Applications and Computational Advances for Solving the QUBO Model

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Abstract

QUBO models have proven to be remarkable for their ability to function as an alternative modeling framework for a wide variety of combinatorial optimization problems. Many studies have underscored the usefulness of the QUBO model to serve as an effective approach for modeling and solving important combinatorial problems. The significance of this unifying nature of the QUBO model is enhanced by the fact that the model can be shown to be equivalent to the Ising model that plays a prominent role in physics and is a major focus of the quantum computing community. Consequently, the broad range of optimization problems approached as QUBO models from the traditional Operations Research community are joined by an important domain of problems with connection to the physics community. Across the board, the QUBO model is used today as an alternative modeling and solution approach for a growing number of important problems found in industry and government. We describe important new applications of this model and sketch fundamental ways to create effective QUBO formulations. We also report computational experience showing the power of recent algorithmic advances.

Keywords: QUBO, Combinatorial optimization, integer programming

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Invited chapter for the forthcoming book, ***The quadratic unconstrained binary optimization problem****, A. P. Punnen (editor), Springer, 2021*

1. Introduction[1]

The field of Combinatorial Optimization (CO) is one of the most important areas in the field of optimization, with practical applications found in every industry, including both the private and public sectors. Generally, these problems are concerned with making wise choices in settings where a large number of yes/no decisions must be made and each set of decisions must satisfy certain constraints while optimizing a corresponding objective function value – like a cost or profit value. Finding good solutions in these settings is extremely difficult as these problems are typically NP-hard. The traditional approach is for the analyst to develop a solution algorithm that is tailored to the mathematical structure of the problem at hand. While this approach has produced good results in certain problem settings, it has the disadvantage that the diversity of applications arising in practice requires the creation of a diversity of solution techniques, each with limited application outside their original intended use.

Early articles such as those by Hammer and Rudeanu (1968), Rosenberg (1975), Hansen, et. al. (1993), and Boros and Hammer (2002) suggested the possible use of what has become known today as the QUBO model. However, only in recent years, through extensive computational work, has the research community demonstrated that the QUBO model can in fact be successfully employed to model and solve an exceptional variety of important CO problems found in industry, science and government, as documented in studies such as Kochenberger et. al. (2004), Kochenberger et. al. (2014), Lucas (2014) and Anthony et. al. (2017). Through special reformulation techniques that are easy to apply, the power of QUBO solvers can be used to efficiently solve many important problems once they are put into the QUBO framework. This approach has proven not only to be competitive with traditional methods, but often superior in performance in terms of both solution time and quality.

It is interesting to note that in recent years the QUBO model has emerged as an underpinning of the quantum computing area known as quantum annealing and Fujitsu's digital annealing, and has become a subject of study in neuromorphic computing. Through these connections, QUBO

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[1] This section draws on material from Glover et al. (2019)

models lie at the heart of experimentation carried out with quantum computers developed by D-Wave Systems and neuromorphic computers developed by IBM. The consequences of these new discoveries linking QUBO models to quantum computing are being explored in initiatives by organizations such as IBM, Google, Amazon, Microsoft, D-Wave and Lockheed Martin in the commercial realm and Los Alamos National Laboratory, Oak Ridge National Laboratory, Lawrence Livermore National Laboratory and NASA's Ames Research Center in the public sector. Computational experience is being amassed by both the classical and the quantum computing communities that highlights not only the potential of the QUBO model but also its effectiveness as an alternative to traditional modeling and solution methodologies.

In section 2 of this chapter, we highlight a diversity of applications that have been reported using the QUBO model. Then, in section 3, we illustrate in the transformation process enabling a classically formulated model to be recast into the form of a QUBO model. Section 4 follows with a summary and some conclusions.

2. Applications of the QUBO model:

Chapter 1 of this book mentioned several applications including the stable set problem, the Ising Spin Glass problem, the circuit layout design problem, and an application regarding detecting and tracking people in a crowded environment. These applications serve to illustrate the diversity of problems that fall under the QUBO umbrella.

In recent years, many other applications of the QUBO model have been reported in the operations research literature. In addition, quantum and quantum inspired computer companies with their QUBO solvers have encouraged exploration of applications, leading to many more accounts of important uses of the QUBO model. All told, the literature in general reports many interesting applications in wide variety of application settings.

In this section we summarize four applications that showcase the usefulness of the QUBO model for modeling and solving important combinatorial optimization problems. Section 2.2 that follows mentions many additional applications recently reported in the literature. References to these applications are provided to enable readers to follow up according to their interests.

Application #1: QUBO and the RNA Folding Problem

Lewis et. al. (2020), report advances derived from the QUBO model applied to the RNA folding problem, by extension of the work of Forester and Greenberg (2008) on quadratic binary models in computational biology.

RNA molecules, which play informational, structural and metabolic roles in all cells, are chains of nucleotides that interact through bases {A, C, G, U} to determine cell functionality and structure. The associated optimization problem seeks to minimize the thermodynamic free energy of a structure by selecting which bases will be paired provided certain constraints are satisfied. Binary variables are associated with potential base pairings and constraints are imposed to limit a variable to one base pair. Additional constraints are included to prohibit selecting base pairs that cross as well as promoting the formation of long RNA stems.

Lewis, et. al. (2020), approach this problem with a series of QUBO models that have proved extremely successful in predicting how base pairings determine RNA secondary structures, and thus facilitating biological functions related to information flow and metabolism. Expensive testing with standard benchmarks underscores the effectiveness of the QUBO approach whose results not only compare favorably with traditional RNA folding programs, but offer an alternative methodology with the potential to lead to improved predictions of RNA folding.

Application #2: QUBO and Vehicle Routing Problem

The Vehicle Routing Problem (VRP) is an important combinatorial optimization problem in which the goal is to find an optimal set of routes for a fleet of vehicles that deliver goods from an origin (depot) to a set of destinations (customers). The VRP is a generalization of the Travelling Salesman Problem (TSP) in which a single vehicle visits all destinations in one continuous path, starting and ending at the depot. Due to their computational challenge, VRPs and TSPs are typically solved by heuristic methods in practice.

Recently the quantum affiliated research community has investigated solving vehicle routing problems as well as TSPs using quantum and quantum inspired technology. For example, Feld et.al. (2018) report results obtained by formulating the vehicle routing problem as a QUBO model to be solved by the D-WAVE quantum annealer. Computational experiments show results comparable to conventional solvers in reasonable amounts of time.

Building on the work of Feld and co-workers, Borowski et. al. (2020) report results obtained from using D-Wave's Leap framework on well-established benchmark test cases, including problem instances based on realistic road networks. They also compared new quantum and hybrid methods with well-known classical algorithms for solving VRP. The experiments indicate that the hybrid quantum annealing methods give promising outcomes and are able to find solutions of similar or even better quality than the classical algorithms.

The application reported by Borowski, et. al. and the solution procedure they employ is limited to small instances compared to practical application. This shortcoming may be overcome by the advances being explored by Wang, et. al. (2020) in their work on TSP and related problems using the AlphaQUBO (2020) solver which can accommodate QUBO models with up to 1,000,000 variables.

<u>Application # 3</u>: QUBO and Machine Learning

Optimizing Gaussian Process Sampling has great promise for enhancing the performance of machine learning methods by improving training set selection. Bottarelli and Farinelli (2019) reported a successful use of the QUBO model for variance reduction in such settings.
Building on this work, Sargent et.al. (2020) at the University of Toronto are developing machine learning models where training set selection is made by optimizing a QUBO model formulated to represent the Gaussian Process posterior function. The overall objective of the research project is to develop enhanced machine learning models to accelerate material discovery with a particular focus on predicting the stability of acidic Oxygen Evolution Reaction electrocatalysts. Early testing based on QUBO solutions obtained from both the Fujitsu Digital Annealer and the AlphaQUBO (2020) solver from Meta-Analytics, Inc. show very encouraging outcomes. Preliminary results indicate that for a database containing 4000 metal oxides structures, the

energy mean absolute error (MAE) obtained from the QUBO model was 0.1 eV/atom less than that given by the conventional method. Further work will address the challenge of developing other QUBO-enhanced regression models like support vector regression.

<u>Application # 4:</u> QUBO and Large-scale Set Partitioning Problems.

The set partitioning problem (SPP) seeks to partition a set of items into subsets such that each item appears in exactly one subset and the cost of the subsets chosen is minimized. This problem appears in many application settings including the airline and other industries. The traditional formulation for SPP is given by

$$\min \sum_{j=1}^{n} c_j x_j$$
$$st$$
$$\sum_{j=1}^{n} a_{ij} x_j = 1 \quad for\ i = 1,\dots m$$

where x_j denotes whether or not subset j is chosen, c_j is the cost of subset j, and the a_{ij} coefficients are 0 or 1 denoting whether or not variable x_j explicitly appears in constraint i. Such models are easily re-cast into an equivalent QUBO model, without adding any new variables, using the standard reformulation procedure given in section 3 of this chapter.

In a recent paper, Du, et. al. (2020) report on a study involving large-scale instances of SPP ranging in size from 10,000 to 100,000 variables and 2,000 to 20,000 constraints. Extensive computational experiments were conducted comparing the traditional model solved by CPLEX and the equivalent QUBO model solved by a modern metaheuristic QUBO solver AlphaQUBO (2020) developed by Meta-Analytics. These are some of the largest QUBO models reported on in the literature. (Detailed computational results from this study are given at the end of section 3 in this chapter).

Both approaches were successful in solving the smaller instances considered. For larger problems, however, CPLEX was unable to find optimal solutions in an allotted time frame of 6 hours and typically reported large gaps when terminating due to the time limit. The QUBO approach on these larger problems, in contrast, found better solutions than the best results produced by CPLEX, often in a few minutes and always within one hour. This study confirms earlier successes of the QUBO model on smaller test problems for SPP reported by Lewis, et.al. (2008).

2.2 Additional applications by category

The vast amount of work going on today extending the use of the QUBO model is creating an ever growing list of QUBO applications. Below we list some to the key applications that have been reported in various categories of problem settings.

Classical Combinatorial Optimization

- Graph Coloring
  - Kochenberger et. al. (2005)
  - Wang et. al. (2013)
- Capital Budgeting Problems
  - Laughhunn, (1970).
- Asset Exchange Problems
  - Glover et. al. (2020)
- Task Allocation Problems (distributed computer systems)
  - Lewis et. al. (2005)
  - Tomasiewicz et. al. (2020)
- Warehouse Location and Product Distribution Problems
  - Ding et. al. (2020)
- Multiple Knapsack Problems
  - Glover et. al. (2002)
  - Forrester and Hunt-Isaak (2020)
- Maximum Independent Set Problems
  - Pardalos and Xue (1999)
  - Kochenberger et.al. (2007)
  - Yarkoni et. al. (2018)
- Maximum Cut Problems
  - Boros and Hammer (1991)
  - Kochenberger et. al. (2013)
  - Wang et. al. (2017)
  - Dunning et. al. (2018)
- Maximum Clique Prolems
  - Pelofske et. al. (2019)
- Constraint Satisfaction Problems (CSPs)
  - Vyskocil and Djidjev (2019)

- Number Partitioning Problems
    - Alidaee et. al. (2005)
- Set Packing Problems
    - Alidaee et. al. (2008)
- Linear Ordering Problems
    - Lewis et. al. (2009)
- Quadratic Assignment Problems.
    - Wang et. al. (2016)
- Clique Partitioning Problems
    - Wang et. al. (2004)
    - Kochenberger et. al. (2005)
    - Shaydulin et. al. (2018)
    - Kochenberger et. al. (2020)
- Satisfiability (SAT) and Max Sat Problems
    - Kochenberger, et. al. (2005)
    - Bonet et. al. (2007)
    - Santra et. al. (2014)
    - Bian et. al. (2017)
- Clustering Problems
    - Kochenberger et. al. (2005)
    - Mniszewski et. al. (2016)
    - Ushijima-Mwesigwa et. al. (2017)
    - Kumar et. al. (2018)
    - Mniszewski et. al. (2018)
    - Bauckhage et. al. (2019)
    - Negre et. al. (2019)

Financial Services

- Portfolio optimization
    - Elsokkary et. al. (2017)
    - Kalra et. al. (2018)
    - Kochenberger et. al. (2019)
    - Cohen et. al. (2020)
- Arbitrage / currency exchange
    - Rosenberg (2016)
- Credit risk assessment & scoring
    - Milne (2017)
    - Egger et. al. (2019)

Transportation

- Route & traffic optimization
    - Neukart et. al. (2017)
    - Feld et al. (2018)
    - Clark et. al. (2019)

    - Ohzeki et. al. (2019)
    - Inoue et. al. (2020)
    - Borowski et. al. (2020)
- Satellite coverage and surveillance
    - Bass et. al. (2017)

Manufacturing

- Product assembly optimization
    - Yarkoni et. al. (2019)
- Autonomous / robotic paths opt.
    - Mehta (2019)
- Job scheduling
    - Alidaee et. al. (1994)
    - Venturelli et. al. (2016)
- Group technology
    - Wang et. al. (2006)

Pharmaceuticals and Related

- Molecular similarity/composition
    - Sahner et al. (2018)
- New drugs and materials discovery
    - Snelling et. al. (2020)
- Computational biology
    - Lewis et. al. (2020)

Network and Energy

- Cybersecurity problems
    - Berwald et al. (2018)
    - Reinhardt et al.(2018)
- Power system design
    - Jones et al. (2020)

Machine learning

- Classical machine learning
    - Glover and Kochenberger (2006)
    - Li. et. al. (2018)
    - Willsch (2020)
- Deep learning
    - Sleeman (2020)

Miscellaneous

- Smelyanskiy et. al. (2012)
- Pakin (2017)
- O'Malley et. al. (2018)

- Aramon et. al. (2019)
- Bottarelli and Farinelli (2019)
- Chang et. al. (2019)
- Rogers and Singleton (2019)

Taken together, the applications highlighted above indicate the widespread diversity of the QUBO model and give a glimpse of what is being reported today and what is to come in the near term The focus on "quantum readiness" as well as the growing appreciation for the usefulness of the QUBO model in general will lead to a continued growth in notable applications in the coming years.

In the next section we provide an overview of the methodology used to convert a traditionally modeled problem into the unified QUBO framework.

3. Creating QUBO Models

While some problems, like the number partitioning problem and the famous Ising spin glass problem, appear naturally in the form of a QUBO model, by far the largest number of problems of interest include additional constraints that must be satisfied as the optimizer searches for good solutions. Such problems can be effectively re-formulated as a QUBO model by introducing <u>quadratic penalties</u> in the objective function as an alternative to explicitly imposing constraints in the classical sense. The penalties are chosen so that the influence of the original constraints on the solution process can alternatively be achieved by the natural functioning of the optimizer as it looks for solutions that avoid incurring the penalties. That is, the penalties are formulated so that they equal zero for feasible solutions and equal some positive penalty amount for infeasible solutions. For a minimization problem, these penalties are added to create an augmented objective function to be minimized. If the penalty terms can be driven to zero, the augmented objective function becomes the original function to be minimized.

For certain types of constraints, quadratic penalties useful for creating QUBO models are known in advance and readily available to be used in transforming a given constrained problem into a

QUBO model. To illustrate the main idea, consider a traditionally constrained problem of the form:

$$\text{Min } x_0 = f(x)$$

subject to the constraint

$$x_1 + x_2 \leq 1$$

where x_1 and x_2 are binary variables. Note that this constraint allows either or neither x variable to be chosen. However, it explicitly precludes both from being chosen (i.e., both cannot be set to 1).

A quadratic penalty that corresponds to our constraint is

$$Px_1x_2$$

where P is a positive scalar. As can be seen, this penalty function is equal to P when both x_1 and x_2 are equal to 1. Otherwise, it is equal to 0. For P chosen sufficiently large, the unconstrained problem

$$\text{minimize } x_0 = f(x) + Px_1x_2$$

has the same optimal solution as the original constrained problem. If f(x) is linear or quadratic, then this unconstrained model will be in the form of a QUBO model, i.e., minimize $x_0 = x^tQx$.

In this example, any optimizer trying to minimize x_0 will tend to avoid solutions having both x_1 and x_2 equal to 1, else a large positive amount will be added to the objective function. This simple constraint ($x_1 + x_2 \leq 1$) arises in many important QUBO applications where the penalty (Px_1x_2) is used as an alternative. See, for instance, the work on the maximum clique and related problems by Pardalos and Xue (1999).

While the example above illustrates the approach of adding penalties to the objective function to create a QUBO model, simple penalties won't always be known in advance and will have to be discovered. The procedure for this is straightforward as shown below.

3.1 Creating QUBO Models: A General Purpose Approach

Consider the general traditionally modeled combinatorial problem

$$\min x_0 = x^t C x$$

$$\text{s.t.} \qquad Ax = b, \;\; x \; binary$$

This model accommodates both quadratic and linear objective functions since the linear case results when C is a diagonal matrix (observing that $x_j^2 = x_j$ when x_j is a 0-1 variable). Under the assumption that A and b have integer components, problems with inequality constraints can always be put in this form by including slack variables and then representing the slack variables by a binary expansion. (For example, this would introduce a slack variable s to convert the inequality $4x_1 + 5x_2 - x_3 \le 6$ to $4x_1 + 5x_2 - x_3 + s = 6$, and since $s \le 7$ (for the case where $x_1 = x_2 = 0$ and $x_3 = 1$), s could be represented by the binary expansion $s_1 + 2s_2 + 4s_3$ where $s_1, s_2,$ and s_3 are additional binary variables. If it is additionally known that at not both x_1 and x_2 can be 0, then s can be at most 3 and can be represented by the expansion $s_1 + 2s_2$. These constrained quadratic optimization models are converted into equivalent unconstrained QUBO models by converting the constraints $Ax = b$ (representing slack variables as x variables) into quadratic penalties to be added to the objective function, following the same re-casting as we illustrated in the discussion that precedes section 3.1.

Specifically, for a positive scalar P, we add a quadratic penalty $P(Ax-b)^t(Ax-b)$ to the objective function to get

$$\begin{aligned} x_0 &= x^t C x + P(Ax-b)^t(Ax-b) \\ &= x^t C x + x^t D x + c \\ &= x^t Q x + c \end{aligned}$$

where the matrix D and the additive constant c result directly from the matrix multiplication indicated. Dropping the additive constant, the equivalent unconstrained version of the constrained problem becomes

$$QUBO: \min x^t Qx, x\ binary$$

This general transformation procedure can in principle be applied to any 0/1 model with a linear or quadratic objective function subject to linear constraints.

Remarks:

1. A suitable choice of the penalty scalar P, as we commented earlier, can always be chosen so that the optimal solution to QUBO is the optimal solution to the original constrained problem. Solutions obtained can always be checked for feasibility to confirm whether or not appropriate penalty choices have been made. Boros and Hammer (2002) give a discussion of this approach which is the basis for establishing the generality of QUBO.
2. For realistic applications, a program, perhaps in Python, will need to be written implementing the Transformation and producing the Q matrix needed for the QUBO model. For small problems we can usually proceed manually as we'll do in example to follow.
3. Note that the additive constant, c, does not impact the optimization and can be ignored during the optimization process. Once the QUBO model has been solved, the constant c can be used to recover the original objective function value. Alternatively, the original objective function value can always be determined by using the optimal x_j found when QUBO is solved.

This general transformation procedure is illustrated by the following example. Consider the set partitioning problem

$$\min y = 3x_1 + 2x_2 + x_3 + x_4 + 3x_5 + 2x_6$$

subject to

$$\begin{aligned} x_1 + x_3 + x_6 &= 1 \\ x_2 + x_3 + x_5 + x_6 &= 1 \\ x_3 + x_4 + x_5 &= 1 \\ x_1 + x_2 + x_4 + x_6 &= 1 \end{aligned}$$

and x binary. Normally, the general Transformation would be embodied in a supporting computer routine and employed to re-cast this problem into an equivalent instance of a QUBO model. For this small example, however, we can proceed manually as follows: The conversion to an equivalent QUBO model involves forming quadratic penalties and adding them to the original objective function. In general, the quadratic penalties to be added (for a minimization problem) are given by $P\sum_i(\sum_{j=1}^{n} a_{ij}x_{ij} - b_i)^2$ where the outer summation is taken over all constraints in the system $Ax = b$.

For our example we have

$$\begin{aligned}\min y = {} & 3x_1 + 2x_2 + x_3 + x_4 + 3x_5 + 2x_6 \\ & + P(x_1 + x_3 + x_6 - 1)^2 + P(x_2 + x_3 + x_5 + x_6 - 1)^2 \\ & + P(x_3 + x_4 + x_5 - 1)^2 + P(x_1 + x_2 + x_4 + x_6 - 1)^2\end{aligned}$$

Arbitrarily taking P to be 10, and recalling that $x_j^2 = x_j$ since our variables are binary, this becomes

$$\begin{aligned}\min x_0 = {} & -17x_1^2 - 18x_2^2 - 29x_3^2 - 19x_4^2 - 17x_5^2 - 28x_6^2 + 20x_1x_2 + 20x_1x_3 + 20x_1x_4 + 40x_1x_6 \\ & + 20x_2x_3 + 20x_2x_4 + 20x_2x_5 + 40x_2x_6 + 20x_3x_4 + 40x_3x_5 + 40x_3x_6 + 20x_4x_5 \\ & + 20x_4x_6 + 20x_5x_6 + 40\end{aligned}$$

Dropping the additive constant 40, we then have our QUBO model

$$\min x^t Qx, \ \ x \ binary$$

where the Q matrix is

$$Q = \begin{bmatrix} -17 & 10 & 10 & 10 & 0 & 20 \\ 10 & -18 & 10 & 10 & 10 & 20 \\ 10 & 10 & -29 & 10 & 20 & 20 \\ 10 & 10 & 10 & -19 & 10 & 10 \\ 0 & 10 & 20 & 10 & -17 & 10 \\ 20 & 20 & 20 & 10 & 10 & -28 \end{bmatrix}$$

Solving this QUBO formulation gives an optimal solution $x_1 = x_5 = 1$ (with all other variables equal to 0) to yield $x_0 = 6$.

As noted in section 2 of this chapter, using the QUBO model for solving large-scale set partitioning problems has proven to be very successful. For detailed examples of re-casting other traditional models into the form of a QUBO model, the reader is referred to Glover, et. al. (2019).

3.2 Illustrative Computational Experience:

As mentioned earlier in this chapter, the QUBO modeling and solution approach has proven to be successful in representing and solving a wide variety of difficult combinatorial optimization problems. We commented in section **3.1** and earlier in section **2.0,** for instance, on the recent study by Yu, et. al. (2020) illustrating such success on large set partitioning problems. The following tables present the main results of this study undertaken on medium, large and very large test problems. Note that the results shown for CPLEX were obtained from the standard linear model for set partitioning while the AlphaQUBO results were obtained from the equivalent QUBO representation.

Table 1: Medium Sized Problems: Comparing AlphaQUBO and CPLEX

				CPLEX		AlphaQUBO	
ID	Vars	Constraints	Density %	OFV	Time(s)	OFV	Time(s)
SPP01a	6,000	1500	25	**10872**	7851	**10872**	53
SPP01b	6,000	1500	50	**6975**	3180	**6975**	6
SPP01c	6,000	3000	25	**22860**	2598	**22860**	275
SPP01d	6,000	3000	50	**14793**	14115	**14793**	12
SPP02a	8,000	2000	25	**14959**	15348	**14959**	34
SPP02b	8,000	2000	50	**9621**	18071	**9621**	74
SPP02c	8,000	4000	25	**30425**	16423	**30425**	95
SPP02d	8,000	4000	50	19882	10191	**19816**	19

As shown in Table 1, both CPLEX and AlphaQUBO found optimal solutions for the first 7 of these modest sized problems. AlphaQUBO obtained a better solution than CPLEX on the last problem and outperformed CPLEX on "time to best" by a wide margin on all 8 problems.

Table 2: Large Sized Problems.

				Cplex		AlphaQUBO	
ID	Vars	Constraints	Density %	OFV	Time(s)	OFV	Time(s)
1	10,000	1,000	25%	**7292**	947	**7292**	378.2
2	10,000	1,000	50	**4543**	1543	**4543**	11.6
3	10,000	5,000	25	**37968**	284	**37968**	5.4
4	10,000	5,000	50	**24297**	8683	**24297**	1337
5	15,000	1,500	25	**10930**	66	**10930**	17.5
6	15,000	1,500	50	7174	2176	**7047**	77
7	15,000	7,500	25	57834	993	**57419**	706.7
8	15,000	7,500	50	37962	2373	**37671**	556.8
9	20,000	2,000	25	**14900**	9833	**14900**	1535.1
10	20,000	2,000	50	**9412**	369	**9412**	3.6
11	20,000	10,000	25	77448	2119	**77198**	1729.1
12	20,000	10,000	50	**50188**	4786	**50188**	5.7
13	25,000	2,500	25	18517	589	**18498**	10
14	25,000	2,550	50	12008	1847	**11923**	813.8
15	25,000	12,500	25	96690	548	**96445**	1474.3
16	25,000	12,500	50	63173	18903	**63156**	98
17	30,000	3,000	25	**22405**	859	**22405**	14.1
18	30,000	3,000	50	**14457**	2507	**14457**	1551.7
19	30,000	15,000	25	115950	16031	**115687**	410.3
20	30,000	15,000	50	76276	17393	**75684**	11.5
21	40,000	4,000	25	30592	2532	**30445**	894.1
22	40,000	4,000	50	19815	7184	**19558**	11.5
23	40,000	20,000	25	155162	19152	**155069**	393.4
24	40,000	20,000	50	**101835**	10286	101835	12.9

Table 2 show that AlphaQUBO quickly found best known solutions for all 24 problems. CPLEX was able to find best known solutions for only 11 of the 24 problems. AlphaQUBO had a "time to best" advantage over CPLEX that typically ranged from 1 to 3 orders of magnitude.

Table 3: Very Large Instances

				Cplex		AlphaQUBO	
ID	Vars	Constraints	Density %	OFV	Time(s)	OFV	Time(s)
spp50k	50,000	10,000	25	76903	18144	**76402**	2315
spp60k	60,000	12,000	25	92293	16060	**91912**	2876
spp70k	70,000	14,000	25	109168	19084	**108112**	272
spp80k	80,000	16,000	25	125139	18600	**123890**	175
spp90k	90,000	18,000	25	140223	15278	**139269**	1804
spp100k	100,000	20,000	25	154694	19509	**154351**	622

For the very large problems of Table 3, CPLEX was unable to find the best known solution to any of these problems in the time limit of 6 hours. AlphaQUBO quickly provided best known solutions for all problems, outperforming CPLEX in terms of solution quality and time. Note that these QUBO models are the largest reported on in the literature to date.

4. Summary and Conclusion:

The remarkable diversity of QUBO applications and the documented successes in solving them effectively highlight the practical importance of these models. The relevance of this area to quantum computing and the discovery of new applications in machine learning, biotechnology, supply chains, portfolio analysis and a host of other realms promises to stimulate further advances in the months ahead. Some of these will mimic and build upon past QUBO successes while others will be completely new as the research community continues to devise creative ways to recast important problems into the QUBO framework.

The applications reported here underscore the success of the QUBO model as a useful alternative to traditional approaches for solving combinatorial optimization problems. As the performance of QUBO solution methods continues to advance, both on the conventional and the quantum side, the practice of employing the QUBO model may be expected to expand as well.

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