Determination of the lower bounds of the goal function for a single-machine scheduling problem on D-Wave quantum annealer

Wrocław University of Science and Technology

Wojciech Bożejko[1] Jarosław Pempera [1] Mariusz Uchroński[2] Mieczysław Wodecki[3]

[1]Department of Control Systems and Mechatronics, WIT, Wrocław University of Technology, Poland
[2] Wroclaw Centre for Networking and Supercomputing, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
[3] Department of Telecommunications and Teleinformatics, WIT, Wrocław University of Science and Technology, Poland

Introduction

- The fundamental problem of using metaheuristics and almost all other approximation methods for difficult discrete optimization problems is the lack of knowledge regarding the quality of the obtained solution. We propose a methodology for efficiently estimating the quality of such approaches by rapidly generating good lower bounds on the optimal value of the objective function using a quantum machine.
- Currently, the two leading types of quantum machines are quantum gate-based computers, developed mainly by IBM and Google, and adiabatic quantum computing (AQC), developed by D-Wave and NEC.
- In AQC, in particular quantum annealing, a starting state of the system modeled in hardware on multiple qubits is prepared as the ground state of the Hamiltonian encoding the solution to the desired optimization problem, to which adiabatic evolution is then applied, aiming at the minimal-energy state of the whole system.
- The model for AQC must be finally written as QUBO – Quadratic Unconstrained Binary Optimization.

Fig. 1. D-Wave Advantage quantum annealer

Formulation of the problem

- In the NP-hard single-machine Total Weighted Tardiness Problem (TWTP, $1||\sum w_i T_i$) there is given a *set of tasks* $\mathcal{J} = \{1, 2, ..., n\}$, which must without interruption be executed on a single machine. The following are associated with each task $i \in \mathcal{J}$: *execution time* p_i, *critical line* d_i, and *weight of penalty function* w_i.
- Let S_i be the starting moment and $C_i = S_i + p_i$ the ending moment of the execution of task $i \in \mathcal{J}$. Then, *tardiness*

  $$T_i = \max\{0, C_i - d_i\}.$$

  The TWTP problem consists in determining the execution schedule of the machine described by S_i, C_i, $i \in \mathcal{J}$ with a minimal *total cost* $\sum_{i=1}^{n} w_i T_i$.
- The task execution schedule described by the sequences S_i, C_i, $i \in \mathcal{J}$ is feasible if the following constraints are met:

$$S_i + p_i \le S_j \vee S_j + p_j \le S_i, \ i \ne j, \ i, j = 1, 2, \ldots, n,$$
$$S_i \ge 0, \quad C_i = S_i + p_i, \quad i = 1, 2, \ldots, n.$$

Lagrange relaxation of the goal function

The Lagrange function with multipliers u_{ij}, v_{ij}, $i, j = 1, 2, \ldots, n$ takes for the vector $S = (S_1, S_2, \ldots, S_n)$ and the matrix $y = [y_{ij}]_{n \times n}$ the form:

$$L(S, y, u, v) = \sum_{i=1}^{n} w_i T_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} u_{ij}(S_i + p_i - S_j -$$
$$K(1 - y_{ij})) + \sum_{i=1}^{n} \sum_{j=i+1}^{n} v_{ij}(S_j + p_j - S_i - K y_{ij}).$$

Transforming this expression we obtain

$$L(S, y, u, v) = \sum_{i=1}^{n} L_i(S_i, u, v) +$$
$$K \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij}(y_{ij}, u, v) + V(u, v), \text{ where}$$
$$L_i(S_i, u, v) = w_i T_i + \alpha_i S_i, \ \alpha_i = \sum_{j=i+1}^{n} (u_{ij} - v_{ij}) + \sum_{j=1}^{i-1} (v_{ji} - u_{ji}),$$
$$Q_{ij}(y_{ij}, u, v) = (u_{ij} - v_{ij}) y_{ij},$$
$$V(u, v) = \sum_{i=1}^{n} p_i \left(\sum_{j=1}^{i-1} v_{ji} + \sum_{j=i+1}^{n} u_{ij} \right).$$

Therefore, when looking for a good lower bound, one should compute

$$LB = \max_{u,v} \min_{S,y} L(S, y, u, v) =$$
$$\max_{u,v} \left(\sum_{i=1}^{n} \min_{0 \le S_i \le T - p_i} L_i(S_i, u, v) + \right.$$
$$\left. + K \sum_{i=1}^{n} \sum_{j=i+1}^{n} \min_{y} Q_{ij}(y_{ij}, u, v) + V(u, v) \right)$$

whereby the maximization with respect to u and v can be approximate, while that with respect to S and y is exact.

Determination of LB on a D-Wave quantum annealer

Let us note that LB can be written as a minimization of the opposite (minus) value, with constraints: $LB =$

$$- \min_{u,v,S,y} \left[- \left(\sum_{i=1}^{n} L_i(S_i, u, v) + K \sum_{i=1}^{n} \sum_{j=i+1}^{n} Q_{ij}(y_{ij}, u, v) + V(u, v) \right) \right]$$

s.t.

$$L_i(S_i, u, v) \le L_i(0, u, v), \ i = 1, 2, \ldots, n,$$
$$L_i(S_i, u, v) \le L_i(1, u, v), \ i = 1, 2, \ldots, n,$$
$$\vdots$$
$$L_i(S_i, u, v) \le L_i(T - p_i, u, v), \ i = 1, 2, \ldots, n,$$

and

$$Q_{ij}(y_{ij}, u, v) \le Q_{ij}(0, u, v), \ i, j = 1, 2, \ldots, n,$$
$$Q_{ij}(y_{ij}, u, v) \le Q_{ij}(1, u, v), \ i, j = 1, 2, \ldots, n.$$

Algorithm 1: Adding S minimalization constraints to the QUBO model

```
Experimental research
for i = 1, 2, ..., n do
    for t = 0, 1, 2, ..., T − p_i do
        if (t + p_i − d_i > 0) then
            Add constraint L_i(S_i, u, v) ≤ w_i · (t + p_i − d_i) + α_j · t
        else
            Add constraint L_i(S_i, u, v) ≤ w_i · 0 + α_i · t
```

Experimental research

- To verify the effectiveness of the proposed method of determining the lower bound, computational experiments were carried out on the quantum algorithm implemented on the D-WAVE quantum annealer and the algorithm determining the lower bound on a classical silicon computer with an i7-12700H 2.30 GHz processor.
- Analyzing the results, we can conclude that in a significant number of instances, the LB^Q determined by the quantum annealer is significantly greater than the LB^{CPU} determined on a classical computer.
- Comparing the calculation time of a quantum exponent and a classical computer, we can conclude that the time of quantum calculations is from 6 to nearly 140 times shorter than the time of calculations on a classical computer.

Experimental research

Table: The results of experiments.

example	LB^Q	$Time^Q$	LB^{CPU}	$TIME^{CPU}$	Speedup
wt5_40	423	15	0	183	12.20
wt5_41	2153	15	456	140	9.33
wt5_42	1657	15	300	103	6.87
wt5_43	1001	15	10	148	9.87
wt5_44	1588	15	116	115	7.67
wt5_45	2099	15	0	187	12.47
wt5_46	1791	15	604	116	7.73
wt5_47	2443	15	783	147	9.80
wt5_48	3353	15	1138	123	8.20
wt5_49	1578	15	358	100	6.67
wt6_70	469	15	0	202	13.47
wt6_71	3328	15	385	241	16.07
wt6_72	3563	15	290	359	23.93
wt6_73	2630	15	421	178	11.87
wt6_74	3216	15	612	312	20.80
wt6_75	1280	15	0	324	21.60
wt6_76	0	15	0	261	17.40
wt6_77	8	15	0	242	16.13
wt6_78	0	15	0	299	19.93
wt6_79	16	15	0	186	12.40

Experimental research

Table: The results of experiments.

example	LB^Q	$Time^Q$	LB^{CPU}	$TIME^{CPU}$	Speedup
wt7_70	3049	15	15	450	30.00
wt7_71	3635	15	317	582	38.80
wt7_72	1395	15	0	282	18.80
wt7_73	3806	15	62	451	30.07
wt7_74	3117	15	0	420	28.00
wt7_75	2840	15	0	238	15.87
wt7_76	0	15	0	605	40.33
wt7_77	64	15	0	436	29.07
wt7_78	0	15	0	302	20.13
wt7_79	12	15	0	381	25.40
wt8_80	100	15	0	1407	93.80
wt8_81	1271	15	0	1278	85.20
wt8_82	992	15	0	1249	83.27
wt8_83	662	15	0	1576	105.07
wt8_84	292	15	0	945	63.00
wt8_85	481	15	0	1682	112.13
wt8_86	3522	15	0	2053	136.87
wt8_87	1961	15	0	1127	75.13
wt8_88	5529	15	0	1774	118.27
wt8_89	2333	15	0	1512	100.80

Summary

- We propose an algorithm for determining the lower bound on the value of the objective function for the TWTP problem implemented on a D-Wave quantum computer.
- The presented approach can be adapted to estimate the value of the optimal solution of other NP-hard discrete optimization problems, such as Traveling Salesman Problem or multi-machine problems (e.g., flow shop, job shop).
- A natural direction for further research will be to apply the proposed method for determining lower bounds on a quantum machine, together with the (natural) determination of upper bounds by simply solving the problem formulated as QUBO, also on a QPU, to the construction of an exact algorithm based on the Branch and Bound method.
- This will allow – against the intuition associated with the probabilistic nature of computation on QPUs – the generation of truly optimal solutions.