

Graduate School of Fundamental Science and Engineering
Waseda University

博士論文概要
Doctoral Dissertation Synopsis

論文題目
Dissertation Title

Driving Ising Machines

- From QUBO Visualization and Modeling to Hyperparameter Tuning -

イジングマシンの活用方法に関する研究

— QUBO可視化と定式化から
ハイパーパラメータのチューニングまで —

申請者
(Applicant Name)
Matthieu PARIZY
パリジ マチュール

Department of Computer Science and Communications Engineering, Research on Information
System Design

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With climate change and the COVID19 pandemic, sustainability has become a great challenge of this century. To tackle this social issue there are several fields to focus on such as logistics and drug discovery. One of the key common research fields between logistics and drug discovery is Operations Research (OR).

OR is the application of analytical methods to help make better decisions. It has been an active field of research since the 1940s. Breakthroughs such as the Branch-and-Cut algorithm in the 1990s have made linear programming a widely adapted method to solve combinatorial optimization problems encountered in various applications. Certain categories of combinatorial problems remain difficult to tackle and are still actively researched: NP-hard problems.

Ten years ago, the first Quantum Annealer by D-Wave, a dedicated quantum computer architecture to solve Quadratic Unconstrained Binary Optimization problems (QUBO) which are NP-hard, was released. QUBO is represented as a polynomial on binary variables of the second order and quantum annealers find a combination of binary variable values to minimize (or maximize) the polynomial. Since the release of the Quantum Annealer, silicon based dedicated architectures have also emerged to solve QUBOs such as Hitachi's CMOS Annealer or Fujitsu's Digital Annealer (DA). Those quantum and silicon based architectures built to solve QUBOs have been called Ising machines. A common trait to the forementioned Ising machines is they are all related, to a certain extent, to the well-known metaheuristic: Simulated Annealing (SA).

The main characteristic of SA, compared to greedy metaheuristics, is it allows to make decisions when solving a problem which can worsen the current cost value of a solution considered, with a certain probability. Given enough solving time and proper SA parameter setting, SA guarantees to reach optimal solution but the required solving time could be astronomical thus many improvements to SA have been proposed since it was created.

Most of combinatorial optimization problems can be modeled as QUBO, with a varying amount of effort required, thus solving those problems on Ising machines has been actively researched for 10 years, especially comparing solving performance with traditional architecture and algorithms. Regardless of the Ising machine used, it has appeared clearly that depending on how a problem is modeled as QUBO, solving performance can vary greatly. Likewise, solving performance also depends on Ising machine's

hyperparameters, parameters which are used to control the QUBO solving process.

To maximize combinatorial problem-solving performance on Ising machines, this dissertation aims at tackling both the QUBO modeling and the hyperparameter setting parts of the QUBO solving process. This dissertation proposes a QUBO solving visualization technique to help identifying bottlenecks in the solving process to improve the modeling as well as an automated efficient Ising machine hyperparameter tuning framework. This dissertation is organized as follows:

Chapter 1 describes the background and overview of this dissertation.

Chapter 2 proposes a QUBO search space landscape visualization technique which uses two local minima solutions found to represent the multi-dimensional space in between and understand what makes a QUBO hard to solve. This technique is applied to the Quadratic Knapsack Problem (QKP) where the goal is to maximize the value of items inserted in a knapsack. This is known to be an NP-hard problem. Chapter 2 show that moving in and out heavy items from the knapsack is difficult due to the nature of representing linear inequality constraints as QUBO. With this insight, a solution mending method is proposed to help Ising machines stuck in local minima which raises the chances of finding the optimal solution with an Ising machine from only 6.7% to 60.7% for an Ising machine used with the proposed solution mending method. Chapter 2 also compares proposed Ising machine used with solution mending against SA. Results show that SA never reaches optimal solution for all problem instances evaluated on.

Chapter 3 proposes a novel integer variable to binary variables modeling technique. Proposed landscape technique from chapter 2 helped us to identify another bottleneck when solving problems which include integer variables. When using classic encoding methods, those encodings either create large differences in the cost function when changing a binary variable value representing a large integer value, which makes those moves unlikely to happen, or require a large quantity of binary variables, creating both computing complexity and a larger memory footprint. A “base10” encoding is proposed as a tradeoff between all fore-mentioned encodings. Proposed encoding is applied to the Cardinality Constrained Mean Variance Portfolio Optimization Problem (CCMVPOP), an NP-hard problem which uses real number variables. An efficient QUBO model for the CCMVPOP is thus

proposed by first converting real number variables to integer variables using coefficient multiplication with rounding combined with integer to binary variable encoding. Solving performance using the proposed encoding is compared to ones using classic encodings. Results show the time to the best-known solutions can be improved by a factor of up to 10x for several CCMVPOP instances. Results also show the proposed encoding is the only one which allows to reach the best-known solutions for a large CCMVPOP instance.

Chapter 4 proposes a novel Ising machine hyperparameter tuning framework. It is based on machine learning state of the art hyperparameter tuning method called Tree-structured Parzen Estimator (TPE), which is a kind of Bayesian optimization technique. After showing TPE effectiveness extends to Ising machines, as well comparing TPE to random parameter sampling, it proposes an enhanced TPE called “FastConvergence”. “FastConvergence” reduces the time required to find parameters which enable the same level of performance as TPE. Random sampling, TPE, and “FastConvergence” are compared using DA to solve Travel Salesman Problem (TSP) and Quadratic Assignment Problem (QAP), two well-known NP-hard problems often used for Ising machine benchmarking. Results show that the proposed “FastConvergence” can find parameters which give solving performance equivalent or better than TPE with two to three times faster tuning time.

Chapter 5 summarizes the dissertation. In conclusion, performance when solving combinatorial problems using Ising machines vary greatly depending on the QUBO modeling technique as well as the used Ising machine’s hyperparameters. It is thus vital to keep developing bottleneck analysis techniques to inspire future Ising machine architectures and solving algorithm techniques. It is also critical to have robust hyperparameter tuning framework to both maximize Ising machines’ performance but also, in general, have fair comparisons between metaheuristics-based solvers which have highly sensitive parameters, as one could easily disregard some solver in favor of another due to poor or lack of parameter tuning. Continuing to improve the proposed hyperparameter tuning framework is our future work.

List of research achievements for application of Doctor of Engineering, Waseda University

Full Name : Parizy Matthieu

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a. 論文 Academic papers	<p>1. ○<u>M. Parizy</u>, and N. Togawa, “Analysis and Acceleration of the Quadratic Knapsack Problem on an Ising Machine,” IEICE Trans. on Fundamentals of Electronics, Communications and Computer Science, vol. E104.A, no. 11, pp. 1526-1535, Dec. 2021.</p> <p>2. K.Fukada, <u>M. Parizy</u>, and N. Togawa, “A Three-Stage Annealing Method Solving Slot-Placement Problems Using an Ising Machine,” IEEE Access, vol. 9, pp. 134413-134426, 2021.</p>
c. 講演 Lectures 国際学会 (査読あり)	<p>3. ○<u>M. Parizy</u>, N. Kakuko, and N. Togawa, “Fast Hyperparameter Tuning for Ising Machines,” in 2023 IEEE International Conference on Consumer Electronics (ICCE) (2023 ICCE), Las Vegas, Nevada, Jan. 2023.</p> <p>4. ○ <u>M. Parizy</u>, P. Sadowski, and N. Togawa, “Cardinality Constrained Portfolio Optimization on an Ising Machine,” in 2022 IEEE 35th International System-on-Chip Conference (SOCC) (SOCC 2022), Belfast, United Kingdom (Great Britain), Sep. 2022.</p> <p>5. W.Y. Suen, <u>M. Parizy</u>, and H.C. Lau, “Enhancing a QUBO solver via data driven multi-start and its application to vehicle routing problem,” in Proceedings of the Genetic and Evolutionary Computation Conference Companion (GECCO '22), pp.2251—2257, Boston, Massachusetts, Jul. 2022.</p> <p>6. M. Ayodele, R. Allmendinger, M. López-Ibáñez, and <u>M. Parizy</u>, “Multi-objective QUBO solver: bi-objective quadratic assignment problem,” in Proceedings of the Genetic and Evolutionary Computation Conference Companion (GECCO '22), pp.467—475, Boston, Massachusetts, Jul. 2022.</p>
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e. そのた 招待論文	<p>9. 宮澤俊之, 小山純平, <u>Matthieu Parizy</u>, “第三世代デジタルアニーラーハイブリッドソルバ技術とその性能-,” 日本オペレーションズ・リサーチ学会 機関誌 特集イジングマシンとOR, vol. 67, no. 6, pp. 312–319, Jun. 2022.</p>
特許	<p>10. 覚幸典弘, <u>パリジマチュウ</u>, “情報処理装置、情報処理方法およびプログラム”, 出願番号2021-192401</p> <p>11. 覚幸典弘, <u>パリジマチュウ</u>, “情報処理方法、情報処理プログラム、および情報処理装置”, 出願番号 2022-106092</p>