A continuous reformulation of the quadratic unconstrained binary optimization problem

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Abstract

In this paper we consider the Quadratic Unconstrained Binary Optimization (QUBO) Problem. Using a suitable function and penalty parameter we can reformulate the original QUBO problem as a continuous program. It is shown that the problem of large size can be reduced to two constraints. A new convex formulation is then proposed.

1   Introduction

In this paper we consider the quadratic unconstrained binary optimization (QUBO) problem:

$$\left. \begin{array}{l} f(x) = x^T Q x + c^T x = \displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} q_{ij} x_i x_j + \sum_{i=1}^{n} c_i x_i \rightarrow \min \\[4mm] \text{subject to } x_i \in \{0,1\}, \forall i = 1,2,\ldots,n, \end{array} \right\} \qquad (1)$$

where Q is a $n \times n$ real symmetric matrix, but not necessarily positive semidefinite, c is a constant vector: $c = (c_1, c_2, \ldots, c_n)^T \in \Re^n$ and x is an n-vector of binary variables: $x \in \{0,1\}^n$. The superscript "T" indicates transposition. $\Re^n$ is the Euclidean space of n-dimensional column vectors with the inner product $x^T y = \displaystyle\sum_{i=1}^{n} x_i y_i$ and $\Re$ denote the set of real numbers.

The problem considered by quadratic programming (1) occurs in different applications [1], [2], [3]. There are several problems of decisions whose modeling is reduced to the binary quadratic optimization. Such problems are frequently found in *Operations Research,* in *Graph Theory,* in *Economic Science* and in other areas [4], [5]. The QUBO problem is a problem of combinatorial optimization and is well known as *NP – hard* [6] and so, is difficult to solve. For example, the well studied *max-cut problem* is a problem of QUBO.

There were developed and proposed different methods of solving and various relaxation techniques of the considered problem:

- Semidefinite Relaxation [7]
- Lagrangian Relaxations [7]
- Linearization Techniques [8], [9]
- Convex – programming Relaxation [10], [11], [12], [13]
- Heuristic Methods [4], [14].

The simplest relaxation technique is the continuous relaxation that consists in replacing the discrete conditions $x_i \in \{0,1\}, i = 1,2,\ldots,n$ with continuous constraints $0 \le x_i \le 1$ for all $i = 1,2,\ldots,n$.

In the present paper are considered some representations of the binary set $\{0,1\}^n$ by means of which continuous reformulations for the QUBO problem could be obtained. But there are many large dimension problems at practical applications which are intractable.

This paper is organized as follows: in Section 2 we extend a well-known result on representation the constraints $x_i \in \{0,1\}, i = 1,2,\ldots,n$; in the third Section we show how one can considerably

reduce a big number of simple constraints $0 \le x_i \le 1, i = 1, 2, \ldots, n,$ to only two convex constraints. In Section 4, by means of penalization parameters, the initial problem is reduced to a known problem in literature - *DC problem*.

2   Continuous Reformulation of QUBO Problem

The QUBO problem can be transformed into a continuous optimization problem, represented the binary set $\{0,1\}^n$ through inequations system:

$$\left. \begin{array}{l} p(x) \le 0, \\ 0 \le x \le e, \end{array} \right\} \tag{2}$$

where $e = (1, 1, \cdots, 1)^T$ is the vector, all components of which are equal to one and $p(x): \Re^n \to \Re$ is a continuous function that checks the inequality and the equality:

$$\left. \begin{array}{l} p(x) \ge 0, \forall x \in [0,1]^n, \\ p(x) = 0 \text{ and } \text{ if and only if } x \in \{0,1\}^n. \end{array} \right\} \tag{3}$$

Acting as $p(x)$ with the above properties (3) has been proposed and used the concave functions [15], [16]:

$$p(x) = \sum_{i=1}^{n} x_i (1 - x_i) = x^T (e - x)$$

or

$$p(x) = \sum_{i=1}^{n} \min(x_i, 1 - x_i) .$$

There is infinity of such functions. In what follows, we would propose three other continuous functions with similar features.
Let the function

$$p(u) = (1-u)|1-u| + u|u| - (1-2u)^2 = \begin{cases} 2u(1-2u), \text{if } u \le 0, \\ 2u(1-u), \text{if } 0 \le u \le 1, \\ 2u(3-2u) - 2, \text{if } u \ge 1. \end{cases} \tag{4}$$

Function $p(u)$ is a concave function, continuously differentiable to derivatives:

$$p'(u) = \begin{cases} 2(1-4u), \text{if } u \le 0, \\ 2(1-2u), \text{if } 0 \le u \le 1, \\ 2(3-3u) - 2, \text{if } u \ge 1. \end{cases}$$

It is found easily that the function

$$p_1(x) = \sum_{i=1}^{n} \left[(1-x_i)|1-x_i| + x_i|x_i| - (1-2x_i)^2 \right] \tag{5}$$

has the required properties.
Another function would be

$$p(u) = 1 - |2u - 1| = \begin{cases} 2u, \text{if } u \le \dfrac{1}{2}, \\ 2(1-u), \text{if } u \ge \dfrac{1}{2}, \end{cases} \tag{6}$$

which generates the function

$$p_2(x) = \sum_{i=1}^{n} \left[1 - |2x_i - 1| \right]. \tag{7}$$

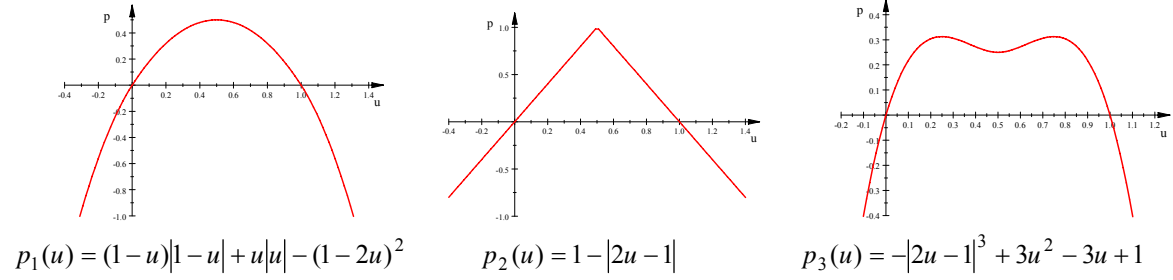We bring another example of a function $p(u)$ that is twice continuously differentiable but is not concave on the interval $[0,1]$:

$$p(u) = -|2u-1|^3 + 3u^2 - 3u + 1 = \begin{cases} u(8u^2 - 9u), \text{if } u \le \dfrac{1}{2}, \\ -8u^3 + 15u^2 - 9u + 2, \text{if } u \ge \dfrac{1}{2}. \end{cases} \tag{8}$$

which generates the function

$$p_3(x) = \sum_{i=1}^{n}\left[-|2x_i - 1|^3 + 3x_i^2 - 3x_i + 1\right]. \tag{9}$$

Graphs functions (4), (6) and (8) are presented below (Fig. 1):

$$p_1(u) = (1-u)|1-u| + u|u| - (1-2u)^2 \qquad p_2(u) = 1 - |2u-1| \qquad p_3(u) = -|2u-1|^3 + 3u^2 - 3u + 1$$

Fig. 1.The graphs of $p_1(u)$**,** $p_1(u)$ **and** $p_3(u)$**.**

Using the functions (5), (7) or (9), quadratic programming problem (1) can be representing in the equivalent form:

$$\left. \begin{aligned} & f(x) = x^T Q x + c^T x \to \min \\ & \text{subject to } p_1(x) \le 0, \\ & \text{or} \qquad\quad p_2(x) \le 0, \\ & \text{or} \qquad\quad p_3(x) \le 0, \\ & \text{and} \qquad\quad 0 \le x \le e. \end{aligned} \right\} \tag{10}$$

We mentioned that $p_s(x) = 0$, $s = 1, s = 2$ or $s = 3$ for any $0 \le x_i \le 1$, $i = 1, 2, \ldots, n$.

3   Reducing the Number of Constraints

The problem (10) includes $2n$ simple constraints:

$$\left. \begin{aligned} & x_i \ge 0, i = 1, 2, \ldots, n, \\ & x_i \le 1, i = 1, 2, \ldots, n. \end{aligned} \right\}$$

For sufficiently large n there are some major problems in solving the problem (10).
In what follows we will show how we can reduce these $2n$ simple restriction to only two convex constraints.
The constraint $u \ge 0$ is equivalent to inequation $\gamma_1(u) \le 0$ or with the inequation $\gamma_2(u) \le 0$, and the constraint $u \le 1$ is equivalent to $\gamma_3(u) \le 0$ or with $\gamma_4(u) \le 0$ where
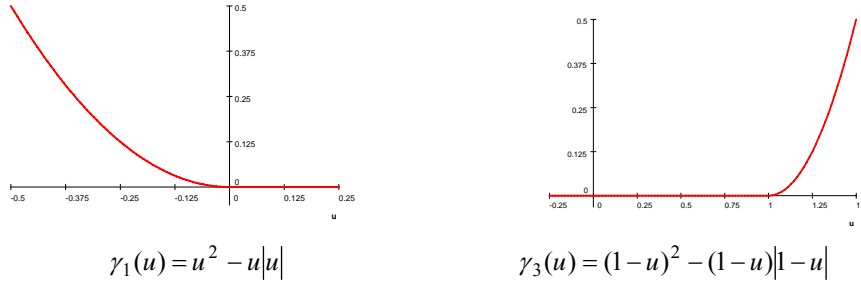
$$\gamma_1(u) = u^2 - u|u| = \begin{cases} 2u^2, \text{if } u \le 0, \\ 0, \text{if } u \ge 0, \end{cases}$$

$$\gamma_2(u) = -u + |u| = \begin{cases} -2u, \text{if } u \le 0, \\ 0, \text{if } u \ge 0, \end{cases}$$

$$\gamma_3(u) = (1-u)^2 - (1-u)|1-u| = \begin{cases} 0, \text{if } u \le 1, \\ 2(1-u)^2, \text{if } u \ge 1, \end{cases}$$

$$\gamma_4(u) = -1 + u + |1-u| = \begin{cases} 0, \text{if } u \le 1, \\ 2(-1+u), \text{if } u \ge 1. \end{cases}$$

The functions $\gamma_1(u)$, $\gamma_2(u), \gamma_3(u)$ and $\gamma_4(u)$ are convex functions for $\forall u \in \Re$, for example, $\gamma_1(u)$ and $\gamma_3(u)$ look like that (Fig. 2):

$$\gamma_1(u) = u^2 - u|u| \qquad\qquad \gamma_3(u) = (1-u)^2 - (1-u)|1-u|$$

Fig. 2.The graphs of $\gamma_1(u)$ and $\gamma_2(u)$

As $x_i^2 - x_i|x_i| \geq 0$ and $-x_i + |x_i| \geq 0$ for $\forall x_i \in \Re$ the restrictions $x_i \geq 0, i = 1,2,\ldots,n$ are equivalent to the constraint $\varphi_1(x) \leq 0$ or $\varphi_2(x) \leq 0$, where
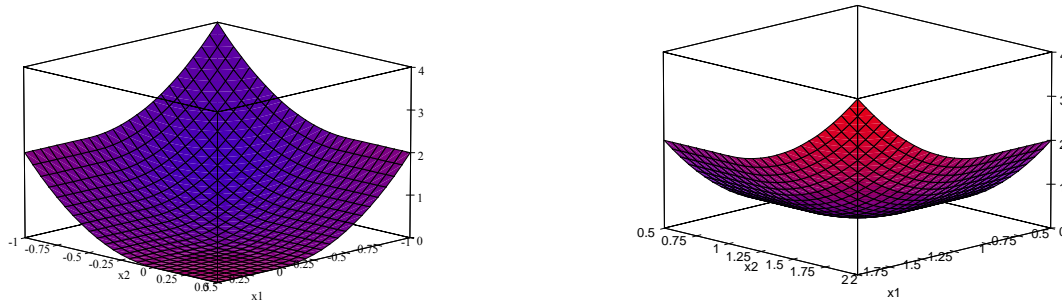
$$\varphi_1(x) = \sum_{i=1}^{n}\left[x_i^2 - x_i|x_i|\right],$$

$$\varphi_2(x) = \sum_{i=1}^{n}\left[-x_i + |x_i|\right]. \tag{11}$$

Similarly it is determined that the conditions $x_i \leq 1, i = 1,2,\ldots,n$ are equivalent to the convex constraint $g_1(x) \leq 0$ or $g_2(x) \leq 0$, where

$$g_1(x) = \sum_{i=1}^{n}\left[(1-x_i)^2 - (1-x_i)|1-x_i|\right],$$

$$g_2(x) = \sum_{i=1}^{n}\left[-1 + x_i + |1-x_i|\right]. \tag{12}$$

The functions $\varphi_1(x)$, $\varphi_2(x)$, $g_1(x)$ and $g_2(x)$ are convex and determines convex set. For example, for $n = 2$ the functions $\varphi_1(x)$ and $g_1(x)$ are as follows (see Fig. 3):

Fig. 3. The graphs of $\varphi_1(x)$ and $\varphi_1(x)$ $g_1(x)$

So the problem (10) which has $(2n+1)$ constrains can be reduced to a problem of optimization only with three constrains:

$$\left.\begin{array}{l} f(x) = x^T Q x + c^T x \rightarrow \min \\ \text{subject to } p_1(x) \leq 0, \\ \qquad\qquad \varphi_1(x) \leq 0, \\ \qquad\qquad g_1(x) \leq 0, \end{array}\right\} \tag{13}$$

or

$$\left. \begin{array}{l} f(x) = x^T Q x + c^T x \to \min \\ \text{subject to } p_2(x) \le 0, \\ \qquad\qquad \varphi_2(x) \le 0, \\ \qquad\qquad g_2(x) \le 0, \end{array} \right\}, \tag{14}$$

where the convex functions $\varphi_1(x)$, $\varphi_2(x)$, $g_1(x)$, $g_2(x)$ are determined by the formulas (11) and (12), while the concave functions $p_1(x)$ and $p_2(x)$ by formulas (5) and respectively (7).

4   Reduction to a DC problem

In problems (13) and (14) the constraints $p_1(x) \le 0$ or $p_2(x) \le 0$ are difficult as they represent non-convex sets. One way to ease the solution of problems (13) and (14) is to penalize these constraints. This can be carried out in such a way: Let us consider the optimization problem obtained from the problem (13):

$$\left. \begin{array}{l} \widetilde{f}(x) = x^T Q x + c^T x - \tau\, p_1(x) \to \min \\ \text{subject to} \\ \qquad\qquad \varphi_1(x) \le 0, \\ \qquad\qquad g_1(x) \le 0, \end{array} \right\} \tag{15}$$

where $\tau > 0$ is a sufficiently large positive number (parameter penalty). If the matrix Q is positive semidefinite then the function $\widetilde{f}(x)$ is represented as the difference of two convex functions and thus the problem (15) becomes a DC (*Difference of Convex Functions*) Programming [17], [18]. It could be found a τ_0 so that for $\forall \tau \ge \tau_0$ the problems (13) and (15) have the same optimal solutions. To solve such problems (15) can be used with success DC Algorithm [18].

5   Conclusions

In this work we are interested in the resolution of quadratic optimization problem in variable binary 0-1. The main idea is to transform QUBO problem into a new problem of optimization with only two convex constraints. The objective function $f(x)$ is reformulated a new function $\widetilde{f}(x)$, convex and equal to $f(x)$ for any admissible solutions QUBO problem. The results obtained with this approach are promising. On all convex functions that we considered $p_1(x)$, $\varphi_1(x)$ and $g_1(x)$ to have been very effective.

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