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Global optimality conditions for quadratic 0-1 optimization problems

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Abstract In the present work, we intend to derive conditions characterizing globally optimal solutions of quadratic 0-1 programming problems. By specializing the problem of maximizing a convex quadratic function under linear constraints, we find explicit global optimality conditions for quadratic 0-1 programming problems, including necessary and sufficient conditions and some necessary conditions. We also present some global optimality conditions for the problem of minimization of half-products.

Keywords Global optimization · Quadratic programming · Global optimality condition · Quadratic 0-1 programming · Half-products

1 Introduction

Quadratic optimization problems cover a large spectrum of situations. They constitute an important part in the field of optimization. These problems can be written as follows:

$$\begin{aligned} &\min\ f(x) = \frac{1}{2}x^T Qx + b^T x \\ &\text{s.t.}\quad x \in C. \end{aligned}$$

The constraints can be given by quadratic functions, linear functions or integers. Such problems have many diverse applications, see e.g.,[1,7,8,14,23]. Due to the importance of quadratic 0-1 problems, various approaches for solving these problems have been developed, see e.g., [9,13,20–22]. But tackling them from the global optimality and duality viewpoints is not as yet at hand. However, some situations are well understood. When there is only one quadratic constraint $g(x) = \frac{1}{2}x^T Q_1 x + b_1^T x \leq 0$, J.J. More obtained the sufficient and necessary condition of $\bar{x}$ being a global solution of (P) was that the KKT conditions held at $\bar{x}$ and $Q + \overline{\mu} Q_1$ was positive semidefinite, see [19]. This result has been explored by PENG-Jiming and YUAN-Yaxiang for the case where (P) has two general quadratic inequality

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constraints in [24] in 1997. In [6], G. Danninger considered the concave quadratic problems and reformulated a global optimality criterion into copositivity conditions. In 2001, by using the term of $\varepsilon - subdifferentials$ of convex functions and $\varepsilon - normal$ directions, J.-B. Hiriart-Urruty derived conditions characterizing a globally optimal solution for the problem of maximizing a convex quadratic function under several convex quadratic constraints in [11]. In 2000, with regard to the quadratic problems with binary constraints, A. Beck and M. Teboulle established a sufficient and a necessary global optimality conditions, which are expressed in a simple way in terms of the problem's data. In the literature [15–18], some global optimality conditions have been given recently.

In this paper, we pursue the goal of characterizing the global solutions of a quadratic optimization problem. We emphasize nonconvex optimization problems presenting some specific structures like quadratic 0-1 programming problems. There is a necessary and sufficient condition for a feasible point to be a global maximizer of a convex quadratic function under linear constraints. Through this work, we intend to derive conditions characterizing globally optimal solutions in the problem of quadratic 0-1 programming problems. We find explicit global optimality conditions of it, including necessary and sufficient conditions and some necessary conditions. The necessary conditions can be checked rather easily and actually implemented. It is interesting that some necessary conditions expressed here are given with lower dimensions than the primal problem. We notice that there is some relations between our results and the results in [2]. If we weaken the sufficient condition in [2], complemented with another condition, the sufficient global optimality condition given by A. Beck and M. Teboulle becomes a necessary and sufficient global optimality condition of quadratic 0-1 problem. Also the necessary condition in [2] can be modified as a necessary and sufficient condition by combining with another condition which is mixed first and second order information about the data.

This paper consists of five sections. Section one is an introduction. With some known results, section two discusses global optimality conditions in maximizing a convex quadratic function under linear constraints or box constraints. Some global optimality conditions of quadratic 0-1 programming problems are given in section three. Section four discusses the problem of minimization of half-products, which is a classical class quadratic 0-1 optimization problem. Furthermore, in section five, we try to reduce the dimensions in our global optimality conditions and give some necessary conditions for quadratic 0-1 programming which may be helpful to taken away some feasible points from the set of the global solutions.

Throughout this paper, we will use the following notations and definitions. For a vector $x \in R^n$, the Euclidean norm $(l_2 - norm)$ and $l_\infty - norm$ are denoted, respectively, by $\|x\| := (\sum_{i=1}^n x_i^2)^{1/2}$ and $\|x\|_\infty := max_{1\le i\le n}|x_i|$. Let $\{e_i\}_{i=1}^n$ be the canonical basis of R^n, and let the vector of all 1's be denoted by e, i.e., $e = (1, \dots, 1)^T$. Also we denote $\lambda_1(\cdot)$ as the largest eigenvalue of a matrix and $\lambda_n(\cdot)$ as the smallest eigenvalue of it.

2 Quadratic programming with linear constraints

In this section, we consider the problem of maximizing the convex quadratic function under linear constraints. This can be viewed as a particular case of the general situation where a convex function is maximized over a convex set. Let $f : R^n \to R$ be convex and let C be a nonempty closed convex set in R^n. Two mathematical objects are useful in deriving optimality conditions in the problem of maximizing f over C, refer to [10].

Definition 2.1 For $\varepsilon \geq 0$, the $\varepsilon - subdifferential$ of f at $\bar{x}$, denoted as $\partial_\varepsilon f(\bar{x})$, is the set of $d \in R^n$ satisfying $f(x) \geq f(\bar{x}) + d^T(x - \bar{x}) - \varepsilon, \forall x \in R^n$.

Definition 2.2 For $\varepsilon \geq 0$, the $\varepsilon - normal$ directions to C at $\bar{x} \in C$, denoted as $N_\varepsilon(C, \bar{x})$, is the set of $d \in R^n$ satisfying $d^T(x - \bar{x}) \leq \varepsilon$ for all $x \in C$.

The following general result characterizes a global maximizer $\bar{x} \in C$ of f over C.

Theorem 2.3 [10] *If $f(x)$ is convex and C is a nonempty closed convex set, then $\bar{x} \in C$ is a global maximizer of f over C if and only if for all $\varepsilon > 0$,*

$$\partial_\varepsilon f(\bar{x}) \subset N_\varepsilon(C, \bar{x}).$$

Instead of using the rough definitions (2.1) (2.2), an alternate way of exploiting Theorem 2.3 is to go through the support functions of $\partial_\varepsilon f(\bar{x})$ and $N_\varepsilon(C, \bar{x})$.

Definition 2.4 The support function of $\partial_\varepsilon f(\bar{x})$, denoted as $f'_\varepsilon(\bar{x}, \cdot)$, is the so called ε-directional derivative of f at $\bar{x}$:

$$d \in R^n \mapsto f'_\varepsilon(\bar{x}, d) = \inf_{t>0} \frac{f(\bar{x} + td) - f(\bar{x}) + \varepsilon}{t}.$$

Definition 2.5 The support function of $N_\varepsilon(C, \bar{x})$, denoted as $(I_c)'_\varepsilon(\bar{x}, \cdot)$, is the so called ε-directional derivative of the indicator function I_c at $\bar{x}$:

$$d \in R^n \mapsto (I_c)'_\varepsilon(\bar{x}, d) = \inf \left\{ \frac{\varepsilon}{t} : t > 0, \bar{x} + td \in C \right\}.$$

So Theorem 2.3 can be reformulated by making use of above support functions.

Theorem 2.6 [11] *If f(x) is convex and C is a nonempty closed convex set in R^n, then $\bar{x} \in C$ is a global maximizer of f over C if and only if for all $\varepsilon > 0$*

$$f'_\varepsilon(\bar{x}, d) \leq (I_c)'_\varepsilon(\bar{x}, d).$$

In [6] and [3], following quadratic minimization problem was discussed

$$\begin{aligned} (P_0)\ \max\ & f(x) = \frac{1}{2}x^T Qx + b^T x \\ \text{s.t.}\ \ & Ax \leq c, \end{aligned}$$

where Q is a positive semidefinite matrix. For this special quadratic case, G. Danninger proved Theorem 2.3 directly and reformulated the global optimality condition into copositivity conditions in [6]. Similarly, for the following quadratic programming problem

$$(P)\quad \begin{array}{ll} \max & f(x) = \frac{1}{2}x^T Qx + b^T x \\ \text{s.t.} & a_j^T x \leq b_j,\ j = 1, \ldots, m, \\ & a_j^T x = b_j,\ j = m+1, \ldots, s, \end{array}$$

the feasible set is $C = \{x : a_j^T x \leq b_j, j = 1, \ldots, m; a_j^T x = b_j, j = m+1, \ldots, s\}$, and it is a closed and convex set. For the convenience of following discussion, we reformulate G. Danninger's results for problem (P) here.

For $\bar{x} \in C$ and $d \in R^n$, from [6] and [3], by Theorem 2.6, $f'_\varepsilon(\bar{x}, d) \leq (I_C)'_\varepsilon(\bar{x}, d)$ means

$$d^T(Q\bar{x} + b) + \sqrt{2\varepsilon d^T Qd} \leq \frac{\varepsilon}{t_d}, \quad \text{for all } \varepsilon > 0, \tag{1}$$

where

$$\begin{aligned} t_d &= \sup\{t > 0 : \bar{x} + td \in C\} \\ &= \sup\{t > 0 : ta_j^T d \le b_j - a_j^T \bar{x},\ j = 1, \ldots, m; \\ &\qquad ta_j^T d = 0,\ j = m+1, \ldots, s\}. \end{aligned}$$

Denote $I(\bar{x}) = \{j : a_j\bar{x} = b_j, 1 \le j \le m\}$. For $j \in I(\bar{x})$, $b_j - a_j^T\bar{x} = 0$, so when $a_j^T d \le 0$, $ta_j^T d \le b_j - a_j^T \bar{x}$ will hold for $t \in (0, +\infty)$. For $j \notin I(\bar{x})$, $1 \le j \le m$, we have $b_j - a_j^T\bar{x} > 0$. If $a_j^T d \le 0$, $ta_j^T d \le b_j - a_j^T\bar{x}$ always holds for $t \in (0, +\infty)$. If $a_j^T d > 0$, then $ta_j^T d \le b_j - a_j\bar{x}$ holds for $t \in \left(0, \dfrac{b_j - a_j^T\bar{x}}{a_j^T d}\right)$. For $j = m+1, \ldots, s$, only when $a_j^T d = 0$, $\bar{x} + td \in C$ holds for $t \in (0, +\infty)$. So we can denote $T(\bar{x}) = \{d \in R^n : a_j^T d \le 0, j \in I(\bar{x}); a_j^T d = 0, j = m+1, \ldots, s\}$ and for $d \in T(\bar{x})$, let $J_d = \{j : a_j^T d > 0, j \notin I(\bar{x}), 1 \le j \le m\}$. Then for $d \in T(\bar{x})$, $t_d = \min_{j\in J_d} \dfrac{b_j - a_j^T\bar{x}}{a_j^T d}$ if $J_d \ne \emptyset$; and $t_d = +\infty$ if $J_d = \emptyset$.

Obviously t_d should be finite otherwise (1) will not hold for all $\varepsilon > 0$. Thus when $J_d \ne \emptyset$, let $\alpha = \sqrt{\varepsilon}$, $\psi(\alpha) = d^T(Q\bar{x} + b) + \alpha\sqrt{2d^T Qd} - \dfrac{\alpha^2}{t_d}$. The inequality (1) becomes

$$\psi(\alpha) \le 0 \ \text{ for all } \alpha > 0. \tag{2}$$

We can prove here (2) is equivalent to

$$\psi(\alpha) \le 0 \text{ for all } \alpha \in R. \tag{3}$$

(3) holds if and only if

$$\Delta = \left(\sqrt{2d^T Qd}\right)^2 - 4\left(-\frac{1}{t_d}\right) d^T(Q\bar{x} + b) \le 0. \tag{4}$$

It is obvious that (4) can be written as

$$d^T Qd \le \frac{-2d^T(Q\bar{x} + b)}{t_d}.$$

Moreover, $d^T(Q\bar{x} + b) \le 0$ is necessary to ensure the above inequality holding because Q is positive semidefinite.

We recapitulate the above arguments in the following theorem and a full proof for problem (P_0) can be found in [6].

Theorem 2.7 *Consider the problem (P). If Q is a positive semidefinite matrix, then a feasible point $\bar{x}$ is a global solution of (P) if and only if for $d \in T(\bar{x})$ such that $J_d \ne \emptyset$, the following two conditions hold:*

(2.7.1) $\quad d^T(Q\bar{x} + b) \le 0$;

(2.7.2) $\quad d^T Qd \le \dfrac{-2d^T(Q\bar{x} + b)}{t_d}$, $t_d = \min_{j\in J_d} \dfrac{b_j - a_j^T\bar{x}}{a_j^T d}$,

where $I(\bar{x}) = \{j : a_j\bar{x} = b_j, 1 \le j \le m\}$, $J_d = \{j : a_j^T d > 0, j \notin I(\bar{x}), 1 \le j \le m\}$, $T(\bar{x}) = \{d \in R^n : a_j^T d \le 0, j \in I(\bar{x}); a_j^T d = 0, j = m+1, \ldots, s\}$.

Example Consider following problem

$$\begin{aligned} &\max\ f(x) = x_1^2 + x_2^2 \\ &\text{s.t.}\quad x_1 + 4x_2 \le 6, x_1 \le 2, x_1, x_2 \ge 0. \end{aligned}$$

Here $Q = 2I$, $b = 0$. There are four constrains: $g_1(x) = x_1 + 4x_2 \le 6$, $g_2(x) = x_1 \le 2$, $g_3(x) = -x_1 \le 0$, and $g_4(x) = -x_2 \le 0$. $a_1 = (1, 4)^T$, $a_2 = (1, 0)^T$, $a_3 = (-1, 0)^T$, $a_4 = (0, -1)^T$.

For $\bar{x} = (2, 1)^T$, $I(\bar{x}) = \{1, 2\}$, $T(\bar{x}) = \{d \in R^2 : d_1 + 4d_2 \le 0, d_1 \le 0\}$. If $d \in T(\bar{x})$, then $d^T(Q\bar{x} + b) = 2(2d_1 + d_2) = \frac{1}{2}(7d_1 + d_1 + 4d_2) \le 0$, the condition (2.7.1) holds. Four cases arise in the process of checking the condition (2.7.2).

Case 1: $d_1 = 0$, $d_2 \le -\frac{1}{4}d_1 = 0$. Since $a_3^T d = 0$ and $a_4^T d = -d_2$, we have $J_d = \emptyset$ when $d_2 = 0$, and when $d_2 < 0$, $J_d = \{4\}$, $t_d = \dfrac{0 - a_4^T\bar{x}}{a_4^T d} = -\dfrac{1}{d_2}$. $d^T Qd = 2(d_1^2 + d_2^2) = 2d_2^2$, $\dfrac{-2d^T(Q\bar{x} + b)}{t_d} = 4d_2(2d_1 + d_2) = 4d_2^2$, thus (2.7.2) holds.

Case 2: $2d_2 \le d_1 < 0$. Since $a_3^T d = -d_1 > 0$ and $a_4^T d = -d_2 > 0$, we have $J_d = \{3, 4\}$, $t_d = min\left(\dfrac{0 - a_3^T\bar{x}}{a_3^T d}, \dfrac{0 - a_4^T\bar{x}}{a_4^T d}\right) = min\left(\dfrac{-2}{d_1}, \dfrac{-1}{d_2}\right) = -\dfrac{1}{d_2}$. By $2d_2 - d_1 \le 0$, $d_1(2d_2 - d_1) \ge 0$, $d_2^2 + 4d_1d_2 - d_1^2 = d_2^2 + 2d_1d_2 + d_1(2d_2 - d_1) \ge 0$, thus $d^T Qd = 2(d_1^2 + d_2^2) \le 4d_2(2d_1 + d_2) = \dfrac{-2d^T(Q\bar{x} + b)}{t_d}$, (2.7.2) holds.

Case 3: $d_1 < 2d_2 < 0$. Similar as case 2, $J_d = \{3, 4\}$, but $t_d = -\dfrac{2}{d_1}$. Since $d_1 < 2d_2 < d_2 < 0$, $d_2(d_1 - d_2) > 0$, $d_1^2 + d_1d_2 - d_2^2 = d_1^2 + d_2(d_1 - d_2) > 0$, we also have $d^T Qd = 2(d_1^2 + d_2^2) < 2d_1(2d_1 + d_2) = \dfrac{-2d^T(Q\bar{x} + b)}{t_d}$, (2.7.2) holds.

Case 4: $d_1 < 0 \le d_2 \le -\frac{1}{4}d_1$. Since $a_3^T d = -d_1 > 0$ and $a_4^T d = -d_2 \le 0$, we obtain $J_d = \{3\}$, $t_d = -\dfrac{2}{d_1}$. Hence $d_1d_2 \ge -\frac{1}{4}d_1^2$, $-d_2^2 \ge -\frac{1}{16}d_1^2$, and $d_1^2 + d_1d_2 - d_2^2 \ge d_1^2 - \frac{1}{4}d_1^2 - \frac{1}{16}d_1^2 = \frac{11}{16}d_1^2 \ge 0$. Thus $d^T Qd = 2(d_1^2 + d_2^2) \le 2d_1(2d_1 + d_2) = \dfrac{-2d^T(Q\bar{x} + b)}{t_d}$, (2.7.2) holds.

Now for all $d \in T(\bar{x})$, the condition (2.7.1) and (2.7.2) hold, $\bar{x} = (2, 1)^T$ is the global maximum.

In fact, $x_1^2 + x_2^2$ is a convex function and the feasible domain is a polytope. If it has an optimal solution, then the optimal solution is attained at a vertex of the polytope. There are four vertices of the polytope: $x^{(1)} = (2, 1)^T$, $x^{(2)} = (2, 0)^T$, $x^{(3)} = (0, 1.5)^T$ and $x^{(4)} = (0, 0)^T$. $f(x^{(1)}) = 5$, $f(x^{(2)}) = 4$, $f(x^{(3)}) = 2.25$, $f(x^{(4)}) = 0$. So $x^{(1)} = (2, 1)^T = \bar{x}$ is the global maximum.

For $x^{(2)} = (2, 0)^T$, $I(x^{(2)}) = \{2, 4\}$, $T(x^{(2)}) = \{d \in R^2 : d_1 \le 0, d_2 \ge 0\}$. Let $d = (0, 1)^T \in T(x^{(2)})$, $J_d = \{1\}$, $d^T Qd = 2 > 0 = \dfrac{-2d^T(Qx^{(2)} + b)}{t_d}$, then the condition (2.7.2) does not hold.

For $x^{(3)} = (0, 1.5)^T$, $I(x^{(3)}) = \{1, 3\}$, $T(x^{(3)}) = \{d \in R^2 : d_1 \ge 0, d_1 + 4d_2 \le 0\}$. Let $d = (2, -1)^T \in T(x^{(3)})$, $J_d = \{2, 4\}$, $t_d = 1$, $d^T Qd = 10 > 6 = -2d^T(Qx^{(3)} + b)$, the condition (2.7.2) does not hold.

For $x^{(4)} = (0,0)^T$, $I(x^{(4)}) = \{3,4\}$, $T(x^{(4)}) = \{d \in R^2 : d_1 \geq 0, d_2 \geq 0\}$. Let $d = (0,1)^T \in T(x^{(4)})$, $J_d = \{1\}$, $d^T Qd = 2 > 0 = \dfrac{-2d^T(Qx^{(4)}+b)}{t_d}$, the condition (2.7.2) does not hold.

This example clearly indicates that the conditions in Theorem 2.7 are sufficient and necessary conditions of a feasible point of problem (P) being a global optimal maximum.

Now we consider a quadratic minimization problem with a concave objective function and box constraints.

$$
\begin{array}{lll}
(P_B) & \min & f(x) = \frac{1}{2}x^T Qx + b^T x \\
 & \text{s.t.} & l_i \leq x_i \leq u_i, i = 1, \ldots, n.
\end{array}
$$

This problem can also be written as follows:

$$
\begin{array}{lll}
(P_{B1}) & \max & -f(x) = \frac{1}{2}x^T(-Q)x - b^T x \\
 & \text{s.t.} & l_i \leq x_i \leq u_i, i = 1, \ldots, n.
\end{array}
$$

where Q is positive semidefinite.

Lemma 2.8 *If $\bar{x} \in R^n$ is a feasible point of problem (P_B), then $T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $\bar{x}_i = u_i$; $d_i \geq 0$ if $\bar{x}_i = l_i\}$. Furthermore, for $d \neq 0$, $d \in T(\bar{x})$, $J_d \neq \emptyset$, and $t_d = min\left\{\min_{d_i>0} \dfrac{u_i - \bar{x}_i}{d_i}, \min_{d_i<0} \dfrac{\bar{x}_i - l_i}{-d_i}\right\}$.*

Proof There are 2n constraints of problem (P_B): the i-th is $-e_i^T x \leq -l_i$, and the n+i-th is $e_i^T x \leq u_i$, $1 \leq i \leq n$. If $\bar{x}_i = u_i$, then $n+i \in I(\bar{x})$. If $\bar{x}_i = l_i$, then $i \in I(\bar{x})$. To the active constraints, the following inequalities should hold if d is a vector of $T(\bar{x})$ denoted in Theorem 2.7: $e_i^T d \leq 0$, for $n+i \in I(\bar{x})$; and $-e_i^T d \leq 0$, for $i \in I(\bar{x})$. All these mean $d_i \leq 0$, if $\bar{x}_i = u_i$; and $d_i \geq 0$, if $\bar{x}_i = l_i$. So here $T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $\bar{x}_i = u_i$; $d_i \geq 0$ if $\bar{x}_i = l_i\}$.

Furthermore, let $d \neq 0, d \in T(\bar{x})$. If $d_i > 0$, then $\bar{x}_i \neq u_i$, the n+i-th constraint $e_i^T x \leq u_i$ is inactive, $n+i \notin I(\bar{x})$. Since $e_i^T d > 0$, we have $n+i \in J_d$. Also if $d_i < 0$, we have $\bar{x}_i \neq l_i$ and $i \in J_d$. Thus the set J_d denoted in the Theorem 2.7 is nonempty when $d \neq 0$.

Suppose $d \in T(\bar{x})$. If $d_i = 0$, then $-e_i^T d = e_i^T d = 0$, $i \notin J_d$, $n+i \notin J_d$. Thus if $j = n+i \in J_d$, then $d_i \neq 0$ and $\dfrac{b_j - a_j^T\bar{x}}{a_j^T d} = \dfrac{u_i - e_i^T\bar{x}}{e_i^T d} = \dfrac{u_i - \bar{x}_i}{d_i}$. If $j = i \in J_d$, then $d_i \neq 0$ and $\dfrac{b_j - a_j^T\bar{x}}{a_j^T d} = \dfrac{-l_i - (-e_i^T)\bar{x}}{-e_i^T d} = \dfrac{\bar{x}_i - l_i}{-d_i}$. So

$$
t_d = \min_{j \in J_d} \frac{b_j - a_j^T\bar{x}}{a_j^T d} = \min_{1 \leq i \leq n}\left\{\min_{d_i>0} \frac{u_i - \bar{x}_i}{d_i}, \min_{d_i<0} \frac{\bar{x}_i - l_i}{-d_i}\right\}.
$$

The proof is completed.

Theorem 2.9 *Consider problem (P_B) with Q a negative semidefinite symmetric matrix. A feasible point $\bar{x}$ is a global minimizer of (P_B) if and only if for all $d \in T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $\bar{x}_i = u_i$; $d_i \geq 0$ if $\bar{x}_i = l_i\}$, the following two inequalities hold:*
(2.9.1) $d^T(Q\bar{x} + b) \geq 0$;
(2.9.2) $-d^T Qd \leq \dfrac{2d^T(Q\bar{x}+b)}{t_d}$, $t_d = \min_{1 \leq i \leq n, d_i \neq 0}\left\{\dfrac{u_i - l_i}{|d_i|}\right\}$.

Proof Over a polytope, a concave function attains its minimum at a vertex of the polytope. What we need to do, is to discuss the points satisfying $x_i = u_i$ or $x_i = l_i$ for all $1 \le i \le n$. Suppose $\bar{x}$ is a vertex, by Lemma 2.8, for all $d \in T(\bar{x})$, $\bar{x}_i = l_i$ when $d_i > 0$ and $\bar{x}_i = u_i$ when $d_i < 0$. So $t_d = \min_{1\le i\le n, d_i\neq 0}\left\{\frac{u_i - l_i}{|d_i|}\right\}$. Thus from Theorem 2.7 and the equivalence of (P_B) and (P_{B1}), we can obtain the conclusion.

Corollary 2.10 *Consider problem (P_B) with Q a negative semidefinite symmetric matrix. If $\bar{x}$ is a vertex satisfying*
(2.10.1) $-\lambda_n(Q)(u_i - l_i) + 2(Q\bar{x} + b)_i \le 0$, *if* $\bar{x}_i = u_i$*;*
(2.10.2) $-\lambda_n(Q)(u_i - l_i) - 2(Q\bar{x} + b)_i \le 0$, *if* $\bar{x}_i = l_i$*,*
then $\bar{x}$ is a global minimizer of problem (P_B).

Proof Let $\bar{x}$ be a vertex and $d \in T(\bar{x})$. If $d_i \neq 0$, then $t_d \le \frac{u_i - l_i}{|d_i|}$. Since $\lambda_n(Q) \le 0$, if $\bar{x}_i = u_i$, $(Q\bar{x} + b)_i \le \frac{1}{2}\lambda_n(Q)(u_i - l_i) \le 0$. By Lemma 2.8, $d_i \le 0$, thus $d_i(Q\bar{x} + b)_i \ge 0$, $\frac{d_i(Q\bar{x} + b)_i}{t_d} \ge \frac{\lambda_n(Q)}{2t_d} d_i(u_i - l_i) \ge -\frac{1}{2}\lambda_n(Q)d_i^2$. If $\bar{x}_i = l_i$, by (2.10.2) and $d_i \ge 0$, we have $d_i(Q\bar{x} + b)_i \ge 0$, $\frac{d_i(Q\bar{x} + b)_i}{t_d} \ge -\frac{\lambda_n(Q)}{2t_d} d_i(u_i - l_i) \ge -\frac{1}{2}\lambda_n(Q)d_i^2$. Thus $d^T(\bar{x} + b) \ge 0$ and

$$\frac{2d^T(Q\bar{x} + b)}{t_d} \ge -\lambda_n(Q)\sum_{1\le i\le n} d_i^2 = -\left(\min_{y\neq 0}\frac{y^T Q y}{y^T y}\right)(d^T d) \ge -d^T Q d.$$

By Theorem 2.9, $\bar{x}$ is a global minimizer of problem (P_B).

Corollary 2.11 *Consider problem (P_B) with $Q = (q_{ij})$ a negative semidefinite symmetric matrix. If $\bar{x}$ is a global minimizer of (P_B), then*
(2.11.1) $2(Q\bar{x} + b)_i \ge \max(-q_{ii}(u_i - l_i), 0)$ *if* $x_i = l_i$*;*
(2.11.2) $2(Q\bar{x} + b)_i \le \min(q_{ii}(u_i - l_i), 0)$ *if* $x_i = u_i$*.*

Proof If $\bar{x}_i = u_i$, let $d^{(1)} = -e_i \in T(\bar{x})$. By Lemma 2.8, $t_{d^{(1)}} = u_i - l_i$. From (2.9.1), $d^{(1)}(Q\bar{x}+b) = -(Q\bar{x}+b)_i \ge 0$. From (2.9.2), $d^{(1)T}(-Q)d^{(1)} = -q_{ii} \le \frac{2d^{(1)}(Q\bar{x} + b)}{t_{d^{(1)}}} = \frac{-2(Q\bar{x} + b)_i}{u_i - l_i}$.

If $\bar{x}_i = l_i$, let $d^{(2)} = e_i \in T(\bar{x})$, $t_{d^{(2)}} = u_i - l_i$. By Theorem 2.9, $d^{(2)}(Q\bar{x} + b) = (Q\bar{x} + b)_i \ge 0$, $d^{(2)T}(-Q)d^{(2)} = -q_{ii} \le \frac{2d^{(2)}(Q\bar{x} + b)}{t_{d^{(2)}}} = \frac{2(Q\bar{x} + b)_i}{u_i - l_i}$. Thus (2.11.1) and (2.11.2) hold and the proof is completed.

The above necessary condition and sufficient condition are obtained by the necessary and sufficient condition directly. These conditions can also be obtained from the results in [15]. In that paper, the authors presented necessary conditions and sufficient conditions for a given feasible point to be a global minimizer of the difference of quadratic and convex functions subject to bounds on the variables.

3 Quadratic 0-1 programming

Now we focus our attention on the problem of quadratic 0-1 programming

$$(D)\quad \min\ f(x) = \frac{1}{2}x^T Q x + b^T x \quad \text{s.t.}\ x \in \{0, 1\}^n.$$

For $\bar{x} \in \{0, 1\}^n$, we denote $E(\bar{x}) = \{i : \bar{x}_i = 1, i = 1, \ldots, n\}$, $N_0 = \{1, \ldots, n\}$.

Theorem 3.1 *Consider problem (D) with Q a negative semidefinite symmetric matrix. $\bar{x} \in \{0, 1\}^n$, then $\bar{x}$ is a global minimizer of (D) if and only if for all $d \in T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $i \in E(\bar{x})$; $d_i \geq 0$ if $i \in N_0 \backslash E(\bar{x})\}$, the following two inequalities hold:*
(3.1.1) $d^T(Q\bar{x} + b) \geq 0$;
(3.1.2) $-d^T Qd \leq 2 \parallel d \parallel_\infty d^T(Q\bar{x} + b)$.

Proof Suppose $0 \leq \bar{x} \leq e$, by Lemma 2.8, for all $i = 1, \ldots, n$, $u_i = 1$ and $l_i = 0$, $T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $\bar{x}_i = 1$; $d_i \geq 0$ if $\bar{x}_i = 0\}$. If $d \in T(\bar{x})$, $d \neq 0$, $t_d = \frac{1}{\|d\|_\infty}$. Thus (3.1.1) and (3.1.2) can be obtained from Theorem 2.9 and the proof is completed.

We denote $T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $\bar{x}_i = 1$; $d_i \geq 0$ if $\bar{x}_i = 0\} = \{d \in R^n : d_i \leq 0$ if $i \in E(\bar{x})$; $d_i \geq 0$ if $i \in N_0 \backslash E(\bar{x})\}$ for problem (D) in this section.

Now suppose Q is a real symmetric matrix and $\lambda_1(Q)$ is the largest eigenvalue of Q. If $\lambda_1(Q) > 0$, then the problem (D) isn't a negative semidefinite problem. But $Q - \lambda_1(Q)I$ becomes a negative semidefinite matrix. When $x \in \{0, 1\}^n$, we have $x^T x = e^T x$. So problem (D) can be written as following:

$$(D) \quad \begin{array}{l} \min\ f(x) = \frac{1}{2}x^T(Q - \lambda_1(Q)I)x + (b + \frac{1}{2}\lambda_1(Q)e)^T x \\ \text{s.t.} \quad x \in \{0, 1\}^n, \end{array}$$

which is a negative semidefinite quadratic 0-1 programming. The following result is then an immediate consequence of Theorem 3.1.

Theorem 3.2 *Consider problem (D) with Q a real symmetric matrix. Let $\bar{x} \in \{0, 1\}^n$. Then $\bar{x}$ is a global solution of problem (D) if and only if for all $d \in T(\bar{x})$, the following two conditions hold:*
(3.2.1) $d^T[Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)] \geq 0$;
(3.2.2) $-d^T Qd + \lambda_1(Q)\|d\|^2 \leq 2\|d\|_\infty d^T\left[Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)\right]$.

Remark 1 If we choose $\mu \leq -\lambda_1(Q)$, then $Q + \mu I$ will be negative semidefinite. Thus $\lambda_1(Q)$ in Theorem 3.2 can be replaced by μ.

Remark 2 As we know, $\lambda_n(Q)I - Q$ is also a negative semidifinite matrix. But $\frac{1}{2}x^T(\lambda_n(Q) I - Q)x - (b + \frac{1}{2}\lambda_n(Q)e)^T x = -f(x)$ for $x \in \{0, 1\}^n$. So we can get similar results for solving the problem $max\{\frac{1}{2}x^T Qx + b^T x : x \in \{0, 1\}^n\}$.

In classical optimality theory, the first-order necessary condition is often expressed with the help of a multiplier. Here condition (3.2.1) is a first-order condition but the vector d can be removed from it without any dual variables.

Lemma 3.3 *Consider problem (D) with Q a real symmetric matrix. Let $\bar{x} \in \{0, 1\}^n$, $\bar{X}$ be the diagonal matrix with the ith element $\bar{x}_i$, $T(\bar{x}) = \{d \in R^n : d_i \leq 0$ if $i \in E(\bar{x})$; $d_i \geq 0$ if $i \in N_0 \backslash E(\bar{x})\}$. Then the following conditions are equivalent:*
(3.2.1) $d^T[Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)] \geq 0$, $d \in T(\bar{x})$;
(3.2.3) $Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right) \in T(\bar{x})$;
(3.2.4) $2(2\bar{X} - I)(Q\bar{x} + b) \leq \lambda_1(Q)e$.

Proof Let $p = Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)$. (3.2.3) means for $i \in E(\bar{x})$, $p_i \leq 0$; and for $i \in N_0 \backslash E(\bar{x})$, $p_i \geq 0$. So (3.2.1) can be gotten from (3.2.3). If (3.2.1) holds while (3.2.3) doesn't hold, suppose $\exists i_0 \in E(\bar{x})$, $p_{i_o} > 0$, let $d = -e_{i_0}$, then $d^T p < 0$ will contradict with (3.2.1). So (3.2.3) always holds when (3.2.1) holds.

Since $i \in E(\bar{x}) \Leftrightarrow \bar{x}_i = 1 \Leftrightarrow 2\bar{x}_i - 1 = 1$; and $i \in N_0 \backslash E(\bar{x}) \Leftrightarrow \bar{x}_i = 0 \Leftrightarrow 2\bar{x}_i - 1 = -1$, then (3.2.3) is equivalent to $(2\bar{x}_i - 1)p_i \leq 0$, $\forall i = 1, \ldots, n$. That is $(2\bar{X} - I)[Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)] \leq 0$. Furthermore, when $\bar{x} \in \{0, 1\}^n$, $(2\bar{X} - I)^2 = I$. Thus

$$\begin{aligned}&(2\bar{X} - I)\left(Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)\right)\\ &\quad = (2\bar{X} - I)(Q\bar{x} + b + \frac{1}{2}\lambda_1(Q)(I - 2\bar{X})e)\\ &\quad = (2\bar{X} - I)(Q\bar{x} + b) - \frac{1}{2}\lambda_1(Q)e \leq 0.\end{aligned}$$

Condition (3.2.4) is gotten and the proof is completed.

In [2], the authors obtained a sufficient global optimality condition for the problem $\min\left\{\frac{1}{2}x^T Qx + b^T x : x \in \{-1, 1\}^n\right\}$. The condition was expressed as [SC]: $\bar{X}Q\bar{X}e + \bar{X}b \leq \lambda_n(Q)e$. Similarly, for the problem (D): $\min\{\frac{1}{2}x^T Qx + b^T x : x \in \{0, 1\}^n\}$, if $\bar{x} \in \{0, 1\}^n$ and

$$[\mathrm{SC}] \qquad 2(2\bar{X} - I)(Q\bar{x} + b) \leq \lambda_n(Q)e$$

holds, then $\bar{x}$ is a global solution of (D). By Lemma 3.3, we notice that there is some relations between [SC] and Theorem 3.2 in a hidden form. If we weaken [SC] to (3.2.4), complemented with (3.2.2), the sufficient global optimality condition given by A.Beck and M.Teboulle becomes a necessary and sufficient global optimality condition for quadratic 0-1 problems.

Furthermore, A.Beck and M.Teboulle also gave a necessary condition for $\min\{\frac{1}{2}x^T Qx + b^T x : x \in \{-1, 1\}^n\}$. That is [NC]: $\bar{X}Q\bar{X}e + \bar{X}b \leq Diag(Q)e$, where $Diag(Q)$ denotes the diagonal matrix with entries q_{ii}. With the help of this result, Theorem 3.2 can be modified as follows:

Theorem 3.4 *Consider problem (D) with Q a real symmetric matrix. Let $\bar{x} \in \{0, 1\}^n$. Then $\bar{x}$ is a global solution of problem (D) if and only if the following two conditions hold:*
(3.4.1) $2(2\bar{X} - I)(Q\bar{x} + b) \leq Diag(Q)e$;
(3.2.2) $-d^T Qd + \lambda_1(Q)\|d\|^2 \leq 2\|d\|_\infty d^T\left[Q\bar{x} + b + \lambda_1(Q)\left(\frac{1}{2}e - \bar{x}\right)\right]$, $d \in T(\bar{x})$.

Proof For a real matrix Q, for $i = 1, \ldots, n$, $\lambda_1(Q) = \max_{\|y\|=1} y^T Qy \geq e_i^T Qe_i = q_{ii}$. If (3.4.1) holds, then we have $2(2\bar{X} - I)(Q\bar{x} + b) \leq Diag(Q)e \leq \lambda_1(Q)e$. Thus when (3.4.1) and (3.2.2) hold, the conditions in Theorem 3.2 are satisfied and $\bar{x}$ is a global solution of (D).

Conversely, If $\bar{x}$ is a global minimum of (D), then $\forall z \in \{0, 1\}^n$, $q(\bar{x}) \leq q(z)$. Let $z = z_1 := (1 - 2\bar{x}_1)e_1 + \bar{x} = (1 - \bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n) \in \{0, 1\}^n$, $e_1 = (1, 0, \ldots, 0)^T$, then from $(1 - 2\bar{x}_1)^2 = 1$,

$$\begin{aligned}q(\bar{x}) &= \frac{1}{2}\bar{x}^T Q\bar{x} + b^T\bar{x}\\ &\leq q(z_1) = \frac{1}{2}((1 - 2\bar{x}_1)e_1 + \bar{x})^T Q((1 - 2\bar{x}_1)e_1 + \bar{x}) + b^T((1 - 2\bar{x}_1)e_1 + \bar{x})\\ &= \frac{1}{2}\left((1 - 2\bar{x}_1)^2 e_1^T Qe_1 + 2(1 - 2\bar{x}_1)e_1^T Q\bar{x} + \bar{x}^T Q\bar{x}\right) + (1 - 2\bar{x}_1)b^T e_1 + b^T\bar{x}\\ &= q(\bar{x}) + \frac{1}{2}e_1^T Qe_1 + (1 - 2\bar{x}_1)e_1^T Q\bar{x} + (1 - 2\bar{x}_1)b^T e_1.\end{aligned}$$

Since $e_1^T Q e_1 = q_{11}$, the inequality reduces to $2(2\bar{x}_1 - 1)(Q\bar{x} + b)^T e_1 \leq q_{11}$. For $i = 1, \ldots, n$, we can get $2(2\bar{x}_i - 1)(Q\bar{x} + b)^T e_i \leq q_{ii}$ similarly. So (3.4.1) holds and the proof is completed.

The condition (3.4.1) is only a necessary condition. This is illustrated by the following example.

Example Consider the problem (D) with $Q = \begin{pmatrix} -2 & 3 & 5 \\ 3 & -8 & -1 \\ 5 & -1 & 9 \end{pmatrix}$, and $b = (-2, 3, -1)^T$. The global solution is $\bar{x} = (1, 0, 0)^T$. $\lambda_1(Q) = 10.9343$, $\lambda_2 = -2.2102$, $\lambda_3 = -9.7241$. For $y = (0, 1, 0)^T$, $2(2Y - I)(Qy + b) = (-2, -10, 4)^T \leq Diag(Q)e \leq \lambda_1(Q)e$. So all the first-order conditions are satisfied. But y isn't a global solution since (3.2.2) doesn't hold if we let $d = (2.5, -3, 0.1)^T$.

Next theorem shows that in the case where Q is a diagonal matrix, (3.4.1) becomes necessary and sufficient for global optimality. For related results, see [15].

Theorem 3.5 *Consider problem (D) with $Q = (q_{ii})$ a diagonal matrix. Let $\bar{x} \in \{0, 1\}^n$. Then $\bar{x}$ is a global solution of problem (D) if and only if (3.4.1) holds, i.e. $2(2\bar{X} - I)(Q\bar{x} + b) \leq Qe$.*

Proof For $\bar{x} \in \{0, 1\}^n, d \in T(\bar{x})$, denote $||d||_\infty = |d_k|, q_{ss} = max_{1 \leq i \leq n}(q_{ii})$, then $\lambda_1(Q) = q_{ss}$. Suppose $2(2\bar{X} - I)(Q\bar{x} + b) \leq Qe$ holds. If $\bar{x}_i = 1$, then $d_i \leq 0$ and $2(Q\bar{x} + b)_i \leq q_{ii}$, $2|d_k|d_i(Q\bar{x} + b)_i \geq |d_k|d_i q_{ii} \geq |d_i|d_i q_{ii} = -d_i^2 q_{ii}$. If $\bar{x}_i = 0$, then $d_i \geq 0$ and $-2(Q\bar{x} + b)_i \leq q_{ii}$, $2|d_k|d_i(Q\bar{x} + b)_i \geq -|d_k|d_i q_{ii} \geq -|d_i|d_i q_{ii} = -d_i^2 q_{ii}$. Thus

$$2||d||_\infty d^T(Q\bar{x} + b) = 2|d_k|d^T(Q\bar{x} + b) = \sum_{1 \leq i \leq n} 2|d_k|d_i(Q\bar{x} + b)_i \geq -d^T Qd. \quad (5)$$

Furthermore, if $\bar{x}_i = 0$, then $d_i \geq 0$, $d_i\left(\frac{1}{2} - \bar{x}_i\right) = \frac{d_i}{2}$. If $\bar{x}_i = 1$, then $d_i \leq 0$, $d_i\left(\frac{1}{2} - \bar{x}_i\right) = \frac{-d_i}{2} = \frac{|d_i|}{2}$. So $2d^T\left(\frac{1}{2}e - \bar{x}\right) = \sum_{1 \leq i \leq n} |d_i|$.

$$2||d||_\infty \lambda_1(Q) d^T\left(\frac{1}{2}e - \bar{x}\right) = |d_k| q_{ss} \sum_{1 \leq i \leq n} |d_i| \geq q_{ss} \sum_{1 \leq i \leq n} d_i^2 = \lambda_1(Q)||d||^2. \quad (6)$$

By (5) and (6), we obtain

$$2||d||_\infty d^T(Q\bar{x} + b) + 2||d||_\infty \lambda_1(Q) d^T\left(\frac{1}{2}e - \bar{x}\right) \geq -d^T Qd + \lambda_1(Q)||d||^2.$$

So when Q is a diagonal matrix, (3.2.2) will hold if (3.4.1) holds. The result can be obtained by Theorem 3.4 and the proof is completed.

Now we establish some global necessary conditions as corollaries of Theorem 3.2.

Corollary 3.6 *Consider problem (D) with $Q = (q_{ij})$ a real symmetric matrix. If $\bar{x} \in \{0, 1\}^n$ is a global minimum of problem (D) and $q = (q_{11}, \ldots, q_{nn})^T$, then*

(3.6.1) $\left(\frac{1}{2}e - \bar{x}\right) \in T(\bar{x})$,

(3.6.2) $2(Q\bar{x} + b) + (I - 2\bar{X})q \in T(\bar{x})$,

(3.6.3) $2(Q\bar{x} + b) + (I - 2\bar{X})\alpha \in T(\bar{x})$, *for all* $\alpha \in R^n$, $\alpha \geq q$,

(3.6.4) $2(Q\bar{x} + b) + \lambda_1(Q)(e - 2\bar{x}) \in T(\bar{x})$.

Proof For $\bar{x} \in \{0,1\}^n$, (3.6.1) holds obviously. If $\bar{x}$ is a global minimum of problem (D), by (3.4.1), $2(2\bar{x}_i - 1)(Q\bar{x}+b)_i - q_{ii} \le 0$ holds for all $1 \le i \le n$. If $i \in E(\bar{x})$, $\bar{x}_i = 1$, then $2(Q\bar{x}+b)_i - q_{ii} \le 0$. If $i \in N_0 \backslash E(\bar{x})$, $\bar{x}_i = 0$, then $2(Q\bar{x}+b)_i + q_{ii} \ge 0$. Thus (3.6.2) holds. Since $\alpha_i \ge q_{ii}$, $-\alpha_i \le -q_{ii}$, (3.6.3) also holds. (3.6.4) will hold if we set $\alpha = \lambda_1(Q)e$ in (3.6.3). That completes the proof.

These vectors are special elements of $T(\bar{x})$. They can be used to check the conditions in Theorem 3.2. The necessary conditions presented in next theorem are some results expressed in a simple way.

Theorem 3.7 *Consider problem (D) with $Q = (q_{ij})$ a real symmetric matrix. Suppose $\alpha \in R^n$, $\alpha \ge q = (q_{11},\ldots,q_{nn})^T$. If $\bar{x} \in \{0,1\}^n$ is a global minimum of problem (D), then we have*
(3.7.1) $2(e-2\bar{x})^T(Q\bar{x}+b) + n\lambda_1(Q) \ge 0,$
(3.7.2) $(e-2\bar{x})^T(Qe+2b) \ge 0,$
(3.7.3) $2\|Q\bar{x}+b\|^2 + (Q\bar{x}+b)^T(I-2\bar{X})(\lambda_1(Q)e+q) + \frac{1}{2}\lambda_1(Q)q^Te \ge 0,$
(3.7.4) $2\|Q\bar{x}+b\|^2 + (Q\bar{x}+b)^T(I-2\bar{X})(\lambda_1(Q)e+\alpha) + \frac{1}{2}\lambda_1(Q)\alpha^Te \ge 0.$

Proof If $\bar{x} \in \{0,1\}^n$ is a global minimum of problem (D), from $\left(\frac{1}{2}e-\bar{x}\right) \in T(\bar{x})$ and (3.2.1),

$$\left(\frac{1}{2}e-\bar{x}\right)^T\left[(Q\bar{x}+b)+\lambda_1(Q)\left(\frac{1}{2}e-\bar{x}\right)\right] = \left(\frac{1}{2}e-\bar{x}\right)^T(Q\bar{x}+b)+\frac{1}{4}n\lambda_1(Q) \ge 0.$$

So the condition (3.7.1) holds. From condition (3.2.2), we have

$$-\left(\frac{1}{2}e-\bar{x}\right)^T Q\left(\frac{1}{2}e-\bar{x}\right) + \lambda_1(Q)\|\tfrac{1}{2}e-\bar{x}\|^2 \le \left[\left(\frac{1}{2}e-\bar{x}\right)^T(Q\bar{x}+b)+\frac{1}{4}n\lambda_1(Q)\right]$$
$$\left(\frac{1}{2}e-\bar{x}\right)^T\left[(Q\bar{x}+b)+Q\left(\frac{1}{2}e-\bar{x}\right)\right] \ge 0$$
$$(e-2\bar{x})^T(Qe+2b) \ge 0.$$

(3.7.2) holds. Furthermore, by (3.6.2) and (3.2.1),

$$\begin{aligned}&\left[2(Q\bar{x}+b)+(I-2\bar{X})q\right]^T\left[(Q\bar{x}+b)+\lambda_1(Q)\left(\frac{1}{2}e-\bar{x}\right)\right]\\ &\quad= 2\|Q\bar{x}+b\|^2+\lambda_1(Q)(Q\bar{x}+b)^T(e-2\bar{x})\\ &\qquad+q^T(I-2\bar{X})(Q\bar{x}+b)+\frac{1}{2}\lambda_1(Q)q^T(I-2\bar{X})(e-2\bar{x})\\ &\quad= 2\|Q\bar{x}+b\|^2+(Q\bar{x}+b)^T(I-2\bar{X})(\lambda_1(Q)e+q)+\frac{1}{2}\lambda_1(Q)q^Te \ge 0.\end{aligned}$$

(3.7.3) holds. (3.7.4) can be proved similarly. Thus we get the necessary conditions expressed in the theorem and the proof is completed.

4 Minimization of half-products

In this section, we consider half-products, a special subclass of quadratic pseudo-Boolean functions, defined by multilinear polynomial expressions of the following form

$$h(x) = \sum_{1\le i<j\le n} a_i b_j x_i x_j - \sum_{i=1}^{n} c_i x_i,$$

where $a = (a_1,\ldots,a_n)^T$, $b = (b_1,\ldots,b_n)^T$ and $c = (c_1,\ldots,c_n)^T$ are non-negative integer vectors. Pseudo-Boolean functions appearing in polynomial representation play a major role in optimization models in a variety of areas. It can be shown that the minimization of half-products is NP-hard.

Denote $A = diag(a)$, $B = \begin{pmatrix} 0 & b_2 & b_3 & \dots & b_n \\ 0 & 0 & b_3 & \dots, & b_n \\ & \dots & & & \\ 0 & 0 & 0 & \dots & b_n \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}$, and $H = AB + B^T A$,

then H is a symmetric matrix and the problem of minimization of half-products can be expressed as follows:

$$
\begin{array}{lll}
(HPP) & \min & h(x) = \frac{1}{2}x^T Hx - c^T x \\
& \text{s.t.} & x \in \{0, 1\}^n.
\end{array}
$$

The results in section three can be applied to problem (HPP). Since the necessary conditions can be checked easily and actually implemented, here we present some necessary conditions especially. By (3.2.1), (3.7.1) (3.7.2) (3.7.3) and $Diag(H) = O$, it is easy to obtain the next theorem.

Theorem 4.1 *If $\bar{x}$ is a global minimizer of (HPP), then*
(4.1.1) $(2\bar{X} - I)(H\bar{x} - c) \leq 0$;
(4.1.2) $2(e - 2\bar{x})^T(H\bar{x} - c) + n\lambda_1(H) \geq 0$;
(4.1.3) $(e - 2\bar{x})^T(He - 2c) \geq 0$;
(4.1.4) $2||H\bar{x} - c||^2 + \lambda_1(H)(H\bar{x} - c)^T(e - 2\bar{x}) \geq 0$.

To give a more detailed overview of all these results, we deliver following theorem.

Theorem 4.2 *If $\bar{x}$ is a global minimizer of (HPP), $\beta = Be$, then*
(4.2.1) $a^T\beta - c^T(e - 2\bar{x}) \geq 0$;
(4.2.2) $(A\bar{x})^T\beta + (B\bar{x})^T a \leq a^T\beta - c^T(e - 2\bar{x})$;
(4.2.3) $a^T(B\bar{x}) + \beta^T(A\bar{x}) - 4(A\bar{x})^T(B\bar{x}) \geq (e - 2\bar{x})^T c - \frac{n}{2}\lambda_1(H)$;
(4.2.4) $4(A\bar{x})^T(B\bar{x}) + 2(e - 2\bar{x})^T c \leq a^T\beta + \frac{n}{2}\lambda_1(H)$.

Proof If $\bar{x} \in \{0, 1\}^n$ is a global minimum of problem (HPP), by (4.1.3),

$$
\begin{aligned}
(e - 2\bar{x})^T He &= e^T(ABe + B^T Ae) - 2\bar{x}^T(ABe + B^T Ae) \\
&= a^T\beta + \beta^T a - 2(A\bar{x})^T\beta - 2(B\bar{x})^T a \\
&= 2a^T\beta - 2(A\bar{x})^T\beta - 2(B\bar{x})^T a \\
&\geq 2c^T(e - 2\bar{x}).
\end{aligned}
$$

Since $a = Ae \geq 0$, $\beta = Be \geq 0$, $\bar{x} \in \{0, 1\}^n$, then

$$0 \leq (A\bar{x})^T\beta + (B\bar{x})^T a \leq a^T\beta - c^T(e - 2\bar{x}).$$

(4.2.1) and (4.2.2) hold. Also, by (4.1.2),

$$
\begin{aligned}
(e - 2\bar{x})^T H\bar{x} &= e^T(AB\bar{x} + B^T A\bar{x}) - 2\bar{x}^T(AB\bar{x} + B^T A\bar{x}) \\
&= a^T B\bar{x} + \beta^T A\bar{x} - 2(A\bar{x})^T(B\bar{x}) - 2(B\bar{x})^T(A\bar{x}) \\
&= a^T B\bar{x} + \beta^T A\bar{x} - 4(A\bar{x})^T(B\bar{x}) \\
&\geq c^T(e - 2\bar{x}) - \frac{n}{2}\lambda_1(H).
\end{aligned}
$$

Thus we obtain (4.2.3). Furthermore, by (4.2.2) and (4.2.3), (4.2.4) can be obtained immediately.

Since for $\bar{x} \in \{0, 1\}^n$, $(H\bar{x})_i = b_i \sum_{1\le j<i}(a_j\bar{x}_j) + a_i \sum_{i<j\le n}(b_j\bar{x}_j)$, some corollaries can be drawn from (4.1.1) and (4.1.2).

Corollary 4.3 *If $\bar{x}$ is a global minimizer of (HPP), then for $1 \le i \le n$,*

$$b_i \sum_{1\le j<i}(a_j\bar{x}_j) + a_i \sum_{i<j\le n}(b_j\bar{x}_j) \le c_i, \quad if \;\; \bar{x}_i = 1;$$
$$b_i \sum_{1\le j<i}(a_j\bar{x}_j) + a_i \sum_{i<j\le n}(b_j\bar{x}_j) \ge c_i, \quad if \;\; \bar{x}_i = 0.$$

Corollary 4.4 *If $\bar{x}$ is a global minimizer of (HPP), then*

$$\sum_{i<j,\bar{x}_i=\bar{x}_j=1}(-2a_ib_j) + \sum_{i<j,\bar{x}_i\ne\bar{x}_j} a_ib_j \ge 2\sum_{\bar{x}_i=0} c_i - 2\sum_{\bar{x}_i=1} c_i - n\lambda_1(H).$$

Proof $(e-2\bar{x})^T c = \sum_{\bar{x}_i=0} c_i - \sum_{\bar{x}_i=1} c_i$. By (4.1.2),

$$\begin{aligned}
(e-2\bar{x})^T H\bar{x} &= \sum_{1\le i\le n}\left(\sum_{j<i}(1-2\bar{x}_i)\bar{x}_j b_i a_j + \sum_{j>i}(1-2\bar{x}_i)\bar{x}_j a_i b_j\right)\\
&= \sum_{1\le i\le n}\left(\sum_{j<i,\bar{x}_i=\bar{x}_j=1} -b_ia_j + \sum_{j<i,\bar{x}_i=0,\bar{x}_j=1} b_ia_j + \sum_{j>i,\bar{x}_i=\bar{x}_j=1} -a_ib_j\right.\\
&\qquad \left. + \sum_{j>i,\bar{x}_i=0,\bar{x}_j=1} a_ib_j\right)\\
&= \sum_{1\le i\le n}\left(\sum_{i<j,\bar{x}_i=\bar{x}_j=1} -a_ib_j + \sum_{i<j,\bar{x}_j=0,\bar{x}_i=1} a_ib_j + \sum_{i<j,\bar{x}_i=\bar{x}_j=1} -a_ib_j\right.\\
&\qquad \left. + \sum_{i<j,\bar{x}_i=0,\bar{x}_j=1} a_ib_j\right)\\
&= \sum_{i<j,\bar{x}_i=\bar{x}_j=1}(-2a_ib_j) + \sum_{i<j,\bar{x}_i\ne\bar{x}_j} a_ib_j \ge 2\sum_{\bar{x}_i=0} c_i - 2\sum_{\bar{x}_i=1} c_i - n\lambda_1(H).
\end{aligned}$$

The proof is completed.

5 Further results of quadratic 0-1 programming

In many quadratic integer programming problems, if the dimensions of the matrixes are quite big, both the speed and the accuracy of calculation will be influenced by the size of the problems. In this section, we try to reduce the dimensions expressed in our global optimality conditions. We will give some necessary global optimality conditions of quadratic 0-1 programming problems which may be used easier than those in last section.

First, for $\bar{x} \in \{0, 1\}^n$, $E(\bar{x}) = \{i : \bar{x}_i = 1, i = 1, \ldots, n\}$, let $m = |E(\bar{x})|$. We denote a sub-matrix $\bar{Q}$ of Q and a sub-vector $\bar{b}$ of b as follows: if and only if $i, j \in E(\bar{x})$, q_{ij} and b_i can be remained in $\bar{Q}$ and $\bar{b}$ in original order. Then we consider the following problem:

$$(\bar{D}) \quad \begin{array}{ll} \min & \bar{q}(x) = \frac{1}{2}x^T\bar{Q}x + \bar{b}^T x \\ \text{s.t.} & x \in \{0, 1\}^m. \end{array}$$

We obtain a theorem as follows:

Theorem 5.1 *If $\bar{x}$ is a global solution of problem (D), then $e^{(m)} = (1, 1, \ldots, 1)^T \in R^m$ is a global solution of the problem $(\bar{D})$.*

Proof Suppose the $k_1, k_2, \ldots, k_m$ elements of $\bar{x}$ are 1, and the other elements of $\bar{x}$ are 0. For all $x \in \{0, 1\}^m$, let $y \in \{0, 1\}^n$, of which $y_{k_i} = x_i$, $i = 1, \ldots, m$, and the other elements of y are 0. Then we have $\bar{q}(x) = q(y) \geq q(\bar{x}) = \bar{q}(e^{(m)})$. So $e^{(m)}$ is the global minimum of problem $(\bar{D})$.

In Theorem 5.1, it is clear that $m \leq n$. If $m = n$, then e is the global solution of problem (D). If $m < n$, the dimensions in global optimality conditions of problem (D) can be reduced from n to m by checking whether $e^{(m)}$ is the global solution of problem $(\bar{D})$. For the case e being a global solution, although we can use the results expressed in last section directly, it is interesting to get some further results which may be used easier.

Theorem 5.2 *Consider the problem (D) with Q a real symmetric matrix. Then e is the global minimum of (D) if and only if 0 is the global solution of the following problem*

$$(D_0) \quad \min \quad x^T Q_0 x \qquad s.t. \quad x \in \{0, 1\}^n,$$

where $Q_0 = (q_{ij}^{(0)})$ is an $n \times n$ matrix. For $i, j = 1, \ldots, n$, if $i \neq j$, $q_{ij}^{(0)} = q_{ij}$; if $i = j$, $q_{ii}^{(0)} = q_{ii} - 2b_i - 2\sum_{j=1}^n q_{ij}$.

Proof Let $u = -\frac{1}{2}(Qe + b)$. The elements of the vector u is $u_i = -\frac{1}{2}(\sum_{j=1}^n q_{ij} + b_i)$, $i = 1, \ldots, n$. Let $U = diag(u)$ be the diagonal $n \times n$ matrix with ith diagonal element u_i. Then the diagonal elements of $Q + 4U$ are $q_{ii} - 2(\sum_{j=1}^n q_{ij} + b_i) = q_{ii}^{(0)}$, $i = 1, \ldots, n$. Thus $Q + 4U = Q_0$.

For $y \in \{0, 1\}^n$, $\forall i = 1, \ldots, n$, $y_i^2 = y_i$, and $e - y \in \{0, 1\}^n$.

$$\begin{aligned} y^T Q_0 y &= y^T (Q + 4U) y = y^T Q y + 4\sum_{i=1}^n u_i y_i^2 \\ &= y^T Q y + 4\sum_{i=1}^n u_i y_i = y^T Q y + 4y^T u \\ &= y^T Q y + 4y^T (-\tfrac{1}{2})(Qe + b) = y^T Q y - 2y^T Q e - 2y^T b. \end{aligned}$$

So we have

$$\begin{aligned} q(e - y) - q(e) &= \frac{1}{2}(e - y)^T Q (e - y) + (e - y)^T b - \frac{1}{2} e^T Q e - e^T b \\ &= -y^T Q e + \frac{1}{2} y^T Q y - y^T b \\ &= \frac{1}{2} y^T Q_0 y. \end{aligned}$$

If e is the global minimum of (D), then for all $y \in \{0, 1\}^n$, $q(e - y) - q(e) \geq 0$, which means $y^T Q_0 y \geq 0$. Conversely, if 0 is the global minimum of problem (D_0), then for all $y \in \{0, 1\}^n$, $y^T Q_0 y \geq 0$ implies $q(e - y) \geq q(e)$. Thus we know e is the global minimum of problem (D) because y is arbitrary in $\{0, 1\}^n$. That completes the proof.

Corollary 5.3 *Under the hypotheses posed in Theorem 5.2, if Q_0 is positive semidefinite on R^n ($Q_0 \succeq 0$), or all the elements of Q_0, $q_{ij}^{(0)} \geq 0$ ($Q_0 \geq 0$), then e is the global minimum of problem (D).*

The proof is simple. We also can say "0 is the global solution of problem (D_0)" means "Q_0 is positive semidefinite on $\{0, 1\}^n$". But Q_0 may not be positive semidefinite on R^n even if e is a strict global minimum of problem (D).

Example Let $Q = \begin{pmatrix} -5 & 2 \\ 2 & -6 \end{pmatrix}$, e is the only one global minimum of $q(x) = x^T Qx$ on $\{0, 1\}^n$. But the matrix $Q_0 = \begin{pmatrix} 1 & 2 \\ 2 & 2 \end{pmatrix}$ is indefinite because its eigenvalues are $\lambda_1 = \frac{3+\sqrt{17}}{2}$ and $\lambda_2 = \frac{3-\sqrt{17}}{2}$.

We use the symbols $\bar{Q}$, $\bar{b}$ and $e^{(m)}$ the same as in Theorem 5.1. Similarly, if $\bar{Q} = (\bar{q}_{ij})_{m\times m}$, then $\bar{Q}_0$ denotes an $m \times m$ matrix $(\bar{q}_{ij}^{(0)})$. For $i, j = 1, \ldots, m$, if $i \neq j$, $\bar{q}_{ij}^{(0)} = \bar{q}_{ij}$; if $i = j$, $\bar{q}_{ii}^{(0)} = \bar{q}_{ii} - 2\bar{b}_i - \sum_{j=1}^{n}(\bar{q}_{ij} + \bar{q}_{ji})$. Then we have some necessary conditions.

Theorem 5.4 *Consider the problem (D) with Q a real symmetric matrix. If $\bar{x}$ is a global solution of (D) then the following inequalities hold:*
(5.4.1) $\lambda_1(\bar{Q}_0) > 0$ *or* $\bar{Q} = -2diag(\bar{b})$,
(5.4.2) $e^{(m)T}\bar{Q}_0 e^{(m)} \geq 0$,
(5.4.3) $\bar{Q}e^{(m)} + \bar{b} \leq \frac{1}{2}Diag(\bar{Q})e^{(m)}$,
(5.4.4) $m\lambda_1(\bar{Q}) - 2e^{(m)T}(\bar{Q}e^{(m)} + \bar{b}) \geq 0$.

Proof If $\bar{x}$ is a global minimum of (D), by Theorem 5.1, $e^{(m)}$ is the global solution of $\min\{\frac{1}{2}x^T\bar{Q}x + \bar{b} : x \in R^m\}$. According to (3.4.1), (5.4.3) holds. Condition (5.4.4) can be gotten from (3.7.1) directly.

Moreover, based on theorems in this section, if $\bar{x}$ is a global minimum of (D), then 0 is the global minimum of $min\left\{x^T\bar{Q}_0x : x \in \{0, 1\}^m\right\}$. Thus from the condition (3.7.1), $m\lambda_1(\bar{Q}_0) \geq 0$. If $\lambda_1(\bar{Q}_0) = 0$, then $\bar{Q}_0$ is negative semidefinite. So $x^T\bar{Q}_0x \leq 0$ for all $x \in R^m$. But 0 is the global minimum of $min\left\{x^T\bar{Q}_0x : x \in \{0, 1\}^m\right\}$, $x^T\bar{Q}_0x \geq 0$ for all $x \in \{0, 1\}^m$, thus we must have $x^T\bar{Q}_0x = 0$ for all $x \in \{0, 1\}^m$. $\forall i, j = 1, \ldots, m$, let $x = e_i$ and $x = e_i + e_j$, we can get $\bar{q}_{ii}^{(0)} = 0$ and $\bar{q}_{ij}^{(0)} = 0$. So $\bar{Q}_0 = 0$. If $i \neq j$, $\bar{q}_{ij}^{(0)} = \bar{q}_{ij} = 0$. If $i = j$, $\bar{q}_{ii}^{(0)} = \bar{q}_{ii} - 2\bar{b}_i - \sum_{j=1}^{n}(\bar{q}_{ij} + \bar{q}_{ji}) = 0$. So $\bar{q}_{ii} = -2\bar{b}_{ii}$ and $\bar{Q} = -2diag(\bar{b})$. Thus (5.4.1) will hold when $\bar{x}$ is a global minimum of (D). Again from (3.7.2), we can get (5.4.2) immediately since 0 is the global minimum of $min\{x^T\bar{Q}_0x : x \in \{0, 1\}^m\}$. That completes the proof.

All the conditions in Theorem 5.4 are expressed in a simple way without the vector d. The condition (5.4.2) and (5.4.3) need not calculate the eigenvalues. That will be convenient to use. Let's review the example in Sect. 3.

Example Consider the problem (D) with $Q = \begin{pmatrix} -2 & 3 & 5 \\ 3 & -8 & -1 \\ 5 & -1 & 9 \end{pmatrix}$, and $b = (-2, 3, -1)^T$. The global solution is $\bar{x} = (1, 0, 0)^T$. For $x^{(1)} = (1, 1, 0)$, $\bar{Q} = \begin{pmatrix} -2 & 3 \\ 3 & -8 \end{pmatrix}$, $\bar{b} = (-2, 3)^T$. $\bar{Q}_0 = \begin{pmatrix} 0 & 3 \\ 3 & -14 \end{pmatrix}$, $e^T\bar{Q}_0e = -8 < 0$. Thus $x^{(1)}$ is not a global solution. Also we know (5.4.2) does not hold for $x^{(2)} = (0, 1, 1)^T$ and neither (5.4.3) does for $x^{(3)} = (1, 0, 1)^T$ and $x^{(4)} = (1, 1, 1)^T$. For $x^{(5)} = (0, 0, 1)^T$, $\bar{Q} = 9$ and $\bar{b} = -1$. So 1 is not the global solution of $\bar{q}(x) = \frac{9}{2}x^2 - x$. So most feasible points in this problem, except $y = (0, 1, 0)^T$, would be taken away from the set of the global minima in a simple way.

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