On physical and physics-motivated QUBO–Ising heuristics: applications and perspectives

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GPU Day 2023. Wigner RCP

Outline

- QUBO - Ising - MaxCut
- Solution methods overview
- Railway application 1: direct quanutm annealing
- Result analysis (statistical)
- Railway application 2: hybrid quantum anneling
- Result analysis (OR)
- Outlook: What next?

QUBO

$$\begin{array}{ll} \text{min.} & \mathbf{x}^\top Q\mathbf{x} \\ \text{s.t.} & \mathbf{x} \in \{0,1\}^N \end{array}$$

- Wlg: Q symmetric or upper triangular
- NP-hard
- Covers all linear $0-1$ LPs...
- penalty methods needed for constraints
  c.f. e.g.
  Gusmeroli & Wiegele, Discrete Optimization vol. 44, 100622 (2022).

(Recall: LP)

Linear program:

$$\begin{aligned} \text{min.} \quad & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} \quad & \mathbf{A}\,\mathbf{x} \leq 0 \\ & \mathbf{x} \geq 0 \end{aligned}$$

- Lead to the establishment of a scientific field.
- If your only tool is a hammer then every problem looks like a nail.

Ising vs. QUBO

$$\begin{aligned} \text{min.} \quad & \mathbf{x}^\top Q \mathbf{x} \\ \text{s.t.} \quad & \mathbf{x} \in \{0,1\}^N \end{aligned}$$

variables

$$s_i := 2x_i - 1 \in \{-1, 1\} \qquad x_i = \frac{1+s_i}{2}$$

objective

$$\text{min.} \quad \mathbf{s}^\top J \mathbf{s} + \mathbf{h}\mathbf{s} = \mathbf{x}^\top Q \mathbf{x} + C$$

$$i \neq j \quad Q_{i,j} = 4J_{i,j}$$

$$Q_{i,i} = -2\sum_j (J_{i,j} + J_{j,i}) + 4J_{i,i} + 2h_i$$

$$= -2\sum_{j, i\neq j} (J_{i,j} + J_{j,i}) + 2h_i$$

$$C = -\sum_i h_i + \sum_{i,j} J_{i,j}$$

Ising vs. MaxCut

Max-Cut:

$$\begin{array}{ll} \text{min.} & \mathbf{s}^\top H \mathbf{s} \\ \text{s.t.} & \mathbf{s} \in \{-1, 1\}^N \end{array}$$

- QUBO with ± 1 variables
- Ising without linear term

Solution methods

Exact

- Semidefinite relaxation + cuts, HPC

  Hrga & Povh, Comput Opt. and Appl. **80**, 347 (2021)

- Fortet linearization

  Fortet R.: Revue Française de Recherche Opérationelle **4** 17 (1960.)

Heuristic

Many of them…

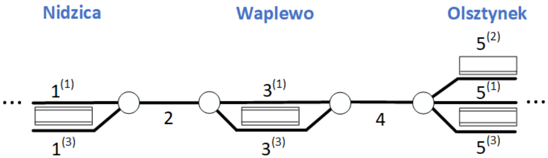
SDP-based

physics motivated: simulated annealing, mean-field annealing, parallel tempering, simulated bifurcation

special & quantum hardware: Toshiba digital annealer, DWave, QAOA

Application: railway conflict management

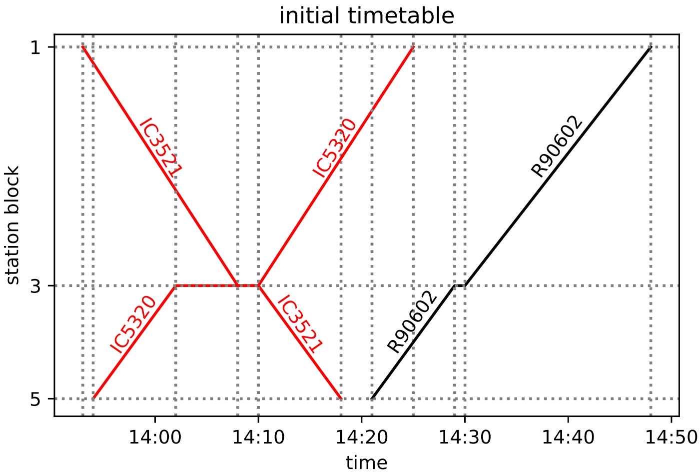
Single-track line. Example: line 206, Poland



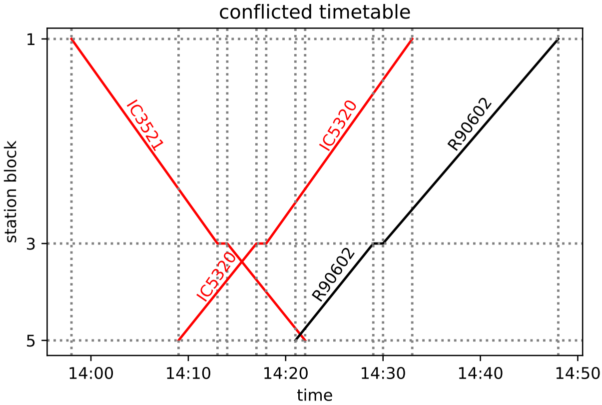
block (track segment): a part of the network that can be occupied by at most 1 train at a time.

Application: railway conflict management

Timetable.



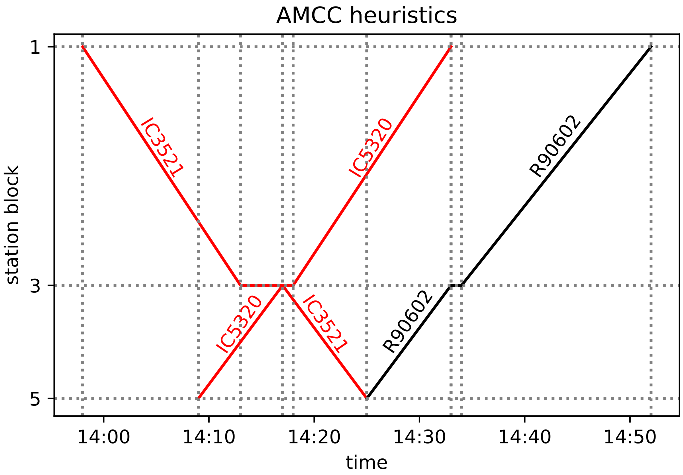
Conflict.



Because of **delays**, all of the trains would meet in block 4.

Solution: (Popular heuristics: First Come First Served, First Leave First Served)

Solution.


AMCC heuristics
station block
1
3
5
time
14:00
14:10
14:20
14:30
14:40
14:50
IC3521
IC5320
IC5320
IC3521
R90602
R90602

Application: railway conflict management

- **Blocking job shop**, scheduling theory notation: $(J_m|r_i, d_i, block|\sum_j w_j T_j)$
- **Jobs:** trains $j \in J$
- **Machines:** blocks, station: $s \in S$, line: $l \in L$
- **Objective:** minimize total weighted tardiness
  : (in other works also: minimize maximum tardiness)

Railway Quantum: model

- Discretized time wth minute resolution
- Variables

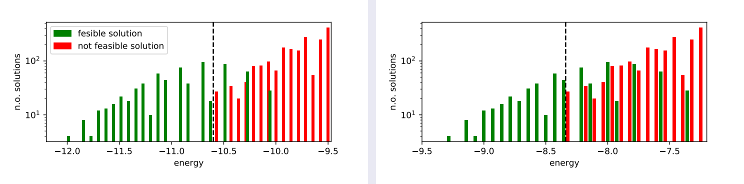
$$x_{s,j,d} = \begin{cases} 1, & d(j,s) = d \\ 0, & \text{otherwise} \end{cases},$$

which take the value of 1 if the train j leaves station block s at delay d, and zero otherwise.

Domino, K., Koniorczyk, M., Krawiec, K., Jałowiecki, K., Deffner, S., Gardas, B, Entropy **25** (2023): 191.

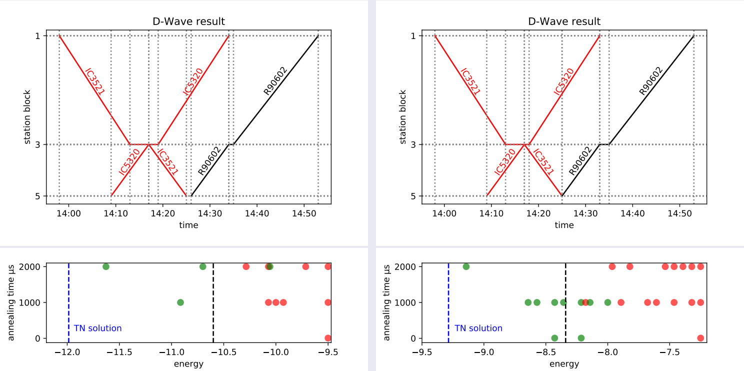
(Originally: https://arxiv.org/abs/2010.08227, from 2020.)

DWave results



Domino, K., Koniorczyk, M., Krawiec, K., Jałowiecki, K., Deffner, S., Gardas, B, Entropy **25** (2023): 191.

DWave results



Domino, K., Koniorczyk, M., Krawiec, K., Jałowiecki, K., Deffner, S., Gardas, B, Entropy **25** (2023): 191.

Railway Quantum: results

Features	line 216	line 191				
		case 1	case 2	case 3	case 4	enlarged
problem size (# logical bits)	48	198	198	198	198	594
# edges	395	1851	2038	2180	1831	5552
density (vs. full graph)	0.35	0.095	0.104	0.111	0.094	0.032
embedding into	Chimera	Chimera	Chimera	Ideal Chimera	Chimera	Pegasus
approximate # physical bits	373	< 2048	< 2048	≈ 2048	< 2048	< 5760

Domino, K., Koniorczyk, M., Krawiec, K., Jałowiecki, K., Deffner, S., Gardas, B, Entropy **25** (2023): 191.

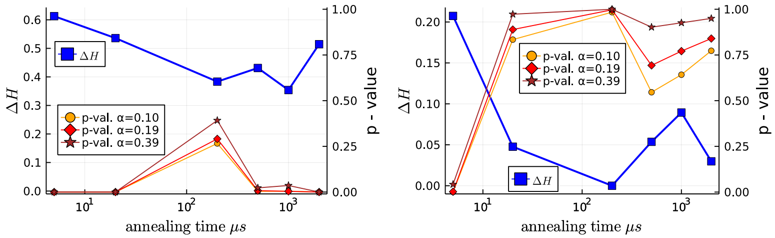
Railway Quantum: lessons learned

- Too few bits.
- Noisy.
- Uncertain if the minimum was sampled.

Have we found the optimum?

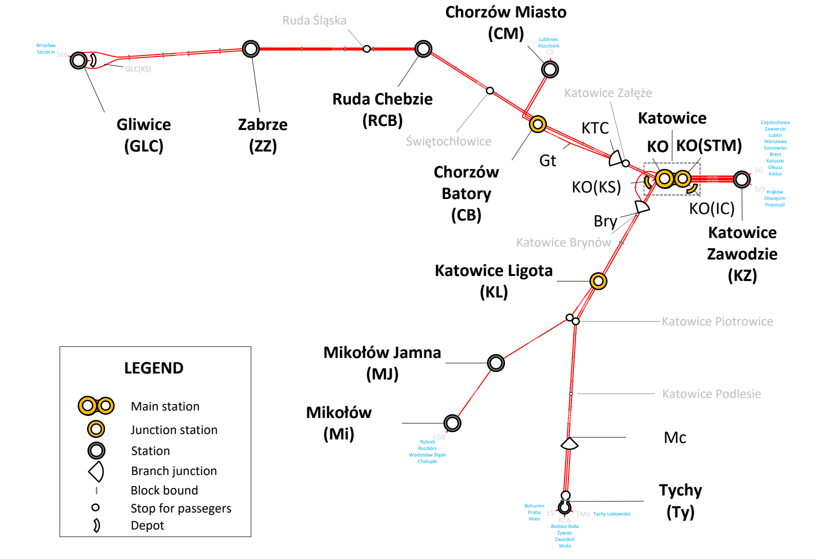
Statistical considerations

- Assumptions on the statistics of Ising-based annealers
- Statistics based on the particular samples
- *p*-value: have we found the optimum?



Domino, K, Koniorczyk M, and Puchała Z. Quantum Information Processing **21** (2022): 288.

Railway Hybrid: network



Koniorczyk M., Krawiec K., Botelho L., Bešinović N.„ Domino K., *to be published*

Railway Hybrid: model & method

- More complex ILP (MILP)
- Integers represented as proper monomials of bits

$$\sum_{l} \gamma_l \beta_l, \qquad \beta_l \in \{0, 1\}$$

- DWave CQM Hybrid
- CPLEX for comparison

Koniorczyk M., Krawiec K., Botelho L., Bešinović N.„ Domino K., *to be published*

Railway Hybrid: results

case	CPLEX			CQM hyb. `t_min` = 20 mean value over 5 realisations		
	#vars / # constr.	obj. × dmax	t [s]	obj. × dmax	comp. time [s]	QPU time [s]
0	556 /1756	0.0	0.072	0.0	20.18	0.029
1	556 / 1756	1.0	0.076	4.0	20.03	0.032
2	556 / 1740	6.0	0.079	6.0	20.22	0.032
3	556 / 1769	7.5	0.085	8.7	19.74	0.032
4	662 / 2210	78.25	0.196	88.75	20.24	0.032
5	662 / 2204	114.75	0.25	139.55	20.26	0.032
6	711 / 2599	91.25	0.41	139.55	20.39	0.032
7	817 / 3029	188.75	7.98	252.95	20.32	0.029
8	817 / 3074	157.75	3.70	268.25	20.24	0.032
9	817 / 3081	185.5	6.51	275.65	20.22	0.032

Koniorczyk M., Krawiec K., Botelho L., Bešinović N.„ Domino K., *to be published*

Railway Hybrid: lessons learned

- The hybrid solver performs well
- Limit on solution time (good for dispatching)
- QPU was used
- Con: black box
- Still no warranty for optimum

Have we found the solution?

Fortet linearization

$$\min \left(\left(\sum_{i=1}^{N} q_{ii} x_i \right) + \sum_{i<j} q_{ij} w_{ij} \right)$$

$$\begin{aligned} \text{s.t.} \quad w_{ij} - x_i \quad & \leq 0 \\ w_{ij} \quad - x_j & \leq 0 \\ -w_{ij} \quad & \leq 0 \\ -w_{ij} + x_i + x_j & \leq 1 \\ x_{ij} & \in \mathbb{Z} \end{aligned}$$

Fortet R.: Revue Française de Recherche Opérationelle 4(14):17–26, 1960.

Have we found the solution?

OR idea

- Fortet linearization (Mixed integer program)
- CPLEX MIPstart
- Duality

Have we found the solution?

instance	best known	DWave total time	DWave QPU time	Dwave problem optimum	simulated bifurcation result	simulated bifurcation time μs	improvement	time diff
1	-4072	2,998,536	42,665	-4072	-4056	44,814,920	16	7%
2	-4064	2,993,910	42,665	-4064	-4028	17,822,222	36	17%
3	-4068	2,991,168	42,665	-4068	-4066	17,863,855	2	17%
4	-4116	2,984,917	0	-4116	-4110	17,716,205	6	17%
5	-4086	2,988,660	42,666	-4086	-4064	17,748,010	22	17%
6	-4202	2,989,141	0	-4202	-4176	18,053,915	26	17%
7	-4162	2,994,115	42,665	-4162	-4142	17,772,211	20	17%
8	-4180	3,002,534	0	-4180	-4178	17,711,459	2	17%
9	-4172	2,995,460	42,663	-4172	-4160	17,793,081	12	17%
10	-4160	3,000,125	42,665	-4160	-4144	35,033,374	16	9%

Comparison of the DWave hybrid and simulated bifurcation results and computational times on the first 10 G-set instances

Have we found the solution?

instance	DWave hybrid optimum	Ising-qubo shift	MILP dual bound	Absolute MIP gap
1	-23248	19176	-31898.17	8650.17
2	-23240	19176	-32561.95	9321.95
3	-23244	19176	-32141.98	8897.98
4	-23292	19176	-31895.24	8603.24
5	-23262	19176	-32134.70	8872.7
6	-4356	154	-14083.58	9727.58
7	-4012	-150	-13728.03	9716.03
8	-4010	-170	-13939.99	9929.99
9	-4108	-64	-13808.79	9700.79
10	-4000	-160	-13796.22	9796.22

MIPstart + duality: lessons learned

- Simulated bifurcation performed well.
  (Phyisics-based heuristics!)
- MIPStart did not help too much
- Duality too slow. Can we improve on that?

Conclusions and outlook

- NISQ devices are best used in hybrid frameworks.
- They offer a valid alternative even in practical problems.
- Orchestration of physical and OR approaches is important.

Thanks to

- Janez Povh,
- all co-authors,
- Wigner GPU lab,
- Development and Innovation, Office within the Quantum Information National Laboratory of Hungary,
- OTKA K133882 and K124351