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Bounds for Binary Integer Programming via Unconstrained Quadratic Pseudo-Boolean Optimization

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Abstract

This research proposes a method for finding bounds in binary integer programming (BIP) and quadratic binary integer programming (QBIP). Our approach utilizes a max-flow technique within the framework of quadratic pseudo-Boolean optimization. We apply Lagrange multipliers to transform these problems into a quadratic pseudo-Boolean format, enabling us to create a corresponding network. We develop sufficient conditions under which a flow can or cannot be established in this network. The upper bound of the original problem is obtained through a feasible flow within the network. Additionally, we provide the optimality conditions for the solutions discussed in this paper. We have derived the closed forms for the various functions and values commonly used in our proposed method, as well as a lower bound for both BIP and QBIP, which can assist in solving these problems. This paper includes examples that illustrate both networks containing flows and those that do not, as well as examples that demonstrate lower and upper bound solutions as identified by our method. Furthermore, since our approach can also be applied to Quadratic Unconstrained Binary Optimization (QUBO), we provide the closed forms for the frequently used functions and values in that context, along with an example showcasing its application to a quadratic unconstrained optimization problem.

Keywords: binary integer programming; quadratic pseudo-Boolean optimization; Lagrange multipliers; max-flow

MSC: 90C10; 90C20

1. Introduction

Several real-world problems can be formulated as a BIP. Some examples are the well-known knapsack problems [1] that provide optimal solutions to transportation problems under consideration in alternative projects and the rectangle blanket problem [2], which involves the determination of an optimum blanket to minimize the non-overlapping area with the given two-dimensional image subject to an upper bound on the total number of rectangles contained in the blanket. BIP also appears in manufacturing problems such as facility location problems [3] to minimize the operating and opening costs of facilities as well as the cost of assigning the customers, scheduling problems [4] to determine the least-cost schedules for vehicles assigned to several depots, production scheduling problems [5] to reduce manufacturing costs, and phasor measurement units (PMUs) [6] that provide real-time voltage and current phasor measurements at the installed locations

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of a power grid system. Since QBIP is a BIP with a quadratic objective function, it has also been applied to many applications, for example, electrical circuit design problems [7] to find a nonoverlapping assignment of rectangular cells to positions on a chip and facility location problems [8] that involve selecting the facility locations from a set of potential locations to balance the trade-off between the facility establishment costs and the distance to end users. The methods for solving these problems have been widely studied by many researchers. They can be classified into two categories: (1) exact methods and (2) heuristic or metaheuristic methods. Since the mentioned problems are NP-hard, the exact method can only yield the optimal solution in small-size problems. Heuristic and metaheuristic methods are often used to take care of larger problems but can only find good, not necessarily the best, solutions for large-size problems.

In both BIP and QBIP, the lower bounds and the upper bounds of the problems are usually studied to guarantee optimality in the exact methods, because finding the bounds of the problems can closer the gaps between the current solution and the optimal solution. The gap is calculated by the absolute difference between the upper and lower bounds. If the gap is within a predefined tolerance, the algorithm returns a solution [9]. For example, branch and bound related algorithms, which are used to find the optimal solution, involve crucial steps to find the bounds of subproblems to reduce the size of a feasible solution set. In 2006, Huang et al. [10] studied four different strategies to estimate the lower bound of the branch and bound algorithm to solve QBIP. Their numerical results indicate that lower bound updating strategies and forcing rules play very important roles in the performance of a branch and bound algorithm. In 2022, Monaci et al. [11] studied a variant of BIP called the 0–1 Time-bomb Knapsack problem and proposed techniques to derive the upper and lower bounds using convex optimization and integer linear programming; the researchers presented three exact approaches based on enumeration, branch and bound, and dynamic programming. They computationally evaluated the performance of their algorithm on large-size instances and claimed that their algorithm is the most efficient way to tackle the problem. In 2023, Theodorakatos et al. [9] studied the PMUs related to measuring power system observability in real time. They proposed BIP, semi-definite programming, and binary polynomial models to determine the optimal number of installed PMUs by using the branch and bound algorithm. The termination criterion of the branch and bound algorithm is adjusted to be equal to $Gap = 0$. Their results showed that the optimal solutions were found in small- and medium-sized instance problems. Recently, Fennich et al. [12] studied the tight upper bounds and lower bounds of QBIP by employing a Breadth-First Search strategy and reduced the average dual-gap by up to 10% for the class of quadratic knapsack instances.

In 2012, Kashan et al. [13] proposed a new artificial bee colony algorithm that is particularly designed for binary optimization. The effectiveness of their algorithm was tested by solving a set of 15 benchmark instances of the uncapacitated facility location problem. Their results were competitive with two studies reported in the literature. In 2013, Bertsimas et al. [14] proposed a local search for solving large, sparse binary optimization problems and provided theoretical properties that guarantee the pseudo-polynomial running times and the complexity of their proposed algorithm. Later, in 2017, Umetani [15] developed a data mining approach for reducing the search space of local search algorithms for BIP. The computational results show that the proposed method improves the performance of the local search algorithm for large-scale set covering and partitioning problems. In 2021, Anacleto et al. [16] improved the processing time of evaluating flip moves in local searches and iterated tabu searches of the quadratic programming problem. In 2023, Djeumou Fomeni [17] proposed a heuristic combining the dynamic programming approach with a local search procedure for finding a good feasible solution. His algorithm can find op-

timal solutions to more than 97% of the standard instances, with optimality gaps for the other instances within 0.1%. Recently, in 2026, Moncayo-Martínez and He [18] studied the formulation of supply chain problems, including facility location and load balancing, as QUBO and solved them by using the quantum approximate optimization algorithm under both noiseless and hardware-calibrated noisy conditions. Their results showed that the unbalanced penalization approach consistently outperforms the slack-variable method, achieving higher feasibility and optimality.

To find the bounds of BIP and QBIP, one can transform the problem into QUBO. The penalty functions used to transform a constrained general problem into a QUBO model are studied in [19]; their work developed tools for integrating classical methods and quantum computing to enhance the practical applications of quantum computing in the future. Since QUBO is an NP-complete problem, large-size instances can be solved using metaheuristics [20] to obtain good solutions.

The general BIP can be formulated as

$$\begin{aligned} &\text{Minimize (or Maximize) } f(x) = \textstyle\sum_{i=1}^{n} c_i x_i \\ &\text{Subject to } \textstyle\sum_{j=1}^{m} a_{ij} x_j \leq b_i \text{ for } i = 1, \ldots, n, \\ &\qquad x_i \in \{0,1\} \text{for all } i = 1, \ldots, n. \end{aligned}$$

Whereas the QBIP can be formulated as

$$\begin{aligned} &\text{Minimize (or Maximize) } f(x) = \textstyle\sum_{j=1}^{m} \sum_{i=1}^{n} c_{ij} x_i x_j \\ &\text{Subject to } \textstyle\sum_{j=1}^{m} a_{ij} x_j \leq b_i \text{ for } i = 1, \ldots, n, \\ &\qquad x_i \in \{0,\ 1\} \text{for all } i = 1, \ldots, n. \end{aligned}$$

These problems can eventually be transformed into QUBO using the Lagrange multiplier and the objective function of BIP or QBIP, and all the constraints can be written in the form of the function $G(x, l)$, which is defined by

$$G(x,l) = f(x) + \sum_{i=1}^{n} l_i \Big(\sum_{j=1}^{m} a_{ij} x_j - b_i\Big),$$

where l_i are the Lagrange multipliers and the variables x_j are binary. It can be seen that $G(x, l)$ is a quadratic pseudo-Boolean function.

Among the works on quadratic pseudo-Boolean optimization, in 1984, Hammer et al. [21] studied a quadratic unconstrained binary maximization problem in which the problem was considered in various forms, e.g., the primal problem of maximization, the pseudo-Boolean complementation problem, the discrete Rhys 0–1 linear program, the weighted stability problem of SAM graphs, and their relaxations. Quadratic unconstrained pseudo-Boolean optimization was used to find the bounds of this problem. Optimality conditions were proposed, and the problems could be executed in polynomial time.

Optimization of the quadratic pseudo-Boolean function can be written following their work in the form of QUBO as

$$\max_x f(x) = \sum_{j=1}^{m} \sum_{i=1}^{n} c_{ij} x_i x_j$$

After the transformation, BIP and QBIP can be transformed into QUBO as

$$\min_x x^T Q x = \min_x \left\{ f(x) + \sum_{i=1}^{m} u_i r_i(x) \right\}$$

where $f(x)$ is the objective function, $r_i\ (x), i = 1, 2, \ldots, m$ are the constraints, and u_i are the Lagrange multipliers.

General pseudo-Boolean optimization was used to find the bounds in the work by Boros and Hammer [22]. They presented a brief overview of the theoretical and algorithmic aspects of pseudo-Boolean functions. Later, in 2008, Boros et al. [23] proposed a maximum cut graph–theoretic approach to provide the bounds. They constructed an iterated roof dual bound of QUBO, which can be computed using a network flow formulation. The computational results showed that the bounds obtained were significantly better than the bounds computed from the then-existing works. In 2017, Anthony et al. [24] studied the quadratizations of pseudo-Boolean functions that are similar to QUBO and derived the lower and upper bounds for the number of auxiliary variables required in the smallest possible quadratization of arbitrary functions. In the same year, Lewis and Glover [25] conducted a study on strategies for reducing the size of the QUBO matrix by identifying the variables whose optimal values can be predetermined. Their approach enhanced both the quality of the solutions and the execution times, utilizing an exact algorithm alongside a tabu search metaheuristic. The findings indicated that while the quality of the solutions achieved within reasonable time constraints was notable, optimal results could not be guaranteed when employing the metaheuristic approach.

Heuristic methods for solving QUBO include the simulated annealing algorithm by Alkhamis et al. [26]. Their work in 1998 started with an initial solution, explored easily reached neighboring solutions and then selected the best among them according to which one improved the solution with $O(n^2)$ computational time. Later, in 2000, there was a genetic local search algorithm by Katayama et al. [27] that combined a genetic algorithm and a local search to solve large instances of 2500 variables. Then, in the year 2002, a greedy algorithm and two local search algorithms were created by Merz and Freisleben [28] to solve the unconstrained binary quadratic programming problem (BQP). The algorithm started with constructing feasible solutions and adding random components to a deterministic greedy heuristic to improve the feasible solution. In the year 2007, Boros et al. [29] also constructed a local-search-based heuristic for QUBO starting with a feasible fractional initial point that can be improved by rounding or switching the values of one variable.

Then, in 2020, deep-reinforcement-learning-based heuristics were developed by Chen et al. [30]. The processes involve the solution construction using a neural network model and solution improvement using two variants of deep reinforcement learning. Metaheuristic methods for finding the solution of QUBO are widely studied. For example, in 2014, Liefooghe et al. [31] proposed a hybrid metaheuristic that combines an elitist evolutionary multi-objective optimization algorithm and a tabu search procedure by using an achievement scalarizing function for the multi-objective case of QUBO. Recently, in 2024, Pérez Armas et al. [32] transformed a mixed integer linear program into QUBO and solved QUBO for small- and medium-sized instances using a quantum annealing method and compared their results with what existed in the literature. Moreover, in 2025, Liu et al. [33] proposed a new open-source quantum-inspired metaheuristic algorithm that combines scatter search, adaptive tenure tabu search, and path-relinking. The performance of their proposed algorithm was highly competitive in both solution quality and computational efficiency when compared with the leading metaheuristic QUBO solvers.

In this research, we propose a method for finding a bound for BIP using the max-flow approach on QUBO. First, BIP is transformed into the QUBO form using the Lagrange multipliers and some relaxations. A bound or, if possible, a solution for this problem is obtained via the max-flow approach of the corresponding network. In order to use the max-flow approach to find the bound, one has to construct a network from the quadratic unconstrained pseudo-Boolean optimization problem. Since the constructed network does

not necessarily contain a flow, which is essential, and eventually gives the bound for the solution, sufficient conditions for the network to have such flow or not are proposed, along with some illustrative examples. The feasibility of the bound found by the proposed method is considered to identify a lower or an upper bound for the problem. Some examples and the closed forms of the frequently used functions and values used in the proposed method are also given in this paper.

The remainder of this paper is structured as follows. Section 2 describes the model formulation, consisting of the problem statement and the network construction. The problem statement includes the definition of BIP, the transformation BIP to QUBO via the Lagrange multipliers and the closed form of the transformation, while the network construction includes the definition of the network corresponding to the bi-form, the definition of the flows and their complement flows and the propositions related to the bound of BIP. Section 3 is a step-by-step algorithm for finding a lower bound of BIP and applied to QBIP. The conclusions are discussed in the last section.

2. Model Formulation

2.1. Problem Statement

In this research, we consider a constrained binary integer programming problem

$$\begin{aligned} &\min_x f(x) = c_0 + \textstyle\sum_{i=1}^{n} c_i x_i \\ &s.t.\ \ r(x) \leq 0 \\ &\quad x_i \in \{0,\ 1\} \text{for all } i = 1, \ldots, n, \end{aligned} \tag{1}$$

where $r(x) = (r_1(x),\ \ldots,\ r_m(x))$ and $r_1(x),\ \ldots,\ r_m(x)$ are linear functions.

The Lagrangian function of Problem (1) is

$$\begin{aligned} L(x,u) &= f(x) + u^t r(x) \\ &= f(x) + \textstyle\sum_{j=1}^{m} u_j r_j(x). \end{aligned}$$

Problem (1) can be rewritten in unconstrained binary integer programming using the Lagrangian function as

$$\min_{x,u} L(x,u) = f(x) + \textstyle\sum_{j=1}^{m} u_j r_j(x), \tag{2}$$

where $u_j \geq 0$ for $j = 1,\ \ldots,\ m$.

Problem (2) is a quadratic function, since its last term is a summation of the products between $r_j(x)$ and u_j where $r_j(x)$ and u_j are linear. We can see that Problem (1) has been transformed into a quadratic unconstrained optimization problem. To change (2) into a quadratic unconstrained binary optimization problem, (2) is relaxed to a quadratic pseudo-Boolean function by $u_j = \{0,\ 1\}$, for $j = 1,\ \ldots,\ m$. Then, u_j is substituted with x_i for $i = n + 1, \ldots, n + m$. Hence, the QUBO for this problem can be formulated as

$$\min_x L(x) = f(x) + \textstyle\sum_{i=n+1}^{n+m} x_i r_i(x) \tag{3}$$

where $x = (x_1,\ \ldots,\ x_n,\ x_{n+1},\ \ldots,\ x_{n+m})$, $f(x)$ and $r(x)$ are linear, and $L(x)$ is in a quadratic pseudo-Boolean form.

Note that QBIP can also be transformed into QUBO and may be analyzed using the method constructed in this work.

Developed thoroughly in Hammer et al. [21], the following definitions and remarks have been modified and extended to solve (1).

Definition 1. *A quadratic pseudo-Boolean*

$$L(x) = c_0 + \sum_{j=1}^{n+m} c_j x_j + \sum_{1\le i\le n} \sum_{n+1\le j\le n+m} c_{ij} x_i x_j \tag{4}$$

where c_0, c_j, c_{ij} are constants and x_i, x_j are binary.

Definition 2.

$$\widetilde{L}(x) = L(x) \tag{5}$$

where $x_i x_j = \frac{1}{2}(x_i x_j + \overline{x}_i \overline{x}_j) + \frac{1}{2}(x_i + x_j) - \frac{1}{2}$,
$-x_i x_j = \frac{1}{2}(x_i \overline{x}_j + \overline{x}_i x_j) - \frac{1}{2}(x_i + x_j)$,
$x_i = x_0 x_i + \overline{x}_0 \overline{x}_i$,
$-x_i = x_0 \overline{x}_i + \overline{x}_0 x_i - 1$.

The term $x_i\ \overline{x}_j + \overline{x}_i\ x_j$ is called a *positive bi-term*, and $x_i\ x_j + \overline{x}_i\ \overline{x}_j$ is called a *negative bi-term*. We can write

$$\widetilde{L}(x) = C + \sum_{(i,j)\in E^+} c_{ij}(x_i \overline{x}_j + \overline{x}_i x_j) + \sum_{(i,j)\in E^-} c_{ij}(x_i x_j + \overline{x}_i \overline{x}_j)$$

where C is constant, $c_{ij} \ge 0$, E^+ is the set of positive bi-terms, and E^- is the set of negative bi-terms; or

$$\widetilde{L}(x_0, \ldots, x_{n+m}) = C + \phi(x_0, \ldots, x_{n+m}) \tag{6}$$

where C is constant and ϕ is called a *bi-form*, which is the collection of bi-terms.

Example 1. *Consider the following problem:*

$$\begin{aligned} \min_x\ & f(x) = 2x_1 + 2x_2 - 3x_3 - x_4 \\ \text{s.t.}\ & x_1 + x_3 - 1 \le 0 \\ & x_2 + x_3 - 1 \le 0 \\ & x_1 + x_2 + x_4 - 1 \le 0 \\ & x_i \in \{0,\ 1\}. \end{aligned} \tag{7}$$

A quadratic pseudo-Boolean function of Equation (7) is

$$\begin{aligned} L(x) \quad &= 2x_1 + 2x_2 - 3x_3 - x_4 + x_1x_5 + x_3x_5 - x_5 + x_2x_6 + x_3x_6 - x_6 + x_1x_7 + x_2x_7 \\ &\quad + x_4x_7 - x_7. \end{aligned}$$

From Definition 2, its bi-form is

$$\begin{aligned} \widetilde{L}(x) \quad &= -6 + 3(x_0x_1 + \overline{x}_0\overline{x}_1) + 3(x_0x_2 + \overline{x}_0\overline{x}_2) + 2(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_0\overline{x}_4 + \overline{x}_0x_4) \\ &\quad + \tfrac{1}{2}(x_0x_7 + \overline{x}_0\overline{x}_7) + \tfrac{1}{2}(x_1x_5 + \overline{x}_1\overline{x}_5) + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5) + \tfrac{1}{2}(x_2x_6 + \overline{x}_2\overline{x}_6) \\ &\quad + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) + \tfrac{1}{2}(x_1x_7 + \overline{x}_1\overline{x}_7) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7). \end{aligned}$$

Since $\widetilde{L}(x) = C + \phi(x)$, $C = -6$ and

$$\begin{aligned} \phi \quad &= 3(x_0x_1 + \overline{x}_0\overline{x}_1) + 3(x_0x_2 + \overline{x}_0\overline{x}_2) + 2(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_0\overline{x}_4 + \overline{x}_0x_4) \\ &\quad + \tfrac{1}{2}(x_0x_7 + \overline{x}_0\overline{x}_7) + \tfrac{1}{2}(x_1x_5 + \overline{x}_1\overline{x}_5) + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5) + \tfrac{1}{2}(x_2x_6 + \overline{x}_2\overline{x}_6) \\ &\quad + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) + \tfrac{1}{2}(x_1x_7 + \overline{x}_1\overline{x}_7) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7). \end{aligned}$$

Definition 3. *Call $x_r = 1$ a root of ϕ. We have*

$$\min_{(x_1,x_2,\ldots,x_{n+m})\in\{0,\,1\}^{n+m}} L(x_1,\ldots,x_{n+m}) = C + \min_{(x_0,x_1,x_2,\ldots,x_{n+m})\in\{0,\,1\}^{n+m+1}} \phi(x_0,x_1,\ldots,x_{n+m}). \tag{8}$$

The proof of Equation (8) is trivial, as proved in [21].

Example 2. *Consider the $L(x)$ of Equation (7) from Example 1.*
We find that $x_0 = 1$ is a root of ϕ.

Proposition 1. *The constant C in Equation (8) can be written in a closed form as*

$$C = c_0 - \sum_{\substack{i=1 \\ c_i+\sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}<0}}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \tag{9}$$

Proof. From Equation (4), $L(x) = c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{j=n+1}^{n+m} c_{ij} x_i x_j$ is a quadratic pseudo-Boolean function. From Definition 2, the constant terms appear only when the coefficients c_i of x_i and c_{ij} of $x_i x_j$ are less than and greater than zero, respectively.

For $c_{ij} > 0$, substitute $c_{ij}\, x_i x_j = \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \frac{|c_{ij}|}{2} x_i + \frac{|c_{ij}|}{2} x_j - \frac{|c_{ij}|}{2}$. We obtain

$$\begin{aligned} L(x) \;&= c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_j \\ &\quad - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} c_{ij} x_i x_j \\ &= c_0 + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \sum_{i=1}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) x_i - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \\ &\quad + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} c_{ij} x_i x_j. \end{aligned}$$

For the coefficient of x_i:
If $c_i < -\sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}$, we have the coefficient of $x_i < 0$. We then substitute as follows:

$$-\left| c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right| x_i = \left| c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right| (x_0 \overline{x}_i + \overline{x}_0 x_i) - \left| c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right|$$

Thus, we obtain

$$
\begin{aligned}
L(x) \quad &= c_0 + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) + \sum_{\substack{i=1 \\ c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} > 0}}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) x_i \\
&+ \sum_{\substack{i=1 \\ c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} < 0}}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) (x_0 \overline{x}_i + \overline{x}_0 x_i) - \sum_{\substack{i=1 \\ c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} < 0}}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) \\
&- \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} c_{ij} x_i x_j.
\end{aligned}
$$

Thus, we obtain the constant

$$
C = c_0 - \sum_{\substack{i=1 \\ c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} < 0}}^{n+m} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \right) - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}.
$$

□

Example 3. *Consider Equation (7) from Example 1.*
Using the closed form of Equation (9), we obtain

$$
C = c_0 - \sum_{i=1}^{7} \left| c_i + \sum_{\substack{j=5 \\ c_{ij}>0}}^{7} \frac{|c_{ij}|}{2} \right| - \sum_{i=1}^{4} \sum_{\substack{j=5 \\ c_{ij}>0}}^{7} \frac{|c_{ij}|}{2} = 0 - \left(\frac{5}{2} \right) - \left(\frac{7}{2} \right) = -6,
$$

which is the same as that obtained in Example 1.

Proposition 2. *$\widetilde{L}(x)$ can be written in the closed form as*

$$
\begin{aligned}
\widetilde{L}(x) \quad &= c_0 - \sum_{\substack{i=1 \\ \gamma_i<0}}^{n+m} |\gamma_i| - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{\substack{i=1 \\ \gamma_i>0}}^{n+m} |\gamma_i|(x_0 x_i + \overline{x}_0 \overline{x}_i) + \sum_{\substack{i=1 \\ \gamma_i<0}}^{n+m} |\gamma_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) \\
&+ \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j)
\end{aligned} \tag{10}
$$

where

$$\gamma_i = \begin{cases} c_i + \sum\limits_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} - \sum\limits_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}, \; i = 1, \ldots, n, \\ c_i + \sum\limits_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ji}|}{2} - \sum\limits_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ji}|}{2}, i = n+1, \ldots, n+m. \end{cases}$$

Proof. From Equation (4), $L(x) = c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{j=n+1}^{n+m} c_{ij} x_i x_j$.

From Definition 2, if $c_{ij} > 0$, substitute

$$c_{ij}\, x_i x_j = \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \frac{|c_{ij}|}{2} x_i + \frac{|c_{ij}|}{2} x_j - \frac{|c_{ij}|}{2}$$

to obtain

$$\begin{aligned} L(x) \;= c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_j \\ - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} c_{ij} x_i x_j. \end{aligned}$$

For $c_{ij} < 0$, substitute $-|c_{ij}|\, x_i x_j = \frac{|c_{ij}|}{2}\left(x_i \overline{x}_j + \overline{x}_i x_j\right) - \frac{|c_{ij}|}{2} x_i - \frac{|c_{ij}|}{2} x_j$, and we obtain

$$\begin{aligned} L(x) \;&= c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} x_j \\ &\quad - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i \overline{x}_j + \overline{x}_i x_j\right) - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2} x_i - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2} x_j. \\ &= c_0 + \sum_{i=1}^{n} \left(c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} - \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2} \right) x_i + \sum_{i=n+1}^{n+m} \left(c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ji}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ji}|}{2} \right) x_i \\ &\quad + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i x_j + \overline{x}_i \overline{x}_j\right) - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i \overline{x}_j + \overline{x}_i x_j\right). \end{aligned}$$

For $i = 1, \ldots, n$, let $\gamma_i = c_i + \sum_{\substack{j=n+1 \\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} - \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}$. For $i = n+1, \ldots, n+m$, let $\gamma_i = c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ji}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ji}|}{2}$.

If $\gamma_i > 0$, substitute $|\gamma_i|\, x_i = |\gamma_i|(x_0 x_i + \overline{x}_0 \overline{x}_i)$, and if $\gamma_i < 0$, substitute $-|\gamma_i|\, x_i = |\gamma_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) - |\gamma_i|$. We then obtain

$$\begin{aligned}
\widetilde{L}(x) &= c_0 + \sum_{\substack{i=1\\ \gamma_i>0}}^{n} |\gamma_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=n+1\\ \gamma_i>0}}^{n+m} |\gamma_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1\\ \gamma_i<0}}^{n} (|\gamma_i|(x_0\overline{x}_i + \overline{x}_0x_i) - |\gamma_i|) \\
&+ \sum_{\substack{i=n+1\\ \gamma_i<0}}^{n+m} (|\gamma_i|(x_0\overline{x}_i + \overline{x}_0x_i) - |\gamma_i|) + \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) - \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \\
&+ \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j) \\
&= c_0 - \sum_{\substack{i=1\\ \gamma_i<0}}^{n+m} |\gamma_i| - \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} + \sum_{\substack{i=1\\ \gamma_i>0}}^{n+m} |\gamma_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1\\ \gamma_i<0}}^{n+m} |\gamma_i|(x_0\overline{x}_i + \overline{x}_0x_i) \\
&+ \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j).
\end{aligned}$$

Thus, we obtain $\widetilde{L}(x) = C + \phi$ where

$$\begin{aligned}
C &= c_0 - \sum_{\substack{i=1\\ \gamma_i<0}}^{n+m} |\gamma_i| - \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} \\
&= c_0 - \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} - \sum_{\substack{i=1\\ c_i - \frac{|c_{ij}|}{2} < 0}}^{n} \sum_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \left| c_i - \frac{|c_{ij}|}{2} \right| - \sum_{\substack{j=1\\ c_j - \frac{|c_{ij}|}{2} < 0}}^{n} \sum_{\substack{i=n+1\\ c_{ij}<0}}^{n+m} \left| c_j - \frac{|c_{ij}|}{2} \right|, \\
\phi &= \sum_{\substack{i=1\\ \gamma_i>0}}^{n+m} |\gamma_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1\\ \gamma_i<0}}^{n+m} |\gamma_i|(x_0\overline{x}_i + \overline{x}_0x_i) + \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) \\
&+ \sum_{i=1}^{n} \sum_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j)
\end{aligned}$$

and

$$\gamma_i = \begin{cases} c_i + \sum\limits_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2} - \sum\limits_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}, \ i = 1, \ldots, n \\ c_i + \sum\limits_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ji}|}{2} - \sum\limits_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ji}|}{2}, i = n+1, \ldots, n+m \end{cases} \tag{11}$$

□

In fact, $L(x)$ in (4) is a QUBO. Hence, for a general QUBO, $Q(x)$, we can develop a closed form for its bi-form, as in the following corollary. Suppose a general QUBO can be written as

$$Q(x) = c_0 + \sum_{i=1}^{n} c_i x_i + \sum_{1\le i\le n} \sum_{1\le j\le n} c_{ij} x_i x_j.$$

Corollary 1. *The bi-form, $\widetilde{Q}(x)$, of a general QUBO, $Q(x)$, can be written in a closed form as*

$$\begin{aligned}\widetilde{Q}(x) \;= c_0 - \sum_{\substack{i=1\\ \delta_i<0}}^{n} |\delta_i| - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} + \sum_{\substack{i=1\\ \delta_i>0}}^{n} |\delta_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1\\ \delta_i<0}}^{n} |\delta_i|(x_0\overline{x}_i + \overline{x}_0x_i)\\ + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j)\end{aligned}$$

where

$$\delta_i = c_i + \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2},\ i = 1, .., n.$$

Proof. From $Q(x) = c_0 + \sum_{i=1}^{n} c_ix_i + \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij}x_ix_j$, and Definition 2, if $c_{ij} > 0$, substitute $c_{ij}\, x_ix_j = \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \frac{|c_{ij}|}{2}x_i + \frac{|c_{ij}|}{2}x_j - \frac{|c_{ij}|}{2}$, we have

$$\begin{aligned}Q(x) \;= c_0 + \sum_{i=1}^{n} c_ix_i + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}x_i + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}x_j\\ - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} c_{ij}x_ix_j.\end{aligned}$$

For $c_{ij} < 0$, substitute $-|c_{ij}|\, x_ix_j = \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j) - \frac{|c_{ij}|}{2}x_i - \frac{|c_{ij}|}{2}x_j$, and we then obtain

$$\begin{aligned}L(x) \;= c_0 + \sum_{i=1}^{n} c_ix_i + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}x_i + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}x_j\\ - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j) - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}x_i - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}x_j\\ = c_0 + \sum_{i=1}^{n} \left(c_i + \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2} \right) x_i + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) - \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}\\ + \sum_{i=1}^{n} \sum_{\substack{j=1\\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j).\end{aligned}$$

For $i = 1, \ldots, n$, let $\delta_i = c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}$.

If $\delta_i > 0$, substitute $|\delta_i|\ x_i = |\delta_i|(x_0 x_i + \overline{x}_0 \overline{x}_i)$, and if $\delta_i < 0$, substitute $-|\delta_i|\ x_i = |\delta_i|(x_i \overline{x}_0 + \overline{x}_i x_0) - |\delta_i|$. We then obtain

$$\begin{aligned}
\widetilde{Q}(x) &= c_0 + \sum_{\substack{i=1 \\ \delta_i>0}}^{n} |\delta_i|(x_0 x_i + \overline{x}_0 \overline{x}_i) + \sum_{\substack{i=1 \\ \delta_i<0}}^{n} (|\delta_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) - |\delta_i|) \\
&\quad + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) \\
&= c_0 - \sum_{\substack{i=1 \\ \delta_i<0}}^{n} |\delta_i| - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} + \sum_{\substack{i=1 \\ \delta_i>0}}^{n} |\delta_i|(x_0 x_i + \overline{x}_0 \overline{x}_i) + \sum_{\substack{i=1 \\ \delta_i<0}}^{n} |\delta_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) \\
&\quad + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j).
\end{aligned}$$

Thus, we obtain $\widetilde{Q}(x) = C + \phi$, where

$$\begin{aligned}
C &= c_0 - \sum_{\substack{i=1 \\ \delta_i<0}}^{n} |\delta_i| - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} \\
&= c_0 - \sum_{i=1}^{n} \left| c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2} \right| - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}, \\
\phi &= \sum_{\substack{i=1 \\ \delta_i>0}}^{n} |\delta_i|(x_0 x_i + \overline{x}_0 \overline{x}_i) + \sum_{\substack{i=1 \\ \delta_i<0}}^{n} |\delta_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) \\
&\quad + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j),
\end{aligned}$$

and

$$\delta_i = c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2},\ i = 1, \ldots, n.$$

□

Example 4. *From Example 1,* $L(x) = 2x_1 + 2x_2 - 3x_3 - x_4 + x_1x_5 + x_3x_5 - x_5 + x_2x_6 + x_3x_6 - x_6 + x_1x_7 + x_2x_7 + x_4x_7 - x_7$ *and* $C = -6$ *from Example 3.*

$$\begin{aligned}
\gamma_1 &= c_1 + \tfrac{c_{15}}{2} + \tfrac{c_{17}}{2} = 2 + \tfrac{1}{2} + \tfrac{1}{2} = 3,\\
\gamma_2 &= c_2 + \tfrac{c_{26}}{2} + \tfrac{c_{27}}{2} = 2 + \tfrac{1}{2} + \tfrac{1}{2} = 3,\\
\gamma_3 &= c_3 + \tfrac{c_{35}}{2} + \tfrac{c_{36}}{2} = -3 + \tfrac{1}{2} + \tfrac{1}{2} = -2,\\
\gamma_4 &= c_4 + \tfrac{c_{47}}{2} = -1 + \tfrac{1}{2} = -\tfrac{1}{2},\\
\gamma_5 &= c_5 + \tfrac{c_{15}}{2} + \tfrac{c_{35}}{2} = -1 + \tfrac{1}{2} + \tfrac{1}{2} = 0,\\
\gamma_6 &= c_6 + \tfrac{c_{26}}{2} + \tfrac{c_{36}}{2} = -1 + \tfrac{1}{2} + \tfrac{1}{2} = 0, \text{ and}\\
\gamma_7 &= c_7 + \tfrac{c_{17}}{2} + \tfrac{c_{27}}{2} + \tfrac{c_{47}}{2} = -1 + \tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2} = \tfrac{1}{2}.
\end{aligned}$$

From Proposition 2, using the closed form in Equation (10), we have

$$\begin{aligned}
\phi \;=\; & \sum_{\substack{i=1\\ \gamma_i>0}}^{n+m} |\gamma_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1\\ \gamma_i<0}}^{n+m} |\gamma_i|(x_0\overline{x}_i + \overline{x}_0x_i) + \sum_{i=1}^{n}\sum_{\substack{j=n+1\\ c_{ij}>0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_ix_j + \overline{x}_i\overline{x}_j\right)\\
& + \sum_{i=1}^{n}\sum_{\substack{j=n+1\\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}\left(x_i\overline{x}_j + \overline{x}_ix_j\right)\\
= {} & 3(x_0x_1 + \overline{x}_0\overline{x}_1) + 3(x_0x_2 + \overline{x}_0\overline{x}_2) + 2(\overline{x}_0x_3 + x_0\overline{x}_3) + \frac{1}{2}(\overline{x}_4x_0 + \overline{x}_0x_4)\\
& + \frac{1}{2}(x_0x_7 + \overline{x}_0\overline{x}_7) + \frac{1}{2}(x_1x_5 + \overline{x}_1\overline{x}_5) + \frac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5) + \frac{1}{2}(x_2x_6 + \overline{x}_2\overline{x}_6)\\
& + \frac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) + \frac{1}{2}(x_1x_7 + \overline{x}_1\overline{x}_7) + \frac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \frac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7)
\end{aligned}$$

as obtained in Example 1.

2.2. Network Construction

A network N, with $2(n+m)+2$ vertices corresponding to a bi-form ϕ, can be constructed depending on the chosen root. Recall that a root of ϕ is a variable with a value equal to one. After a root of ϕ is chosen, a network N is constructed; then, a lower bound of (8) can be computed using a maximum-flow problem via a network N. Note that a root of ϕ can be at any arbitrary variable.

Definition 4. *Given a bi-form*

$$\phi(x_0, x_1, \ldots, x_{n+m}) = \sum_{(i,j)\in E^+} c_{ij}\left(x_i\overline{x}_j + \overline{x}_ix_j\right) + \sum_{(i,j)\in E^-} c_{ij}\left(x_ix_j + \overline{x}_i\overline{x}_j\right).$$

A network $N = (V, A)$ corresponding to a bi-formϕ, is constructed with $2(n+m)+2$ vertices, having a root at x_r. The vertices of the constructed network are defined as $V = \{0, \overline{0}, 1, \overline{1}, \ldots, n+m, \overline{n+m}\}$. Every positive bi-term $(i,j) = x_i\overline{x}_j + \overline{x}_ix_j$ will be an edge e connected between i and j and an edge e' between $\overline{i}$ and $\overline{j}$ in the network. The negative bi-term $(i,j) = x_ix_j + \overline{x}_i\overline{x}_j$ will be an edge e between i and $\overline{j}$ and an edge e' between $\overline{i}$ and j. The capacities of edge e and e' in N are $\left(\frac{1}{2}\right)c_{ij}$.

Definition 5. *Let a flow from r to $\overline{r}$ in N through the vertices $\{u_1, u_2, u_3, \ldots, u_{p-2}, u_{p-1}, u_p\}$ be a flow starting at a vertex r, i.e., $u_1 = r$, and ending at a vertex $\overline{r}$, i.e., $u_p = \overline{r}$. Denote the flow F_i, $i = 1, \ldots, t$ with values f_i.*

A complement flow from r to $\overline{r}$ in N through the vertices $\{\overline{u}_p, \overline{u}_{p-1}, \overline{u}_{p-2}, \ldots, \overline{u}_3, \overline{u}_2, \overline{u}_1\}$ is a flow starting at a vertex $\overline{u}_p = r$, through a vertex $\overline{u}_{p-1}, \overline{u}_{p-2}, \ldots, \overline{u}_3, \overline{u}_2$, and ending at a vertex $\overline{u}_1 = \overline{r}$. Denote the complement flow $\overline{F}_i, i = 1, \ldots, t$ be (i.e., $\overline{u}_p = r$, $\overline{u}_1 = \overline{r}$) with values f_i. A flow together with a complement flow is called a bi-flow.

Definition 6. *A feasible solution of (8), ζ, is a collection of ζ_i where ζ_i is the total flow on the ith bi-flow with the edge in the bi-flow. That is,*

$$\zeta_i = 2f_i,\ N_i = \{(j,k)|(j,k) \text{ is an edge in a flow } F_i \text{ and } \overline{F}_i\}.$$

Example 5. *Consider the Equation (7) in Example 1. Then, construct a network corresponding to the bi-form ϕ, as shown in Figure 1. Let the root of bi-form ϕ be x_0; we obtain the flows and their complement flows from Definition 5 as follows:*

$$\begin{array}{l} F_1 : 0 \to \overline{1} \to 5 \to \overline{3} \to \overline{0},\ f_1 = \frac{1}{4},\ \overline{F}_1 : 0 \to 3 \to \overline{5} \to 1 \to \overline{0},\ f_1 = \frac{1}{4}, \\ F_2 : 0 \to \overline{2} \to 7 \to \overline{4} \to \overline{0},\ f_2 = \frac{1}{4},\ \overline{F}_2 : 0 \to 4 \to \overline{7} \to 2 \to \overline{0},\ f_2 = \frac{1}{4}, \\ F_3 : 0 \to \overline{1} \to 7 \to \overline{0},\ f_3 = \frac{1}{4},\ \overline{F}_3 : 0 \to \overline{7} \to 1 \to \overline{0},\ f_3 = \frac{1}{4}, \\ F_4 : 0 \to \overline{2} \to 6 \to \overline{3} \to \overline{0},\ f_4 = \frac{1}{4},\ \overline{F}_4 : 0 \to 3 \to \overline{6} \to 2 \to \overline{0},\ f_4 = \frac{1}{4}. \end{array}$$

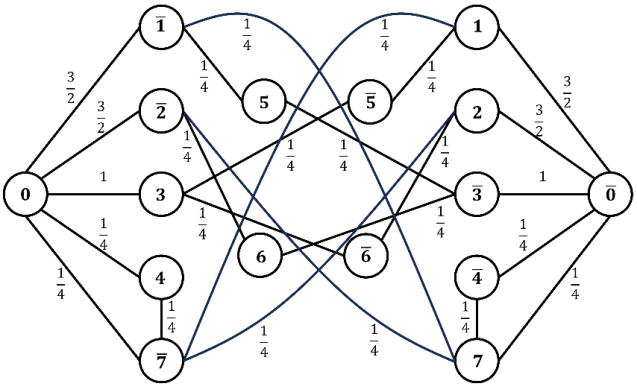


Figure 1. Network N corresponding to the bi-form ϕ in Example 4.

Hence, from Definition 6,

$$\zeta = \begin{cases} \frac{1}{2},\ N_1 = [(0,1),(1,5),(5,3),(3,0)], \\ \frac{1}{2},\ N_2 = [(0,7),(7,1),(1,0)], \\ \frac{1}{2},\ N_3 = [(0,2),(2,7),(7,4),(4,0)], \\ \frac{1}{2},\ N_4 = [(0,2),(2,6),(6,3),(3,0)], \\ 0\ , \text{ otherwise.} \end{cases}$$

Definition 7. *Let the root of a given bi-form ϕ be x_r, $r = 0, 1, \ldots, n+m$, then the problem*

$$\min_{(x_0,x_1,\ldots,x_{n+m}) \in \{0,\ 1\}^{n+m+1}} \widetilde{L} = C + \phi \tag{12}$$

has a lower bound $\rho(L_r) = C + \sum_{i=1}^{t} \zeta_i$.

Note that $\min_{(x_0,x_1,\ldots,x_{n+m}) \in \{0,\ 1\}^{n+m+1}} \widetilde{L} \geq \max_{r \in \{0,\ 1,\ldots,n+m\}} \rho(L_r)$.

Remark 1. $\max_{r \in \{0,\ 1,\ldots,n+m\}} \rho(L_r) \geq \rho(L_r)$ *for all r.*

Definition 8. *Given a bi-form ϕ and a feasible solution ζ, we shall define the ζ decomposition of ϕ as*

$$\phi = h_\zeta + g_\zeta + \phi'_\zeta,$$

where $h_\zeta = \sum_{i=1}^{t} \zeta_i N_i$, g_ζ *is the remaining bi-form of* $\phi - h_\zeta$ *containing* x_r, *and* ϕ'_ζ *is the remaining bi-form of* $\phi - h_\zeta$.

From the Persistency theorem in [23], if ζ is an optimal solution, then at any minimum point x^* of ϕ, we have $g_\zeta(x^*) = 0$. Observing that each of the terms of $g_\zeta(x)$ is nonnegative, and that $x_r = 1$ if the root of ϕ is at x_r, we can find an x that makes $g_\zeta(x) = 0$. Since $L(x) = f(x)$ from (1), and since we are minimizing $f(x)$, some of the unknown variables left can be observed by minimizing $L(x)$. If x is a feasible solution for (1), x is an upper bound of (1). If x is not feasible, $\rho(L_r)$ is a lower bound of (1). If ϕ'_ζ is not equal to zero, a network N corresponding to ϕ'_ζ is constructed with a new root to start the next iteration.

Proposition 3. *Let* $\hat{x}$ *be a solution found from* $g_\zeta(x) = 0$, *with the unknown variables observed by minimizing* $L(x)$. *If* $\hat{x}$ *is not feasible for (1), then* $L(\hat{x})$ *is a lower bound of (1).*

Proof. Since $\hat{x}$ is not feasible for (1), (1) can be solved by minimizing $L(x)$. From Remark 1, we have $\min\limits_{\sim} L = \min L \geq \max\rho(L_r) \geq \rho(L_r) = L(\hat{x})$. Hence, $L(\hat{x})$ is a lower bound of $\min\limits_{\sim} L$. Therefore, $L(\hat{x})$ is also a lower bound of (1). □

Example 6. *Consider the following problem*

$$\begin{aligned} &\min_x f(x) = 3x_1 + x_2 - 2x_3 - x_4 - 5x_5 \\ \text{s.t. } & x_1 + x_3 + x_5 - 1 \leq 0 \\ & x_2 + x_4 - 1 \leq 0 \\ & x_1 + x_3 + x_4 - 1 \leq 0 \\ & x_i \in \{0,\ 1\}. \end{aligned} \tag{13}$$

A quadratic pseudo-Boolean function of (13) is

$$\begin{aligned} L(x) \quad &= 3x_1 + x_2 - 2x_3 - x_4 - 5x_5 + x_1x_6 + x_3x_6 + x_5x_6 - x_6 + x_2x_7 + x_4x_7 - x_7 + x_1x_8 \\ &+ x_3x_8 + x_4x_8 - x_8, \end{aligned}$$

and its bi-form is

$$\begin{aligned} \widetilde{L}(x) \quad &= -\tfrac{19}{2} + 4(x_0x_1 + \overline{x}_0\overline{x}_1) + \tfrac{3}{2}(x_0x_2 + \overline{x}_0\overline{x}_2) + (x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{9}{2}(x_0\overline{x}_5 + \overline{x}_0x_5) \\ &+ \tfrac{1}{2}(x_0x_6 + \overline{x}_0\overline{x}_6) + \tfrac{1}{2}(x_0x_8 + \overline{x}_0\overline{x}_8) + \tfrac{1}{2}(x_1x_6 + \overline{x}_1\overline{x}_6) + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) \\ &+ \tfrac{1}{2}(x_5x_6 + \overline{x}_5\overline{x}_6) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) + \tfrac{1}{2}(x_1x_8 + \overline{x}_1\overline{x}_8) \\ &+ \tfrac{1}{2}(x_3x_8 + \overline{x}_3\overline{x}_8) + \tfrac{1}{2}(x_4x_8 + \overline{x}_4\overline{x}_8). \end{aligned}$$

Since $\widetilde{L} = C + \phi,\ C = -\frac{19}{2}$ *and*

$$\begin{aligned} \phi \quad &= 4(x_0x_1 + \overline{x}_0\overline{x}_1) + \tfrac{3}{2}(x_0x_2 + \overline{x}_0\overline{x}_2) + (x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{9}{2}(x_0\overline{x}_5 + \overline{x}_0x_5) \\ &+ \tfrac{1}{2}(x_0x_6 + \overline{x}_0\overline{x}_6) + \tfrac{1}{2}(x_0x_8 + \overline{x}_0\overline{x}_8) + \tfrac{1}{2}(x_1x_6 + \overline{x}_1\overline{x}_6) + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) \\ &+ \tfrac{1}{2}(x_5x_6 + \overline{x}_5\overline{x}_6) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) + \tfrac{1}{2}(x_1x_8 + \overline{x}_1\overline{x}_8) \\ &+ \tfrac{1}{2}(x_3x_8 + \overline{x}_3\overline{x}_8) + \tfrac{1}{2}(x_4x_8 + \overline{x}_4\overline{x}_8). \end{aligned}$$

The flows and their complement flows with the root of bi-form ϕ *being* x_0 *are as follows:*

$F_1 : 0 \to \overline{1} \to 6 \to \overline{0},\ f_1 = \frac{1}{4},\ \overline{F}_1 : 0 \to \overline{6} \to 1 \to \overline{0},\ f_1 = \frac{1}{4},$
$F_2 : 0 \to \overline{1} \to 8 \to \overline{0},\ f_2 = \frac{1}{4},\ \overline{F}_2 : 0 \to \overline{8} \to 1 \to \overline{0},\ f_2 = \frac{1}{4},$
$F_3 : 0 \to \overline{2} \to 7 \to \overline{4} \to 8 \to \overline{3} \to \overline{0},\ f_3 = \frac{1}{4},\ \overline{F}_3 : 0 \to 3 \to \overline{8} \to 4 \to \overline{7} \to 2 \to \overline{0},\ f_3 = \frac{1}{4}.$

Hence,

$$\zeta = \begin{cases} \frac{1}{2},\ N_1 = [(0,1),(1,6),(6,0)], \\ \frac{1}{2},\ N_2 = [(0,1),(1,8),(8,0)]\ , \\ \frac{1}{2},\ N_3 = [(0,2),(2,7),(7,4),(4,8),(8,3),(3,0)], \\ 0,\ \text{otherwise.} \end{cases}$$

The lower bound for $\underset{\sim}{\min}\, L(x)$ *is* $\rho(L_0) = -\frac{19}{2} + \frac{3}{2} = -8$.
We can decompose ϕ *into* $\phi = h_\zeta + g_\zeta + \phi'_\zeta$, *where*

$$\begin{aligned} h_\zeta &= (x_0x_1 + \overline{x}_0\overline{x}_1) + \tfrac{1}{2}(x_0x_2 + \overline{x}_0\overline{x}_2) + \tfrac{1}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_0x_6 + \overline{x}_0\overline{x}_6) \\ &\quad + \tfrac{1}{2}(x_0x_8 + \overline{x}_0\overline{x}_8) + \tfrac{1}{2}(x_1x_6 + \overline{x}_1\overline{x}_6) + \tfrac{1}{2}(x_1x_8 + \overline{x}_1\overline{x}_8) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) \\ &\quad + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) + \tfrac{1}{2}(x_3x_8 + \overline{x}_3\overline{x}_8) + \tfrac{1}{2}(x_4x_8 + \overline{x}_4\overline{x}_8), \\ g_\zeta &= 3(x_0x_1 + \overline{x}_0\overline{x}_1) + (x_0x_2 + \overline{x}_0\overline{x}_2) + \tfrac{1}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{9}{2}(x_0\overline{x}_5 + \overline{x}_0x_5) \\ &\quad + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) + \tfrac{1}{2}(x_5x_6 + \overline{x}_5\overline{x}_6), \end{aligned}$$

and $\phi'_\zeta = 0$.

Setting $g_\zeta = 0$, *since each of the components of* g_ζ *is nonnegative, we consequently obtain* $x_0 = 1$, $x_1 = 0$, $x_2 = 0$, $x_3 = 1$, $x_5 = 1$, *and* $x_6 = 0$. *Substitute* $\hat{x} = (0,\ 0,\ 1, x_4, 1,\ 0, x_7, x_8)$ *in* $L(x)$; *at this point, minimizing* $L(\hat{x})$ *will lead to* $x_4 = 0, x_7 = 1$ *and* x_8 *being unrestricted.*

The solution, $(x_1, x_2, x_3, x_4, x_5, x_6, x_7) = (0,0,1,0,1,0,1)$, *with* x_8 *unrestricted, is infeasible since the first constraint of Problem (13) is not satisfied. Hence, the lower bound of Problem (13) found by this algorithm is* -8.

Proposition 4. *$\hat{x}$ is a solution found from $g_\zeta(x) = 0$, along with the feasibility of (1) ($r(\hat{x}) \le 0$). The upper bound of (1) is $L(\hat{x})$.*

Proof. Since $\hat{x}$ is feasible for (1) and (1) is a minimization problem, if $\hat{x}$ is not optimal for (1), i.e., there exists a feasible solution x such that $f(x) \le f(\hat{x})$, then $f(\hat{x}) = L(\hat{x})$ is an upper bound of (1). □

Example 7. *From Example 4, the lower bound for* $\underset{\sim}{\min}\, L(x)$ *is* $\rho(L_0) = -6 + 2 = -4$. *From Definition 8, we can decompose* ϕ *into* $\phi = h_\zeta + g_\zeta + \phi'_\zeta$, *where*

$$\begin{aligned} \phi &= 3(x_0x_1 + \overline{x}_0\overline{x}_1) + 3(x_0x_2 + \overline{x}_0\overline{x}_2) + 2(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_0\overline{x}_4 + \overline{x}_0x_4) \\ &\quad + \tfrac{1}{2}(x_0x_7 + \overline{x}_0\overline{x}_7) + \tfrac{1}{2}(x_1x_5 + \overline{x}_1\overline{x}_5) + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5) + \tfrac{1}{2}(x_2x_6 + \overline{x}_2\overline{x}_6) \\ &\quad + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6) + \tfrac{1}{2}(x_1x_7 + \overline{x}_1\overline{x}_7) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) \\ h_\zeta &= (x_0x_1 + \overline{x}_0\overline{x}_1) + (x_0x_2 + \overline{x}_0\overline{x}_2) + (x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_0\overline{x}_4 + \overline{x}_0x_4) + \tfrac{1}{2}(x_0x_7 + \overline{x}_0\overline{x}_7) \\ &\quad + \tfrac{1}{2}(x_1x_5 + \overline{x}_1\overline{x}_5) + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5) + \tfrac{1}{2}(x_1x_7 + \overline{x}_1\overline{x}_7) + \tfrac{1}{2}(x_2x_7 + \overline{x}_2\overline{x}_7) \\ &\quad + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) + \tfrac{1}{2}(x_2x_6 + \overline{x}_2\overline{x}_6) + \tfrac{1}{2}(x_3x_6 + \overline{x}_3\overline{x}_6), \\ g_\zeta &= 2(x_0x_1 + \overline{x}_0\overline{x}_1) + 2(x_0x_2 + \overline{x}_0\overline{x}_2) + (x_0\overline{x}_3 + \overline{x}_0x_3), \\ \phi'_\zeta &= 0. \end{aligned}$$

Setting $g_\zeta = 0$, *since each of the components of* g_ζ *is nonnegative, and* $x_0 = 1$, *we have* $g_\zeta = 2x_1 + 2x_2 + \overline{x}_3$.

We consequently obtain $x_1 = 0, x_2 = 0$ *and* $x_3 = 1$. *By substituting* $\hat{x} = (1,0,0,\ 1, x_4, x_5, x_6, x_7)$ *into* $L(x)$ *at this point, minimizing* $L(\hat{x})$ *will lead to* $x_4 = 1$, *with* x_5, x_6 *and* x_7 *unrestricted.*

The solution $(x_1, x_2, x_3, x_4) = (0,0,1,1)$ *with* (x_5, x_6, x_7) *unrestricted, is feasible, since the original constraints of the problem are satisfied. The upper bound of Problem (7) found by Proposition 4 is* -4.

Since the upper bound is equal to the lower bound, this solution is optimal.

The following proposition proposes a sufficient condition for the constructed network to not contain a flow from 0 to $\overline{0}$.

Proposition 5. *Let* $L(x) = c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{j=n+1}^{n+m} c_{ij} x_i x_j$ *be a quadratic pseudo-Boolean function. If* $c_{ij} < 0, \forall i, j$, $c_i - \sum_{j=n+1}^{n+m} \frac{|c_{ij}|}{2} < 0$, $i = 1, \ldots, n$, *and* $c_j - \sum_{i=1}^{n} \frac{|c_{ij}|}{2} < 0$, $j = n+1, n+2, \ldots, n+m$, *then the network corresponding to* $L(x)$ *does not contain a flow.*

Proof. Let $L(x) = c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{j=n+1}^{n+m} c_{ij} x_i x_j$ be a quadratic pseudo-Boolean function.

Suppose that $c_{ij} < 0, \forall i, j$. From Definition 2, $c_{ij} x_i x_j = \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) - \frac{|c_{ij}|}{2} x_i - \frac{|c_{ij}|}{2} x_j$. Therefore,

$$\begin{aligned} L(x) &= c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} (x_i \overline{x}_j + \overline{x}_i x_j) - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2} x_i - \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2} x_j \\ &= c_0 + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) + \sum_{i=1}^{n} \left(c_i - \sum_{j=n+1}^{n+m} \frac{|c_{ij}|}{2} \right) x_i + \sum_{j=n+1}^{n+m} \left(c_j - \sum_{i=1}^{n} \frac{|c_{ij}|}{2} \right) x_j. \end{aligned}$$

Assume that $c_i - \sum_{j=n+1}^{n+m} \frac{|c_{ij}|}{2} < 0$, $i = 1, \ldots, n$ and $c_j - \sum_{i=1}^{n} \frac{|c_{ij}|}{2} < 0$, $j = n+1, n+2, \ldots, n+m$.

From Definition 2, $c_i x_i = |c_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) - |c_i|$.

Hence,

$$\begin{aligned} L(x) &= c_0 + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) + \sum_{i=1}^{n} \left| c_i - \sum_{j=n+1}^{n+m} \frac{|c_{ij}|}{2} \right| (x_0 \overline{x}_i + \overline{x}_0 x_i) - \sum_{i=1}^{n} |c_i| \\ &+ \sum_{j=n+1}^{n+m} \left| c_j - \sum_{j=1}^{n} \frac{|c_{ij}|}{2} \right| (x_0 \overline{x}_j + \overline{x}_0 x_j) - \sum_{j=n+1}^{n+m} |c_j| \\ &= C + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij}<0}}^{n+m} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) + \sum_{i=1}^{n} \left| c_i - \sum_{j=n+1}^{n+m} \frac{|c_{ij}|}{2} \right| (x_0 \overline{x}_i + \overline{x}_0 x_i) \\ &+ \sum_{j=n+1}^{n+m} \left| c_j - \sum_{j=1}^{n} \frac{|c_{ij}|}{2} \right| (x_0 \overline{x}_j + \overline{x}_0 x_j) \end{aligned} \tag{14}$$

where $C = c_0 - \sum_{i=1}^{n} |c_i| - \sum_{j=n+1}^{n+m} |c_j|$ is constant. □

Consider the terms $x_0 \overline{x}_i + \overline{x}_0 x_i$, $i = 1, 2, \ldots, n+m$ in (14). The corresponding network is constructed with the vertices $V = \{0, \overline{0}, 1, \overline{1}, ..., n+m, \overline{n+m}\}$ and the edges e between the nodes 0 and i, as well as the edges e' between the vertices $\overline{0}$ and $\overline{i}$, as shown in Figure 2, without capacities. Note that the capacities on the edges e and the edges e' are half of the coefficients of the terms $x_0 \overline{x}_i + \overline{x}_0 x_i$, $i = 1, 2, \ldots, n+m$.

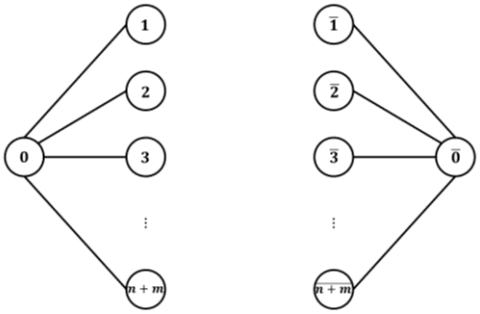


Figure 2. Constructed network from the terms $x_0\overline{x}_i + \overline{x}_0 x_i, i = 1, 2, \ldots, n+m$ in (14).

Similarly, the terms $x_i\overline{x}_j + \overline{x}_i x_j,\ i = 1, 2, \ldots, n, j = n+1, \ldots, n+m$ will create edges e between i and j and edges e' between $\overline{i}$ and $\overline{j}$, as illustrated in Figure 3, without capacities. In addition, note that those capacities on the edges are half of the coefficients of the terms $x_i\overline{x}_j + \overline{x}_i x_j$. Since (14) contains only $x_0\overline{x}_i + \overline{x}_0 x_i$ and $x_i\overline{x}_j + \overline{x}_i x_j$ terms, the network constructed from (14) is not connected, and, as a result, does not contain a flow from vertex 0 to $\overline{0}$.

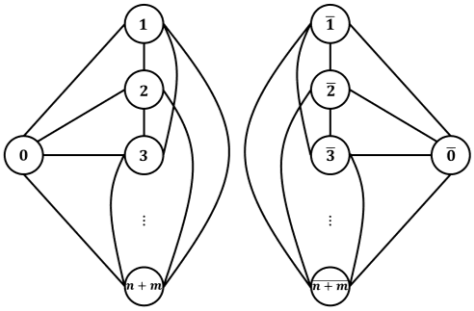


Figure 3. Constructed network corresponding to (14) without capacities.

Example 8. *Consider the following problem:*

$$\begin{aligned}\min f(x) = \quad & -5x_1 - 3x_2 - x_3 - 2x_4 - 4x_5 - x_1x_6 - x_2x_6 - x_5x_6 - x_6 - x_3x_7 - x_4x_7 \\ & -x_5x_7 - x_7 - x_2x_8 - x_3x_8 - x_8.\end{aligned}$$

From Definition 2,

$$\begin{aligned}f(x) \quad & = -5x_1 - 3x_2 - x_3 - 2x_4 - 4x_5 + \tfrac{1}{2}(x_1\overline{x}_6 + \overline{x}_1x_6) - \tfrac{1}{2}x_1 - \tfrac{1}{2}x_6 + \tfrac{1}{2}(x_2\overline{x}_6 + \overline{x}_2x_6) \\ & -\tfrac{1}{2}x_2 - \tfrac{1}{2}x_6 + \tfrac{1}{2}(x_5\overline{x}_6 + \overline{x}_5x_6) - \tfrac{1}{2}x_5 - \tfrac{1}{2}x_6 - x_6 + \tfrac{1}{2}(x_3\overline{x}_7 + \overline{x}_3x_7) - \tfrac{1}{2}x_3 - \tfrac{1}{2}x_7 \\ & +\tfrac{1}{2}(x_4\overline{x}_7 + \overline{x}_4x_7) - \tfrac{1}{2}x_4 - \tfrac{1}{2}x_7 + \tfrac{1}{2}(x_5\overline{x}_7 + \overline{x}_5x_7) - \tfrac{1}{2}x_5 - \tfrac{1}{2}x_7 - x_7 \\ & +\tfrac{1}{2}(x_2\overline{x}_8 + \overline{x}_2x_8) - \tfrac{1}{2}x_2 - \tfrac{1}{2}x_8 + \tfrac{1}{2}(x_3\overline{x}_8 + \overline{x}_3x_8) - \tfrac{1}{2}x_3 - \tfrac{1}{2}x_8 - x_8 \\ & = -\tfrac{11}{2}x_1 - 4x_2 - 2x_3 - \tfrac{5}{2}x_4 - 5x_5 - \tfrac{5}{2}x_6 - \tfrac{5}{2}x_7 - 2x_8 + \tfrac{1}{2}(x_1\overline{x}_6 + \overline{x}_1x_6) \\ & +\tfrac{1}{2}(x_2\overline{x}_6 + \overline{x}_2x_6) + \tfrac{1}{2}(x_5\overline{x}_6 + \overline{x}_5x_6) + \tfrac{1}{2}(x_3\overline{x}_7 + \overline{x}_3x_7) + \tfrac{1}{2}(x_4\overline{x}_7 + \overline{x}_4x_7) \\ & +\tfrac{1}{2}(x_5\overline{x}_7 + \overline{x}_5x_7) + \tfrac{1}{2}(x_2\overline{x}_8 + \overline{x}_2x_8) + \tfrac{1}{2}(x_3\overline{x}_8 + \overline{x}_3x_8) \\ & = \tfrac{11}{2}(x_0\overline{x}_1 + \overline{x}_0x_1) + 4(x_0\overline{x}_2 + \overline{x}_0x_2) + 2(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{5}{2}(x_0\overline{x}_4 + \overline{x}_0x_4) \\ & +5(x_0\overline{x}_5 + \overline{x}_0x_5) + \tfrac{5}{2}(x_0\overline{x}_6 + \overline{x}_0x_6) + \tfrac{5}{2}(x_0\overline{x}_7 + \overline{x}_0x_7) + 2(x_0\overline{x}_8 + \overline{x}_0x_8) - 26 \\ & +\tfrac{1}{2}(x_1\overline{x}_6 + \overline{x}_1x_6) + \tfrac{1}{2}(x_2\overline{x}_6 + \overline{x}_2x_6) + \tfrac{1}{2}(x_5\overline{x}_6 + \overline{x}_5x_6) + \tfrac{1}{2}(x_3\overline{x}_7 + \overline{x}_3x_7) \\ & +\tfrac{1}{2}(x_4\overline{x}_7 + \overline{x}_4x_7) + \tfrac{1}{2}(x_5\overline{x}_7 + \overline{x}_5x_7) + \tfrac{1}{2}(x_2\overline{x}_8 + \overline{x}_2x_8) + \tfrac{1}{2}(x_3\overline{x}_8 + \overline{x}_3x_8).\end{aligned}$$

Let the root of $f(x)$ be x_0. The network corresponding to $f(x)$ is shown in Figure 4. Since the network is not connected, the flow from vertex 0 to $\overline{0}$ cannot be found.

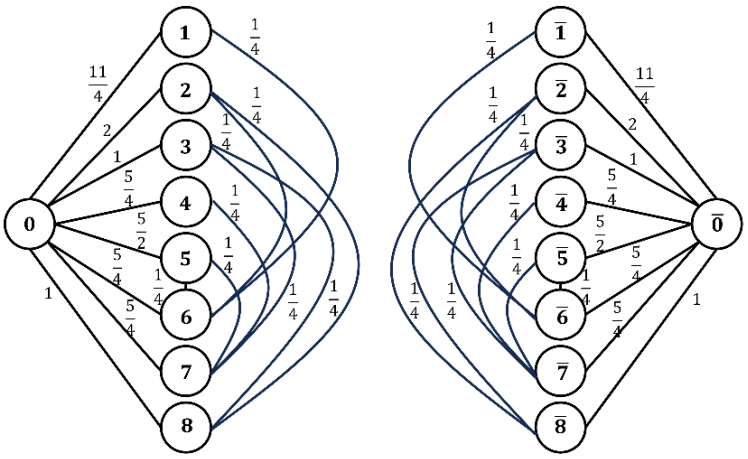


Figure 4. Constructed network not containing a flow, as in Example 8.

The sufficient condition for the network to contain a flow is proposed in the following proposition.

Proposition 6. *Let* $L(x) = c_0 + \sum_{i=1}^{n+m} c_i x_i + \sum_{i=1}^{n} \sum_{j=n+1}^{n+m} c_{ij} x_i x_j$ *be a quadratic pseudo-Boolean function. If there exist* r, s, $1 \le r \le n$, $n+1 \le s \le n+m$, $c_{rs} > 0$, *and there are sequences* $u_1, u_2, \ldots, u_k$ *and* $v_1, v_2, \ldots, v_l$ *with some coefficients that are either positive or negative, then a flow can be found in the network corresponding to* $L(x)$.

Proof. Assume that there exist $c_{rs} > 0$ where $1 \le r \le n$, $n+1 \le s \le n+m$. From Definition 2, $c_{rs} x_r x_s = \frac{c_{rs}}{2}(x_r x_s + \overline{x}_r \overline{x}_s) + \frac{c_{rs}}{2} x_r + \frac{c_{rs}}{2} x_s - \frac{c_{rs}}{2}$, and from (11), the Lagrangian function can be written as

$$\begin{aligned} L(x) \quad = C + & \sum_{\substack{i=1 \\ i \neq r,s \\ \gamma_i > 0}}^{n+m} |\gamma_i|(x_0 x_i + \overline{x}_0 \overline{x}_i) + \sum_{\substack{i=1 \\ i \neq r,s \\ \gamma_i < 0}}^{n+m} |\gamma_i|(x_0 \overline{x}_i + \overline{x}_0 x_i) + \sum_{\substack{i=1 \\ i \neq r}}^{n} \sum_{\substack{j=n+1 \\ j \neq s \\ c_{ij} > 0}}^{n+m} \frac{|c_{ij}|}{2}(x_i x_j + \overline{x}_i \overline{x}_j) \\ & + \sum_{i=1}^{n} \sum_{\substack{j=n+1 \\ c_{ij} < 0}}^{n+m} \frac{|c_{ij}|}{2}(x_i \overline{x}_j + \overline{x}_i x_j) + \frac{c_{rs}}{2}(x_r x_s + \overline{x}_r \overline{x}_s) + \left(c_r + \frac{c_{rs}}{2}\right) x_r + \left(c_s + \frac{c_{rs}}{2}\right) x_s, \end{aligned}$$

where

$$\gamma_i = \begin{cases} c_i + \sum\limits_{\substack{j=n+1 \\ j \neq s \\ c_{ij} > 0}}^{n+m} \frac{|c_{ij}|}{2} - \sum\limits_{\substack{j=n+1 \\ j \neq s \\ c_{ij} < 0}}^{n+m} \frac{|c_{ij}|}{2}, \; i = 1, \ldots, n, \text{ and } i \neq r \\ c_i + \sum\limits_{\substack{j=1 \\ j \neq r \\ c_{ij} > 0}}^{n} \frac{|c_{ji}|}{2} - \sum\limits_{\substack{j=1 \\ j \neq r \\ c_{ij} < 0}}^{n} \frac{|c_{ji}|}{2}, i = n+1, \ldots, n+m, \text{ and } i \neq s \end{cases}$$

and

$$C = c_0 - \sum_{\substack{i=1 \\ \gamma_i < 0}}^{n+m} |\gamma_i| - \sum_{\substack{i=1 \\ i \neq r}}^{n} \sum_{\substack{j=n+1 \\ j \neq s \\ c_{ij} > 0}}^{n+m} \frac{|c_{ij}|}{2} - \frac{c_{rs}}{2}. \tag{15}$$

Consider $L(x)$ in the following two cases.

Case 1:

Suppose that (1) there exists a sequence $u_1, u_2, \ldots, u_k$, where $c_{u_i,u_{i+1}} > 0$, $\forall i \in \{1, 2, \ldots, k-1\}$, $c_{u_k,r} > 0$ and $\gamma_{u_1} > 0$, and (2) there exists a sequence $v_1, v_2, \ldots, v_l$, where $c_{v_i,v_{i+1}} > 0$, $\forall i \in \{1, 2, \ldots, l-1\}$, $c_{v_l,s} > 0$ and $\gamma_{v_1} > 0$.

From Definition 4, the constructed network corresponding to (15) is shown in Figure 5. Since (15) contains the term $x_{u_i}x_{u_{i+1}} + \overline{x}_{u_i}\overline{x}_{u_{i+1}}$, there exist edges between the vertices u_i and $\overline{u}_{i+1}$ and between the vertices $\overline{u}_i$ and u_{i+1}. Moreover, the term $x_{u_k}x_r + \overline{x}_{u_k}\overline{x}_r$ in (15) guarantees that there exists an edge between the vertices u_k and $\overline{r}$ and an edge between $\overline{u}_k$ and r. Finally, the term $x_0x_{u_1} + \overline{x}_0\overline{x}_{u_1}$ in (15) provides that there is an edge between the vertices 0 and $\overline{u}_1$ and an edge between the vertices $\overline{0}$ and u_1. Hence, the vertices $0, \overline{u}_1, u_2, \ldots, u_k, \overline{r}$ in the constructed network are connected, as are the vertices $r, \overline{u}_k, u_{k-1}, \ldots, u_1, \overline{0}$.

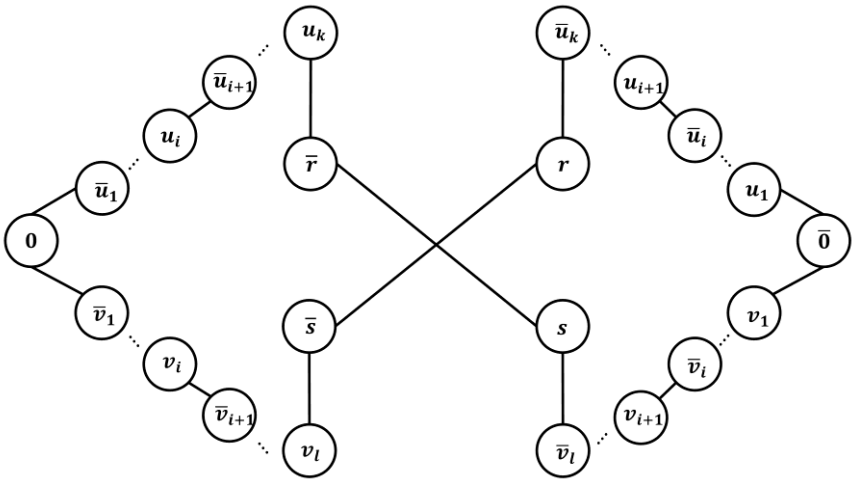


Figure 5. Constructed network from (15) having some sequence with positive coefficients.

Similarly, (15) contains $x_{v_i}x_{v_{i+1}} + \overline{x}_{v_i}\overline{x}_{v_{i+1}}$, $x_{v_l}x_s + \overline{x}_{v_l}\overline{x}_s$, and $x_0x_{v_1} + \overline{x}_0\overline{x}_{v_1}$. Consequently, there are edges between v_i and $\overline{v}_{i+1}$ and between $\overline{v_i}$ and v_{i+1}; edges between v_l and $\overline{s}$ and between $\overline{v_l}$ and s; and edges between 0 and $\overline{v}_1$ and between $\overline{0}$ and v_1. Hence, both $0, \overline{v}_1, v_2, \ldots, v_k, \overline{s}$ and $s, \overline{v}_k, v_{k-1}, \ldots, v_1, \overline{0}$ are connected. Since there are edges between the vertices r and $\overline{s}$ and $\overline{r}$ and s, because of the existence of the term $x_rx_s + \overline{x}_r\overline{x}_s$, the flow from 0 to $\overline{0}$ can be found in this network (see Figure 5).

Case 2:

Suppose that (1) there exists a sequence $u_1, u_2, \ldots, u_k$ where $c_{u_i,u_{i+1}} < 0$, $\forall i \in \{1, 2, \ldots, k-1\}$, $c_{u_k,r} < 0$ and $\gamma_{u_1} < 0$, and (2) there exists a sequence $v_1, v_2, \ldots, v_l$ where $c_{v_i,v_{i+1}} < 0$, $\forall i \in \{1, 2, \ldots, l-1\}$, $c_{v_l,s} < 0$ and $\gamma_{v_1} < 0$.

Similar to Case 1, it can be shown that $0, v_1, v_2, \ldots, v_l, s$ are connected by the edges between v_i, and v_{i+1}, $\forall\, i = 1, \ldots, l-1$, between 0 and v_1, and between v_l and s. Similarly, $0, u_1, u_2, \ldots, u_k, r$; $\overline{r}, \overline{u}_k, \overline{u}_{k-1}, \ldots, \overline{u}_1, \overline{0}$; and $\overline{s}, \overline{v}_l, \overline{v}_{l-1}, \ldots, \overline{v}_1, \overline{0}$ are connected. The existence of the term $x_rx_s + \overline{x}_r\overline{x}_s$ ensures the connection between the four, as seen in Figure 6. Therefore, the flow from 0 to $\overline{0}$ can be found in the constructed network. □

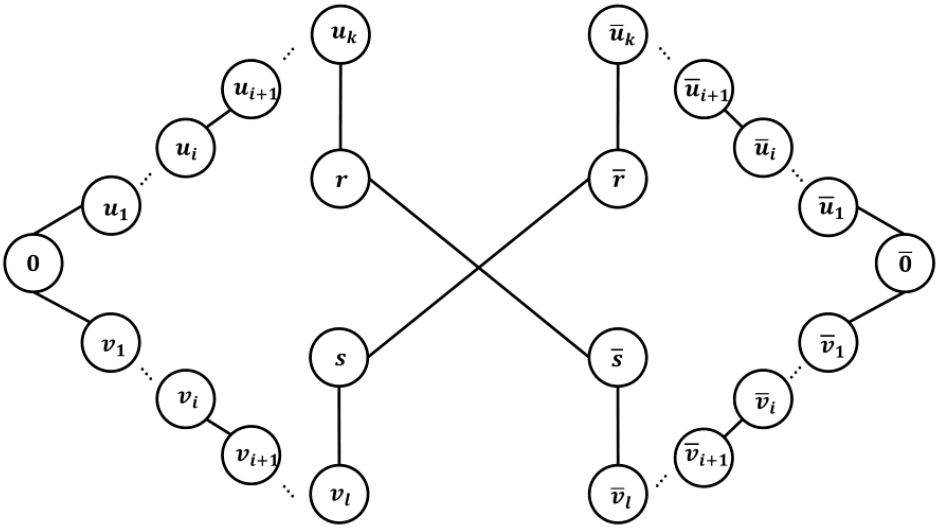


Figure 6. The network constructed from (15) having some sequence with negative coefficients.

3. Algorithm

A step-by-step algorithm for how to find a bound of BIP (1) is as follows.

Step 0: Transform the BIP (1) into a QUBO (3).

Set $\widetilde{L}(x) = L(x)$

Step 1: Find C, as defined in Proposition 1, and the bi-form ϕ of $\widetilde{L}(x)$, as defined in Proposition 2.

Construct a network, N, corresponding to the bi-form ϕ, as defined in Definition 4.

Select k to be a source vertex in network N.

Let a bound of $\widetilde{\min} L(x)$ be $\rho(L) = C$.

Step 2: Find the max-flow ζ from source vertex k to sink vertex $\bar{k}$.

Update the lower bound $\rho(L) = \rho(L) + \zeta$.

Step 3: Decompose a bi-form ϕ as $\phi = h_\zeta + g_\zeta + \phi'_\zeta$.

Find x_i that makes $g_\zeta(x) = 0$.

The remaining x_i is found by minimizing $L(x)$, with the obtained x_i substituted.

Assume x^* is a solution of the problem.

Check the feasibility of x^*.

If x^* is feasible, $\rho(L)$ is an upper bound for (1); otherwise, $\rho(L)$ is a lower bound for (1).

Step 4: Stop, if $\phi'_\zeta = 0$. Otherwise, $\phi = \phi'_\zeta$, repeat Step 1.

The summary of the step-by-step algorithm is shown in a flowchart provided in Figure 7.

The following example shows how to use the closed form in Corollary 1 along with the step-by-step algorithm to find the lower bound of a QUBO problem.

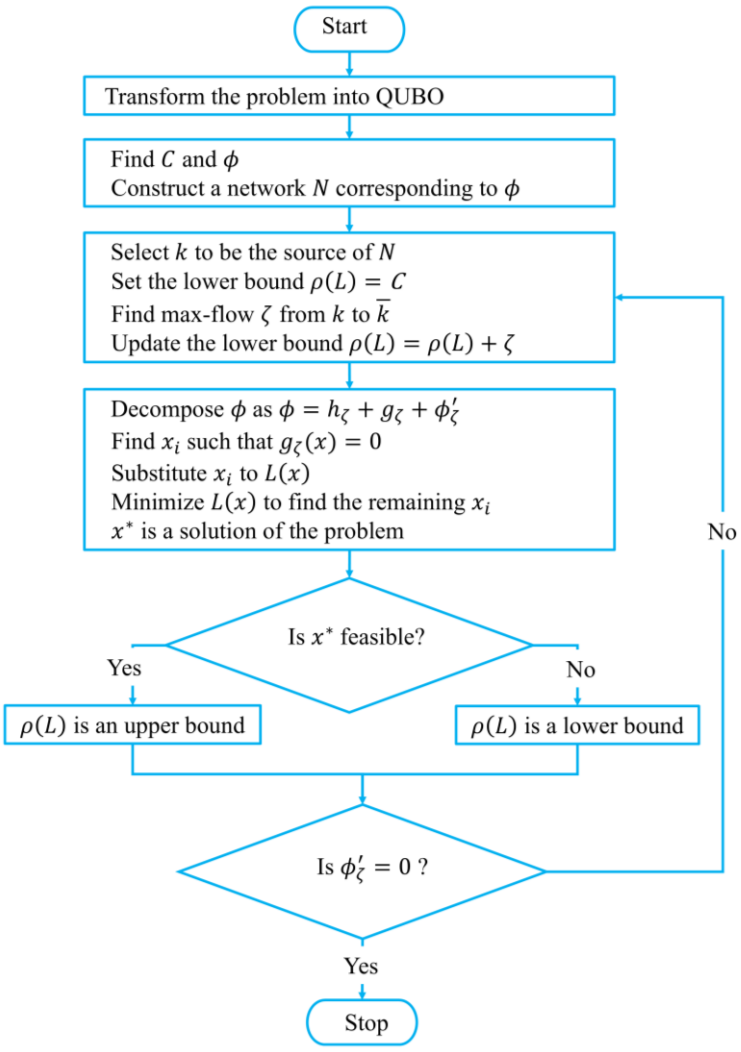


Figure 7. Flowchart of the algorithm for finding the bound of BIP or QBIP.

Example 9. *Consider the following problem:*

$$\begin{aligned}\min f(x) = \quad & -2x_1 - x_3 - 4x_4 - x_6 - 4x_1x_2 - 6x_1x_4 + 4x_2x_3 - 2x_2x_4 - 10x_2x_5 - 8x_3x_4 \\ & -2x_3x_6 - 2x_4x_5 - 12x_4x_6.\end{aligned}$$

Here, $Q(x) = f(x)$.
From Corollary 1,

$$\begin{aligned}\widetilde{Q}(x) \quad = c_0 - & \sum_{\substack{i=1 \\ \delta_i < 0}}^{n} |\delta_i| - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij} > 0}}^{n} \frac{|c_{ij}|}{2} + \sum_{\substack{i=1 \\ \delta_i > 0}}^{n} |\delta_i|(x_0x_i + \overline{x}_0\overline{x}_i) + \sum_{\substack{i=1 \\ \delta_i < 0}}^{n} |\delta_i|(\overline{x}_ix_0 + \overline{x}_0x_i) \\ & + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij} > 0}}^{n} \frac{|c_{ij}|}{2}(x_ix_j + \overline{x}_i\overline{x}_j) + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij} < 0}}^{n} \frac{|c_{ij}|}{2}(x_i\overline{x}_j + \overline{x}_ix_j)\end{aligned}$$

where

$$\delta_i = c_i + \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} - \sum_{\substack{j=1 \\ c_{ij}<0}}^{n} \frac{|c_{ij}|}{2},\ i = 1,..,n.$$

$$\delta_1 = c_1 - \frac{c_{12}}{2} - \frac{c_{14}}{2} = -2-2-3 = -7,$$

$$\delta_2 = c_2 - \frac{c_{12}}{2} + \frac{c_{32}}{2} - \frac{c_{42}}{2} - \frac{c_{52}}{2} = 0-2+2-1-5 = -6,$$

$$\delta_3 = c_3 + \frac{c_{32}}{2} - \frac{c_{34}}{2} - \frac{c_{36}}{2} = -1+2-4-1 = -4,$$

$$\delta_4 = c_4 - \frac{c_{41}}{2} - \frac{c_{42}}{2} - \frac{c_{43}}{2} - \frac{c_{45}}{2} - \frac{c_{46}}{2} = -4-3-1-4-1-6 = -19\ ,$$

$$\delta_5 = c_5 - \frac{c_{52}}{2} - \frac{c_{54}}{2} = 0-5-1 = -6,$$

$$\delta_6 = c_6 - \frac{c_{63}}{2} - \frac{c_{64}}{2} = -1-1-6 = -8\ .$$

$$C = c_0 - \sum_{\substack{i=1 \\ \delta_i<0}}^{n} |\delta_i| - \sum_{i=1}^{n} \sum_{\substack{j=1 \\ c_{ij}>0}}^{n} \frac{|c_{ij}|}{2} = 0-(7+6+4+19+6+8)-2 = -52$$

$$\begin{aligned}\widetilde{Q}(x) \quad &= -52 + 7(x_0\overline{x}_1 + \overline{x}_0x_1) + 6(x_0\overline{x}_2 + \overline{x}_0x_2) + 4(x_0\overline{x}_3 + \overline{x}_0x_3) + 19(x_0\overline{x}_4 + \overline{x}_0x_4)\\ &\quad +6(x_0\overline{x}_5 + \overline{x}_0x_5) + 8(x_0\overline{x}_6 + \overline{x}_0x_6) + 2(x_2x_3 + \overline{x}_2\overline{x}_3) + 2(x_1\overline{x}_2 + \overline{x}_1x_2)\\ &\quad +3(x_1\overline{x}_4 + \overline{x}_1x_4) + (x_2\overline{x}_4 + \overline{x}_2x_4) + 5(x_2\overline{x}_5 + \overline{x}_2x_5) + 4(x_3\overline{x}_4 + \overline{x}_3x_4)\\ &\quad +(x_3\overline{x}_6 + \overline{x}_3x_6) + (x_4\overline{x}_5 + \overline{x}_4x_5) + 6(x_4\overline{x}_6 + \overline{x}_4x_6).\end{aligned}$$

The constructed network corresponding to $\widetilde{Q}(x)$ *is shown in Figure 8.*

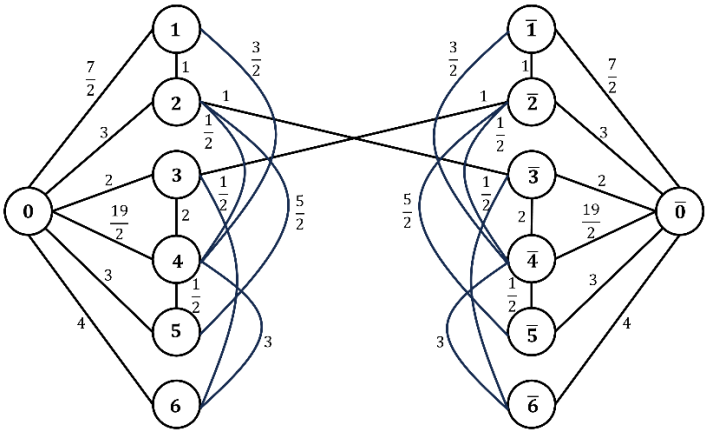


Figure 8. Constructed network containing a flow and a complement flow between 0 and $\overline{0}$ in Example 9.

Let the root of $f(x)$ *be* x_0 *and the lower bound of* $f(x)$ *be* -52.
The flows and their complement flows are as follows:

$$F_1 : 0 \to 2 \to \overline{3} \to \overline{0},\ f_1 = 1,\ \overline{F}_1 : 0 \to 3 \to \overline{2} \to \overline{0},\ f_1 = 1.$$

Thus, $\zeta = \begin{cases} 2, N_1 = [(0,2),(2,3),(3,0)], \\ 0, \text{ otherwise.} \end{cases}$

Hence, the updated lower bound of $f(x)$ *is* $-52+2 = -50$.

The following two examples show how the proposed algorithm works in a quadratic programming problem.

Example 10. *Consider the following problem:*

$$\begin{aligned} \min_x \ & f(x) = -5x_1 - 8x_2 - 6x_3 + 2x_1x_2 + 3x_2x_3 \\ \text{s.t.} \ & x_1 + x_3 - 1 \le 0 \\ & x_2 + x_3 - 1 \le 0 \\ & x_i \in \{0,\ 1\}. \end{aligned} \tag{16}$$

A quadratic pseudo-Boolean function of (16) is

$$L(x) = -5x_1 - 8x_2 - 6x_3 + 2x_1x_2 + 3x_2x_3 + x_1x_4 + x_3x_4 - x_4 + x_2x_5 + x_3x_5 - x_5.$$

From Propositions 1 and 2,

$$\begin{aligned} \widetilde{L} \ &= C + \phi, \text{ where } C = -\tfrac{33}{2} \text{ and} \\ \phi \ &= \tfrac{7}{2}(x_0\overline{x}_1 + \overline{x}_0x_1) + 5(x_0\overline{x}_2 + \overline{x}_0x_2) + \tfrac{7}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_1x_2 + \overline{x}_1\overline{x}_2) \\ &\quad + \tfrac{3}{2}(x_2x_3 + \overline{x}_2\overline{x}_3) + \tfrac{1}{2}(x_1x_4 + \overline{x}_1\overline{x}_4) + \tfrac{1}{2}(x_3x_4 + \overline{x}_3\overline{x}_4) + \tfrac{1}{2}(x_2x_5 + \overline{x}_2\overline{x}_5) \\ &\quad + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5). \end{aligned}$$

The flows and their complement flows with the root of bi-form ϕ being x_0 are as follows:

$$\begin{aligned} &F_1 : 0 \to \overline{1} \to \overline{2} \to \overline{0},\ f_1 = \tfrac{1}{2},\ \overline{F}_1 : 0 \to 2 \to 1 \to \overline{0},\ f_1 = \tfrac{1}{2} \\ &F_2 : 0 \to 1 \to \overline{4} \to 3 \to \overline{2} \to \overline{0},\ f_2 = \tfrac{1}{4},\ \overline{F}_2 : 0 \to 2 \to \overline{3} \to 4 \to \overline{1} \to \overline{0},\ f_2 = \tfrac{1}{4} \\ &F_3 : 0 \to 2 \to \overline{3} \to \overline{0},\ f_3 = \tfrac{1}{2},\ \overline{F}_3 : 0 \to 3 \to \overline{2} \to \overline{0},\ f_3 = \tfrac{1}{2}. \end{aligned}$$

Hence,

$$\zeta = \begin{cases} 1,\ N_1 = [(0,1),(1,2),(2,0)], \\ \dfrac{1}{2},\ N_2 = [(0,1),(1,4),(4,3),(3,2),(2,0)], \\ 1,\ N_3 = [(0,2),(2,3),(3,0)], \\ 0\text{ , otherwise.} \end{cases}$$

The lower bound for $\widetilde{\min}\, L(x)$ *is* $\rho(L_0) = -\frac{33}{2} + \frac{5}{2} = -14$.
We can decompose ϕ *into* $\phi = h_\zeta + g_\zeta + \phi'_\zeta$, *where*

$$\begin{aligned} h_\zeta \ &= \tfrac{3}{2}(x_0\overline{x}_1 + \overline{x}_0x_1) + \tfrac{5}{2}(x_0\overline{x}_2 + \overline{x}_0x_2) + (x_0\overline{x}_3 + \overline{x}_0x_3) + (x_1x_2 + \overline{x}_1\overline{x}_2) \\ &\quad + \tfrac{1}{2}(x_1x_4 + \overline{x}_1\overline{x}_4) + \tfrac{1}{2}(x_3x_4 + \overline{x}_3\overline{x}_4) + \tfrac{3}{2}(x_2x_3 + \overline{x}_2\overline{x}_3), \\ g_\zeta \ &= 2(x_0\overline{x}_1 + \overline{x}_0x_1) + \tfrac{5}{2}(x_0\overline{x}_2 + \overline{x}_0x_2) + \tfrac{5}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{1}{2}(x_2x_5 + \overline{x}_2\overline{x}_5) \\ &\quad + \tfrac{1}{2}(x_3x_5 + \overline{x}_3\overline{x}_5), \end{aligned}$$

and $\phi'_\zeta = 0$.

Setting $g_\zeta = 0$, *we obtain* $x_0 = 1$, $x_1 = 1$, $x_2 = 1$ *and* $x_3 = 1$.

Substitute $\hat{x} = (1,\ 1,\ 1, x_4, x_5)$ *into* $L(x)$. *At this point, minimizing* $L(\hat{x})$ *will lead to* $x_4 = 0$ *and* $x_5 = 0$. *The solution,* $(x_1, x_2, x_3, x_4, x_5) = (1,1,1,0,0)$, *is infeasible, since both the constraints of Problem (16) are not satisfied. Hence, the lower bound of Problem (16) found by this algorithm is* -8. *This bound cannot be updated, since the flow cannot be found in* ϕ'_ζ.

Example 11. *Consider the following problem:*

$$\begin{aligned} \min_x \ & f(x) = 3x_1 - 2x_3 + 5x_4 + 4x_1x_4 - x_1x_5 + 3x_2x_3 - 2x_3x_5 \\ \text{s.t.} \ & x_1 - x_3 - x_5 - 1 \le 0 \\ & -x_2 + x_4 + x_5 - 1 \le 0 \\ & x_3 - x_4 - 1 \le 0 \\ & x_i \in \{0,\ 1\}. \end{aligned} \tag{17}$$

A quadratic pseudo-Boolean function of (17) is

$$L(x) = 3x_1 - 2x_3 + 5x_4 + 4x_1x_4 - x_1x_5 + 3x_2x_3 - 2x_3x_5 + x_1x_6 - x_3x_6 - x_5x_6 - x_6 \\ -x_2x_7 + x_4x_7 + x_5x_7 - x_7 + x_3x_8 - x_4x_8 - x_8.$$

From Propositions 1 and 2,

$$\begin{aligned} \tilde{L} &= C + \phi, \text{ where } C = -\tfrac{23}{2} \text{ and} \\ \phi = \; & 5(x_0x_1 + \overline{x}_0\overline{x}_1) + (x_0x_2 + \overline{x}_0\overline{x}_2) + \tfrac{3}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + 7(x_0x_4 + \overline{x}_0\overline{x}_4) \\ & + \tfrac{3}{2}(x_0\overline{x}_5 + \overline{x}_0x_5) + \tfrac{3}{2}(x_0\overline{x}_6 + \overline{x}_0x_6) + \tfrac{1}{2}(x_0\overline{x}_7 + \overline{x}_0x_7) + (x_0\overline{x}_8 + \overline{x}_0x_8) \\ & + 2(x_1x_4 + \overline{x}_1\overline{x}_4) + \tfrac{1}{2}(x_1\overline{x}_5 + \overline{x}_1x_5) + \tfrac{3}{2}(x_2x_3 + \overline{x}_2\overline{x}_3) + (x_3\overline{x}_5 + \overline{x}_3x_5) \\ & + \tfrac{1}{2}(x_1x_6 + \overline{x}_1\overline{x}_6) + \tfrac{1}{2}(x_3\overline{x}_6 + \overline{x}_3x_6) + \tfrac{1}{2}(x_5\overline{x}_6 + \overline{x}_5x_6) + \tfrac{1}{2}(x_2\overline{x}_7 + \overline{x}_2x_7) \\ & + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) + \tfrac{1}{2}(x_5x_7 + \overline{x}_5\overline{x}_7) + \tfrac{1}{2}(x_3x_8 + \overline{x}_3\overline{x}_8) + \tfrac{1}{2}(x_4\overline{x}_8 + \overline{x}_4x_8). \end{aligned}$$

The flows and their complement flows with the root of bi-form ϕ *being* x_0 *are as follows:*

$$\begin{aligned} &F_1 : 0 \to \overline{1} \to 4 \to \overline{0},\ f_1 = 1,\ \overline{F}_1 : 0 \to \overline{4} \to 1 \to \overline{0},\ f_1 = 1, \\ &F_2 : 0 \to \overline{1} \to \overline{5} \to \overline{0},\ f_2 = \tfrac{1}{4},\ \overline{F}_2 : 0 \to 5 \to 1 \to \overline{0},\ f_2 = \tfrac{1}{4}, \\ &F_3 : 0 \to \overline{2} \to \overline{7} \to \overline{0},\ f_3 = \tfrac{1}{4},\ \overline{F}_3 : 0 \to 7 \to 2 \to \overline{0},\ f_3 = \tfrac{1}{4}, \\ &F_4 : 0 \to 3 \to \overline{8} \to \overline{0},\ f_4 = \tfrac{1}{4},\ \overline{F}_4 : 0 \to 8 \to \overline{3} \to \overline{0},\ f_4 = \tfrac{1}{4}, \\ &F_5 : 0 \to \overline{4} \to 7 \to \overline{5} \to \overline{0},\ f_5 = \tfrac{1}{4},\ \overline{F}_5 : 0 \to 5 \to \overline{7} \to 4 \to \overline{0},\ f_5 = \tfrac{1}{4}, \\ &F_6 : 0 \to 8 \to 4 \to \overline{0},\ f_6 = \tfrac{1}{4},\ \overline{F}_6 : 0 \to \overline{4} \to \overline{8} \to \overline{0},\ f_4 = \tfrac{1}{4}. \end{aligned}$$

Hence,

$$\zeta = \begin{cases} 2,\ N_1 = [(0,1),(1,4),(4,0)], \\ \tfrac{1}{2},\ N_2 = [(0,1),(1,5),(5,0)], \\ \tfrac{1}{2},\ N_3 = [(0,2),(2,7),(7,0)], \\ \tfrac{1}{2},\ N_4 = [(0,3),(3,8),(8,0)], \\ \tfrac{1}{2},\ N_5 = [(0,4),(4,7),(7,5),(5,0)], \\ \tfrac{1}{2},\ N_6 = [(0,8),(8,4),(4,0)], \\ 0, \text{ otherwise.} \end{cases}$$

The lower bound for $\overset{\sim}{\min} L(x)$ *is* $\rho(L_0) = -\frac{23}{2} + \frac{9}{2} = -7$.
We can decompose ϕ *into* $\phi = h_\zeta + g_\zeta + \phi'_\zeta$, *where*

$$\begin{aligned} h_\zeta \; = & \tfrac{5}{2}(x_0x_1 + \overline{x}_0\overline{x}_1) + \tfrac{1}{2}(x_0x_2 + \overline{x}_0\overline{x}_2) + \tfrac{1}{2}(x_0\overline{x}_3 + \overline{x}_0x_3) + 3(x_0x_4 + \overline{x}_0\overline{x}_4) \\ & + (x_0\overline{x}_5 + \overline{x}_0x_5) + \tfrac{1}{2}(x_0\overline{x}_7 + \overline{x}_0x_7) + (x_0\overline{x}_8 + \overline{x}_0x_8) + 2(x_1x_4 + \overline{x}_1\overline{x}_4) \\ & + \tfrac{1}{2}(x_1\overline{x}_5 + \overline{x}_1x_5) + \tfrac{1}{2}(x_2\overline{x}_7 + \overline{x}_2x_7) + \tfrac{1}{2}(x_3x_8 + \overline{x}_3\overline{x}_8) + \tfrac{1}{2}(x_4x_7 + \overline{x}_4\overline{x}_7) \\ & + \tfrac{1}{2}(x_5x_7 + \overline{x}_5\overline{x}_7) + \tfrac{1}{2}(x_4x_8 + \overline{x}_4\overline{x}_8), \\ g_\zeta \; = & \tfrac{5}{2}(x_0x_1 + \overline{x}_0\overline{x}_1) + \tfrac{1}{2}(x_0x_2 + \overline{x}_0\overline{x}_2) + (x_0\overline{x}_3 + \overline{x}_0x_3) + \tfrac{9}{2}(x_0x_4 + \overline{x}_0\overline{x}_4) \\ & + \tfrac{1}{2}(x_0\overline{x}_5 + \overline{x}_0x_5) + \tfrac{3}{2}(x_0\overline{x}_6 + \overline{x}_0x_6) + \tfrac{3}{2}(x_2x_3 + \overline{x}_2\overline{x}_3) + (x_3\overline{x}_5 + \overline{x}_3x_5) \\ & + \tfrac{1}{2}(x_1x_6 + \overline{x}_1\overline{x}_6) + \tfrac{1}{2}(x_3\overline{x}_6 + \overline{x}_3x_6) + \tfrac{1}{2}(x_5\overline{x}_6 + \overline{x}_5x_6), \end{aligned}$$

and $\phi'_\zeta = 0$.

Setting $g_\zeta = 0$, *we obtain* $x_0 = 1,\ x_1 = 0, x_2 = 0,\ x_3 = 1,\ x_4 = 0,\ x_5 = 1$ *and* $x_6 = 1$. *Substitute* $\hat{x} = (0,\ 0,\ 1,\ 0,\ 1,\ 1,\ x_7, x_8)$ *into* $L(x)$. *At this point, minimizing* $L(\hat{x})$ *will lead to* x_7 *and* x_8 *being unrestricted. The solution,* $(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8) = (0,\ 0,\ 1,\ 0,\ 1,\ 1,\ x_7, x_8)$, *is feasible. Hence, the upper bound of Problem (17) found by this algorithm is* -7. *This bound cannot be updated, since the flow cannot be found in* ϕ'_ζ.

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4. Simulation Results

We attempt to solve the star-capacitated vehicle routing problem (SCVRP) [34]; the mathematical model for the SCVRP is formulated as follows.

$$\begin{aligned}
&\min_x f(x) = \sum_{i=1}^{N+K}\sum_{j=1}^{N+K} c_{ij}x_{ij} \\
&\text{s.t.} \sum_{j=1}^{N+K} x_{1j} = K, \\
&\sum_{j=N+1}^{N+K} x_{ij} = 1, \ \ i \in \{2,\ldots,N\} \\
&\sum_{j=1}^{N+K} x_{ij} = 1, \ \ i \in \{2,\ldots,N\} \\
&\sum_{i=1}^{N+K}\sum_{j=N+1}^{N+K} x_{ij} = 0 \\
&\sum_{i=2}^{N+K}\sum_{j=2}^{N} x_{ij} = 0 \\
&\sum_{i=2}^{N} d_i x_{ij} \le q_j, \ \ j \in \{N+1,\ldots,N+K\} \\
&x_{ij} \in \{0,\ 1\}, \quad i \in \{1,\ldots,N+K\}, \quad j \in \{1,\ldots,N+K\},
\end{aligned} \tag{18}$$

where N denotes the number of customers, K denotes the number of centers, x_{ij} denotes the decision variable, d_i denotes the demand of customer i, and q_i denotes the capacity of center i. To apply the proposed algorithm, all the equality constraints are relaxed into inequality constraints:

$$\begin{aligned}
&\sum_{j=1}^{N+K} x_{1j} \le K, \\
&-\sum_{j=1}^{N+K} x_{1j} \le -K, \\
&\sum_{j=N+1}^{N+K} x_{ij} \le 1, \ \ i \in \{2,\ldots,N\} \\
&-\sum_{j=N+1}^{N+K} x_{ij} \le -1, \ \ i \in \{2,\ldots,N\} \\
&\sum_{j=1}^{N+K} x_{ij} \le \ 1, \ \ i \in \{2,\ldots,N\} \\
&-\sum_{j=1}^{N+K} x_{ij} \le -\ 1, \ \ i \in \{2,\ldots,N\} \\
&\sum_{i=1}^{N+K}\sum_{j=N+1}^{N+K} x_{ij} \le 0 \\
&-\sum_{i=1}^{N+K}\sum_{j=N+1}^{N+K} x_{ij} \le 0 \\
&\sum_{i=2}^{N+K}\sum_{j=2}^{N} x_{ij} \le 0 \\
&-\sum_{i=2}^{N+K}\sum_{j=2}^{N} x_{ij} \le 0
\end{aligned}$$

To illustrate the efficiency of the proposed algorithm, 30 real-world instances with 10 customers and 2 centers were tested on an AMD Ryzen 5 3400G processor (3.70 GHz) with 16 GB of RAM. The QUBO formulation of (18) is

$$
\begin{aligned}
L(x) \quad &= \sum_{i=1}^{12}\sum_{j=1}^{12} c_{ij}x_{ij} + u_1\left(\sum_{j=1}^{12} x_{1j} - 2\right) + u_2\left(-\sum_{j=1}^{12} x_{1j} + 2\right) + \sum_{i=3}^{11} u_i\left(\sum_{j=11}^{12} x_{i-1,j} - 1\right) \\
&+ \sum_{i=12}^{20} u_i\left(-\sum_{j=11}^{12} x_{i-10,j} + 1\right) + \sum_{i=21}^{29} u_i\left(\sum_{j=1}^{12} x_{i-19,j} - 1\right) + \sum_{i=30}^{38} u_i\left(-\sum_{j=1}^{12} x_{i-28,j} + 1\right) \\
&+ u_{39}\sum_{i=1}^{12}\sum_{j=11}^{12} x_{ij} + u_{40}\left(-\sum_{i=1}^{12}\sum_{j=11}^{12} x_{ij}\right) + u_{41}\left(\sum_{i=2}^{12}\sum_{j=2}^{10} x_{ij}\right) + u_{42}\left(-\sum_{i=2}^{12}\sum_{j=2}^{10} x_{ij}\right) \\
&+ \sum_{j=43}^{44} u_j\left(\sum_{i=2}^{10} d_i x_{i,j-32} - q_{j-32}\right).
\end{aligned}
$$

where u_i, $i = 1, \ldots 44$, are the Lagrange multipliers for this problem. From Proposition 1, the constant C of each instance is shown in the second column of Table 1. The max-flow ζ obtained from the proposed algorithm is shown in the third column and is applied to derive the lower bound in the last column. We observe that the lower bound obtained from the proposed algorithm overestimates the optimal value. This occurs because the center capacity's constants q_i are considerably larger than the other coefficients, leading to a significantly negative constant C. Depending on the nature of the model, if the coefficients and/or the right-hand side constant values are high, the constant C, and consequently, the lower bound found by our method, will be substantially far from the optimal solution. Moreover, we found that transforming a real-world problem with a mere 10 customer nodes and 2 centers can yield a problem with $12^2 + 44 = 188$ variables. Generally, applying our method to a real-world problem will not be computationally sound. However, selecting an appropriate real-world application may improve the computational outcomes.

Table 1. Lower bounds of real-world instances with 10 customers and 2 centers.

Instance No.	Constant C	Max-Flow ζ	Lower Bound $\rho(L)$
1	−6736	82	−6654
2	−9059	82	−8977
3	−9347	82	−9265
4	−10,836	82	−10,754
5	−3612	231	−3381
6	−5052	290	−4762
7	−7287	82	−7205
8	−9036	82	−8954
9	−10,612	82	−10,530
10	−8317	82	−8235
11	−7030	274	−6756
12	−8643	82	−8561
13	−5568	350	−5218
14	−5642	836	−4806
15	−6565	82	−6483
16	−9386	82	−9304
17	−7245	82	−7163
18	−9914	82	−9832
19	−4426	82	−4344
20	−9182	82	−9100
21	−6147	922	−5225
22	−4422	622	−3800
23	−7281	82	−7199
24	−6741	82	−6659
25	−4715	82	−4633
26	−5526	82	−5444
27	−6779	82	−6697
28	−9036	82	−8954
29	−8100	82	−8018
30	−5998	82	−5916

5. Conclusions

We propose a method for finding the bound of a constrained binary programming problem using quadratic unconstrained pseudo-Boolean optimization. If the network constructed corresponding to a bi-form contains a flow, the proposed method can find the bound of this problem in polynomial time. Sufficient conditions for the coefficients of the problem are given to ensure the existence and the nonexistence of flows in the network. In the case that the flow exists, the bound of the problem is found via the max-flow of the corresponding network. If the solution obtained via quadratic unconstrained pseudo-Boolean optimization is feasible, the optimal solution for the constrained binary problem is found. On the other hand, if the obtained solution is not feasible, the lower bound for the constrained binary programming problem is found.

The difficulties of the method in this work are separated into two parts: (1) constructing a bi-form, $\widetilde{L}$, where we have to substitute the terms $x_i x_j$, $-x_i x_j$, x_i and $-x_i$ as defined in Definition 2 into the quadratic pseudo-Boolean function; (2) constructing a network and finding the max-flow of the corresponding network. Although finding a network from the bi-form and its flows is another challenge to improving the overall efficiency of the algorithm to solve BIP, the second part of the difficulty is not a major concern in this work. In this paper, we focus only on the first part, where we derive all the functions and values used in the proposed method to determine the bounds of the original BIP. Additionally, we provide the closed forms of these functions and values. These closed forms facilitate the use of the algorithm, since they lead to a more efficient bound finding. However, after carefully selecting existing problems that can be transformed into QUBO for computational simulation, the proposed method did not outperform the existing approaches for two specific benchmark problems including the SCVRP [34] and the N-Queen problem [35]. The SCVRP was chosen because it addresses a clustering problem that minimizes transportation costs with one center per cluster and capacity constraints. The N-Queen problem was selected because it can model various real-world problems including parallel memory storage schemes, VLSI testing, traffic control, and deadlock prevention [36]. This lack of improved performance may indicate that the method is not suitable for solving these problems. This issue is common in theoretical advancements in optimization, where the simulation results may not accurately reflect the theoretical improvements. We note that the feasibility is not adjusted in the step-by-step algorithm, and the bound obtained from our proposed algorithm is considerably distant from the optimum. Enhancing the feasibility of the algorithm's bound is essential for future studies.

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