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Hybrid Quantum Branch-and-Bound Method for Quadratic Unconstrained Binary Optimization

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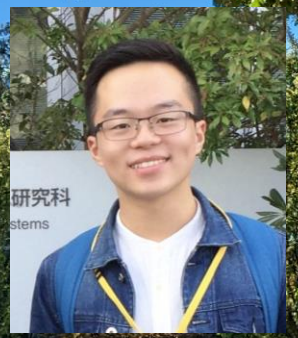


SEQUOIA

Background: QUBO and Quantum Optimization

Quadratic Unconstrained Binary Optimization (QUBO)

- Quadratic objective function
- No Constraints
- Binary variables

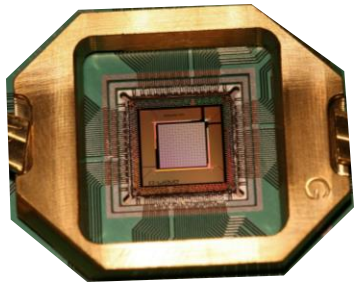
QUBO

$$\min_{\mathbf{x}} \quad \mathbf{x}^\top Q\mathbf{x} + 2l^\top \mathbf{x}$$
$$\text{s.t.} \quad x \in \{0,1\}$$

$\Longleftrightarrow$

Ising Model

$$\min_{\mathbf{s}} \quad \mathbf{s}^\top J\mathbf{s} + 2h^\top \mathbf{s}$$
$$\text{s.t.} \quad s \in \{\pm 1\}$$



Quantum Computer

- Applications
  - Quadratic Assignment Problems
  - Capital Budgeting Problems
  - Task Allocation Problems
  - Maximum Diversity Problems
  - P-Median Problems
  - Quadratic Knapsack Problems

Ref: [1] Glover, F., Kochenberger, G., Hennig, R., & Du, Y. (2022). Quantum bridge analytics I: a tutorial on formulating and using QUBO models. Annals of Operations Research, 314(1), 141-183.
[2] Mohseni, N., McMahon, P. L., & Byrnes, T. (2022). Ising machines as hardware solvers of combinatorial optimization problems. Nature Reviews Physics, 4(6), 363-379.

Algorithms to solve QUBOs

Exact Algorithms[1]

- Branch & Prune method
- Branch & Bound method
- Branch & Cut method
  - *Presolving*
  - *Domain propagation*
  - *Decomposition*
  - *Primal heuristics*
  - *Branching (pseudo-costs* branching)
  - Cutting planes (odd-cycle cuts)

MIQP solvers: CPLEX, Gurobi, SCIP, BARON, etc.

Heuristic & Approximation algorithm[2]

- Simulated annealing
- Tabu search
- Local search
- Scatter search
- Evolutionary algorithm

Heuristic Solvers: Algorithms implemented in MQLib

Quantum methods

- Quantum Alternating Optimization Algorithm (QAOA)
- Quantum Annealing (QA)

Quantum Solver: D-Wave Quantum Annealer

Ref: [1] Kochenberger, G., Hao, J. K., Glover, F., Lewis, M., Lü, Z., Wang, H., & Wang, Y. (2014). The unconstrained binary quadratic programming problem: a survey. Journal of combinatorial optimization, 28, 58-81.
[2] Dunning, I., Gupta, S., & Silberholz, J. (2018). What works best when? A systematic evaluation of heuristics for Max-Cut and QUBO. INFORMS Journal on Computing, 30(3), 608-624.
[3] Abbas, A., Ambainis, A., Augustino, B., Bärtschi, A., Buhrman, H., Coffrin, C., ... & Zoufal, C. (2023). Quantum optimization: Potential, challenges, and the path forward. arXiv preprint arXiv:2312.02279.

Goal: Solve QUBOs to Global Optimality

Branch and Bound

- Provides optimality bounds of the solution
- Can be slow for large problems
- For QUBO, strong cutting planes have not been developed (compared to constrained MIP problems)

Quantum Annealing

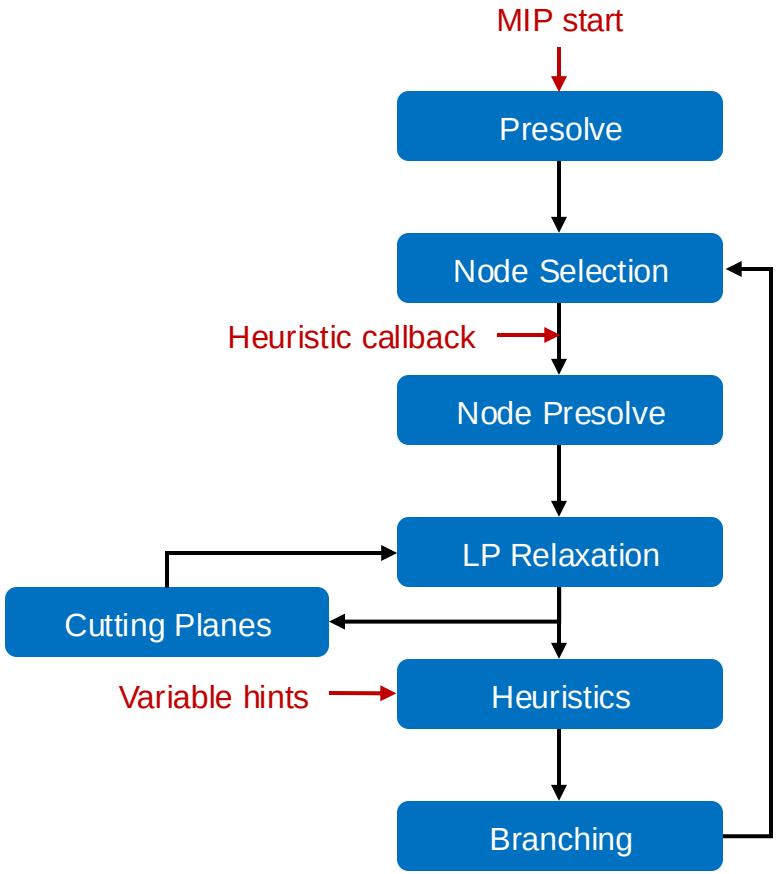
- Does not guarantee optimality
- Potentially more efficient at obtaining good quality solutions for problems up to the number of qubits in the quantum annealer

GUROBI OPTIMIZATION + D-Wave The Quantum Computing Company™

Injecting Solution Information to Gurobi

Three ways to inject solution information into Gurobi

1. **MIP start** ✓
   - Pass a known feasible or partial solution when optimization starts
   - MIP solver will try to reproduce that solution
2. **Heuristic Callbacks** ✓
   - User code called at each node of the branch-and-cut tree
   - Can query relaxation solution, and can inject a feasible solution (or partial solution)
3. **Variable hint**
   - Pass hints about promising values for variables, and the relative priorities of those hints



Branch & Cut method in Gurobi

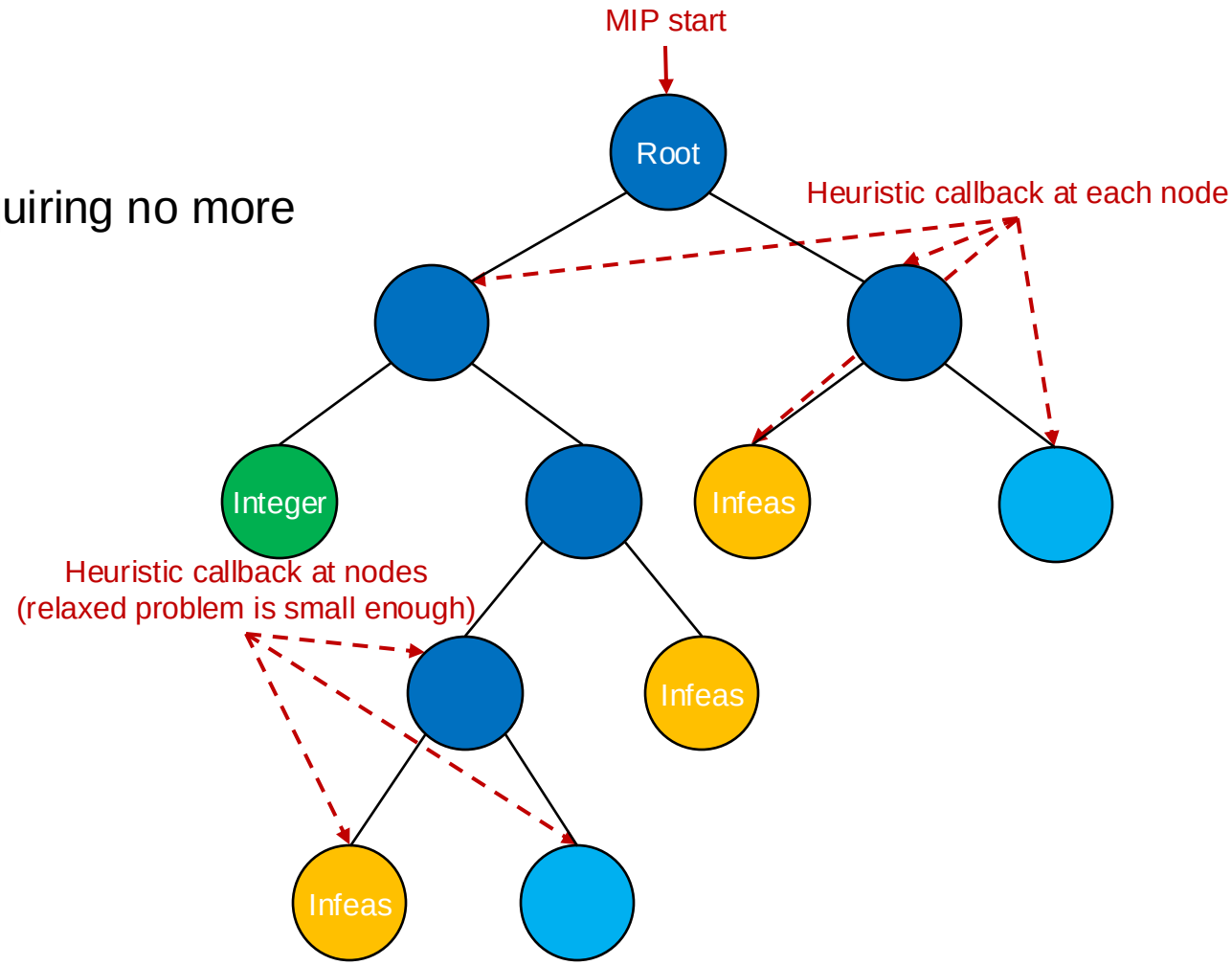
Ref: [1] https://assets.gurobi.com/pdfs/user-events/2017-frankfurt/MIP-Models-and-Heuristics.pdf

Injecting Solution Information to Gurobi

Quantum Processing Unit (QPU) solver

- decomposes a large problem into subproblems requiring no more than the number of qubits available on the QPU.

1. **MIP start** ✓
   - Top 1, 10, 30, 100 heuristic solutions
2. **Heuristic Callbacks** ✓
   - At each node, let the (quantum) heuristic find solutions to it.
   - At nodes where the relaxed problem is small enough for Quantum Computer.
   - Apply QPU solver once. Store the solution pool and provide the solution from the pool at the proper nodes.



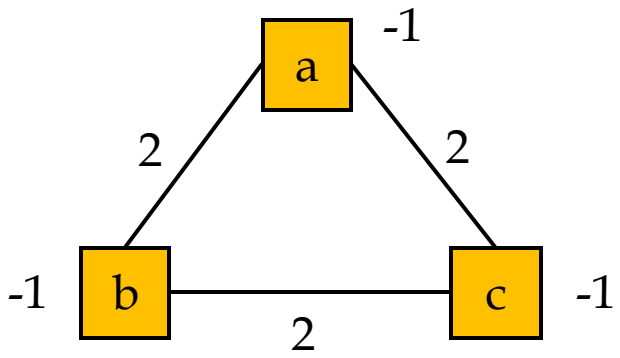
Branch and Bound Tree

Ref: [1] https://assets.gurobi.com/pdfs/user-events/2017-frankfurt/MIP-Models-and-Heuristics.pdf

Branch Priority

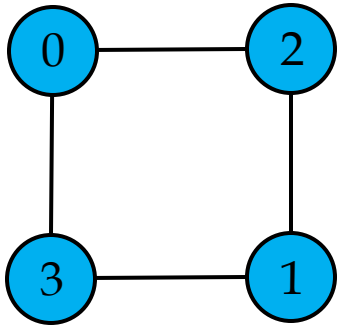
Motivation

- **Embedding**: mapping all the variables of a QUBO problem to the physical qubits on quantum computers.

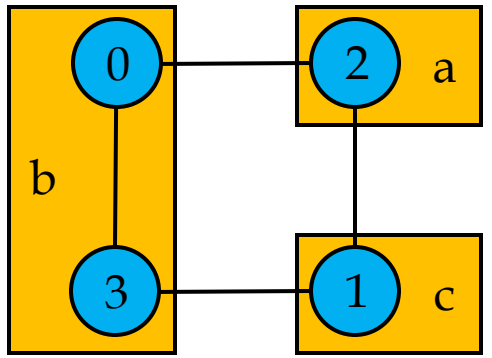


Triangular graph of QUBO

min $2ab+2ac+2bc-a-b-c$



QPU Topology



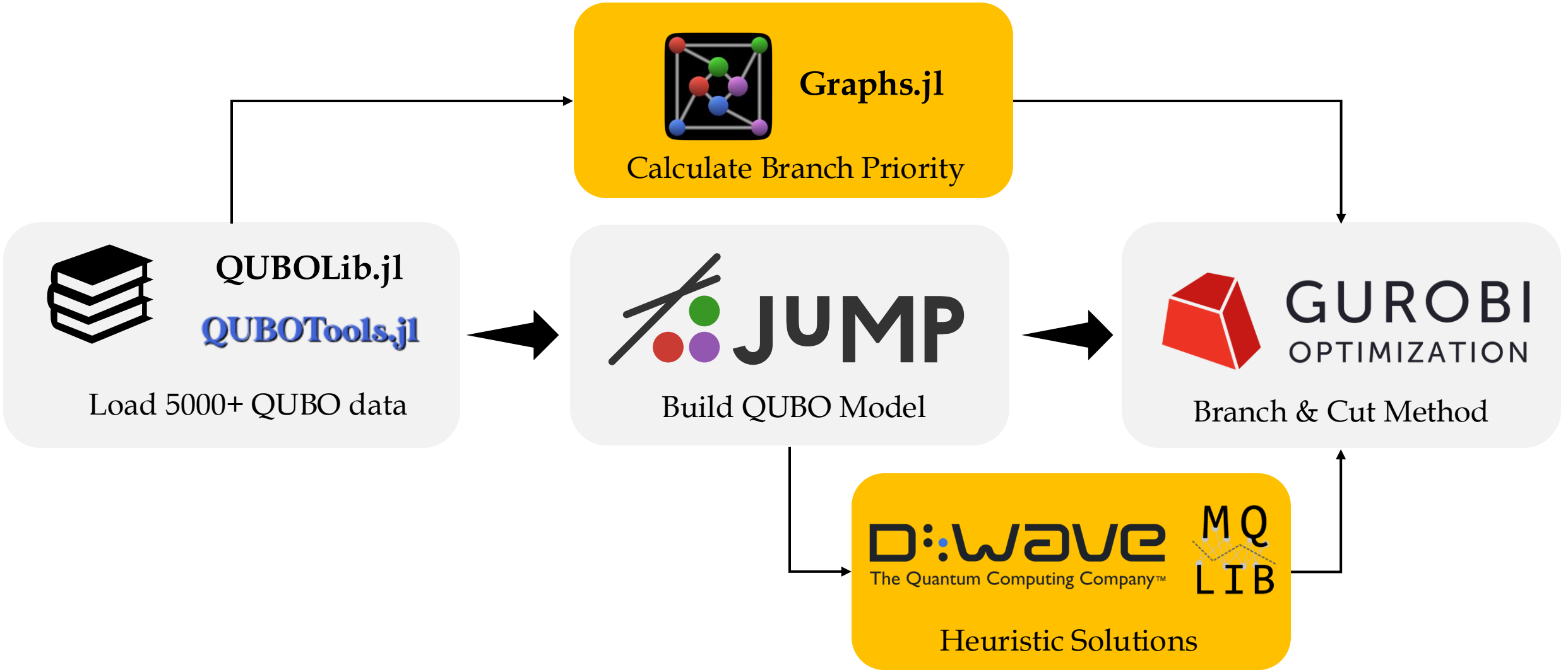
Embedding

Intuition: Fix the most connected variable, and the size of the resulting embedded subproblem will be smaller.

- **Branch Priority** = the degree of the graph induced by matrix **Q**

Ref: [1] https://docs.dwavesys.com/docs/latest/c_gs_7.html#triangle

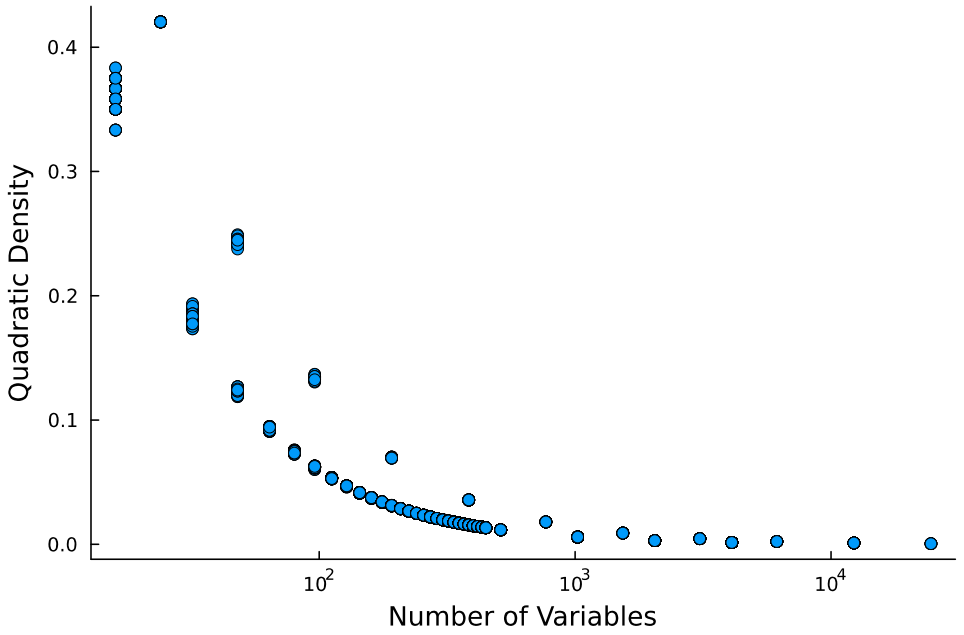
Implementation



Computational Results

- QUBO instances in QUBOLib.jl

Collection	# of instances	# of variables
3-Regular 3-XORSAT Planted Solutions arXiv:2103.08464 (3R3X)	2300	16 ~ 4096
3-Regular 3-XORSAT Planted Solutions arXiv:1903.10928 (3R3X)	3200	16 ~ 4096
5-Regular 5-XORSAT Planted Solutions arXiv:1903.10928 (5R5X)	307	24 ~ 24576



- **Solvability**: Instances take default Gurobi **more than 10 seconds** to solve. (1000)

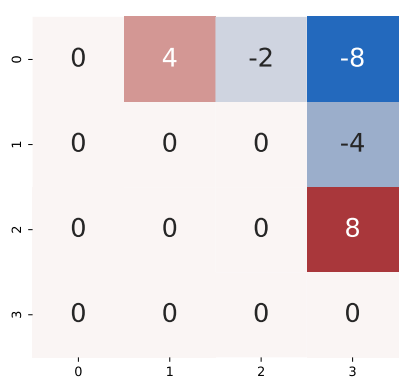
Ref: [1] Kowalsky, M., Albash, T., Hen, I., & Lidar, D. A. (2022). 3-regular three-XORSAT planted solutions benchmark of classical and quantum heuristic optimizers. Quantum Science and Technology, 7(2), 025008.

[2] Hen, I. (2019). Equation planting: a tool for benchmarking Ising machines. Physical Review Applied, 12(1), 011003.

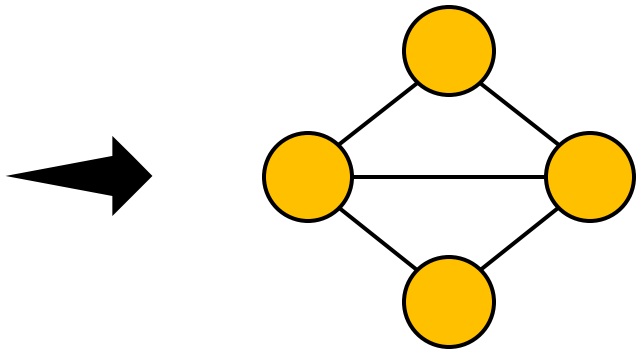
Computational Results

- Benchmark setting
  - **Baseline**: Gurobi 11.0.0 with default parameters
  - Performance index = (experiment - baseline) / baseline
    - Solution time
    - Number of nodes
    - Geometric mean over instances
    - Penalty for failed instances
- For comparison, we apply the following heuristics
  - **Heuristic** methods from MQLib
    (BURER2002, FESTA2002GVNSPR, PALUBECKIS2004bMST3, FESTA2002GPR, FESTA2002GVNS, PALUBECKIS2004bMST2, and etc)
  - **Simulated Annealing** as implemented in dimod.neal V0.5.9.
  - **Quantum Annealing** running on system Advantage 4.1 with 5750 qubits and at least 35000 couplers.

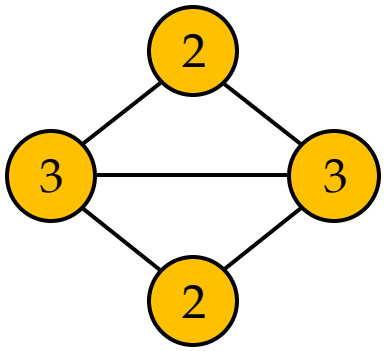
Computational Results – Branch Priority



Q matrix



Generate the graph



Calculate the degree

- Benchmark results

Strategies	Number of Nodes	Solution time
Branch Priority	-22%	-16%

Performance Compare – MQLib Heuristics

We tested 16 heuristic methods in MQLib to provide the heuristic solution to Gurobi.

- **Heuristic callback**: since MQLib only provides the optimal solution, we apply MQLib at each node to solve the subproblem.

Strategies	Heuristic Method	Number of Nodes	Solution time
MIP start (top1)	PALUBECKIS2006 (Best)	-15%	-12%
	FESTA2002G (Worst)	-9%	-5%
	Average MQLib Heuristic	-13%	-7%
	Optimal Solution	-95%	-96%
Heuristic callback	LU 2010 (Best)	-1%	+73%
	FESTA2002GVNSPR (Worst)	+18%	+89%
	Average MQLib Heuristic	+8%	+83%

- Injecting the heuristic solution at MIP start is helpful.
- Triggering heuristic callback at each node is too expensive.

Quantum Annealing & Simulated Annealing

We tested QA and SA in DWave to provide the heuristic solution to Gurobi.

- **Heuristic callback**
  - QUBO heuristic provides the solution pool.
  - Run QUBO heuristic only once and retrieve the solution from the pool at each node.

Strategies	Heuristic Method	Number of Nodes	Solution time
MIP start TOP 1 (TOP 10, TOP 30, TOP 100)	Simulated Annealing	-11% (-12%, -15%, -13%)	-7% (-5%, -10%, -14%)
	Quantum Annealing	-13% (-11%, -11%, -10%)	-6% (-7%, -7%, -4%)
	Quantum Annealing + Embedding	-10% (-15%, -13%, -10%)	-7% (-11%, -8%, -9%)
MIP start + Branch Priority Top 1 (TOP 10, TOP 30, TOP 100)	Simulated Annealing	-20% (-19%, -19%, 20%)	-19% (-13%, -12%, -16%)
	Quantum Annealing	-17% (-19%, -22%, -16%)	-12% (-16%, -11%, -13%)
Heuristic Callback	Simulated Annealing	+1%	+5%
	Quantum Annealing	+4%	+24%
MIP start	Optimal Solution	-95%	-96%

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Thank you!

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