

Goal Seeking Quadratic Unconstrained Binary Optimization

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Abstract

The Quadratic Unconstrained Binary Optimization (QUBO) modeling and solution framework is required for quantum and digital annealers whose goal is the optimization of a well defined metric, the objective function. However, diverse suboptimal solutions may be preferred over harder to implement strict optimal ones. In addition, the decision-maker usually has insights that are not always efficiently translated into the optimization model, such as acceptable target, interval or range values. Multi-criteria decision making is an example of involving the user in the decision process. In this paper, we present two variants of goal-seeking QUBO that minimize the deviation from the goal through a tabu-search based greedy one-flip heuristic. Experimental results illustrate the efficacy of the proposed approach over Constraint Programming for quickly finding a satisficing set of solutions.

Keywords: Quadratic Unconstrained Binary Optimization, pseudo-Boolean optimization, goal seeking, what if, goal programming, quantum computer

1. Introduction

Quadratic Unconstrained Binary Optimization (QUBO) is a popular modeling framework wherein many combinatorial optimization problems are recast into the form $\min x'Qx; x \in \{0, 1\}$ where Q is a symmetric matrix of size n with integer or real components and x is a binary vector (see [1] for more details). Solvers for QUBO focus on finding the best objective function

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in a limited timeframe. However, in many real-life problems, the decision-maker is interested in setting goals for the objective function and generating a set of solutions to consider for implementation, for example, a target time to complete a task, multi-criteria profit, risk, or time-frame targets. In the mixed integer linear programming paradigm, the objective target is modeled as lower and upper bound constraints on the objective function. However for quadratic binary objectives, these constraints are also binary quadratic and are very difficult for conventional linear solvers such as CPLEX and Gurobi. In this short paper, we present two variants of a goal-seeking or target QUBO. In the first case, the target t is exact and we are interested in finding binary vectors x such that $x'Qx = t$. In the second case, the target is uncertain but defined by an interval $[lb, ub]$.

Target QUBO belongs to the class of goal programming under multi-criteria decision making where the objective function $x'Qx$ is provided a goal or target to be achieved and deviation from the target may be seen as the quadratic Taguchi quality loss function ([2]), although other measures such as absolute value are valid. Our implementation utilizes the squared deviation from the goal, which is minimized in the tabu-search heuristic. However, the importance of the magnitude of deviation from the target is typically determined by the decision-maker.

Our proposed model finds utility in four scenarios. First, the settings where we are interested in finding the input parameters that achieve a desired target level benefit from this analysis which is closely related to the “goal-seeking problem” defined in [3] and exemplified in the parameter selection method of Taguchi ([4]). Second, in sensitivity analysis of a discrete event simulation (see [3] for more details).

The third application arises in the context of the Constraint Satisfaction Problem modeled as a QUBO wherein a target number of constraints are specified for satisfaction. While existing solution techniques utilize the minimization of penalty term for unsatisfied clauses, using the goal-based QUBO solver, we could employ the solution technique to specifically search for instances wherein all clauses are satisfied, and the overall penalty goal is zero.

Fourth, target QUBO can be utilized as a tool to solve multi-objective optimization problems. For instance, the model appears as a subproblem for lexicographic optimization where the objectives are sorted from most important to least important ([5]). Thereafter, we find the binary variables satisfying the inequality for the i 'th objective $x'Q_i x \leq f_i^* + \delta_i$ which guar-

antees that the search focused on near-optimal function evaluation f_i^* controlled by a tolerance level δ_i which translates to $x'Q_i x \in [f_i^*, f_i^* + \delta_i]$ in our modeling framework. Thus, the results could be useful for lexicographic optimization wherein we are looking for solutions that are close to the optimal value. Moreover, various objectives can be combined into a weighted multi-objective function. Thus, the various solution techniques proposed for multi-objective QUBO (like [6, 7, 8, 9]) could benefit from our analysis.

The paper is organized as follows. The goal-seeking QUBO model is presented in Section 2. The solution technique and the results are presented in Section 3 and 4, followed by conclusions and future research directions.

2. Model

First, we present the exact goal-seeking QUBO for a deterministic target t . An exact model with quadratic penalties minimizing the squared deviation from the target is $\min (x'Qx - t)^2 = \min (x'Qx)^2 - 2t(x'Qx) + t^2$ wherein the first term has fourth-degree pseudo boolean functions of the form $x_i x_j x_k x_l$ significantly increasing the computational complexity. We could iteratively use Rosenberg quadratization substituting the quadratic subterm $x_i x_j$ with an additional binary variable z_{ij} thereby introducing a penalty term $M(x_i x_j - 2x_i z_{ij} - 2x_j z_{ij} + 3z_{ij})$ for a minimization problem. In this way, we could transform the fourth degree polynomial to a quadratic polynomial and utilize existing QUBO solvers. However, this reformulation leads to a large number of auxiliary variables and penalty terms ([10]).

While the number of auxiliary variables required for the transformation of a fourth degree goal-seeking QUBO is $O(n^2)$, calculating the impact on the achievement function $(x'Qx - t)^2$ as part of a one-flip search routine is fast given that the incremental function evaluation of $x'Qx$ could be done in $O(1)$ ([11]). Thus, selecting the best variable out of one-flip neighborhood is $O(n)$. Only binary vectors that meet the target are collected as part of the search routine and presented to the decision-maker.

A common feature of integer optimization problems is the presence of alternate optima ([12]) and while it may not be practical to enumerate all alternate optima, our solution approach generates a list of binary solution vectors meeting the target value or range. This feature is important to multi-criteria decision-making, wherein the decision-maker selects the preferred solution from the list of pareto optimal solution vectors.

Second, we describe the interval goal-seeking QUBO that seeks to find solution vectors that satisfy $x'Qx \in [lb, ub]$. This is attained by optimizing the achievement function $\min (x'Qx - lb)(x'Qx - ub) = \min (x'Qx)^2 - (lb + ub)(x'Qx) + lb * ub$. Again we face computational difficulties with solving this exact fourth-degree pseudo boolean function involving a large number of auxiliary variables and penalty terms. Alternatively, lower and upper bound constraints on the objective function can be used, but most solvers do not work well with quadratic binary constraints. Thus we integrate the target constraint into the solution method as described in Section 3.

Because of the quadratic nature of the achievement function, the optimal value is achieved at $x'Qx = (lb + ub)/2$. However, in general the achievement function is non-positive as long as $x'Qx \in [lb, ub]$. Moreover, the binary vectors outside this interval lead to a higher penalty term, which increases with the squared distance from the interval bounds. This incentivizes the solver to limit the search to the solution landscape around the interval. Any binary vectors with non-positive function evaluation are easily collected during the search routine. Such vectors satisfying the interval constraint are presented to the decision-maker in descending order according to their objective function.

The following lemma captures the relationship between satisficing vectors and achievement function for either of the variants of goal-seeking QUBO.

Lemma 1. *Achievement function $AF(x_*) \leq 0$ if and only if x_* is a satisficing solution vector.*

Proof. First, the deterministic goal-seeking QUBO has $AF(x) = (x'Qx - t)^2$. Note that this quadratic function is always positive except for the case wherein $x'Qx = t$. Thus, $AF(x) = 0$ only when the binary vector x meets the target t .

Second, any solution vector x for the interval goal-seeking QUBO with $AF(x) = (x'Qx - lb)(x'Qx - ub)$ should have objective function evaluation $x'Qx$ belonging to one of the following three intervals: (i) $(-\infty, lb)$ (ii) $[lb, ub]$ (iii) (ub, ∞) . If $x'Qx \in (-\infty, lb)$, then $(x'Qx - lb)(x'Qx - ub) > 0$ since both of the subterms evaluate to negative values. Similarly, if $x'Qx \in (ub, \infty)$, then $(x'Qx - lb)(x'Qx - ub) > 0$ because both subterms evaluate to positive values. The only scenario wherein $AF(x)$ given by $(x'Qx - lb)(x'Qx - ub) \leq 0$ happens for $x'Qx \in [lb, ub]$ because of the conflicting signs of the two components. \square

3. Solution Technique

Our solution method is summarized in Algorithm 1. We utilize a tabu-search (TS) heuristic for finding the binary vectors that meet the user-defined goals. A neighborhood move is defined by a one-flip i.e. setting x_i to $1 - x_i$ for a specific variable i . The best impact on the objective function $x'Qx$ due to one-flip is calculated in an incremental manner building on a previous solution requiring $O(n)$ ([11]) to select the best one-flip from the n variables in the neighborhood. We start from the all-zero solution and iteratively choose the non-tabu move that leads to the best improvement in the achievement function (AF). In case an improvement in AF is not possible i.e., we reach a local optima, we chose the non-improving and non-tabu move having the least impact on AF . As discussed earlier, AF is defined as $(x'Qx - t)^2$ for deterministic target and $(x'Qx - lb)(x'Qx - ub)$ for interval target.

Algorithm 1 Tabu search heuristic

1: procedure TABU SEARCH(TS)	▷ Returns the set S of satisficing solutions
2: Input: $Q, x_{initial}$	▷ Q matrix and starting solution
3: Input: $TabuList$	▷ Tabu list of fixed length
4: Output: S	▷ Set containing output vectors satisfying target
5: $S \leftarrow \emptyset$	
6: $x_* \leftarrow x_{initial}$	
7: while termination criteria is not met do	
8: $best_{AF} \leftarrow \infty$	
9: for each $x \in Neighborhood(x_*)$ do	▷ For all one flip neighbors of best solution
10: if $x \notin TabuList$ then	▷ Variable is non-tabu
11: if $AF(x) < best_{AF}$ then	▷ Solution vector improves achievement function
12: $x_* \leftarrow x$	
13: $best_{AF} \leftarrow AF(x)$	
14: $TabuList \leftarrow Update(TabuList)$	▷ Remove a variable from the tabu list
15: $TabuList \leftarrow Update(TabuList, x_*)$	▷ Add the best choice variable to the tabu list
16: if $AF(x_*) \leq 0$ then	▷ Solution vector meets the specified target
17: $S \leftarrow S \cup x_*$	▷ Add the solution vector to the output set
18: $S \leftarrow Postprocess(S)$	▷ Remove the duplicates from output set S
19: return S	

To help prevent cycling to previously visited solutions, we define a tabu list consisting of the tabu tenure of the variables that were flipped. Thus, a non-tabu variable x_i is added to the tabu list with maximum tabu tenure if it was the best choice for one-flip. The variable is eventually removed from the tabu list after a fixed number of iterations set by the tabu tenure parameter. Note that this parameter has an impact on the computational performance of the heuristic. In general, as the tabu tenure increases, the chances for cycling reduces while a too large tabu tenure parameter inhibits the ability to reach a target.

Compared to a traditional heuristic wherein we are interested in finding the best solution in a limited runtime, we focus on finding multiple solutions that meet the user-defined objective goal. In this way, we can provide various choices to the decision-maker. The termination criteria in our TS heuristic is the solution runtime and our algorithm might find duplicate solutions due to cycling, so the end of the routine, we run a post-processing method that identifies the unique solutions among the solution set.

The solution quality of target QUBO is assessed by the number of unique solutions obtained by the solver in a limited runtime. Because the tabu tenure parameter has an impact on the solution quality, we conducted preliminary experiments to determine a good setting. For this purpose, we utilized the 2500 node ORLIB instances ([13]). The deterministic target was set at 80% of the best known solutions of the problems (obtained from [14]). In general, smaller tabu tenures lead to quick solutions, but tend to cycle, and the solver is often stuck in local optima. On the other hand, large tabu tenure restricts the neighborhood visited by the solver. Based on preliminary experiments, we observed that tabu tenure between 10 and 20 provides good results on the ORLIB problems and we set the tabu tenure to 10 for the problem set in the following section.

4. Results

For computational experiments, we use the QUBO instances with 2500, 3000 and 4000 variables (presented in [13] and [15]). The solution technique was implemented using C. We also utilize the IBM Constraint Programming (CP) Optimizer for benchmarking with the exact model. The exact non-linear model for the two variants namely $x'Qx = t$ and $x'Qx \geq lb \ \& \ x'Qx \leq ub$ was input to the CP solver using Python DOCPLEX API. The target level is set as a higher percentage of best known solutions (*bks*) namely 80%, 85%, 90% and 95%. The experiments were performed on a 3.40 GHz Intel Core i7 processor with 16 GB RAM running 64 bit Windows 7 OS.

In terms of benchmarking, the IBM CP solver was unable to find any feasible solution for either of the problem variants in 100 seconds and for bigger instances, the size of the exact model was too large in terms of memory requirements. We also tried the default portfolio of solvers provided by MiniZinc ([16]) for the non-linear models, and those also yielded no solutions. Thus, these problems are computationally challenging.

First, we present the results using our heuristic for the exact target QUBO problem $x'Qx = t$ in Table 1. It is evident from the results that as we get closer to bks , the goal-setting problem becomes more challenging and we conclude that the solution landscape for these problems are distributed such that the number of feasible solutions decrease as the target approaches bks .

Table 1: Number of unique solutions for $x'Qx = t$

Instance	80%	85%	90%	95%	Instance	80%	85%	90%	95%
<i>2500.1</i>	31	27	22	15	<i>3000.1</i>	28	22	19	17
<i>2500.2</i>	21	17	8	6	<i>3000.2</i>	61	52	41	30
<i>2500.3</i>	30	25	19	16	<i>3000.3</i>	60	54	45	36
<i>2500.4</i>	36	36	20	19	<i>3000.4</i>	42	33	27	16
<i>2500.5</i>	32	31	30	22	<i>3000.5</i>	31	26	18	14
<i>2500.6</i>	26	24	14	8	<i>4000.1</i>	38	30	24	14
<i>2500.7</i>	60	59	39	31	<i>4000.2</i>	29	18	14	8
<i>2500.8</i>	27	23	16	16	<i>4000.3</i>	33	28	24	12
<i>2500.9</i>	45	37	33	18	<i>4000.4</i>	29	24	19	16
<i>2500.10</i>	33	23	19	8	<i>4000.5</i>	52	50	44	27

Second, we investigate the performance of our heuristic on interval targets i.e. $x'Qx \in [lb, ub]$ in Table 2. For this case, we choose the intervals as (80%, 85%), (85%, 90%), (90%, 95%) and (95%, 100%) of bks . Note that (lb, ub) is equivalent to $[lb + 1, ub - 1]$ for functions with integral coefficients. We again observe from the results that the intervals close to bks do not contain as many feasible solutions. Moreover, the number of unique feasible solutions found while satisfying an interval goal as well as the deterministic goal are dependent on the solution landscape which is problem specific.

The diversity attributes for the set of solution vectors (S) output by the heuristic for a specific target were also analyzed. For this purpose, the hamming distance $h(x, y)$ between two solution vectors x and y given by the number of difference bits was computed for each pair of solution vectors. Thereafter, we calculated the mean hamming distance given by $\sum_{x, y \in S}^{x \neq y} h(x, y) / \binom{|S|}{2}$. The denominator represents the number of unique solution pairs. The mean hamming distance for all output sets was between 1 and 2. The median hamming distance is 1 or 2 while the maximum hamming distance is 2 or 3 bits. Thus the solutions found were not diverse. In other words, alternate optima for a specific target near bks are located in close proximity in the solution landscape. Based on this finding, it is more likely to find the next satisficing binary vector near the current one.

Table 2: Number of unique solutions for $x'Qx \in [lb, ub]$

Instance	(80,85)	(85,90)	(90,95)	(95,100)	Instance	(80,85)	(85,90)	(90,95)	(95,100)
<i>2500.1</i>	29	22	14	10	<i>3000.1</i>	19	15	13	10
<i>2500.2</i>	15	11	7	4	<i>3000.2</i>	42	33	26	16
<i>2500.3</i>	23	23	16	10	<i>3000.3</i>	42	37	27	19
<i>2500.4</i>	32	25	20	13	<i>3000.4</i>	24	22	11	10
<i>2500.5</i>	30	29	17	13	<i>3000.5</i>	17	17	14	8
<i>2500.6</i>	19	14	9	7	<i>4000.1</i>	25	20	12	6
<i>2500.7</i>	52	46	25	16	<i>4000.2</i>	21	10	11	5
<i>2500.8</i>	18	17	15	13	<i>4000.3</i>	18	16	14	8
<i>2500.9</i>	29	24	16	6	<i>4000.4</i>	16	18	9	5
<i>2500.10</i>	22	15	14	5	<i>4000.5</i>	36	29	26	11

5. Conclusions and Future Research

We present a novel model for two variants of goal-seeking QUBO involving either deterministic or uncertain targets. A number of alternate satisficing solutions were obtained using a greedy one-flip tabu search routine. Testing on benchmark instances clearly established the efficacy of our approach compared to state-of-the-art CP solvers which were unable to find solutions to any of the problems in the test set.

Regarding more detailed future research, our technique is easily extendable to multiple targets. For instance, achieving target levels of t_1 or t_2 would require parallelized instances of the routine searching for the two target levels. These threads could operate independently. Moreover, two different objective goals t_1 and t_2 with priorities w_1 and w_2 could be handled by changing the achievement function to $w_1(x'Q_1x - t_1)^2 + w_2(x'Q_2x - t_2)^2$. In this way, we construct the efficient solution frontier by enumerating different choices of w_1 and w_2 . Herein, the weights are determined by relative importance according to the decision-maker and is closely related to weighted or non-preemptive goal programming ([17]).

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