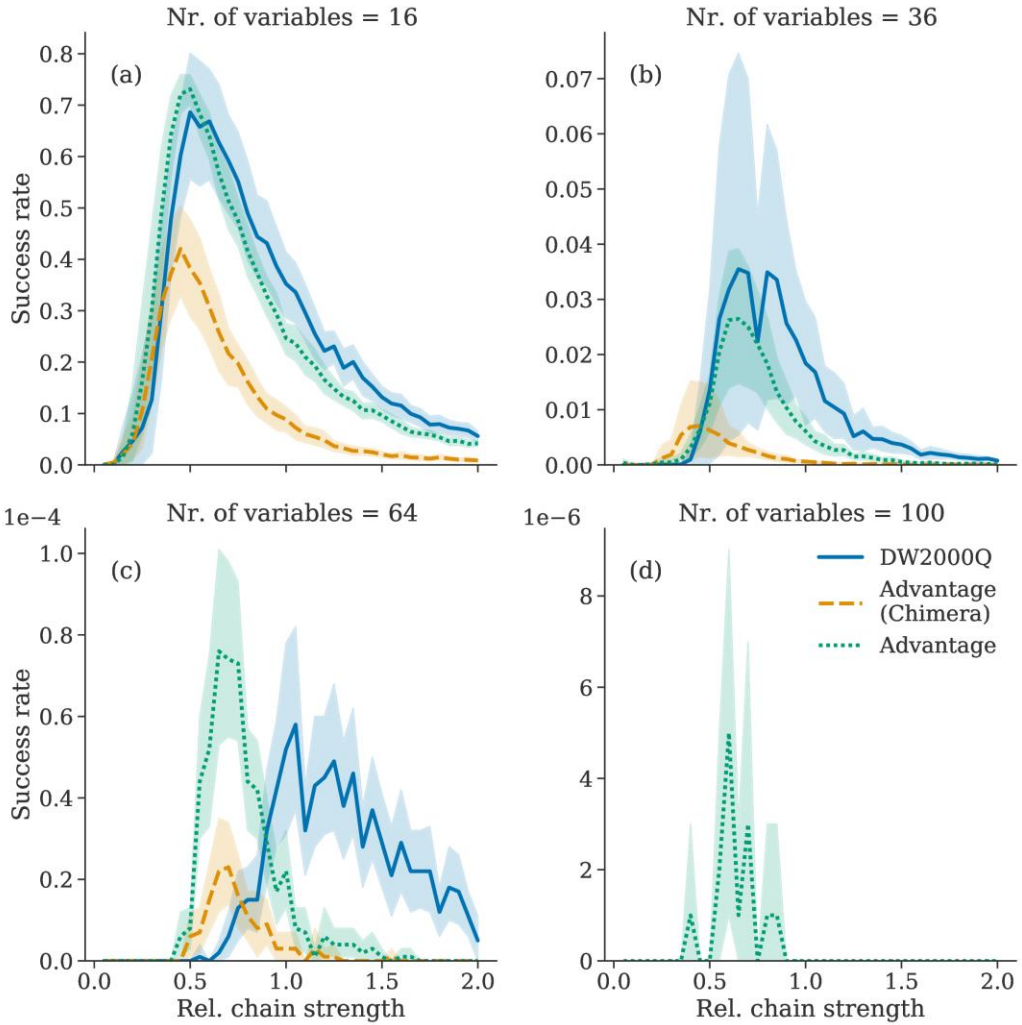


Finding the optimal chain strength: Results



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|)

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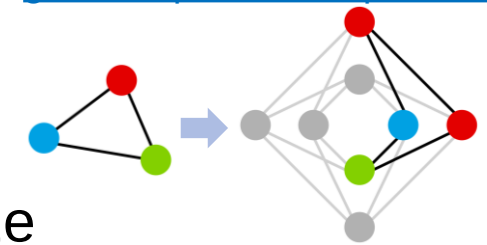
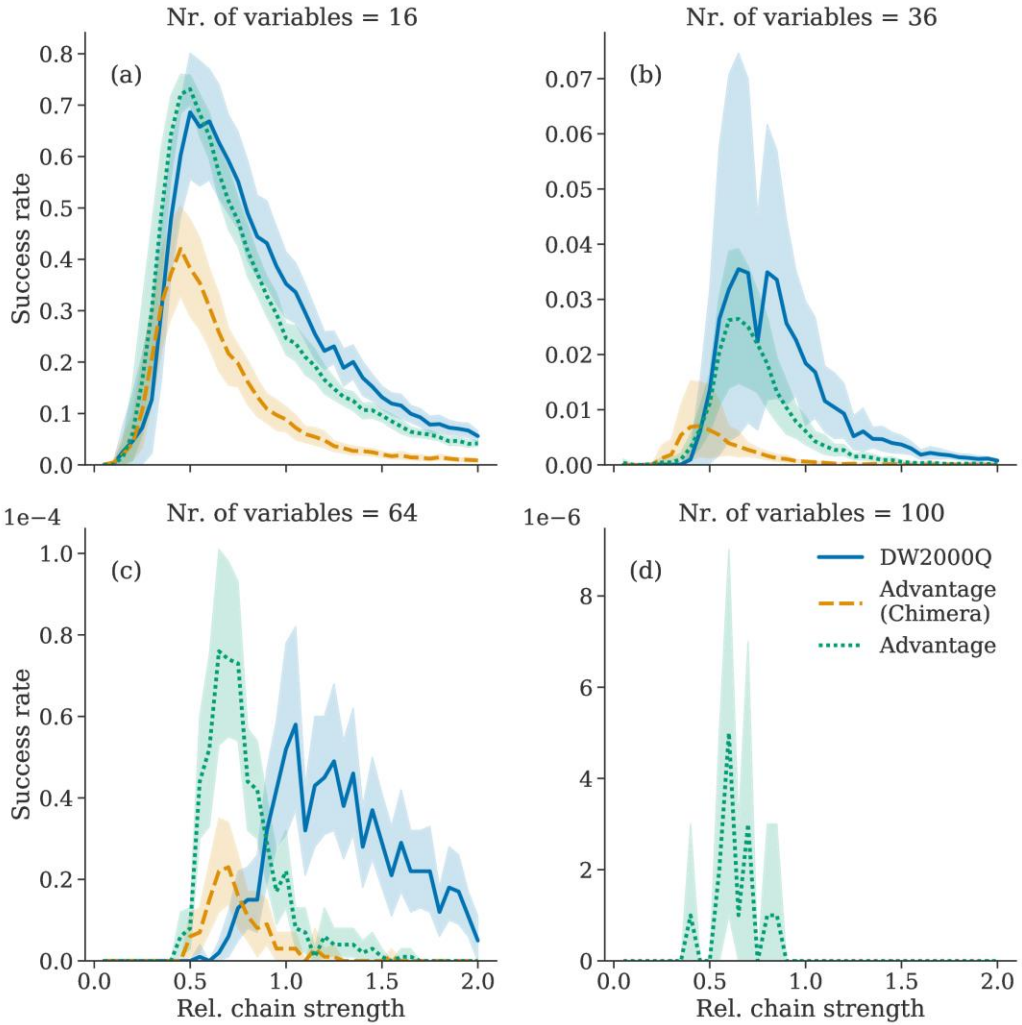
QINP **20**, 305
arXiv:2101.10827
https://jugit.fz-juelich.de/qip/garden-optimization-problem



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

VEGETABLE GARDEN OPTIMIZATION

Gonzalez Calaza et al. (2021)
QINP **20**, 305
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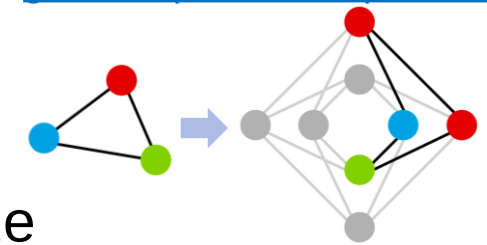

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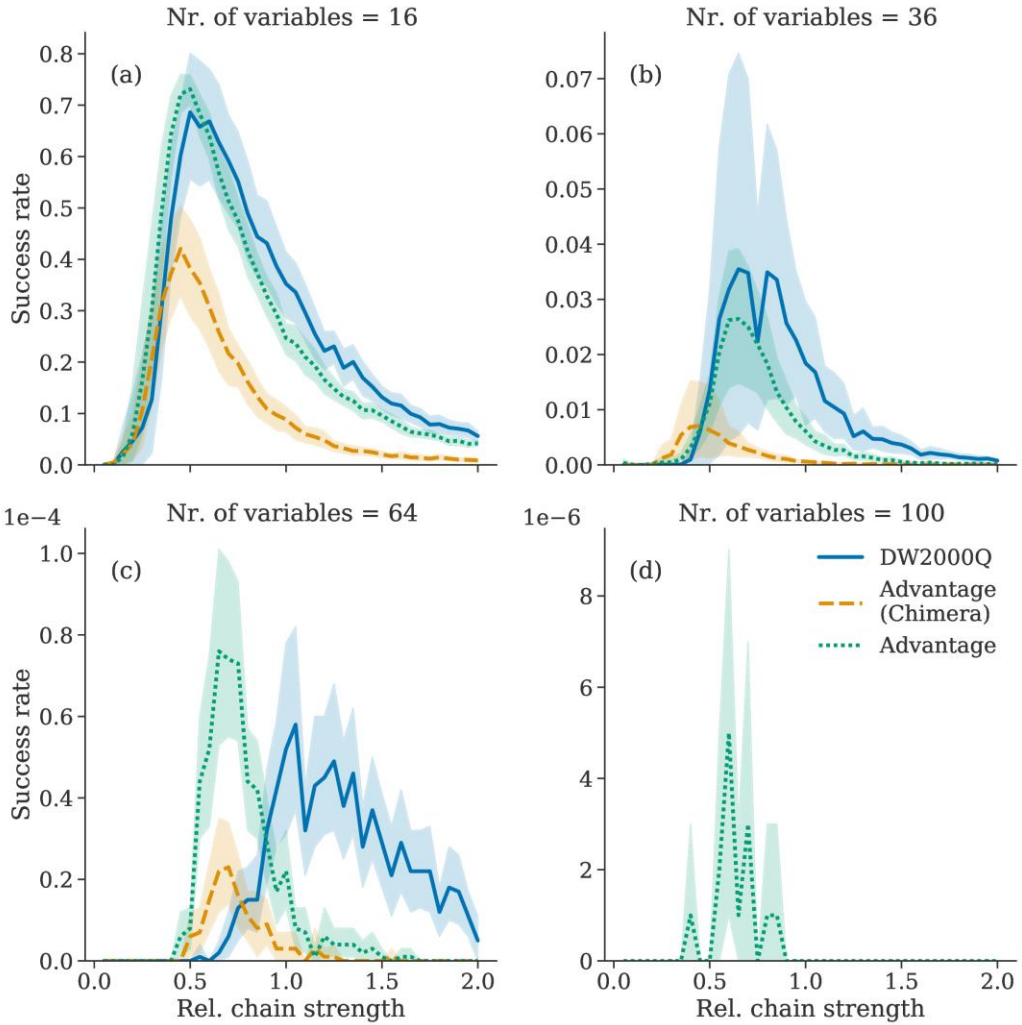

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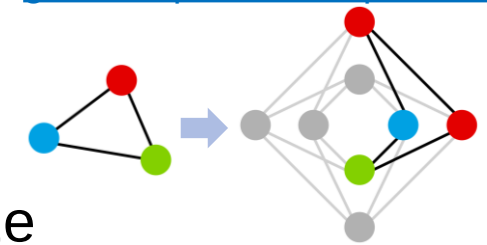

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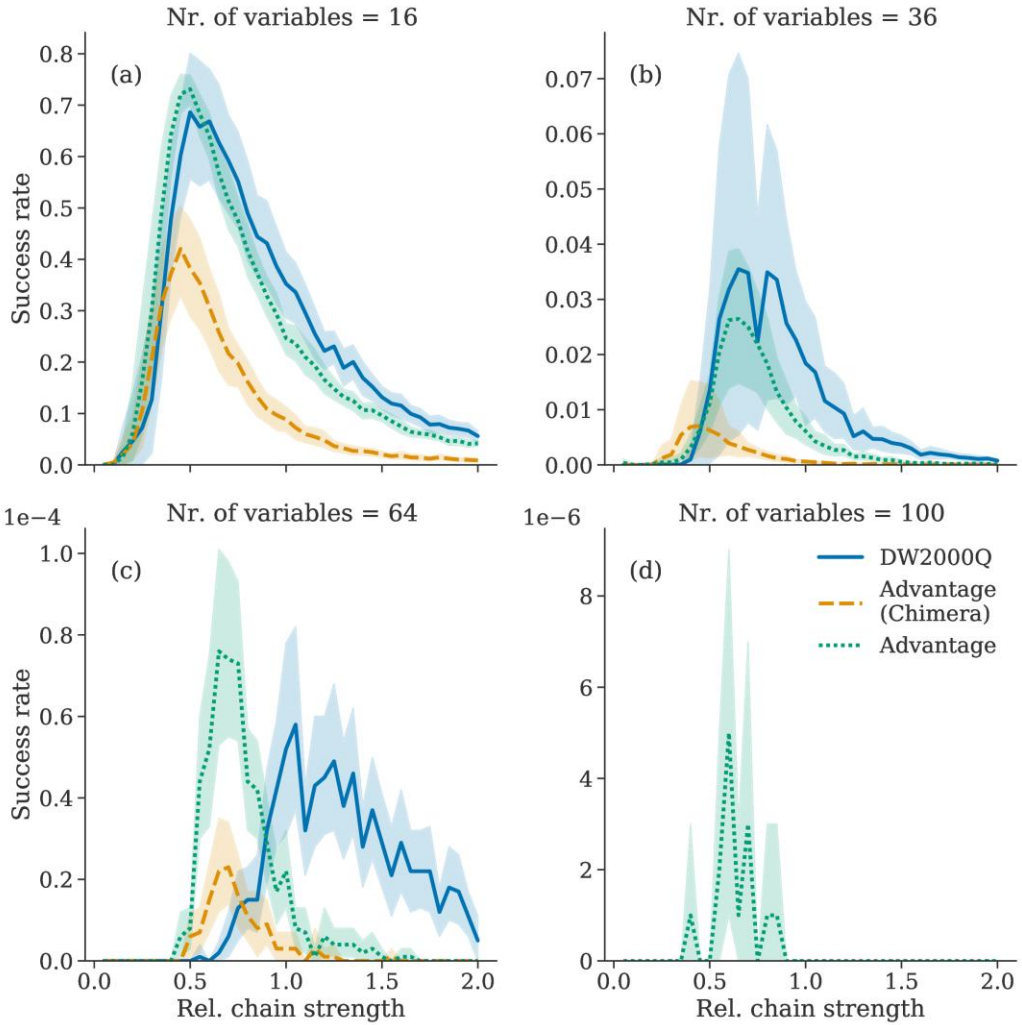

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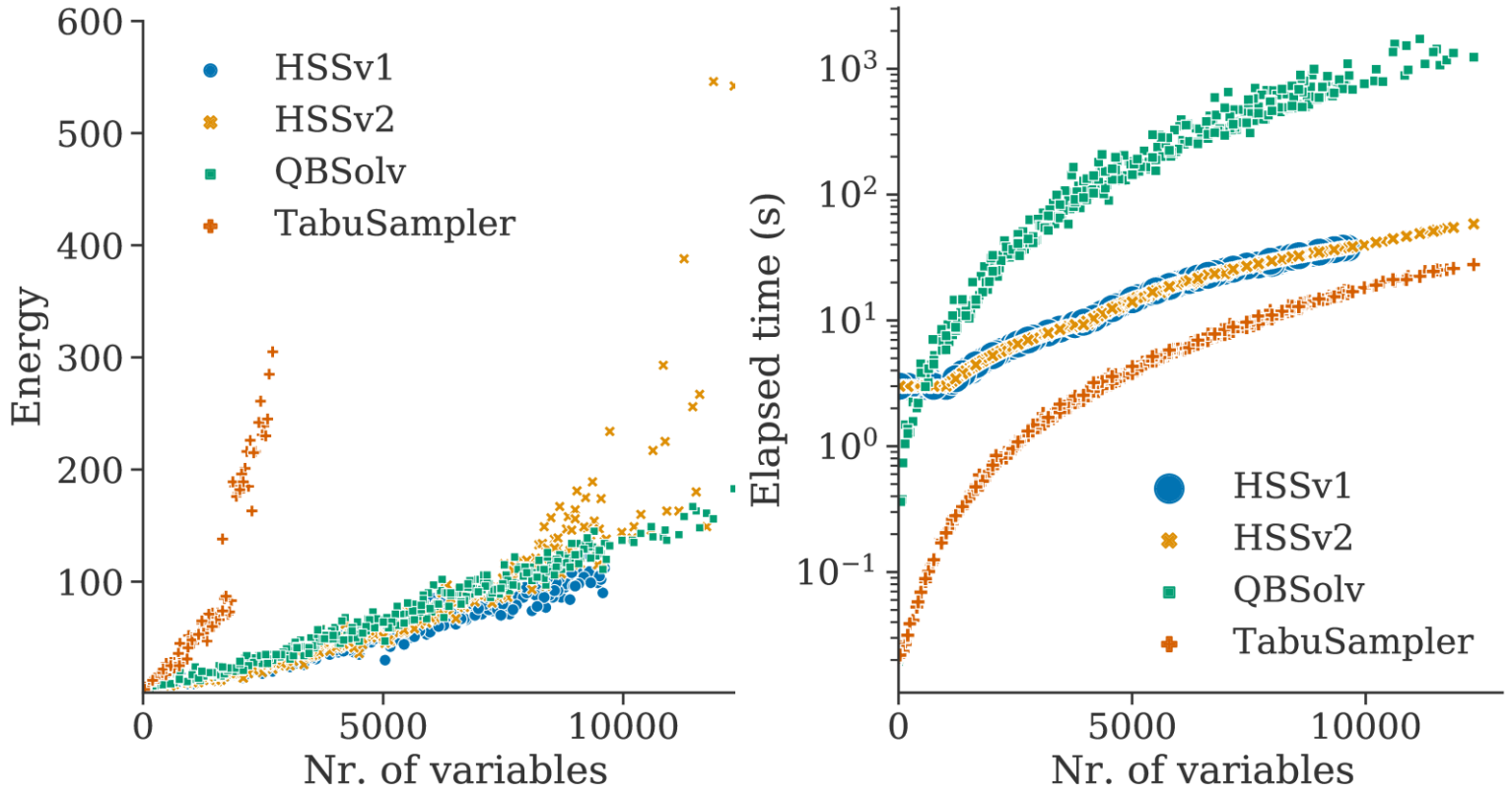
- Longer chains require higher chain strengths

CLASSICAL AND HYBRID SOLVERS

Comparing energies and run times

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



Results:

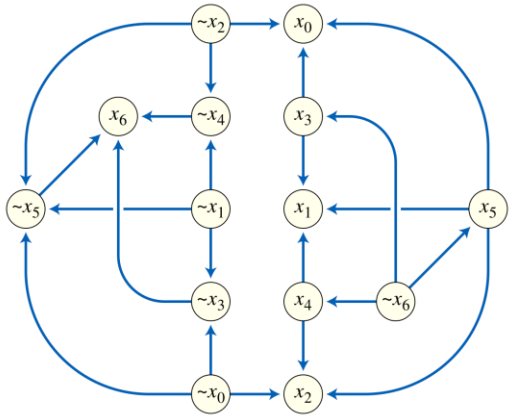
- HSSv1: best but only up to 10k vars.
- HSSv2: same as v1 up to 2k vars., worse later.
- QBSolv: good but very slow.
- TabuSampler: returns unusable results extremely fast.

Conclusion:

- Hybrid solvers outperform classical solvers.

2-SATISFIABILITY

Overview



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

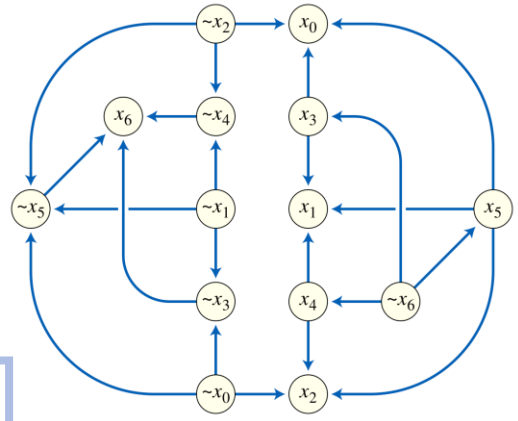
2-SATISFIABILITY

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 $x_i = 0, 1$



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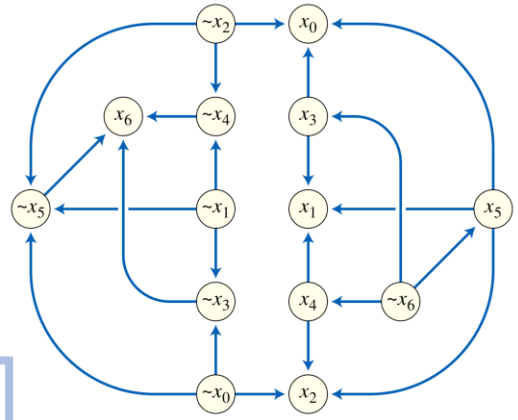

Mehta et al., PRA **105**, 062406 (2022)
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→ find assignment to x_i that makes *F* true

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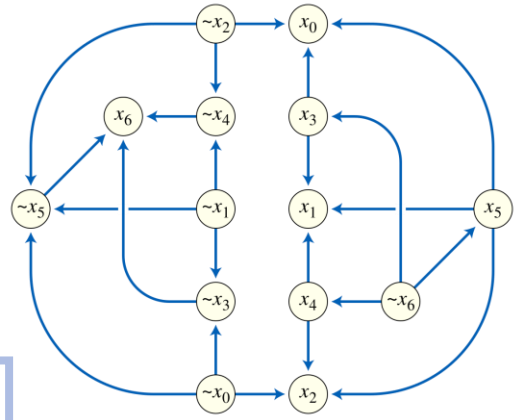

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Ising: $$\min_{s_i = \pm 1} \left(\sum_i h_i s_i + \sum_{i<j} J_{ij} s_i s_j \right)$$

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2-SATISFIABILITY

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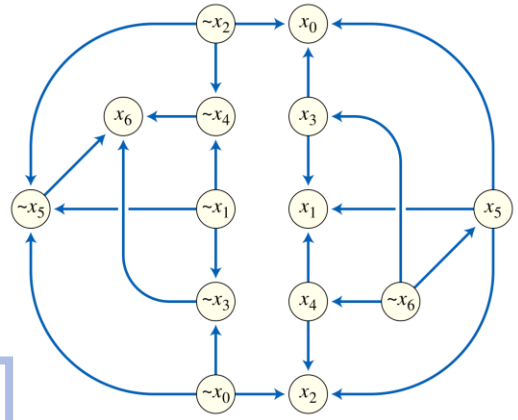

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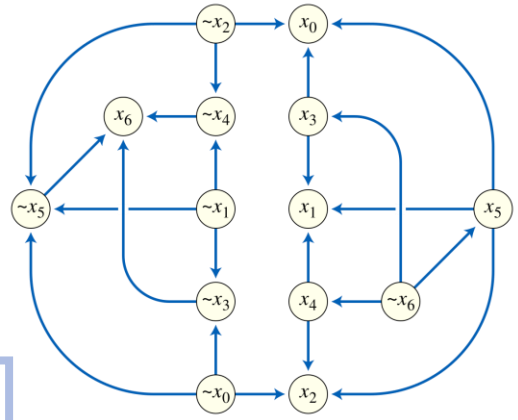

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  - Example for clause $x_1 \vee x_2$: $h_{2SAT} = s_1 s_2 - (s_1 + s_2) + 1$

- "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)
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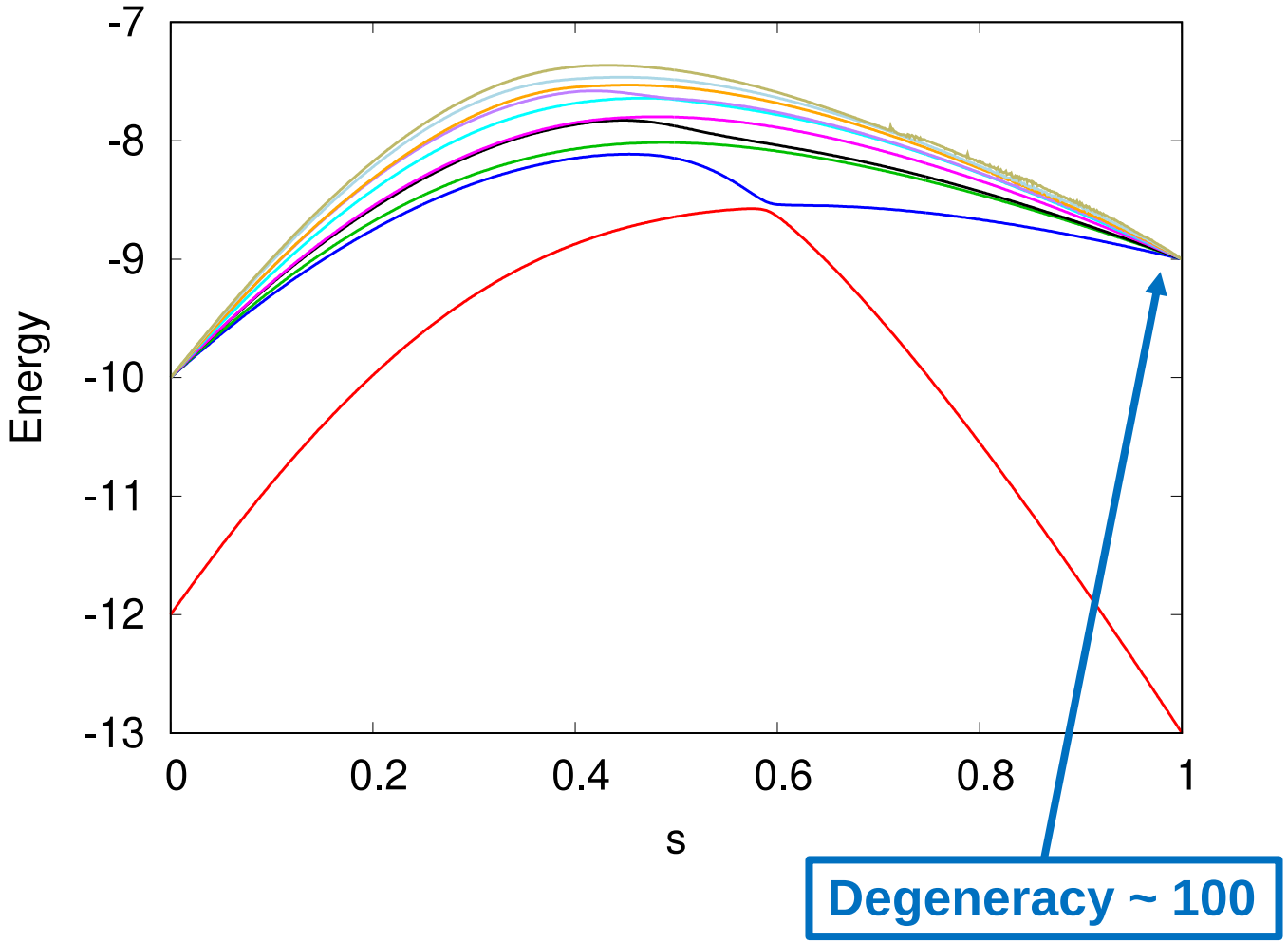
2-SATISFIABILITY

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



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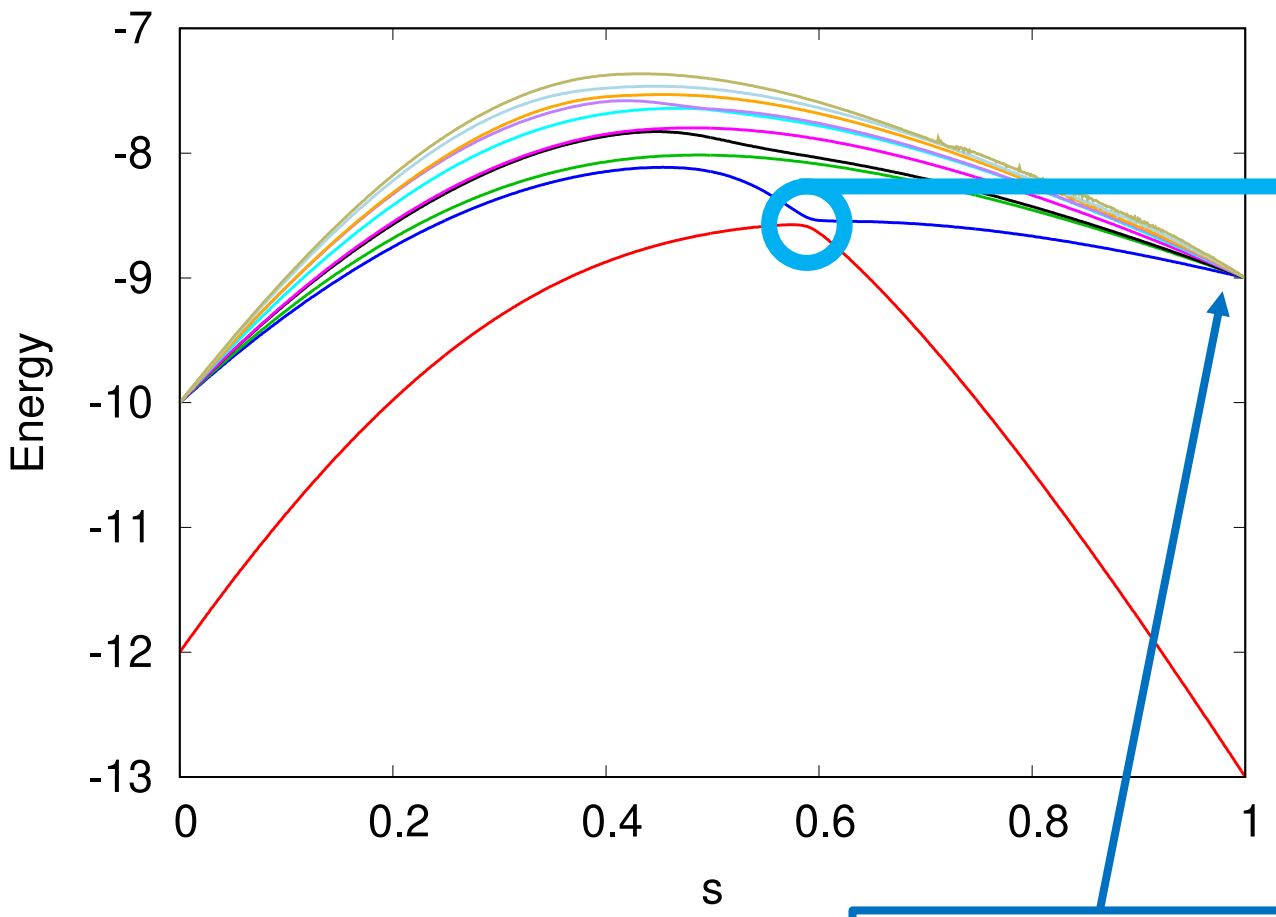
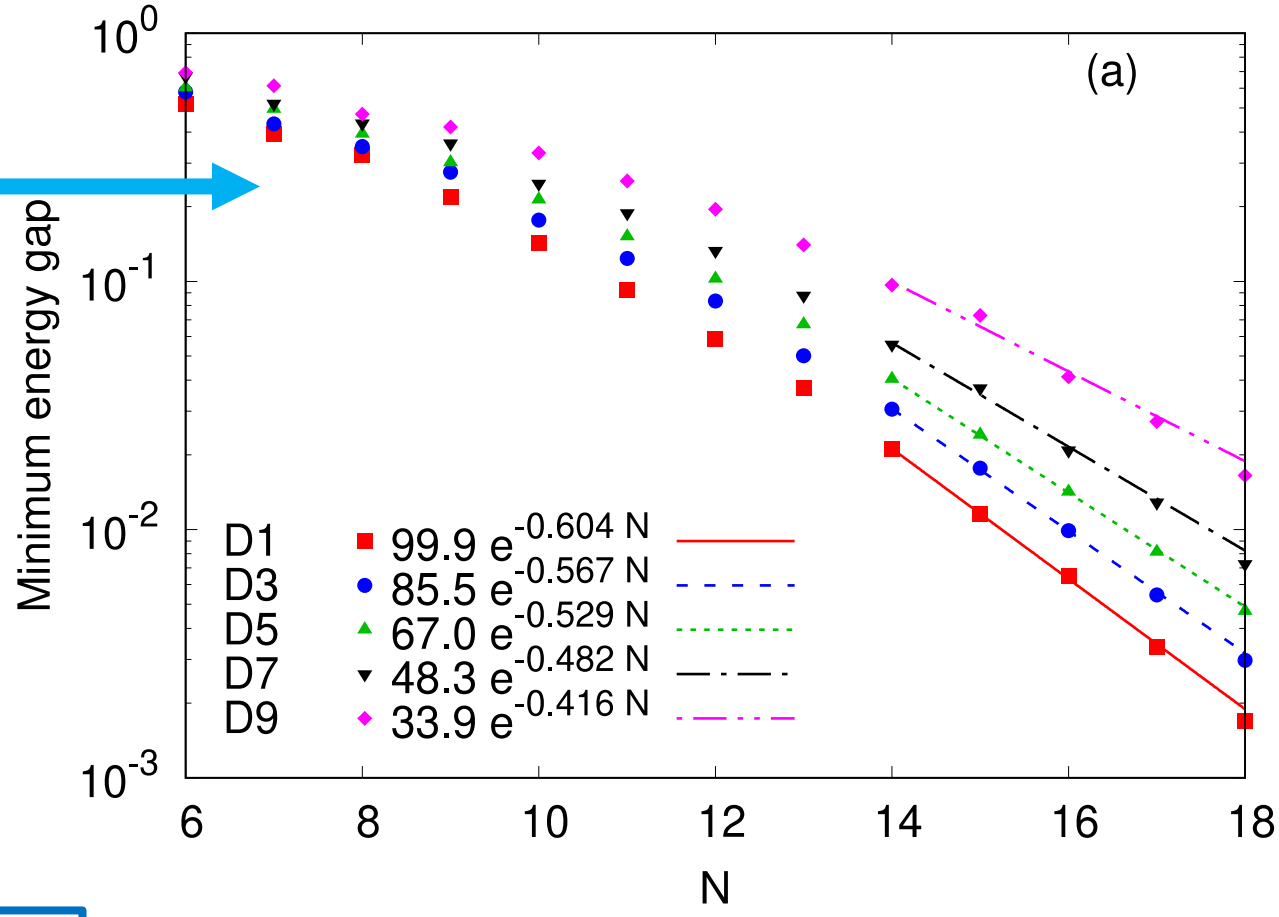
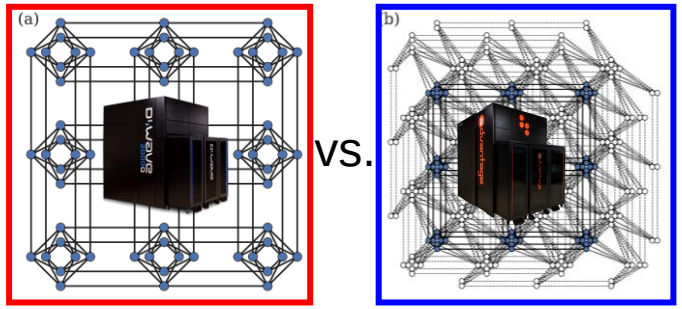




Degeneracy ~ 100

2-SATISFIABILITY: RESULTS

Success rate for 1000 2-SAT problems



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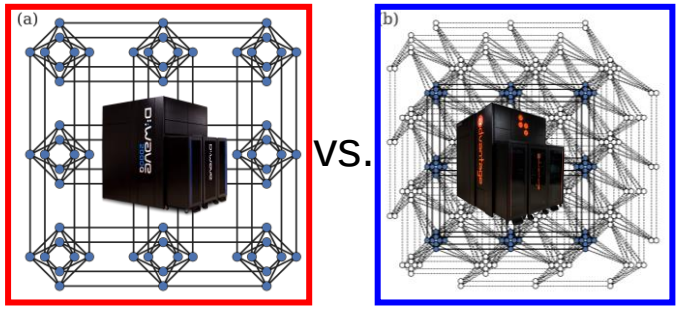

vs.

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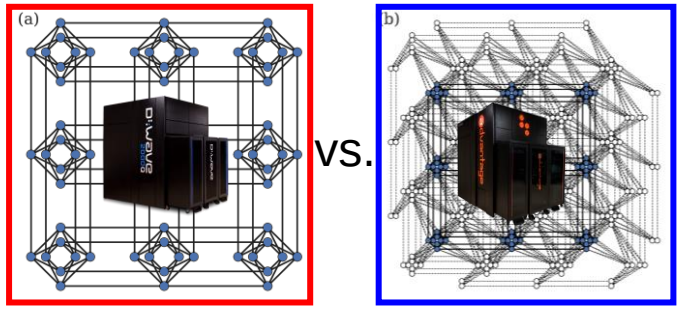

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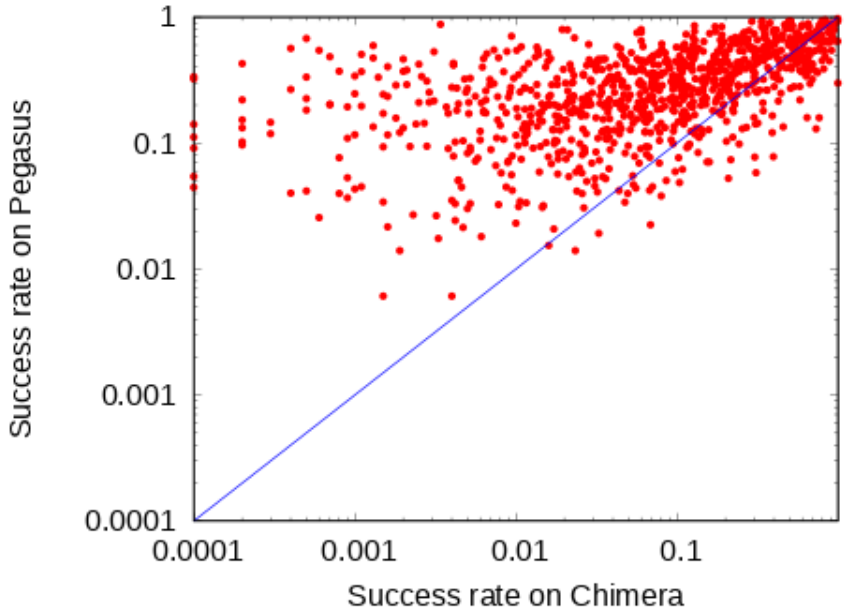
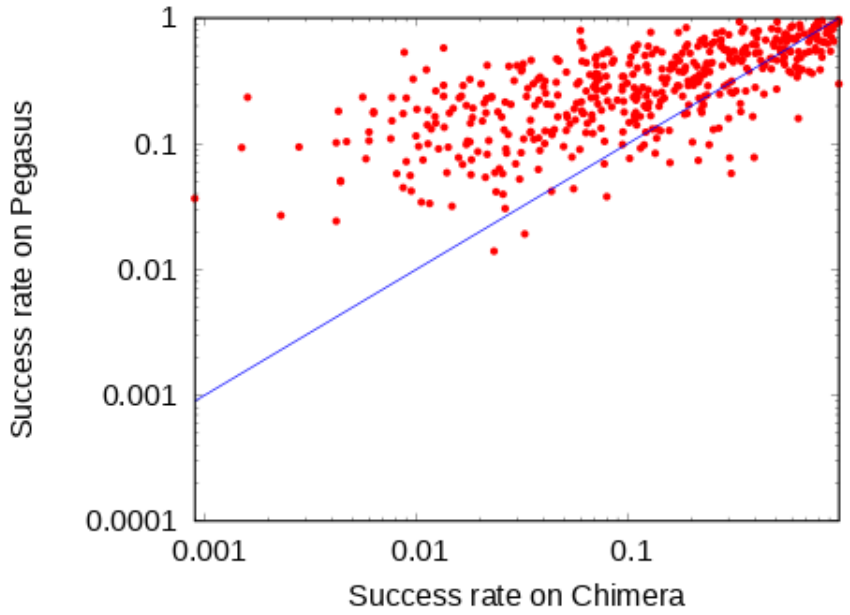
All problems



Problems with direct mapping



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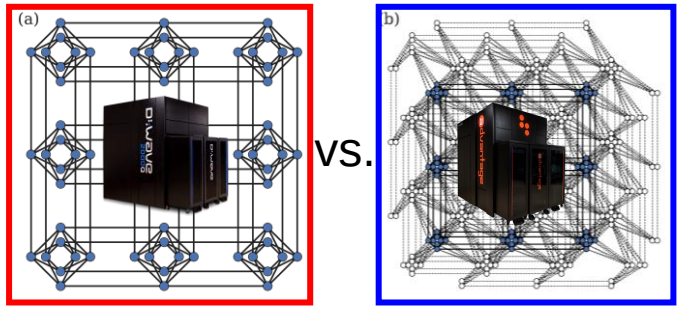

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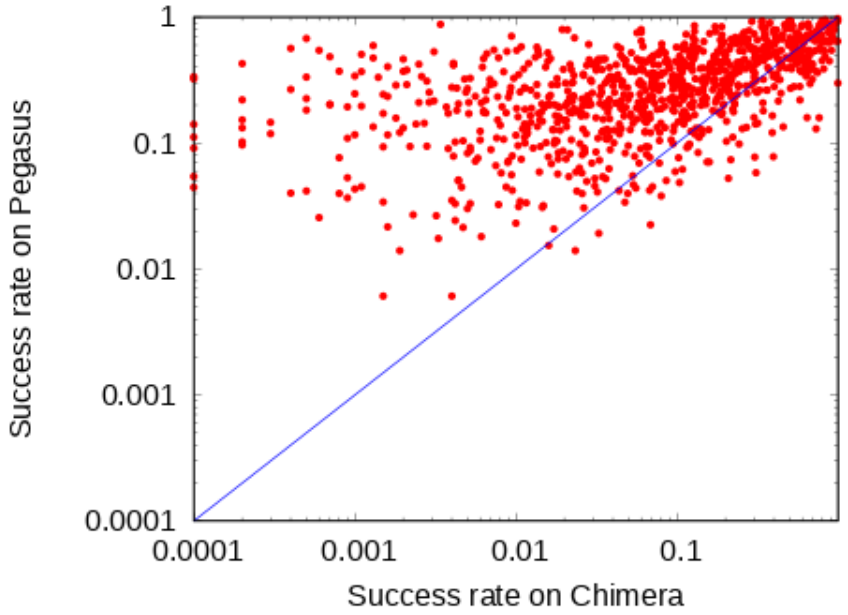

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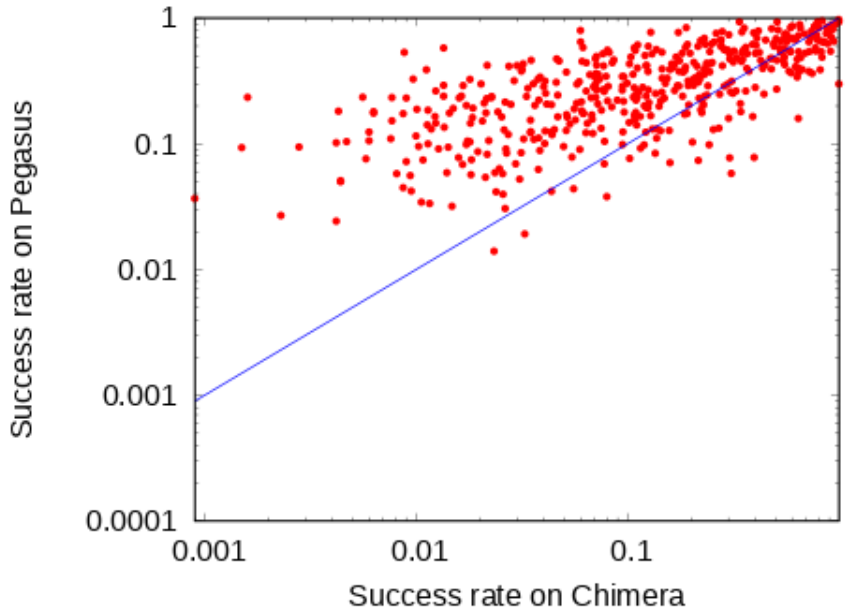
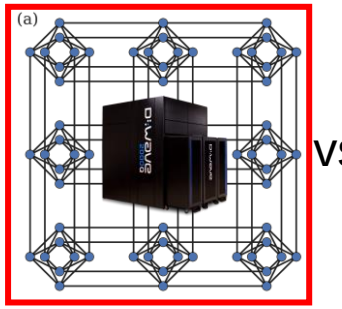


- Largest enhancement for cases that require embedding only on Chimera

2-SATISFIABILITY: RESULTS

Success rate for 1000 2-SAT problems



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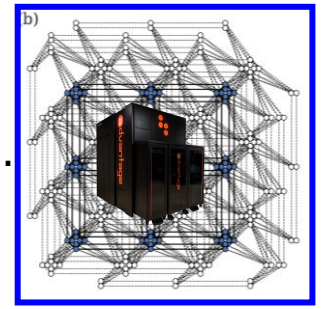

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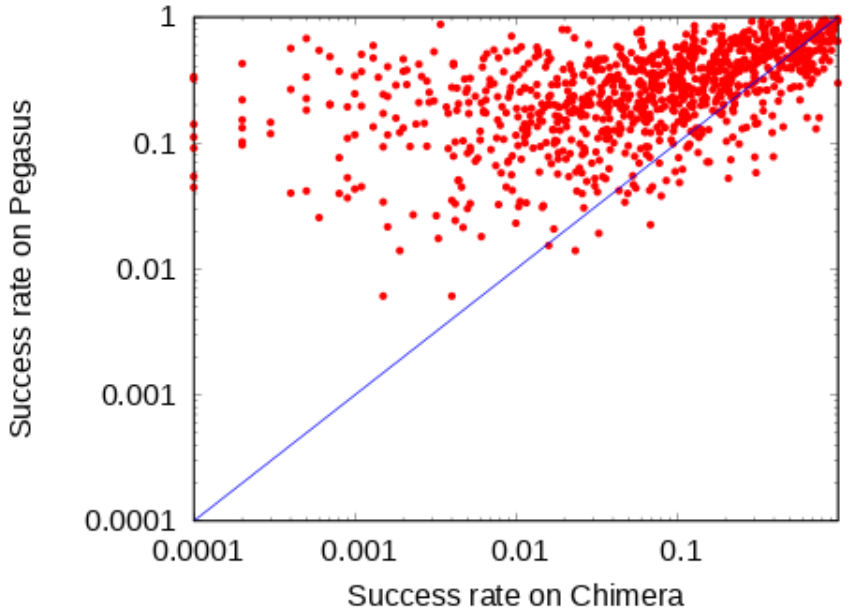

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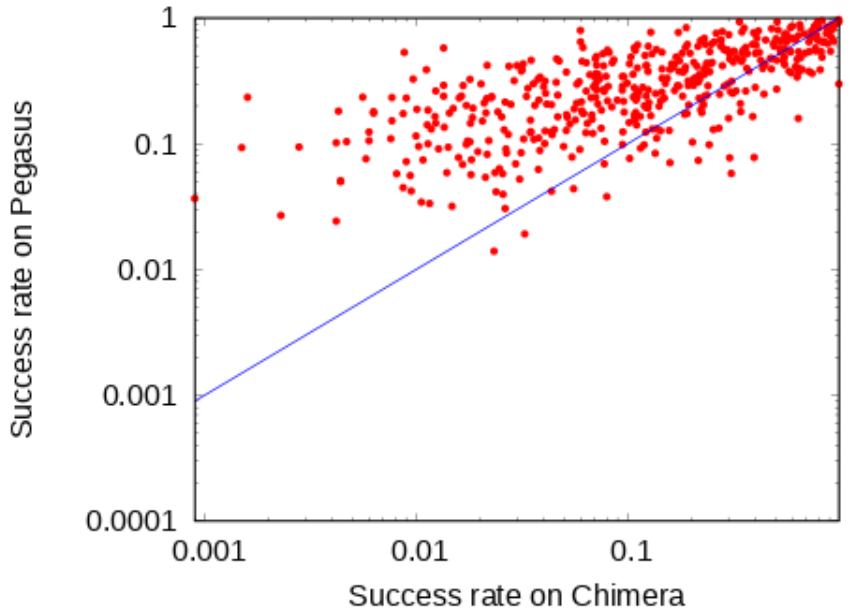
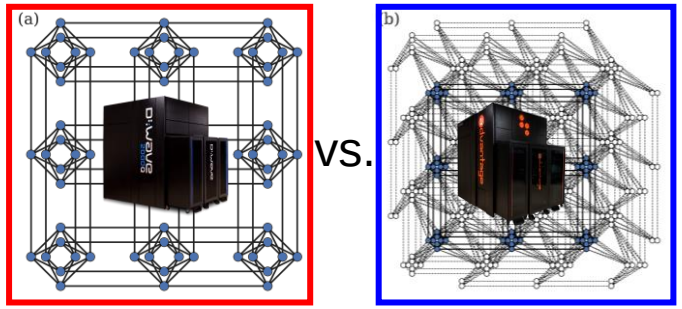


- Largest enhancement for cases that require embedding only on Chimera
  ➔ Improvement due to increased connectivity

2-SATISFIABILITY: RESULTS

Success rate for 2 particular 2-SAT problems



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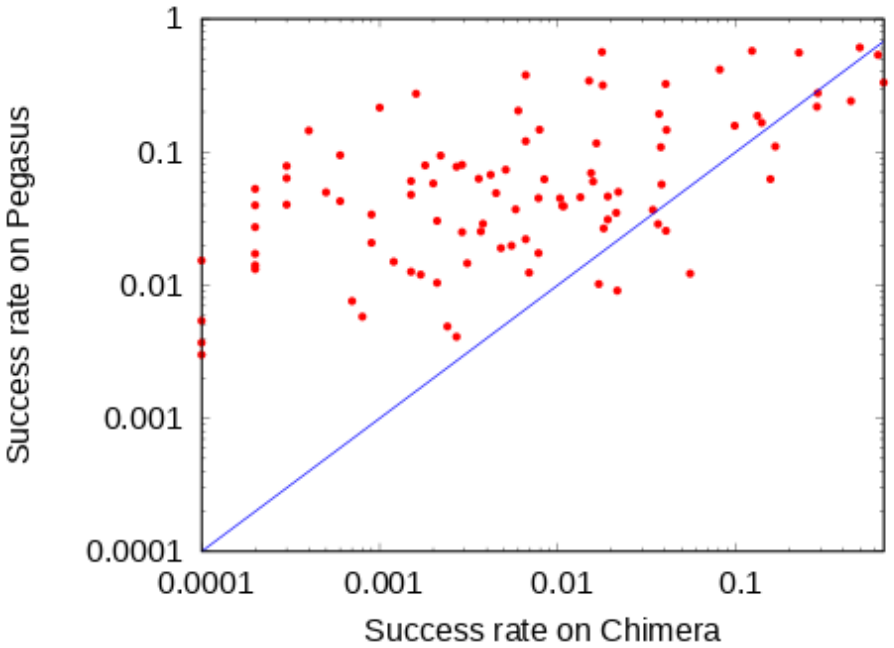
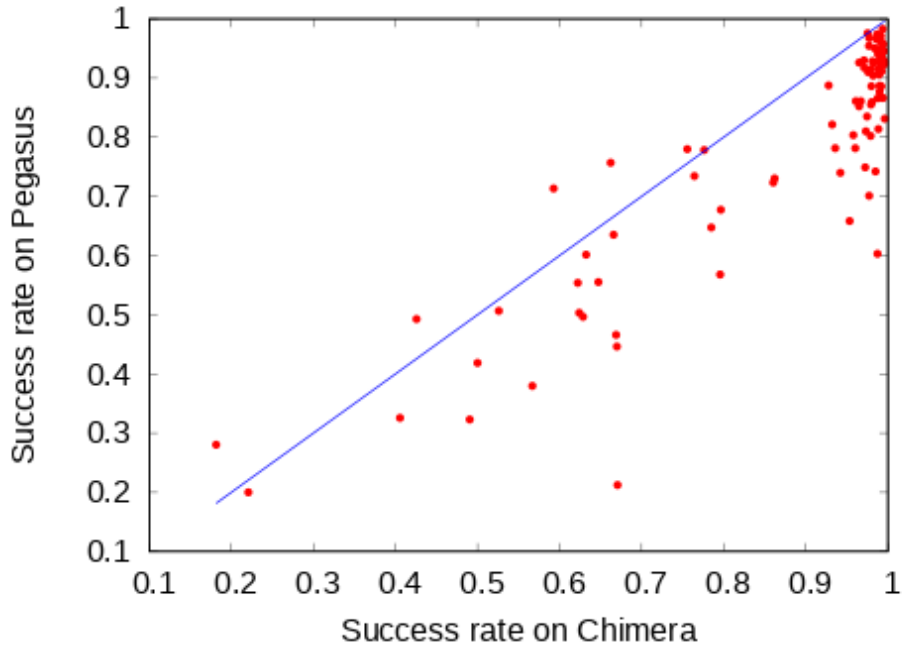
Hard Problem



Easy problem



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

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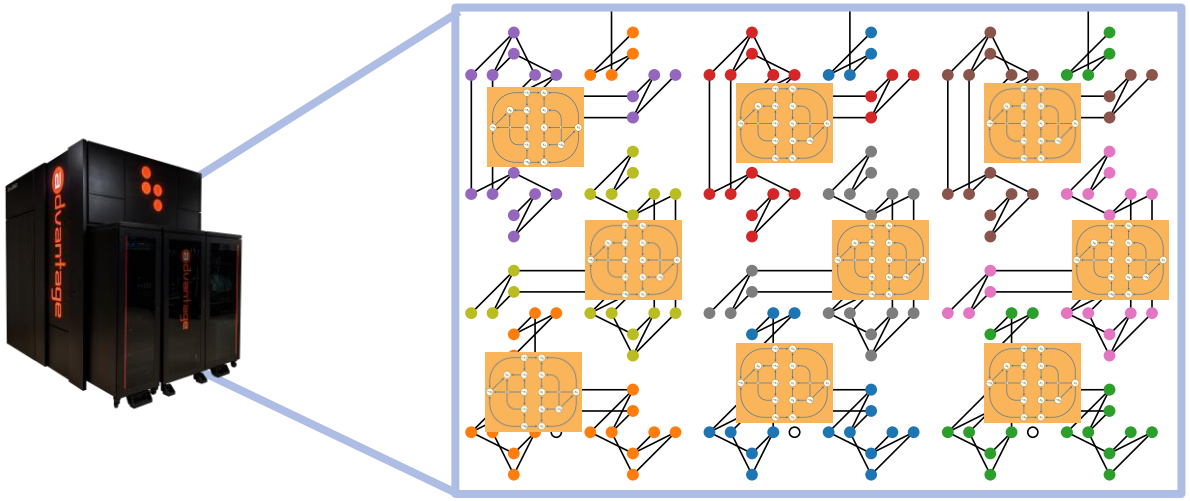
2-SATISFIABILITY: RESULTS

Embed the same problem multiple times



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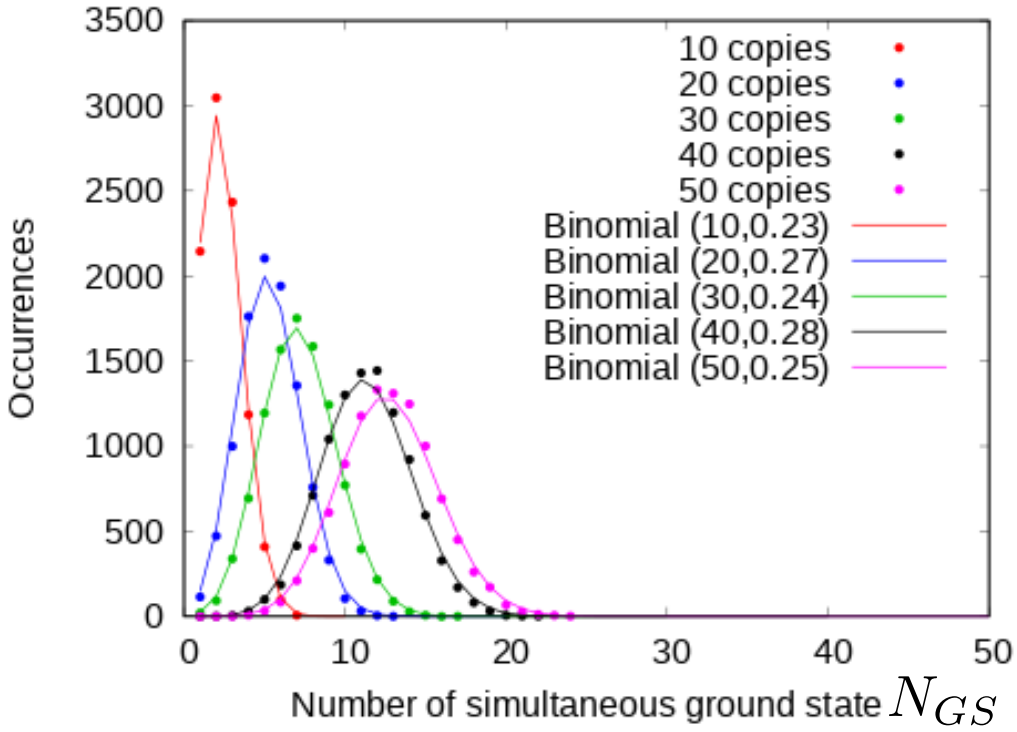

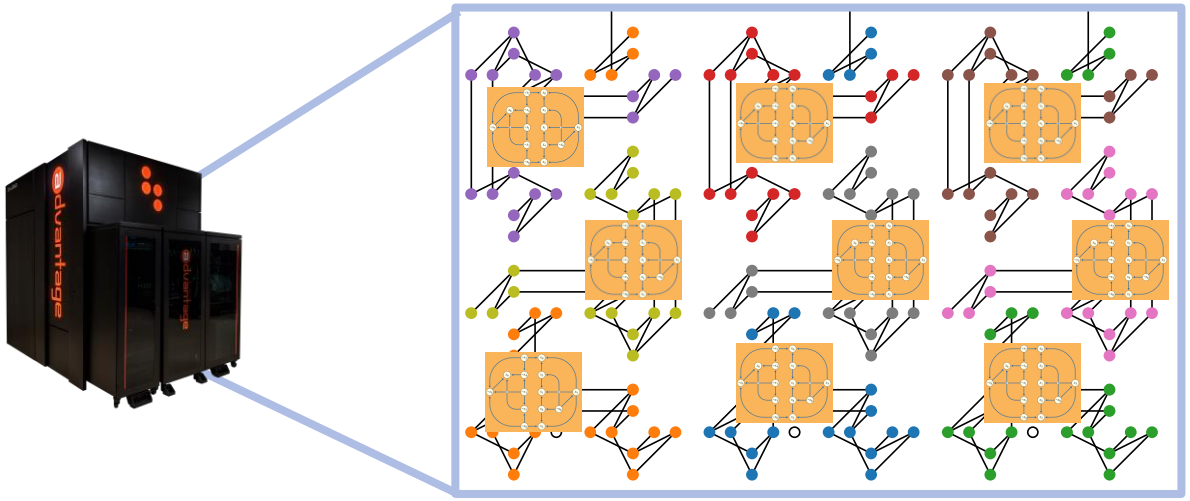

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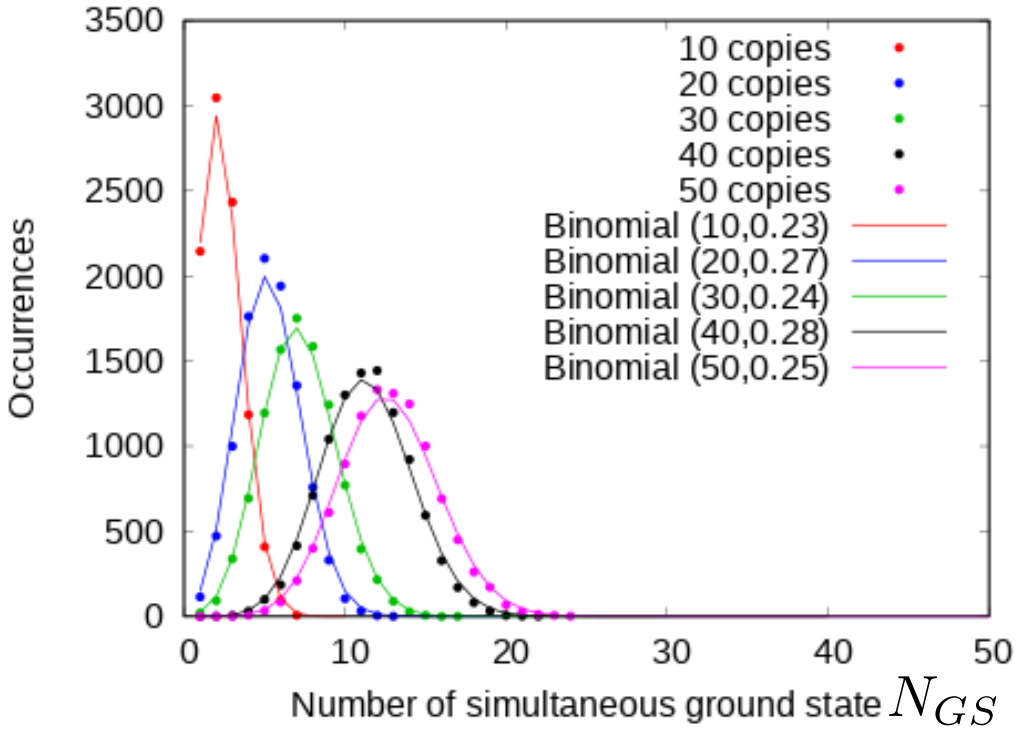

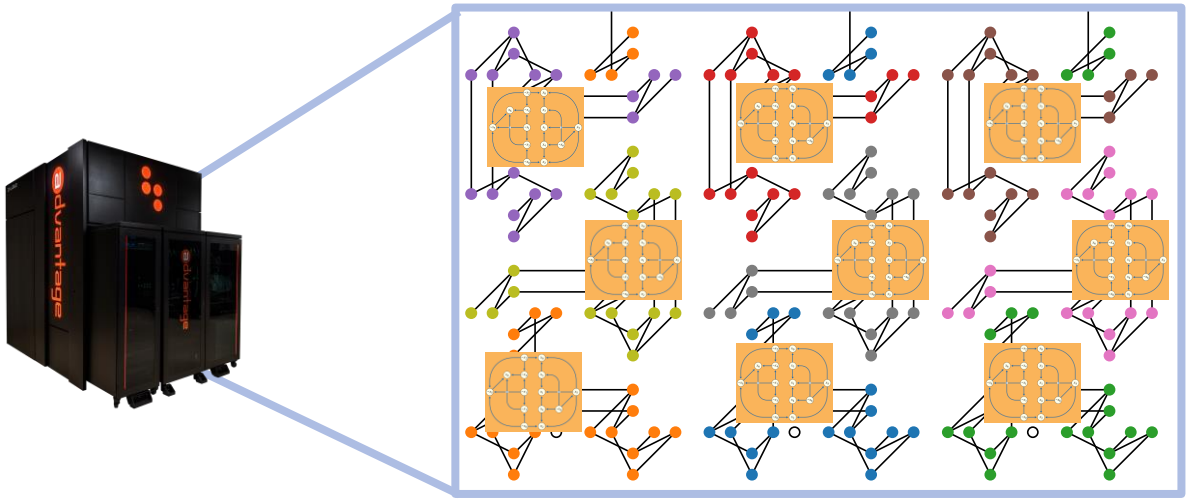

- The occurrence of optimal solutions follows a binomial distribution

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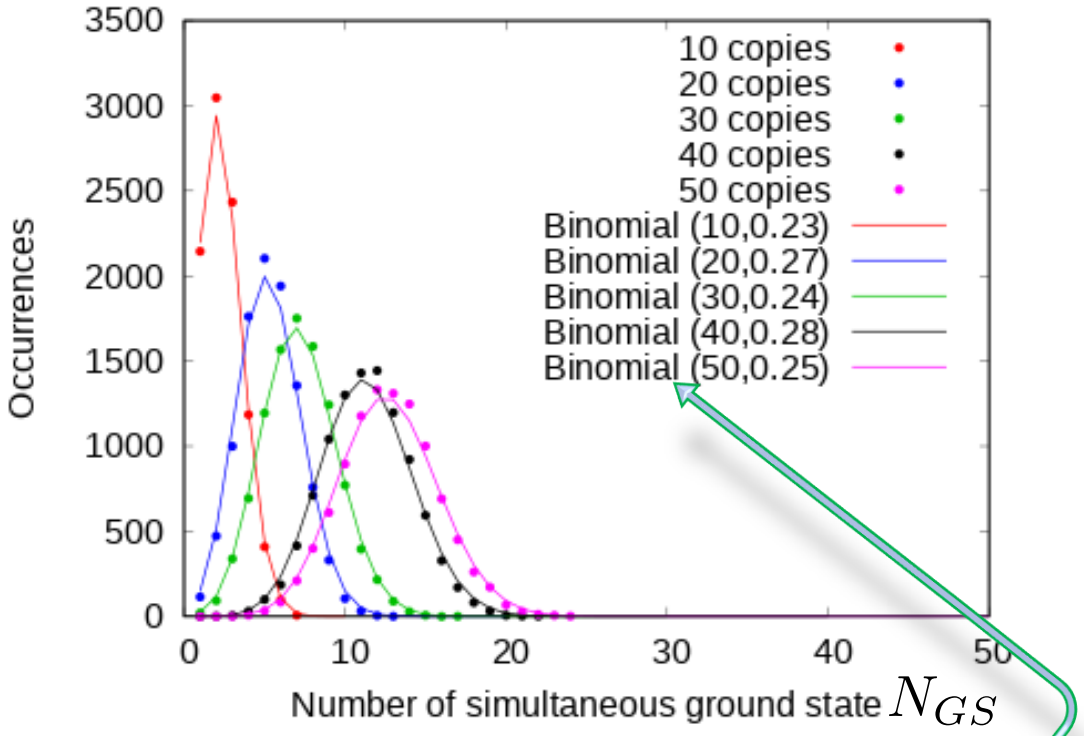
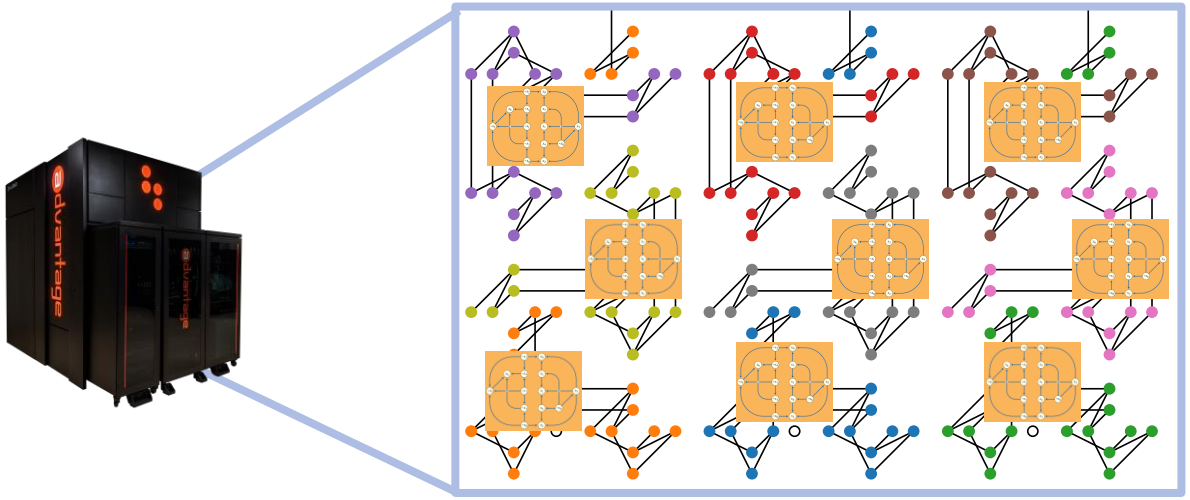


$$\binom{N_{\text{copies}}}{N_{GS}} p^{N_{GS}} (1-p)^{N_{\text{copies}}-N_{GS}}$$

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

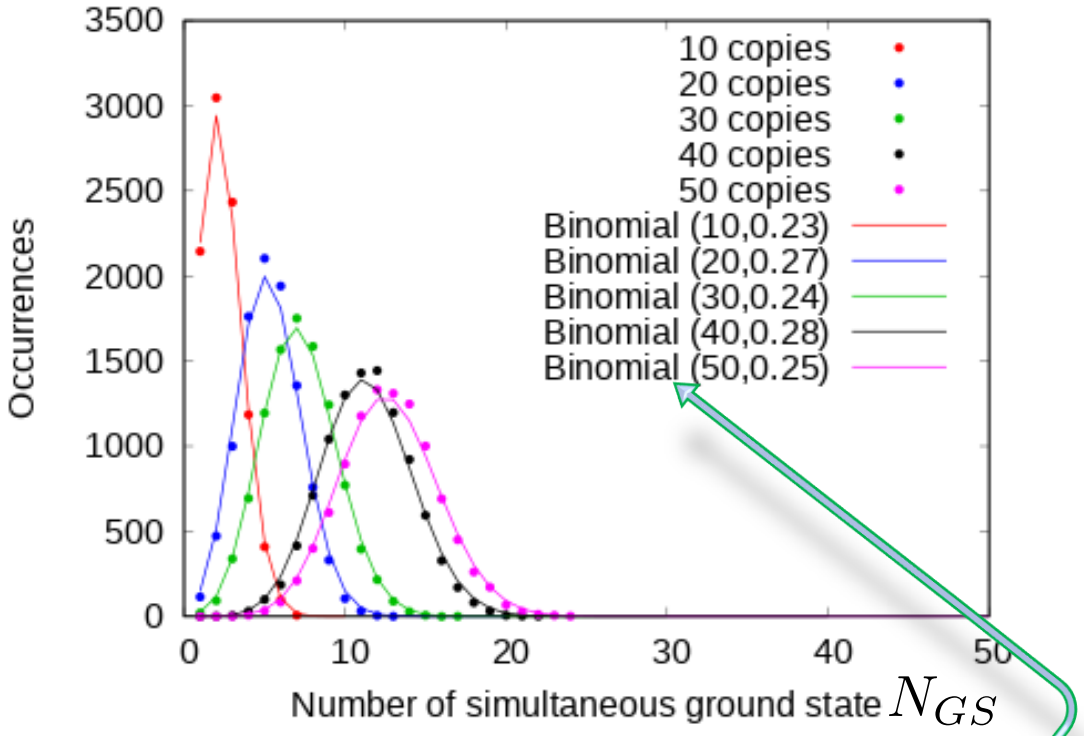


- The occurrence of optimal solutions follows a binomial distribution

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

2-SATISFIABILITY: RESULTS

Embed the same problem multiple times



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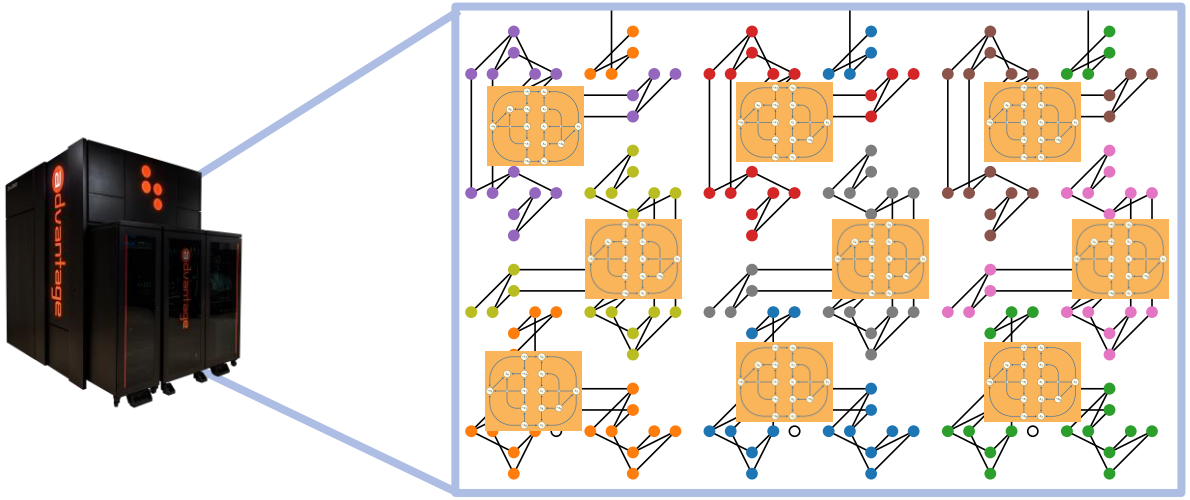

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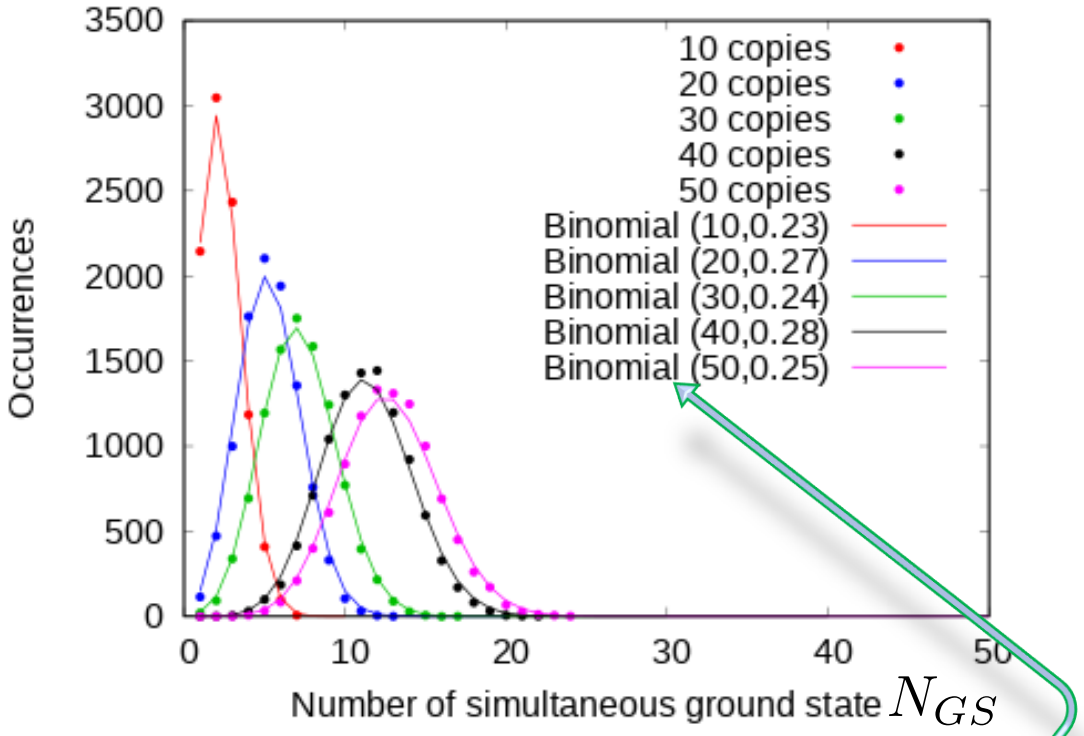

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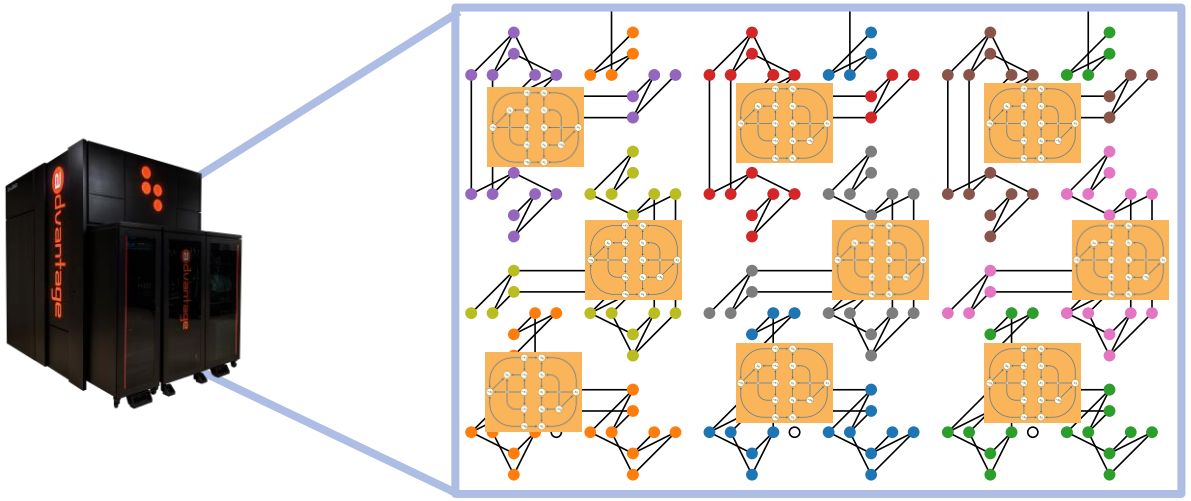

- The occurrence of optimal solutions follows a binomial distribution
- Parts of the solver corresponding to each copy work almost independently
- Note that in no run could all ground states be found simultaneously

QUANTUM SUPPORT VECTOR MACHINES

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

From classical SVM to quantum SVM

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From classical SVM to quantum SVM

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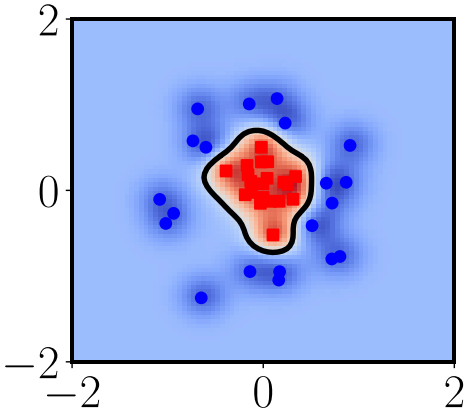

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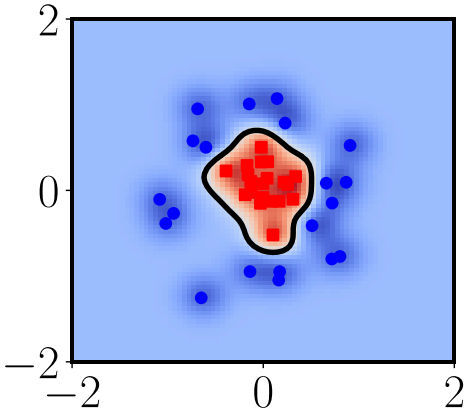

- An SVM is a supervised machine-learning method for binary classification
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Feature vector Label

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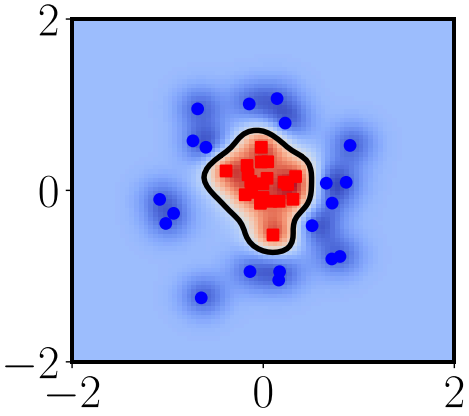

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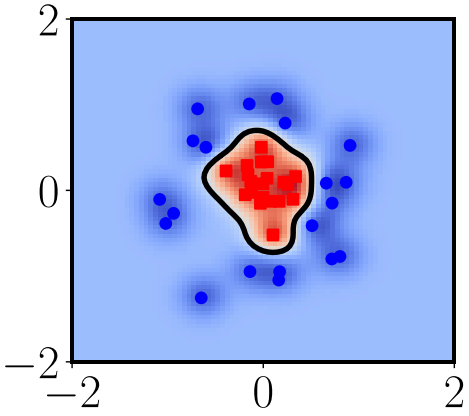

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Continuous problem variables

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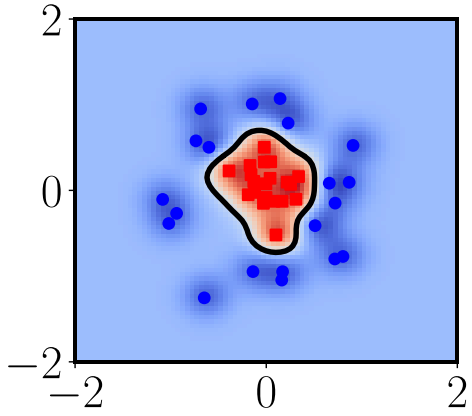

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Kernel function (nonlinear SVM)

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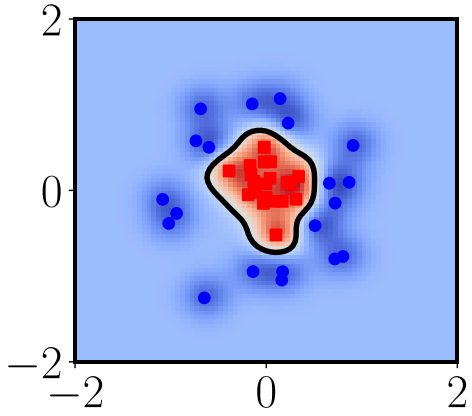

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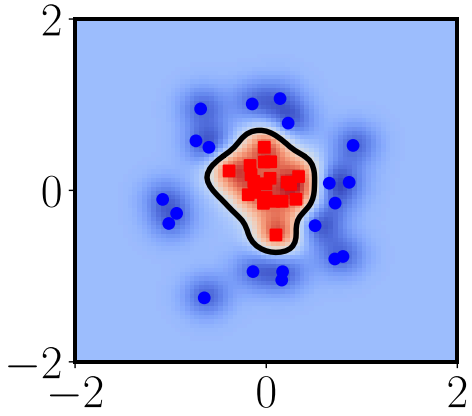

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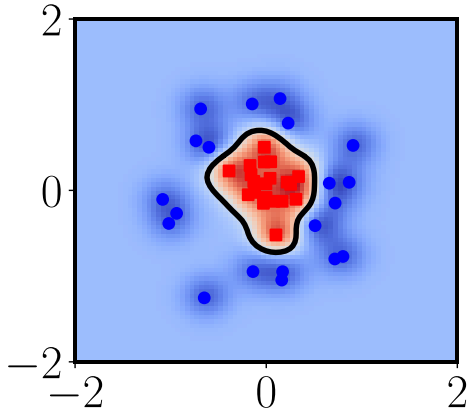

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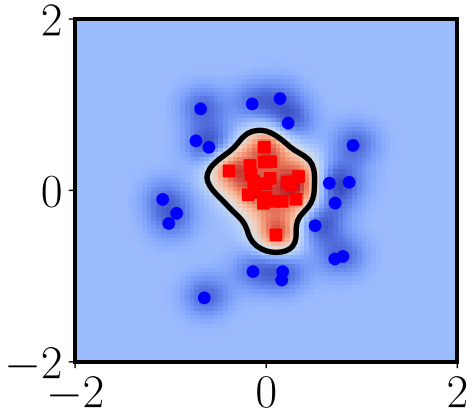

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Base & Exponent

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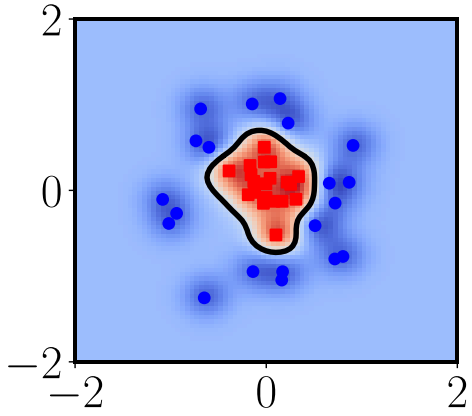

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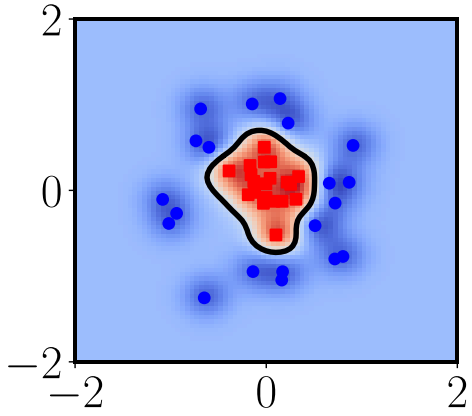

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Number of qubits per problem variable

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

Base & Exponent

QUANTUM SUPPORT VECTOR MACHINES

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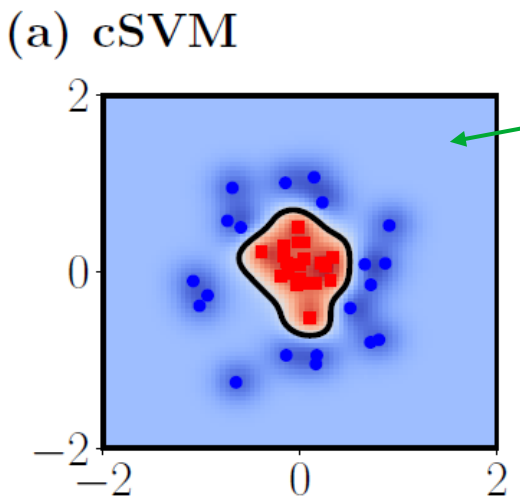
Results



- Classical SVM (**cSVM**) yields the global minimum, but only for the training data

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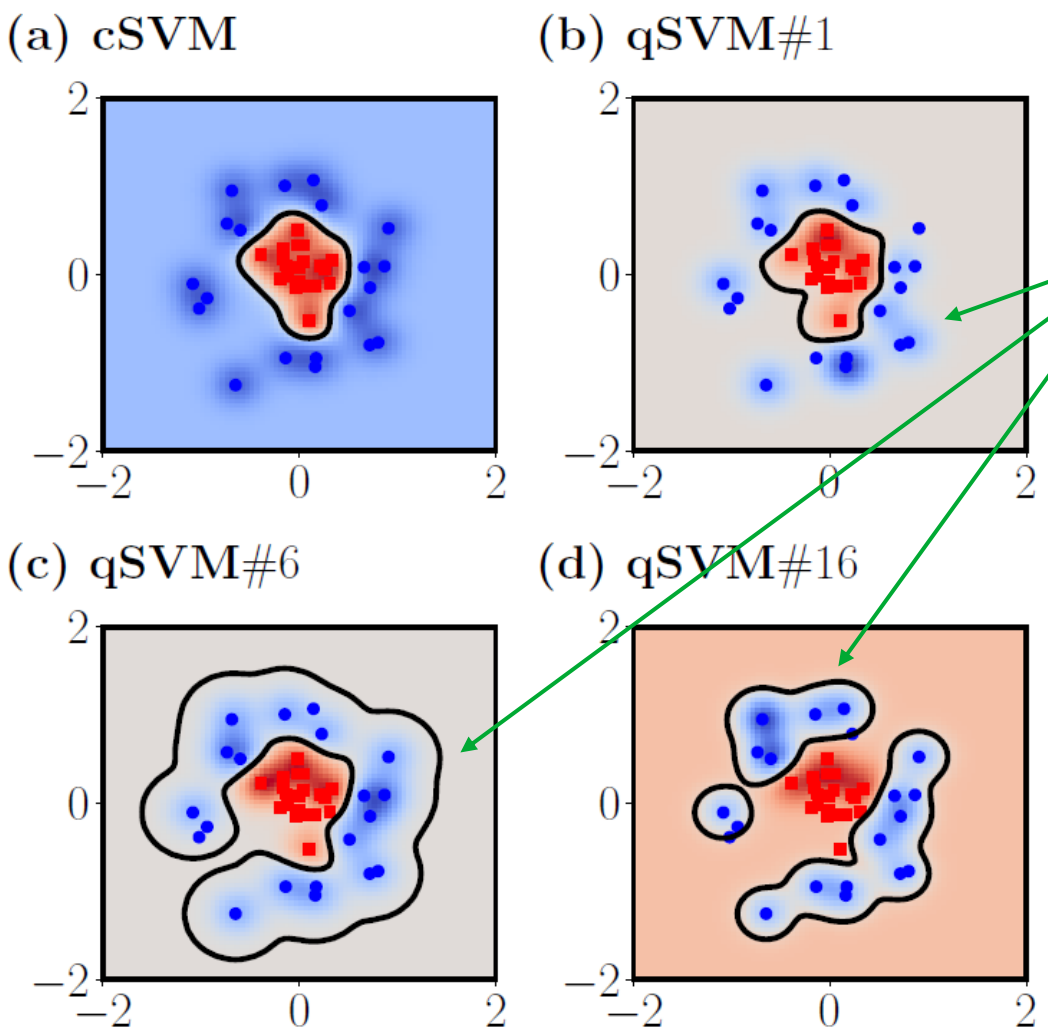

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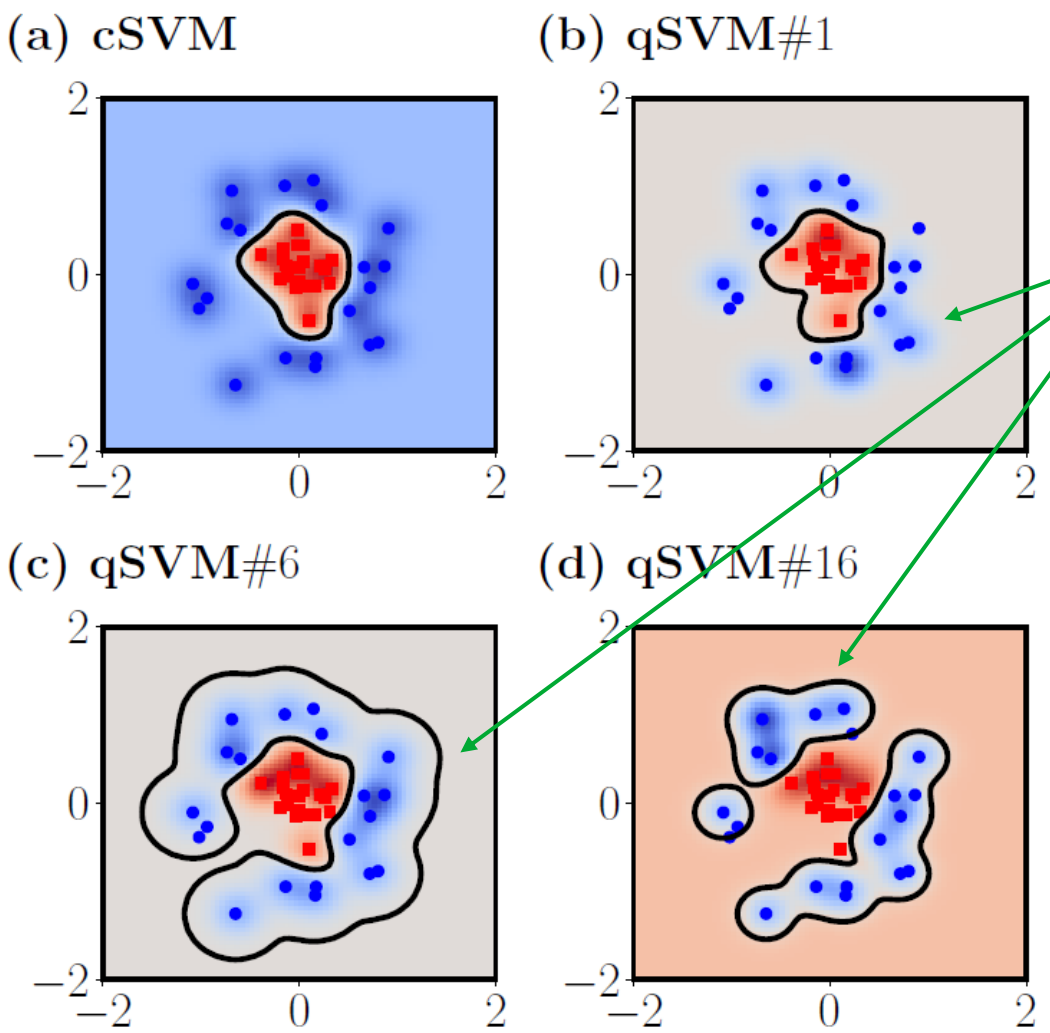

- Classical SVM (**cSVM**) yields the global minimum, but only for the training data
- Quantum SVM (**qSVM**) yields additional low-energy classifiers from ensemble of solutions

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., IGARSS 2022, 4903 (2022)
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QUANTUM SUPPORT VECTOR MACHINES

Application to remote sensing: Results

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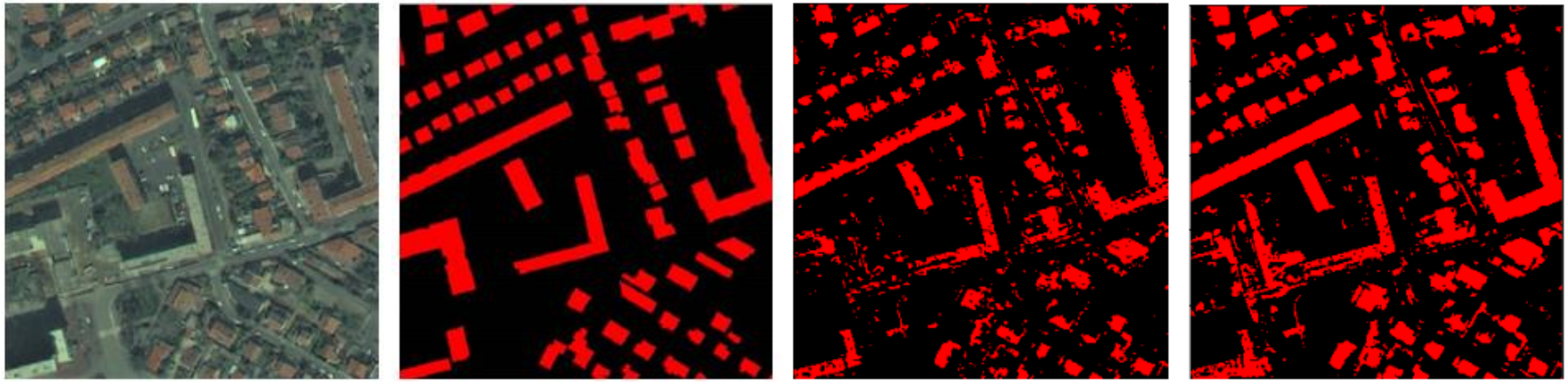
Original | Ground truth | Classical SVM | Quantum SVM



QUANTUM SUPPORT VECTOR MACHINES

Extension to multiple classes

Willsch et al., CPC 248, 107006 (2020)
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Pasetto et al., IGARSS 2022, 4903 (2022)
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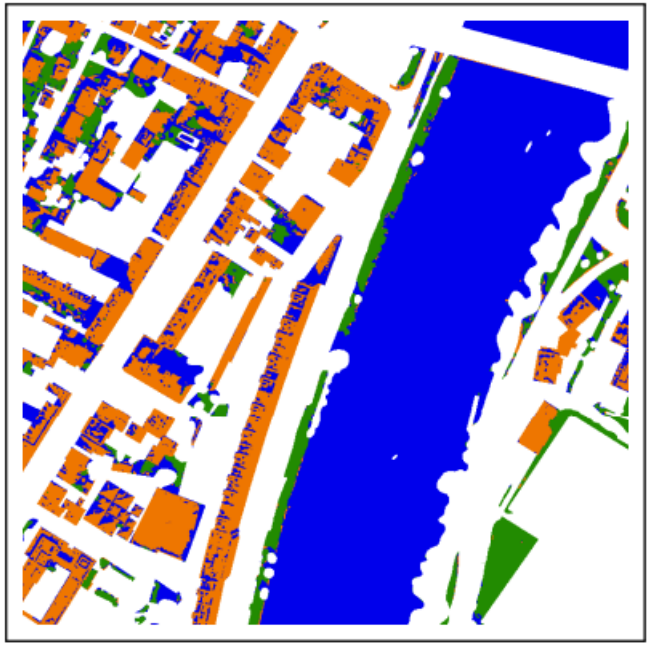
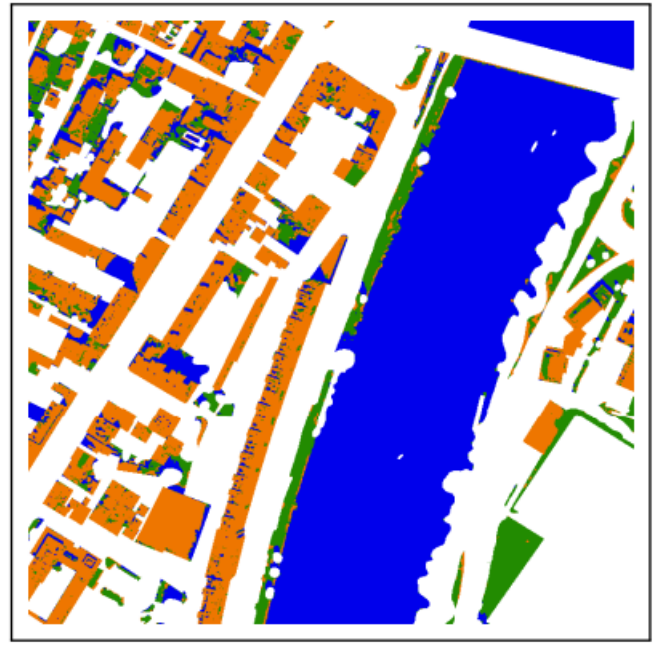
Ground truth



Classical SVM



Quantum SVM

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

QUANTUM BOLTZMANN MACHINES

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

QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

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

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QUANTUM BOLTZMANN MACHINES

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QUANTUM BOLTZMANN MACHINES

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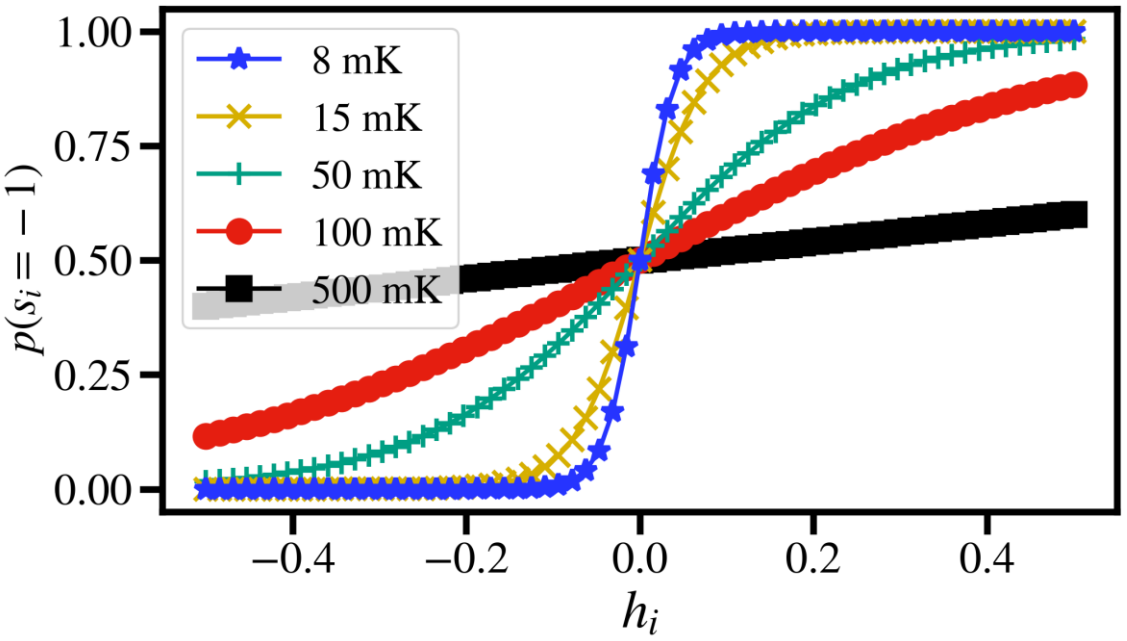

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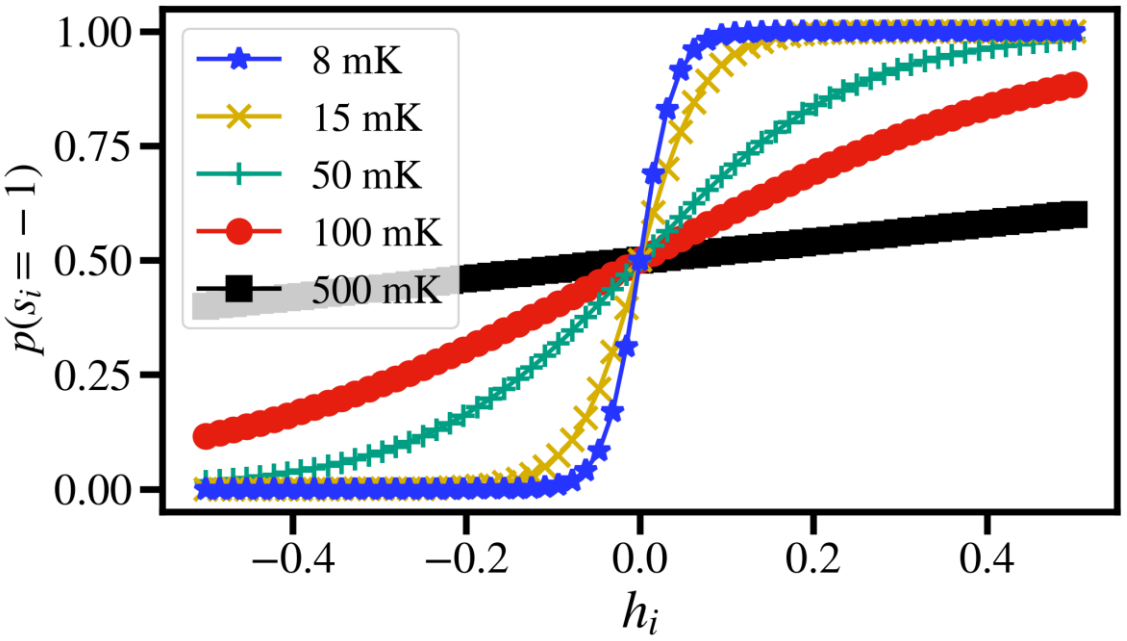
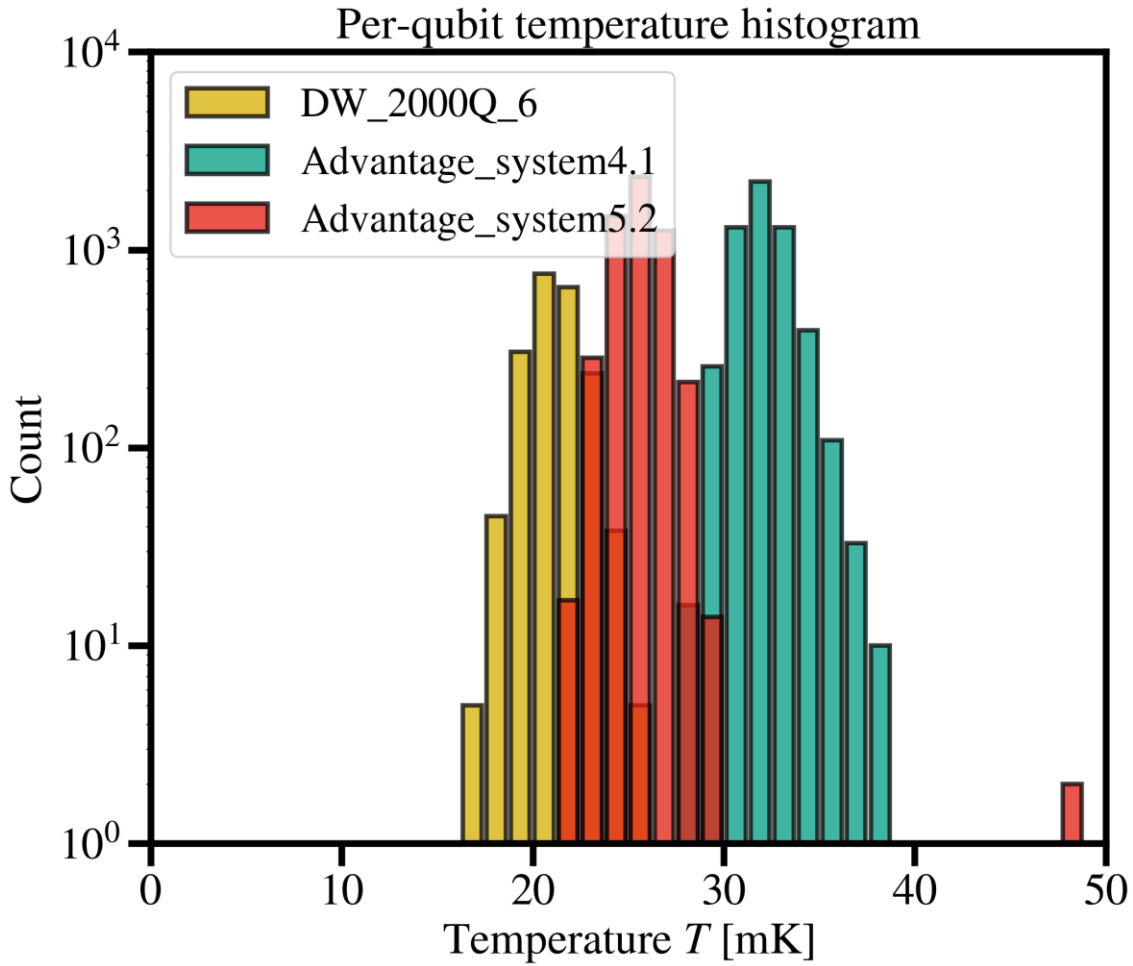


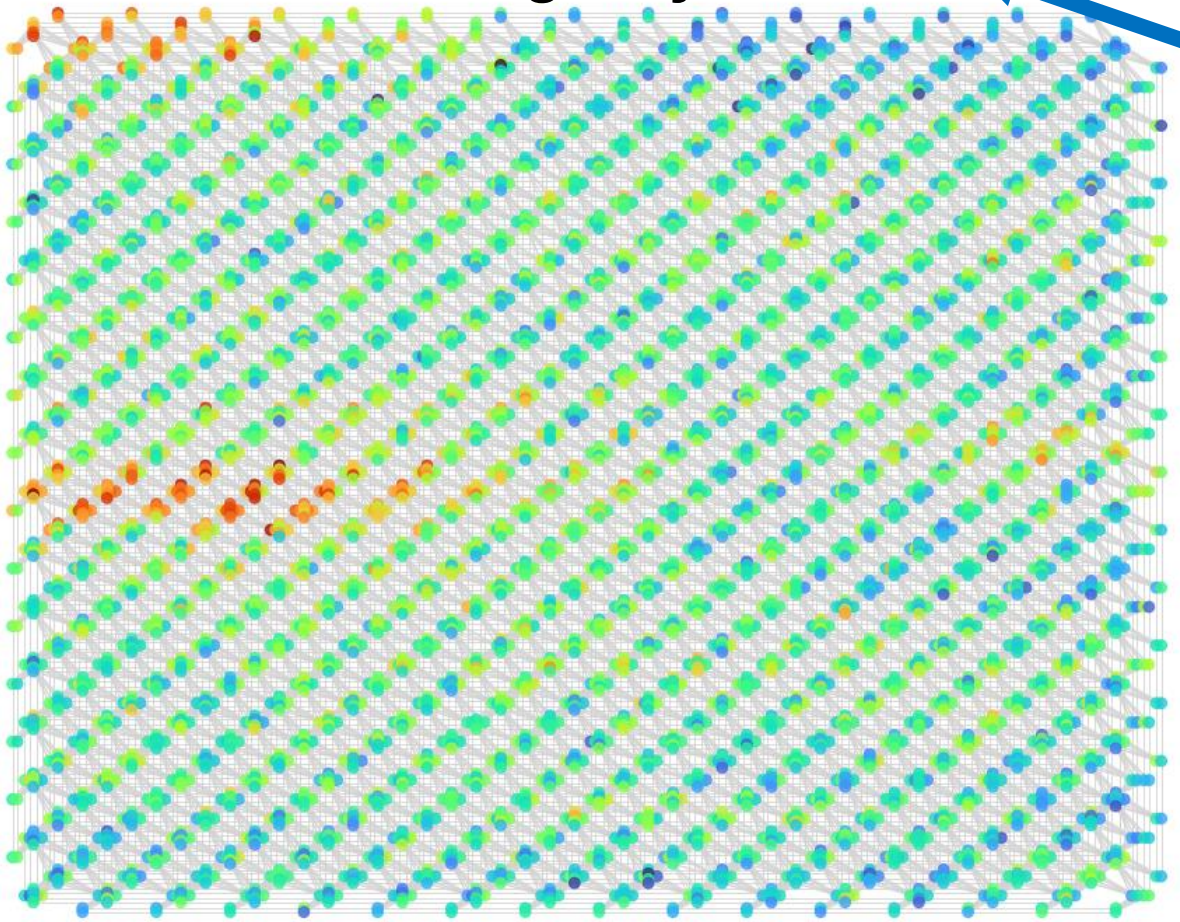


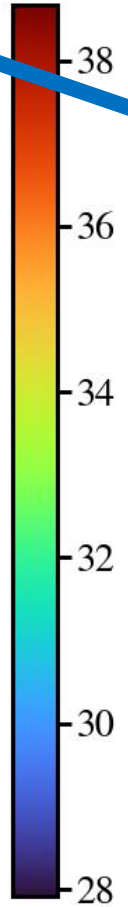
Perot et al. (2022)
https://jugit.fz-juelich.de/qip/qbm-quant-finance

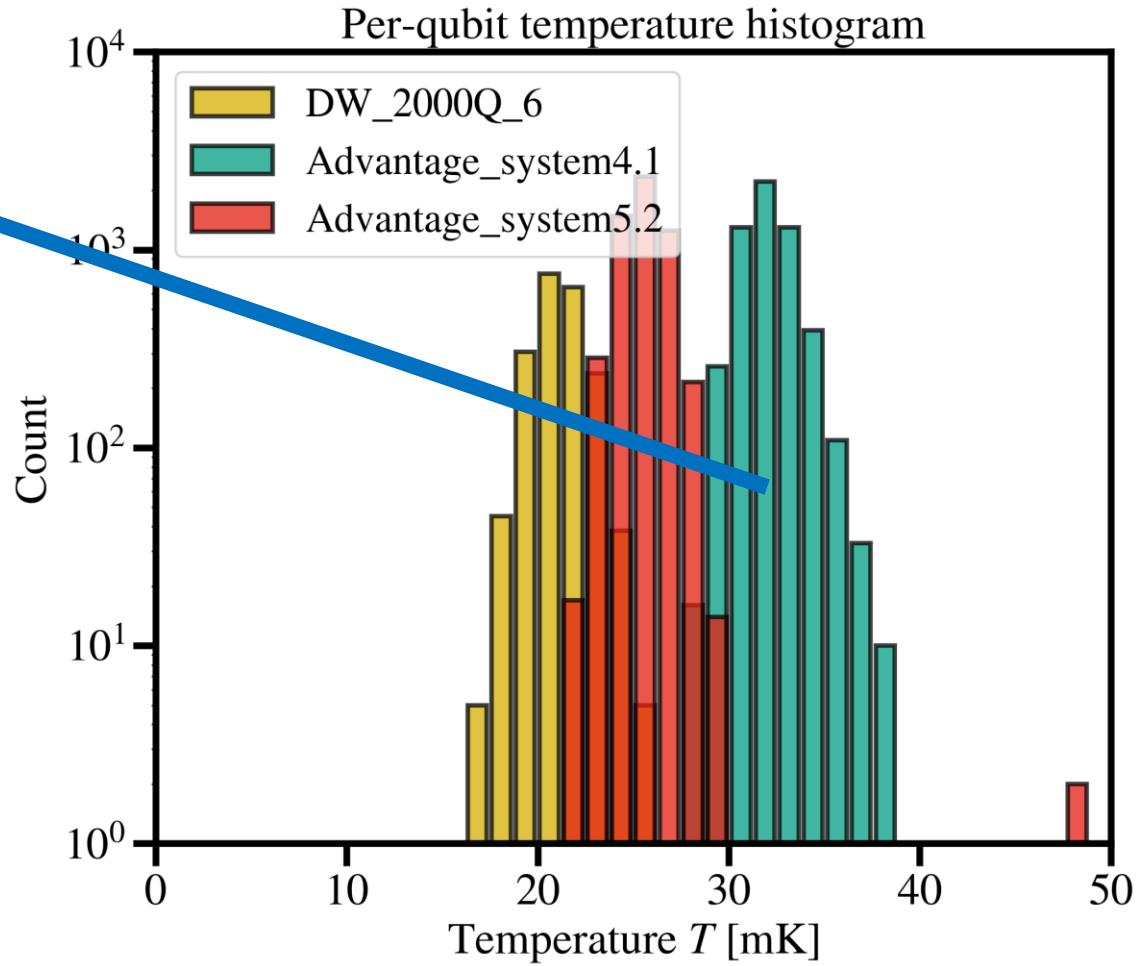
QUANTUM BOLTZMANN MACHINES

Experiment #1: Effective per-qubit temperature distribution

Advantage_system4.1







Perot et al. (2022)
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QUANTUM BOLTZMANN MACHINES

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

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

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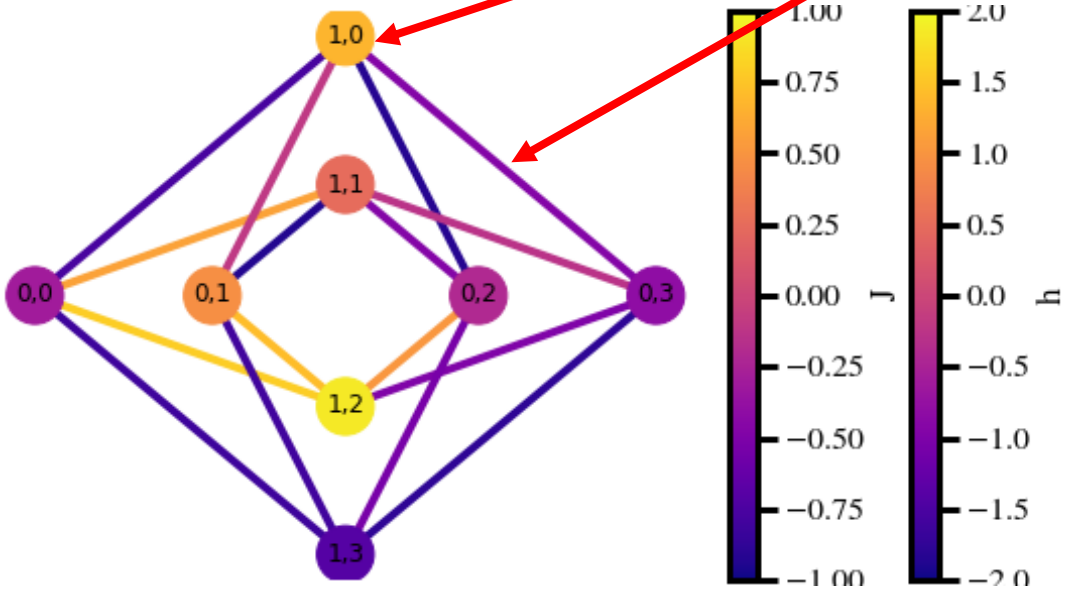

QUANTUM BOLTZMANN MACHINES

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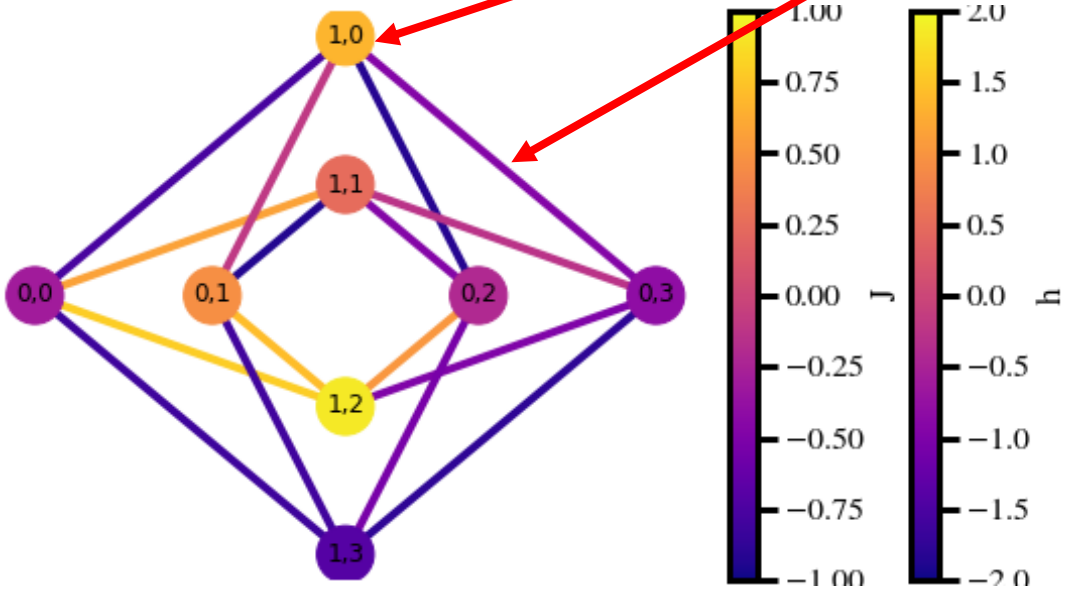

Fit Boltzmann distribution to observed samples at $s = 1$ to infer $\beta = 1/k_B T$:

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

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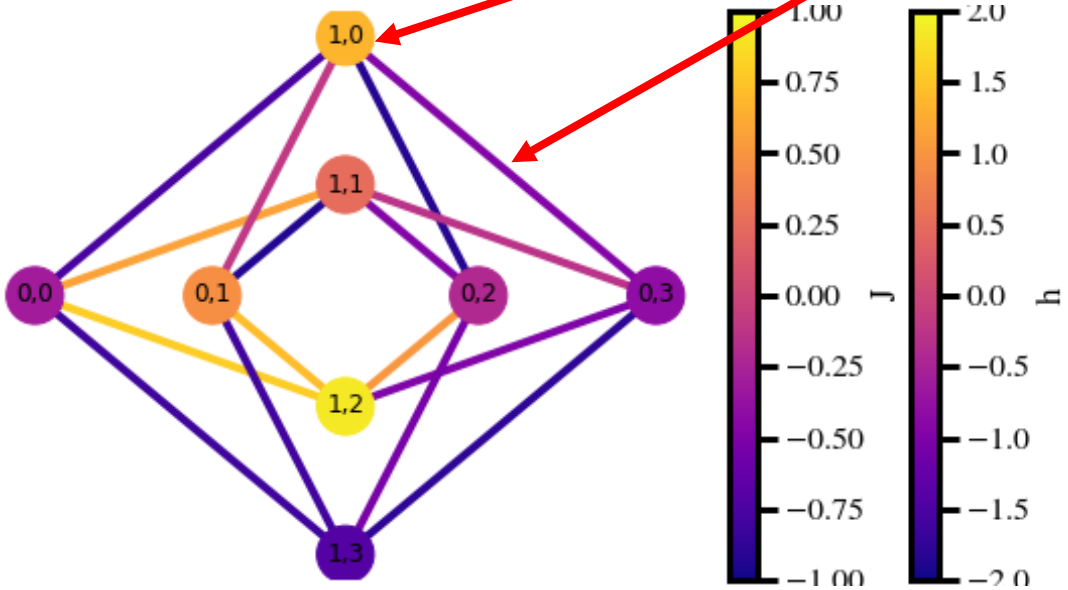

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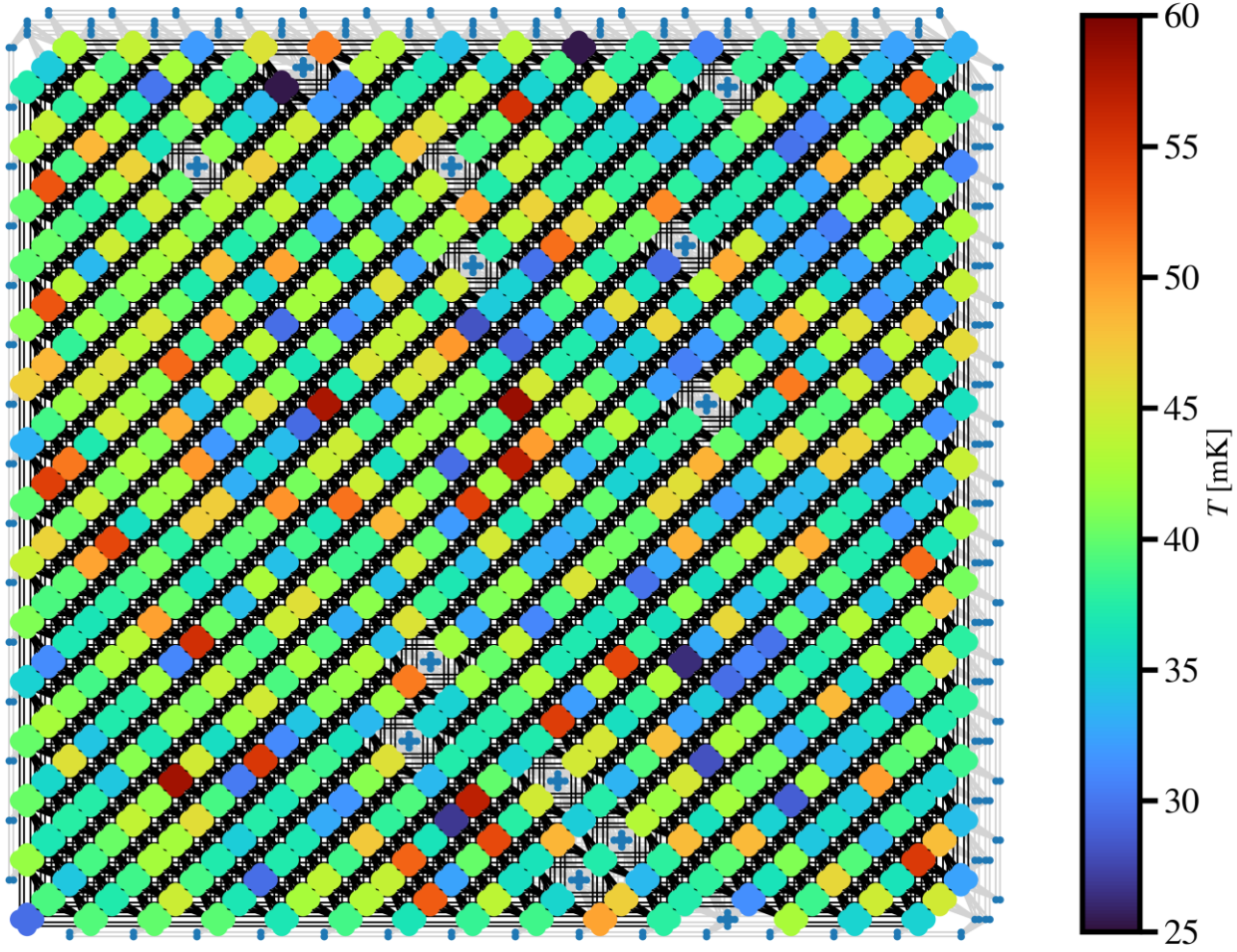

Perot et al. (2022)
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QUANTUM BOLTZMANN MACHINES

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

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

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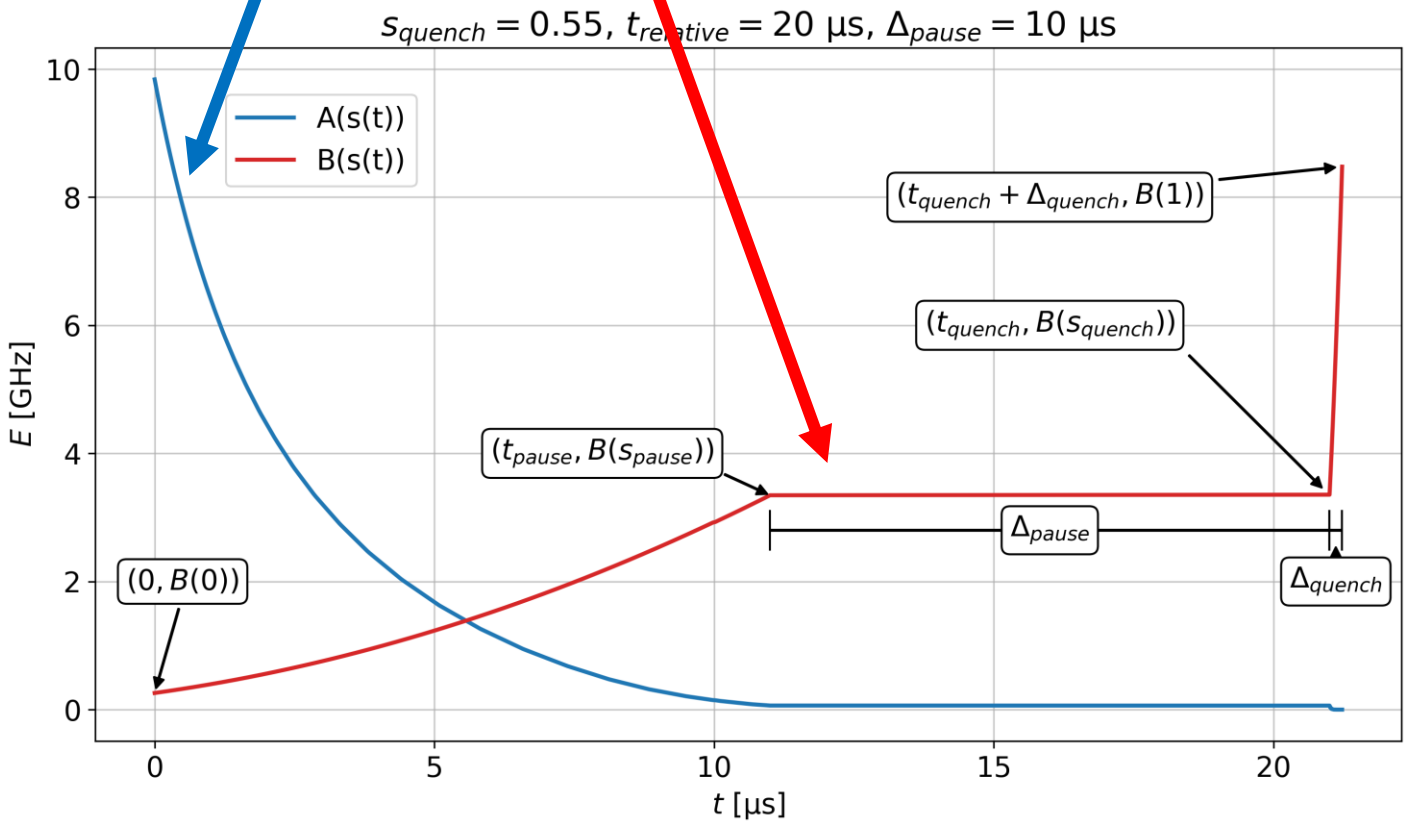

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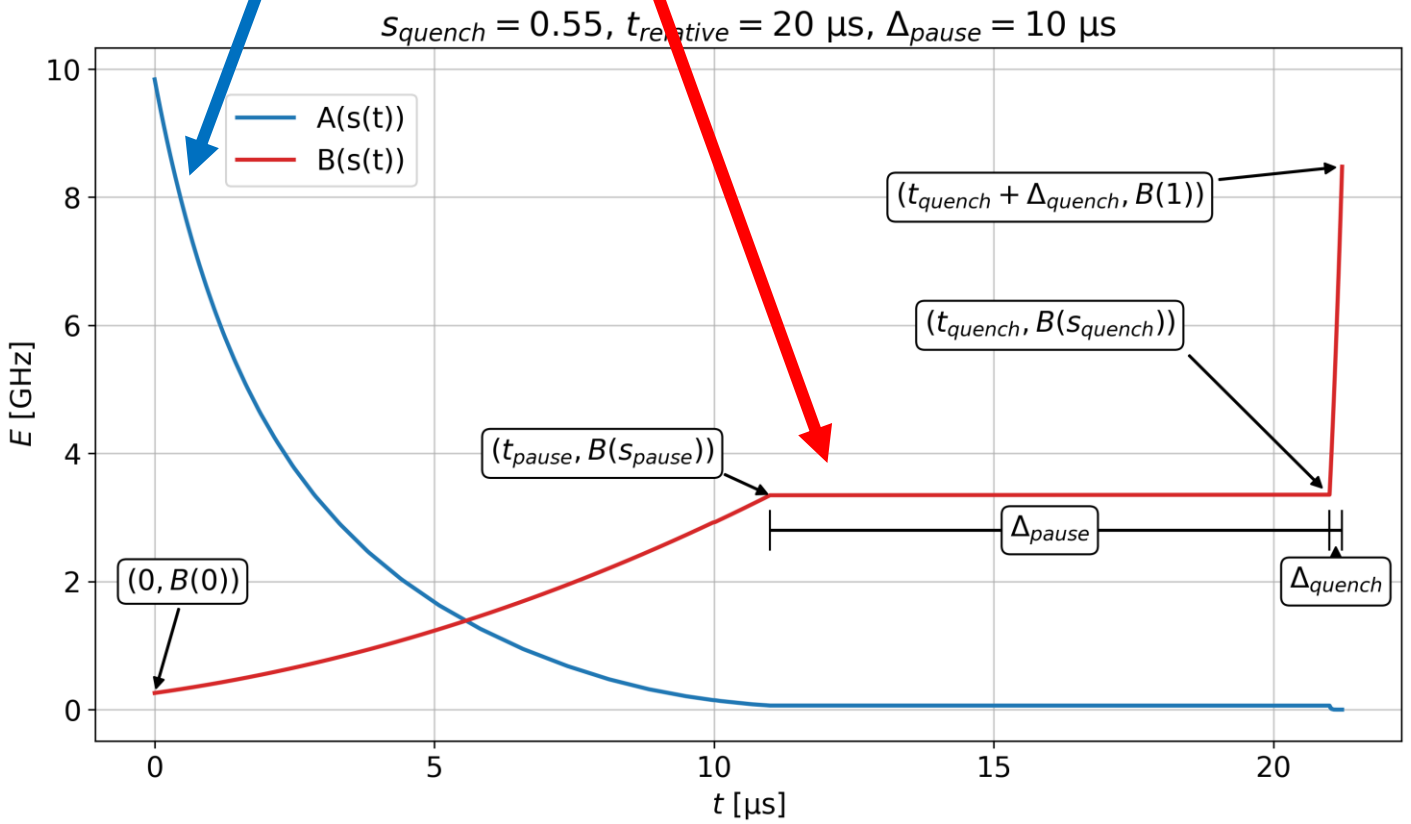

Quantum Boltzmann distribution
at inverse temperature β and time s:

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

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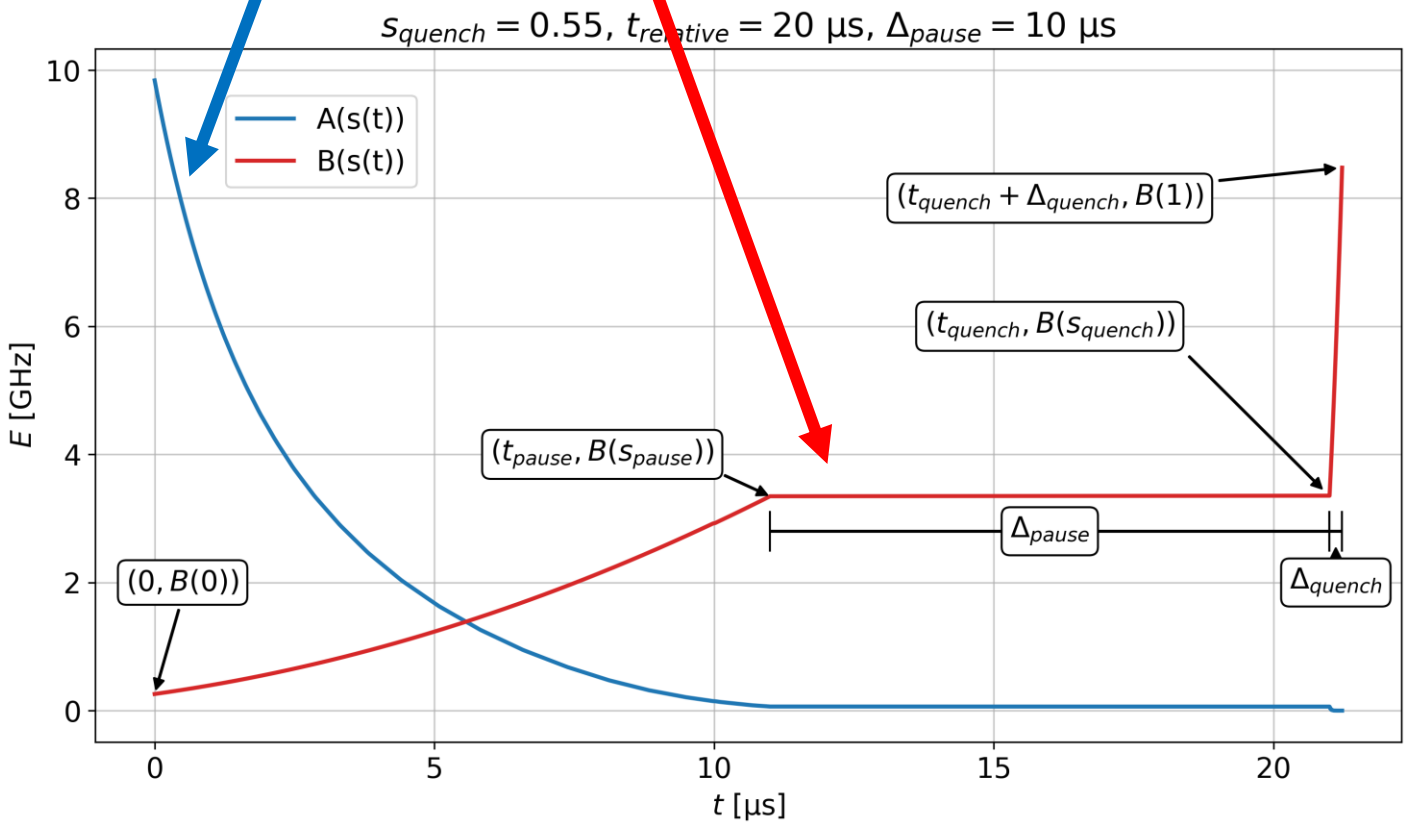
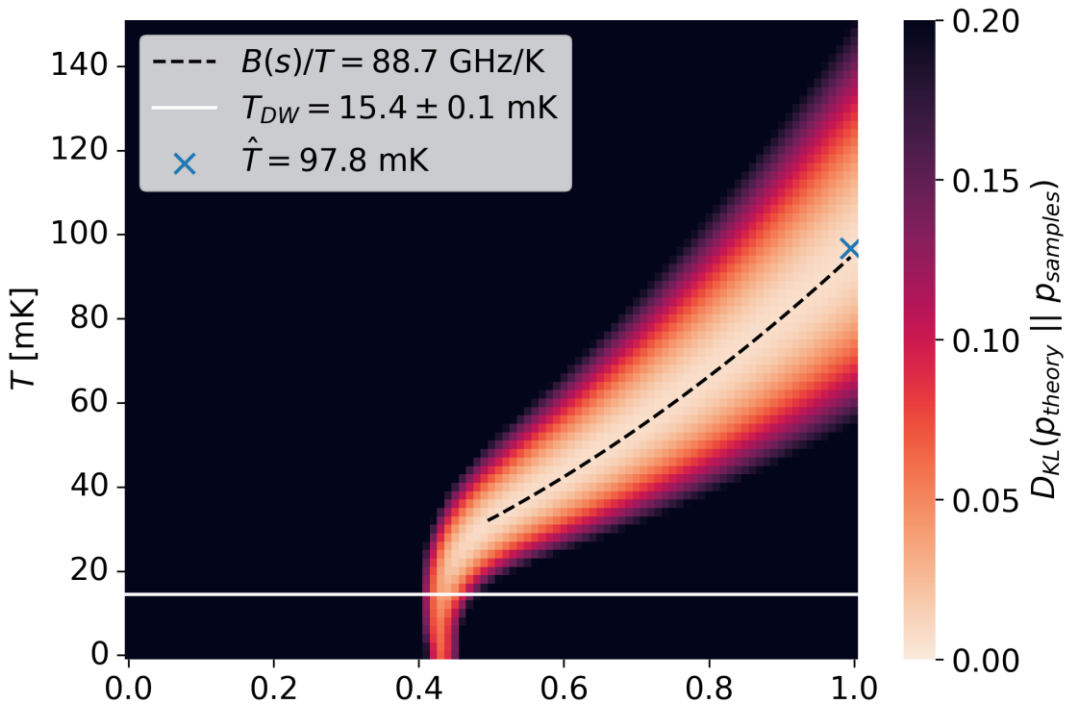




Perot et al. (2022)
https://jugit.fz-juelich.de/qip/qbm-quant-finance

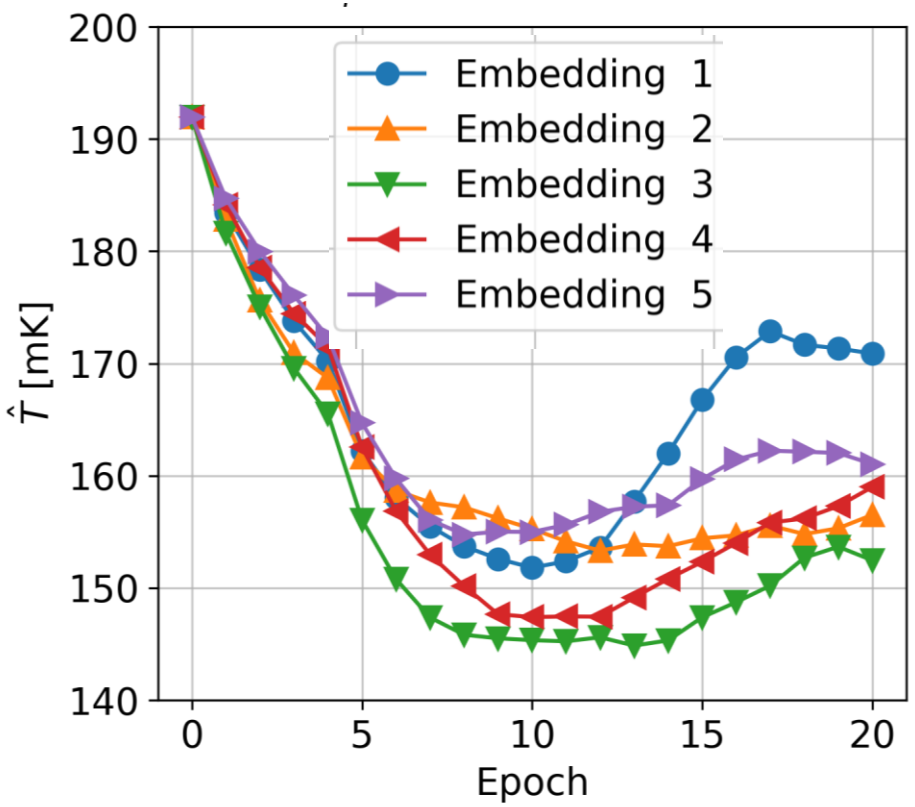
QUANTUM BOLTZMANN MACHINES

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

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)



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

QUANTUM BOLTZMANN MACHINES

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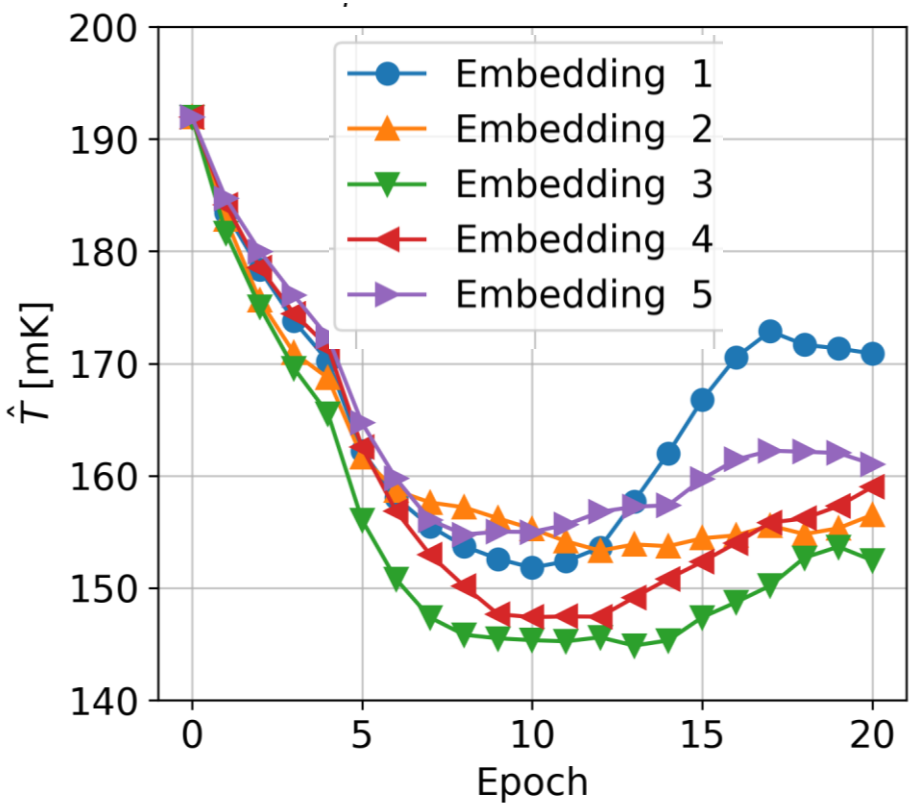

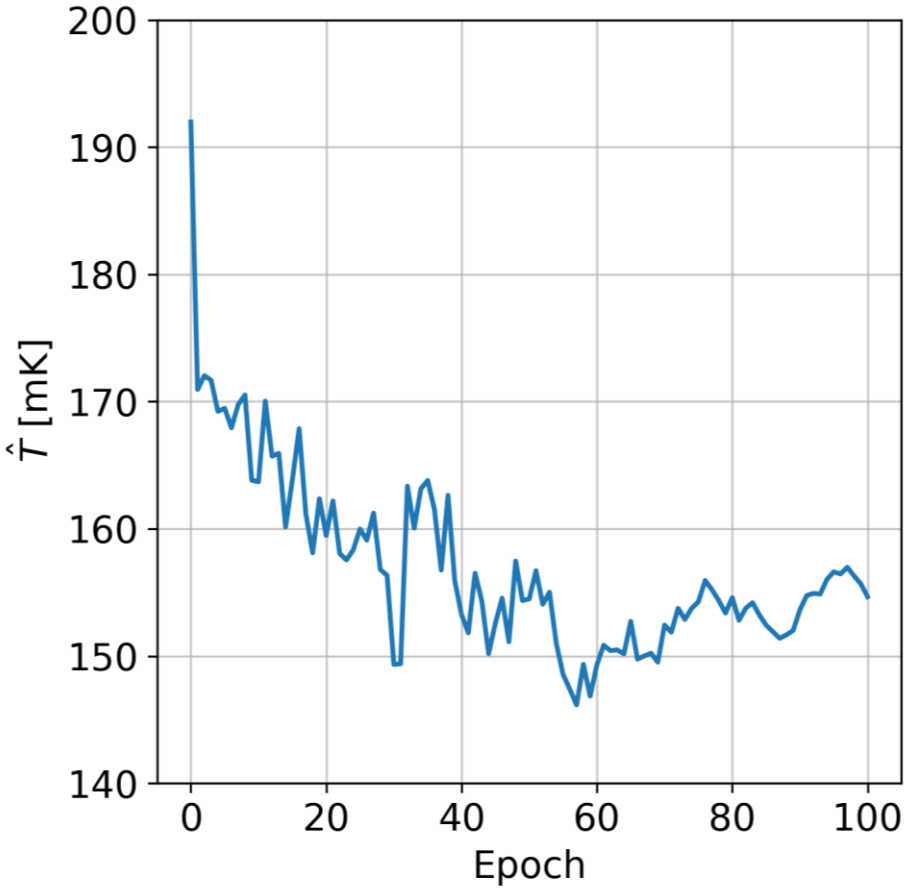

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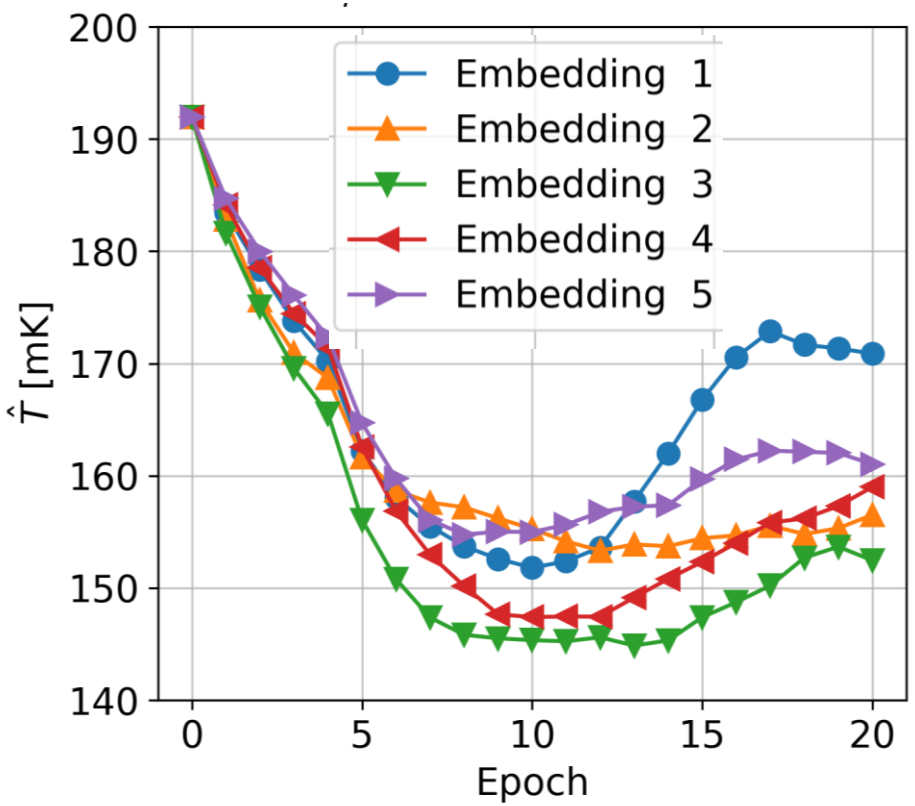
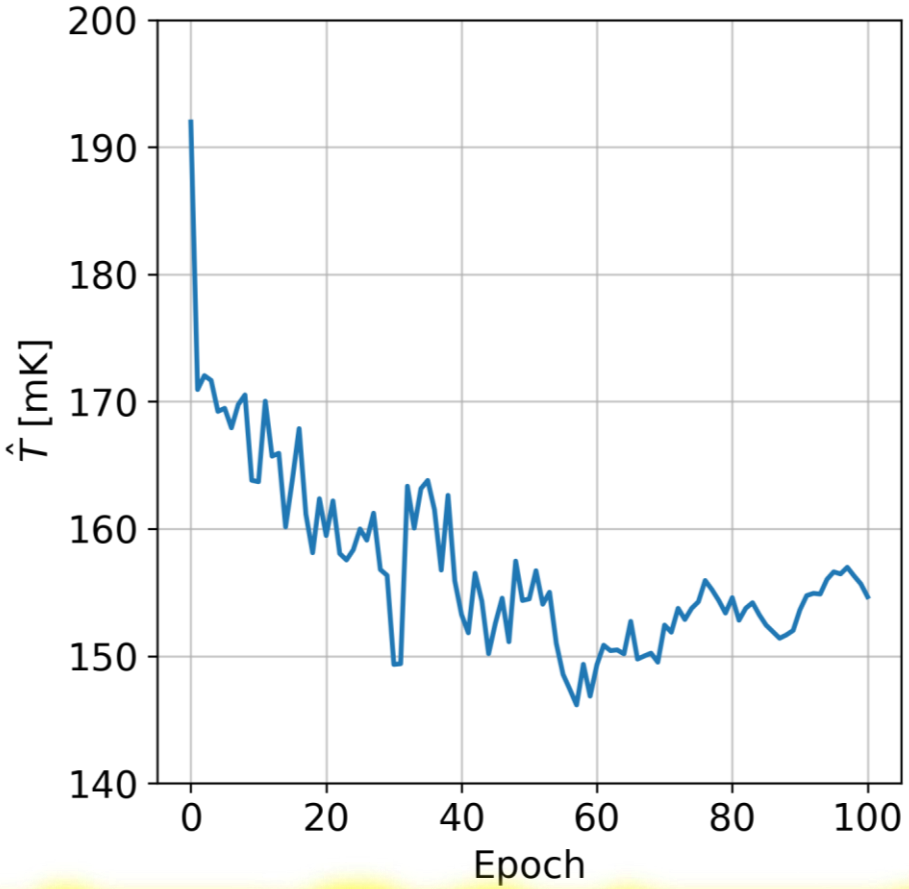
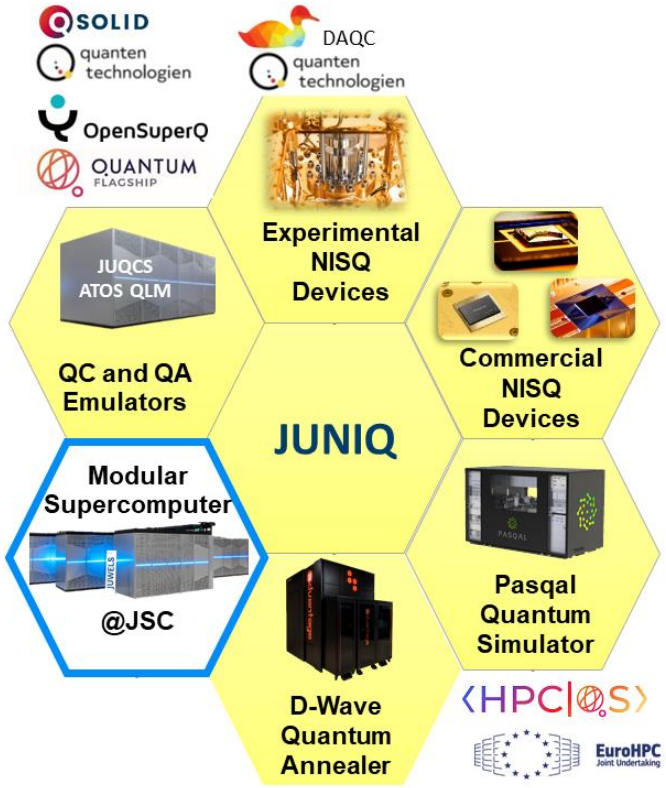




→ Observation: Larger problems ~ larger effective temperature

SUMMARY



JUNIQ Rolling Call:

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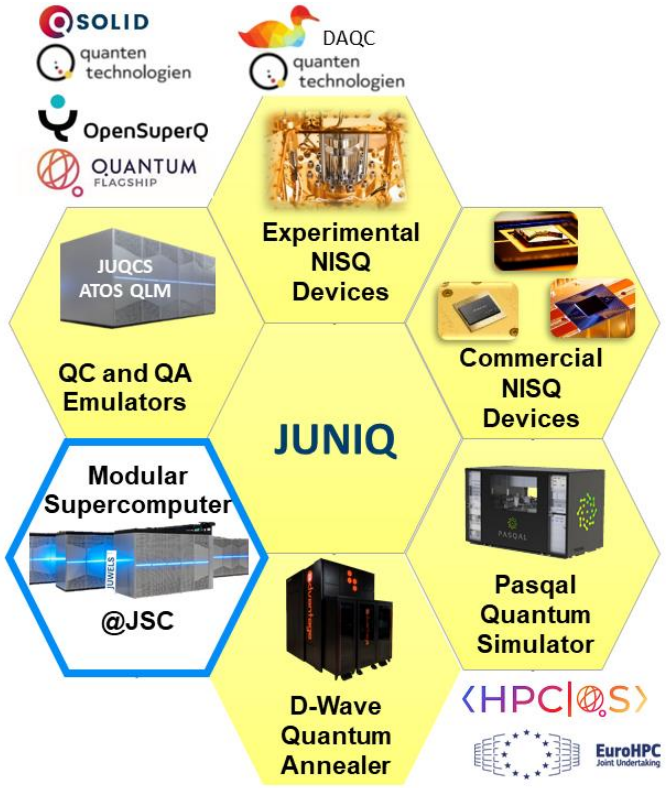
SUMMARY

1. Airline Scheduling



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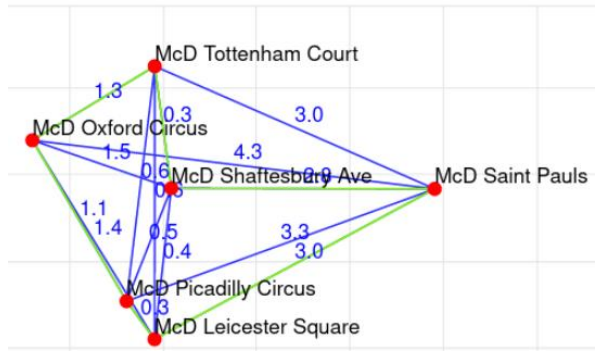
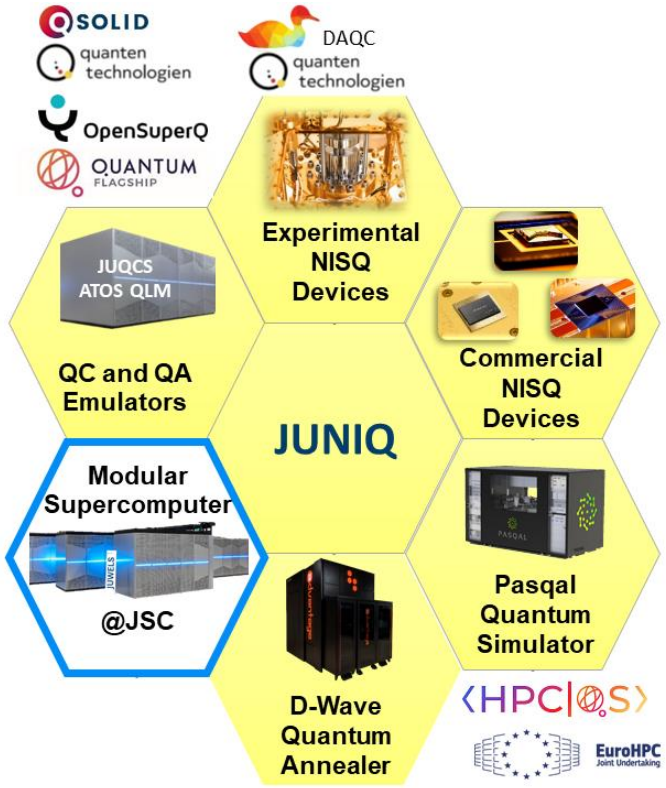
SUMMARY

1. **Airline Scheduling**
2. **Traveling Salesman**





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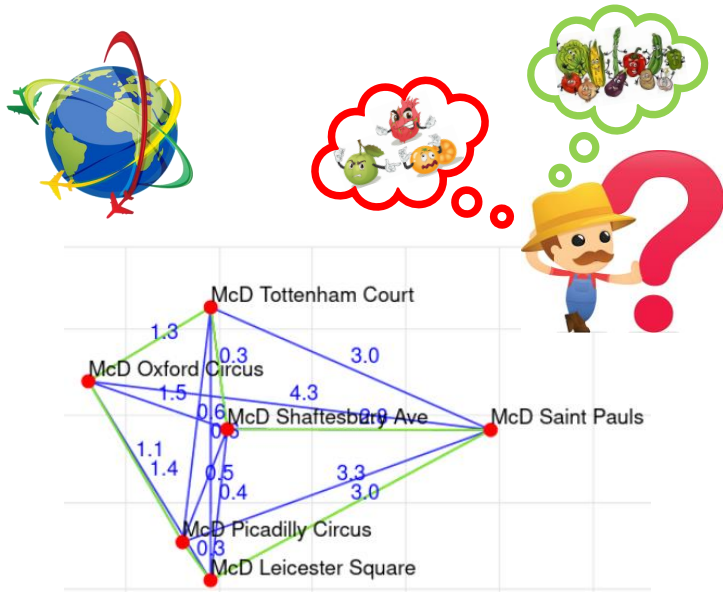
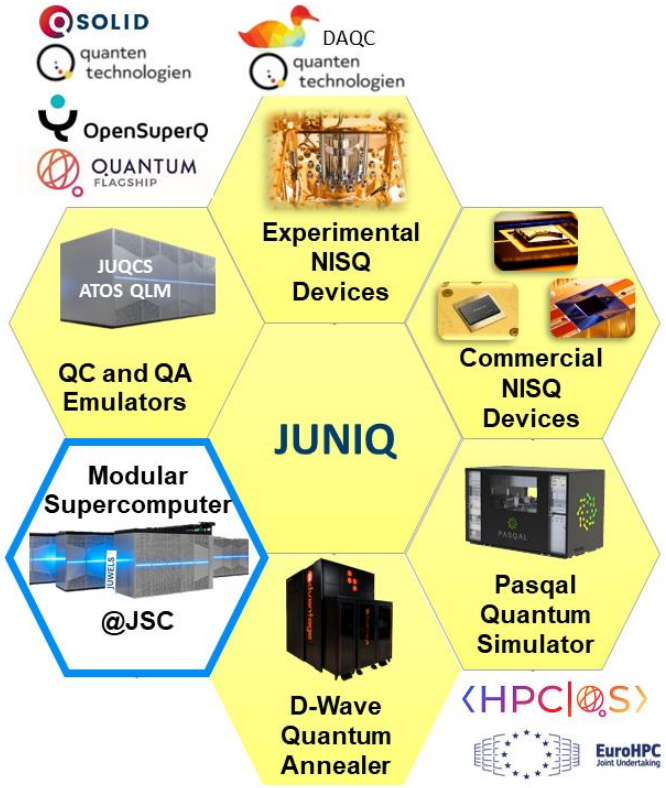
SUMMARY

1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization





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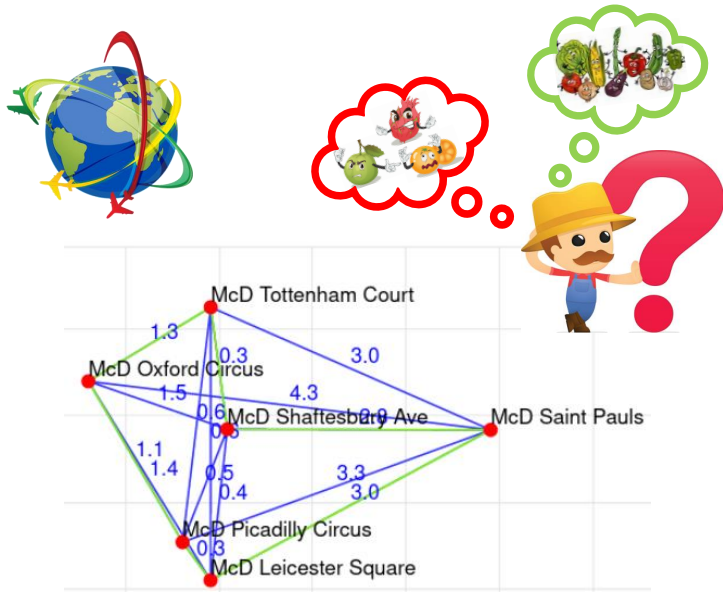
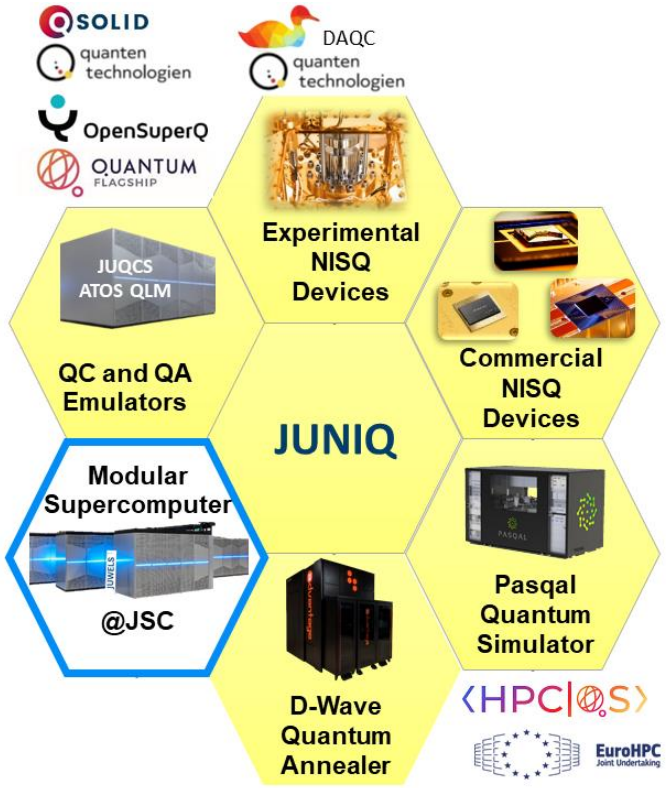
SUMMARY

1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization

optimization problem
with constraints
[increasing complexity]





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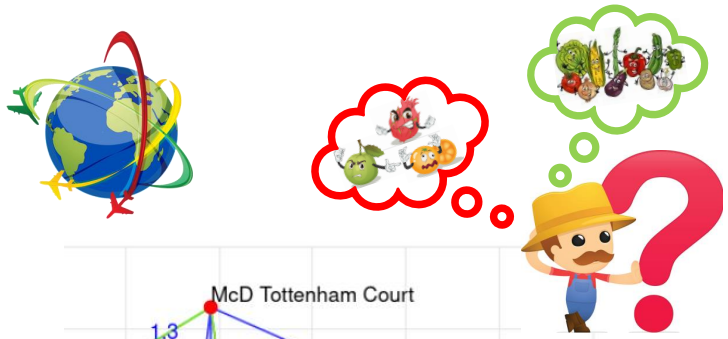
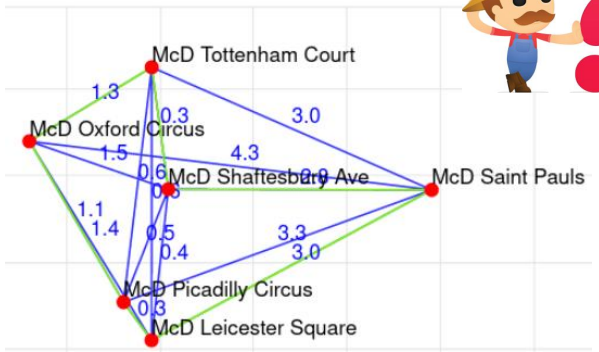
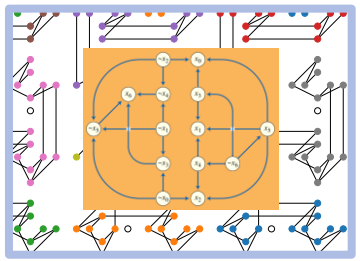
SUMMARY

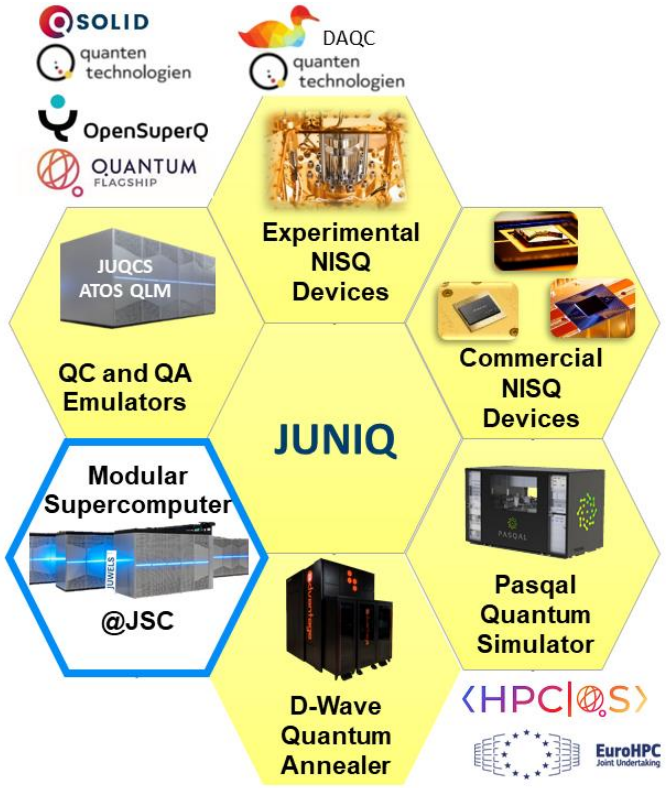
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability

optimization problem
with constraints
[increasing complexity]









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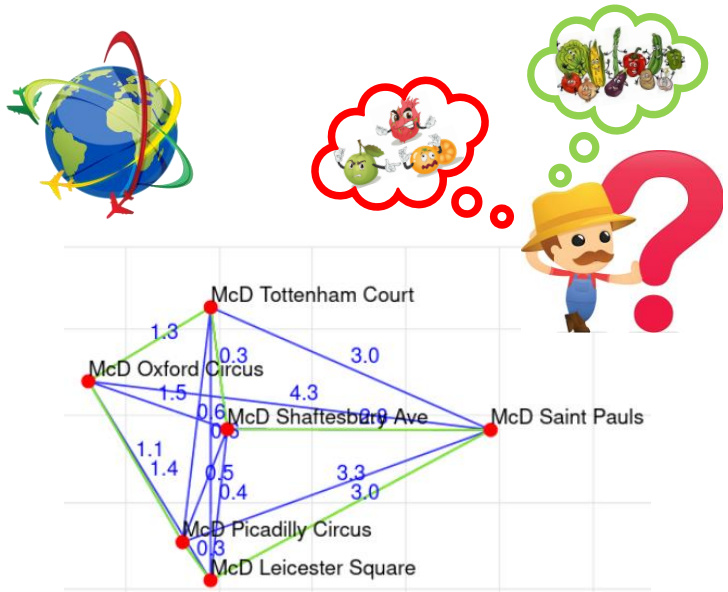
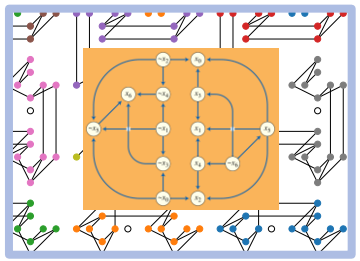
SUMMARY

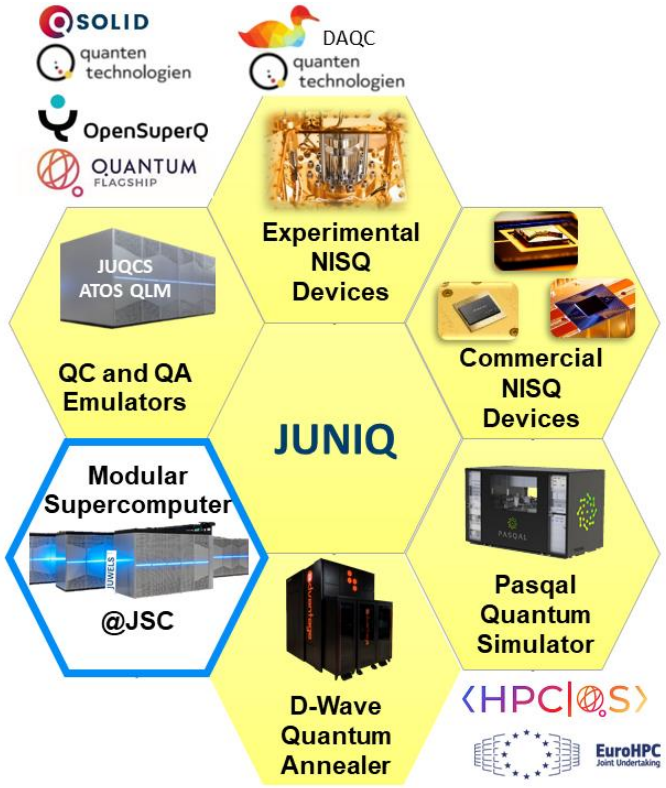
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability

optimization problem with constraints [increasing complexity]

constraints only







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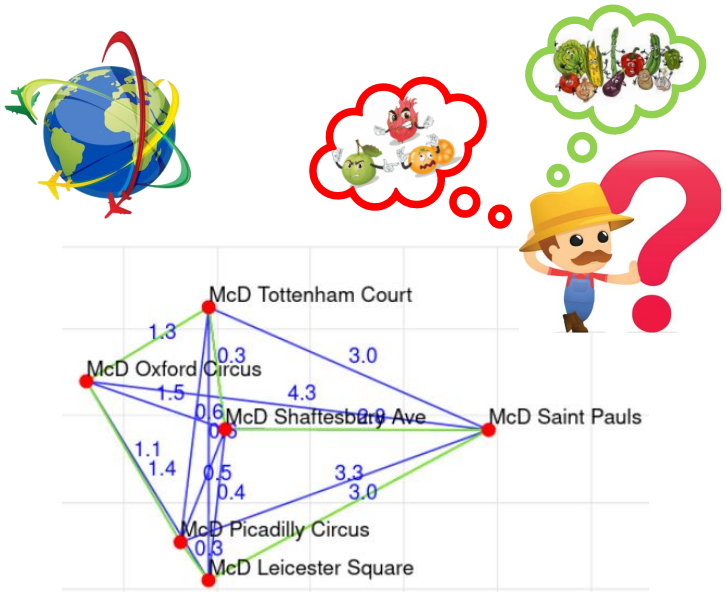
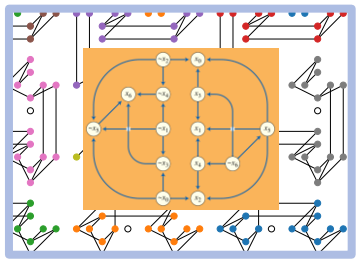
SUMMARY

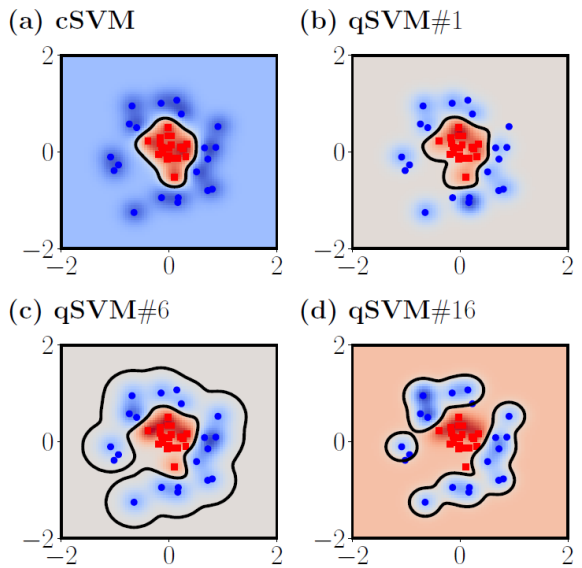
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability
5. QSVM

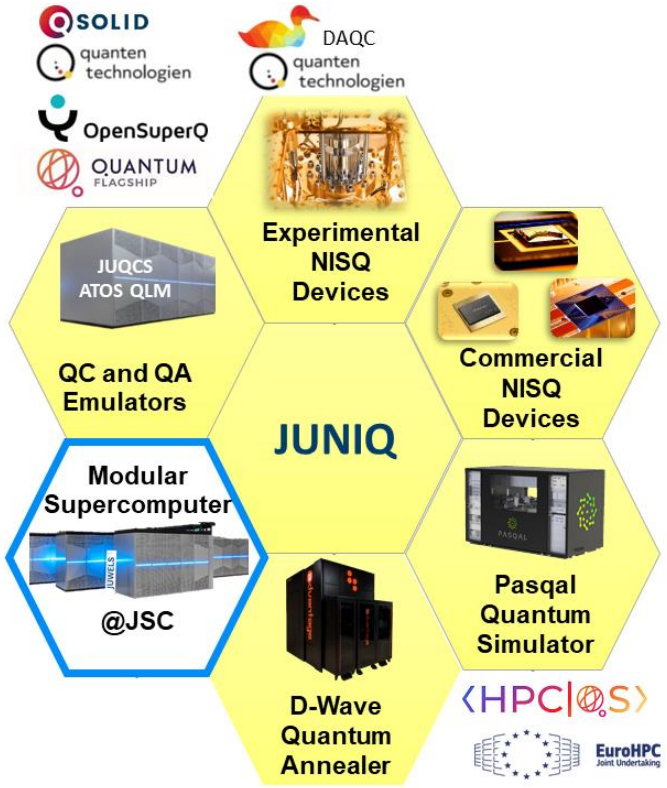
optimization problem with constraints [increasing complexity]

constraints only









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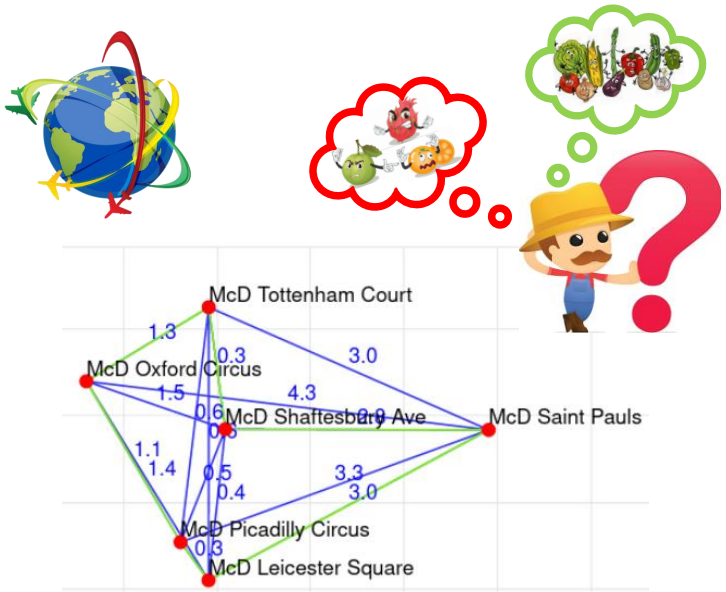
SUMMARY

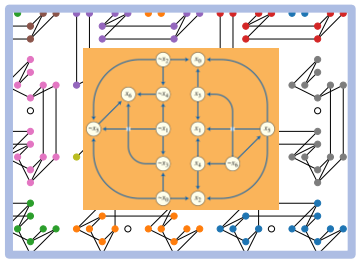
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability
5. QSVM

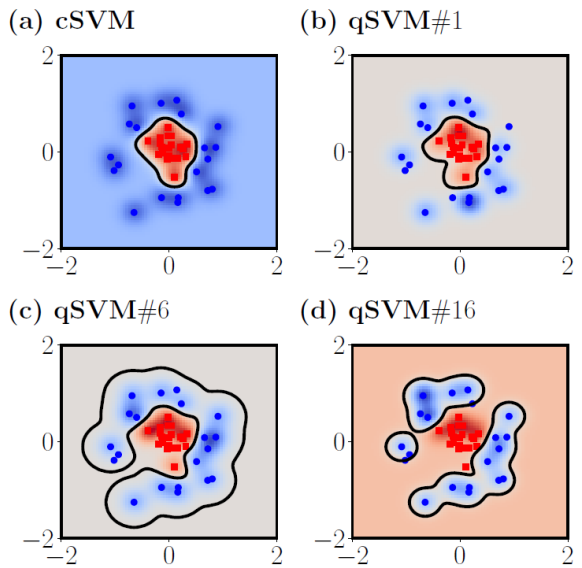
optimization problem with constraints [increasing complexity]

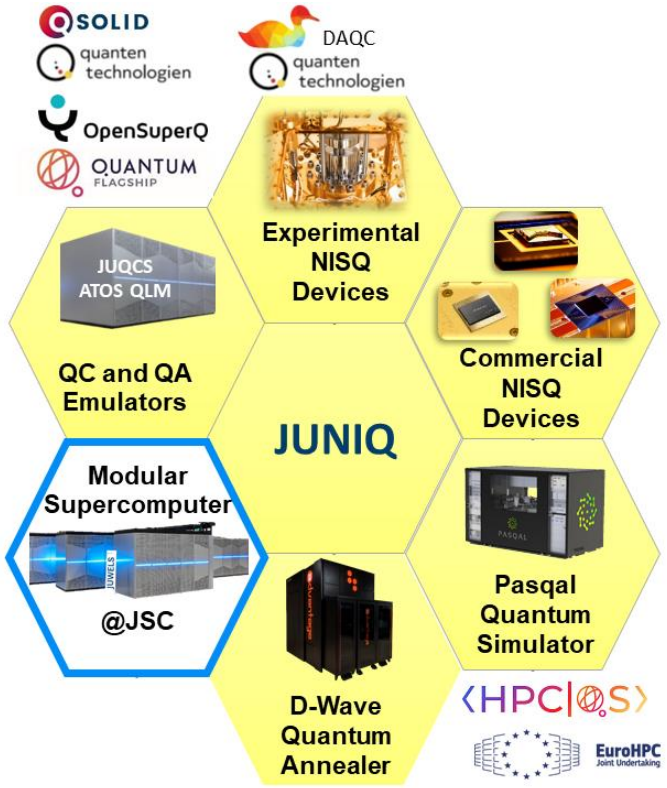
constraints only

optimization only [basically]









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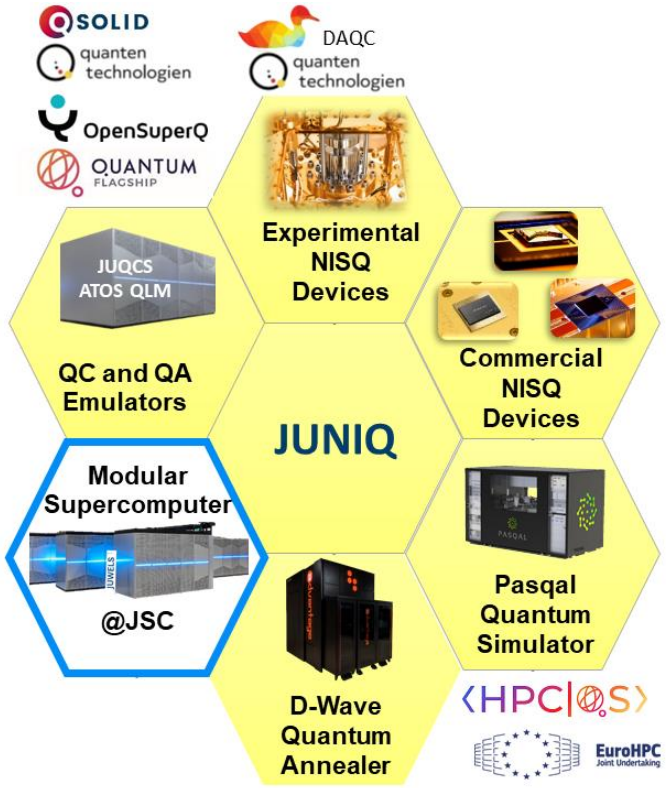
SUMMARY

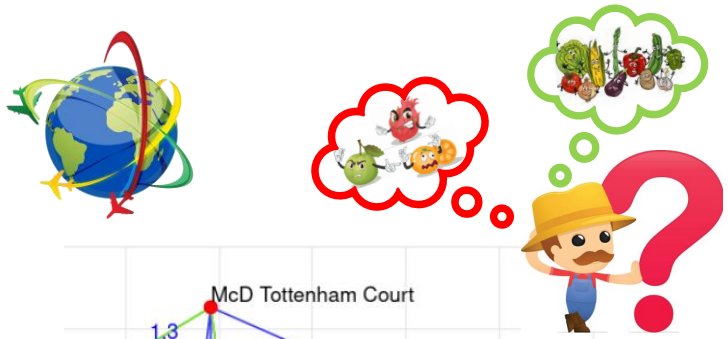
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability
5. QSVM
6. QBM

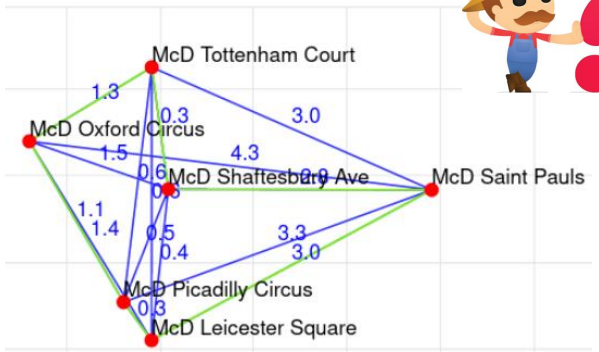
optimization problem with constraints [increasing complexity]

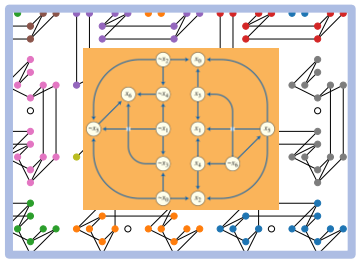
constraints only

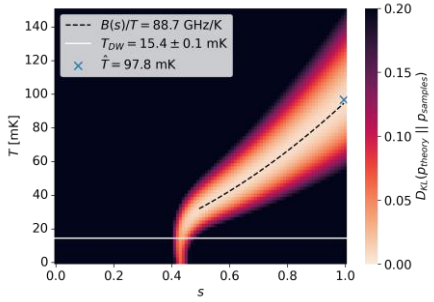
optimization only [basically]

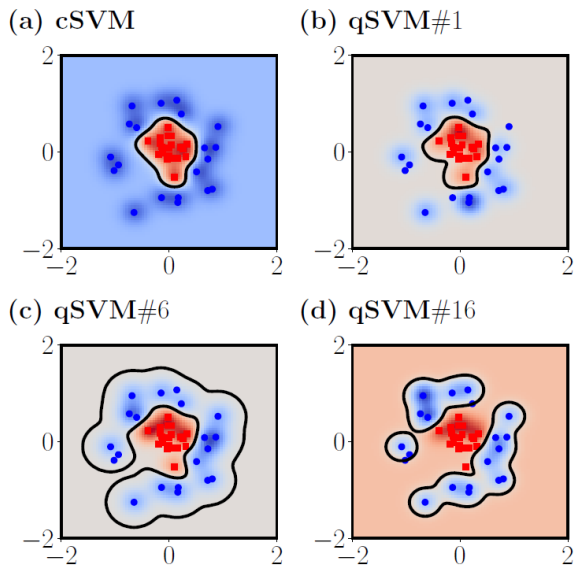












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1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability
5. QSVM
6. QBM

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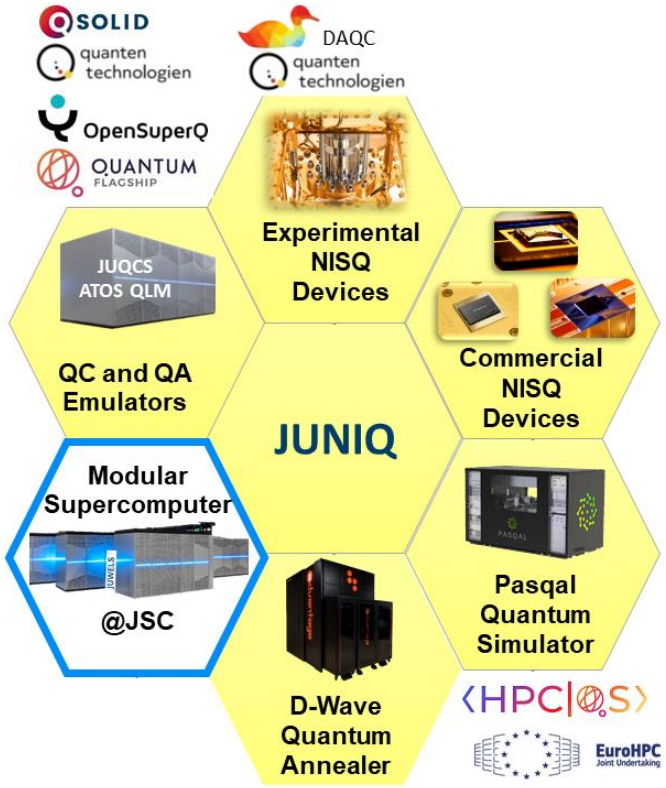

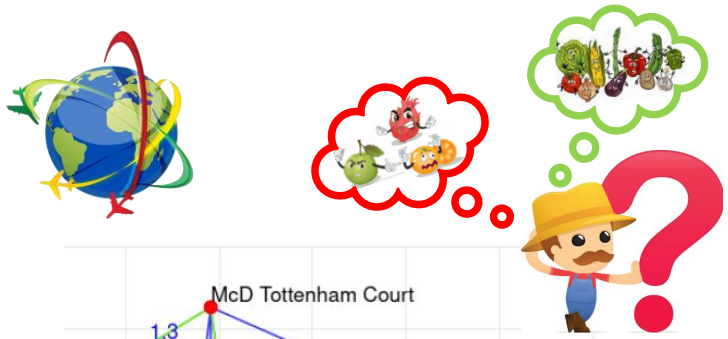

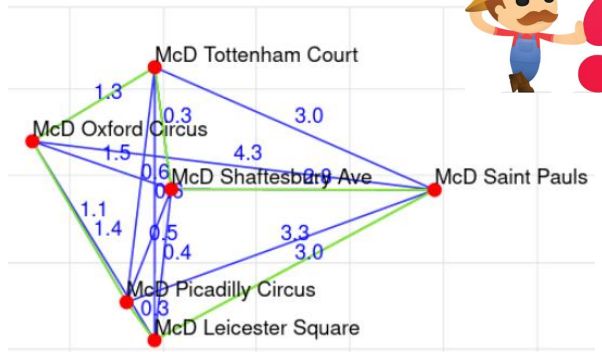

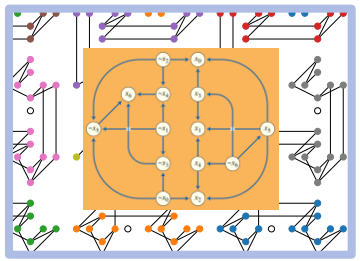

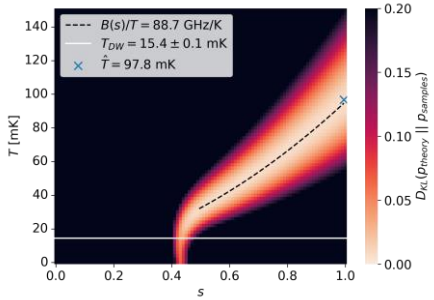

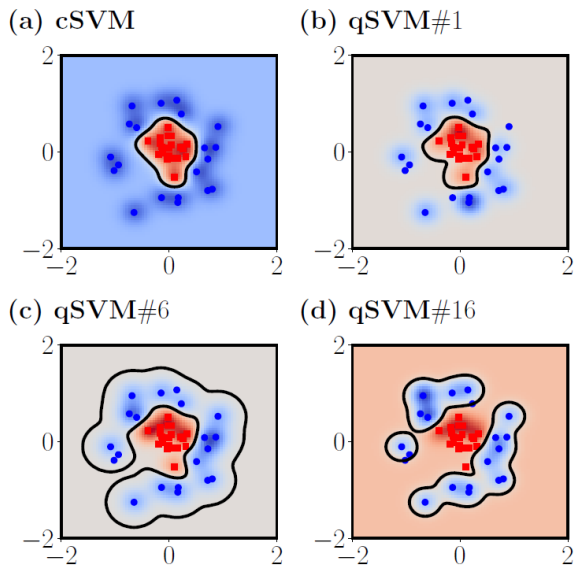

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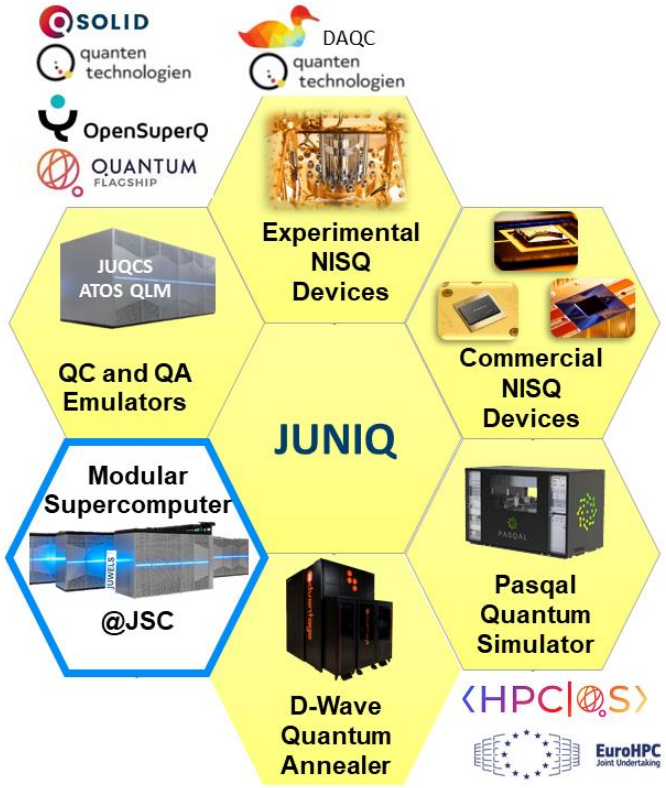

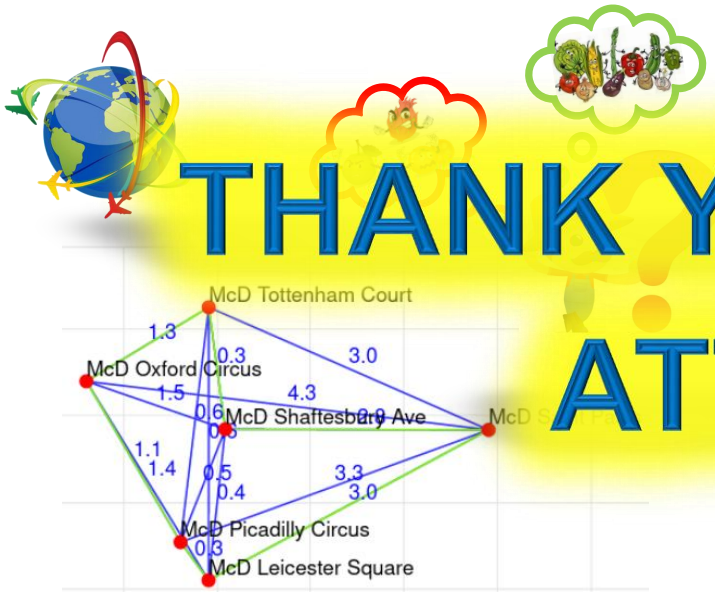

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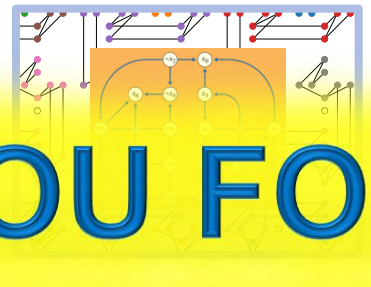

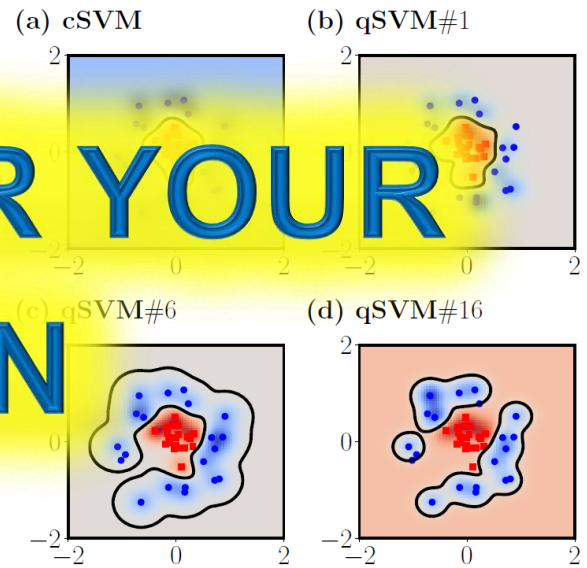

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