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Improved SDP Bounds for Binary Quadratic Programming

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ABSTRACT

As a classical combinatorial problem, the binary quadratic programming problem has many applications in finance, statistics, production management, etc. The state-of-the-art solution for solving this problem accurately is based on branch-and-bound frameworks, with the low bound support of a semi-definite programming (SDP) relaxation. This paper generalizes the spectral bounds in the literature and proposes a sequence of improved SDP bounds for the binary quadratic programming problem. Our method relies on the closest binary points to an affine space, which can be found by reverse enumeration technique.

KEYWORDS: Binary quadratic programming; Semi-definite programming; Reverse enumeration; Branch-and-bound

Introduction

We consider the classical NP-hard binary quadratic programming problem:

$$(BQP)\begin{array}{ll}\min & f(x) \triangleq \frac{1}{2}x^TQx + c^Tx \\ s.t. & x \in \{-1,1\}^n\end{array}$$

for given $Q = Q^T \in \mathbb{R}^{n\times n}$ and $c \in \mathbb{R}^n$. And we denote the binary quadratic programming problem without the linear term by:

$$(BQP0)\begin{array}{ll}\min & x^TQx \\ s.t. & x \in \{-1,1\}^n\end{array}$$

for given $Q = Q^T \in \mathbb{R}^{n\times n}$. It is easy to see that $(BQP0)$ contains the Max-Cut problem as its special case.

The problem (BQP) is a classical combinatorial optimization problem with many applications. Exact solution methods for (BQP) are of a branch-and-bound framework based on various lower bounding techniques and branching rules. One of the most powerful bounds is obtained from semidefinite programming relaxation of (BQP). Algorithms based on SDP relaxations have been proposed for solving (BQP) (see, e.g., [4], [8], [10]).

It is known that the performance of a branch-and-bound algorithm depends a lot on the quality of the bound of its root node. Thus many authors have worked on improved bounds from the SDP bound. Malik et al. [9] investigated the duality gap between maximum cut problem and its semi definite relaxation and showed that the gap can be reduced by computing a reduced-rank binary quadratic problem, which results in a bound tighter than the well known Goemans and Williamson's SDP bound [7]. Ben-Ameur and Neto[2], [3] generalized Malik et al.'s results to binary quadratic problems without the linear term $(BQP0)$ by introducing spectral bounds. Sun et al. [12] generalized Malik et al.'s results to (BQP) with the linear term and the methodology has been extended to binary quadratic problems with linear constraints by Zheng et al. [15]. Xia et al. [13] improved Malik et al. 's results with a weighted distance measure instead of the Euclidean distance measure.

The above improved bounds all rely on the information of the distance of $\{-1,1\}^n$ to an affine space, which can be obtained via the reverse enumeration (see [1], [11]) or other enumeration technique (see [6]).

In this paper, we would review the classical SDP bound for (BQP) in Section 1. In Section 2, we review how we apply the reverse enumeration technique and further develop an algorithm to obtained the 2nd closest point and 3rd closest point and so on to an affine space. In Section 3, we review the bounds for binary quadratic problems without the linear term $(BQP0)$ in [3] and [9]. In Section 4, we will generalize the spectral bounds in [3] to (BQP) and prove the bound in [12] as a special case. In Section 5 we generate a sequence of improved bounds starting from the bound in [12], based on the algorithm developed in Section 3. We conclude in Section 6.

The notations used in this paper are as follows. $Diag(\cdot)$ converts a vector to a diagonal matrix with the i-th component of the vector at the ii-th position of the matrix. $v(\cdot)$ denotes the optimal value of a problem. The dot product between two matrices $Q \bullet X$ denotes the trace of QX. $sign(\cdot)$ change a vector to a sign vector indicating the signs of each component. $dist(\cdot,\cdot)$ denotes the Euclidean distance between two sets. $lin(v^1, \dots, v^n)$ denotes the linear space spanned by $v^1, \dots, v^n$. We index different vectors by superscripts such as $x^1, \dots, x^i$ and refer to the value in specific coordinate of a vector by subscripts such as

$x_1, \ldots, x_n$. Let e denotes the all one vector and $\mathbf{0}$ denotes the all zero vector.

1. The Classical SDP bound

We give a brief review of the classical SDP relaxation for (BQP) in this session. For (BQP), because $x \in \{-1,1\}^n$, $x_i^2 = 1$, the problem (BQP) is equivalent to the following problem

$$(BQP_\lambda) \begin{array}{ll} \min & \frac{1}{2}x^T(Q + 2Diag(\lambda))x - e^T\lambda + c^Tx \\ s.t. & x \in \{-1,1\}^n \end{array}$$

for any $\lambda \in \mathbb{R}^n$. Thus, by making $(Q + Diag(\lambda)) \succcurlyeq 0$, the objective function can always be made convex. Removing the constraints of (BQP_λ), the following value

$$d(\lambda) \triangleq \inf_{x \in \mathbb{R}^n} \{L(x,\lambda) \triangleq \frac{1}{2}x^T(Q + 2Diag(\lambda))x - e^T\lambda + c^Tx\}$$

is a lower bound of the optimal value of (BQP) and (BQP_λ). Thus the best lower bound can be obtained by solving

$$(D) \begin{array}{ll} \max & d(\lambda) \\ s.t. & \lambda \in \mathbb{R}^n \end{array}$$

Actually, $L(x,\lambda)$ is the Lagrangian function and the problem (D) is the Lagrangian dual problem of (BQP). It can be shown that (D) is equivalent to the following problem:

$$\begin{array}{ll} \max & \tau \\ s.t. & \frac{1}{2}x^T(Q + 2Diag(\lambda))x - e^T\lambda + c^Tx \geq \tau \\ & \lambda \in \mathbb{R}^n, \tau \in \mathbb{R} \end{array}$$

which can be formulated as the following SDP problem:

$$(Ds) \begin{array}{ll} \max & \tau \\ s.t. & \begin{pmatrix} Q + 2Diag(\lambda) & c \\ c^T & -2\tau - 2e^T\lambda \end{pmatrix} \succcurlyeq 0 \\ & \lambda \in \mathbb{R}^n, \tau \in \mathbb{R} \end{array}$$

Besides (Ds), we can derive an SDP relaxation for (BQP) directly from the primal point of view. (BQP) is equivalent to the following rank-constrained problem:

$$\begin{array}{ll} \min & \frac{1}{2}Q \bullet X + c^Tx \\ s.t. & X_{ii} = 1, i = 1, \ldots, n \\ & \begin{pmatrix} X & x \\ x & 1 \end{pmatrix} \succcurlyeq 0 \\ & rank\begin{pmatrix} X & x \\ x & 1 \end{pmatrix} = 1 \end{array}$$

Dropping the rank constrained, we obtain the primal SDP relaxation for (BQP):

$$(Ps) \begin{array}{ll} \min & \frac{1}{2}Q \bullet X + c^Tx \\ s.t. & X_{ii} = 1, i = 1, \ldots, n \\ & \begin{pmatrix} X & x \\ x & 1 \end{pmatrix} \succcurlyeq 0 \end{array}$$

It can be shown that (Ps) and (Ds) are conic dual to each other. And because they are strictly feasible, by duality theorem, $v(Ps) = v(Ds)$.

2. Closest Binary Points to an Affine Space

In this section we will review how we apply the reverse enumeration technique and further develop an algorithm to obtain from the binary set the 2nd closest point and 3rd closest point and so on to an affine space.

Firstly, let us look at the following graph.

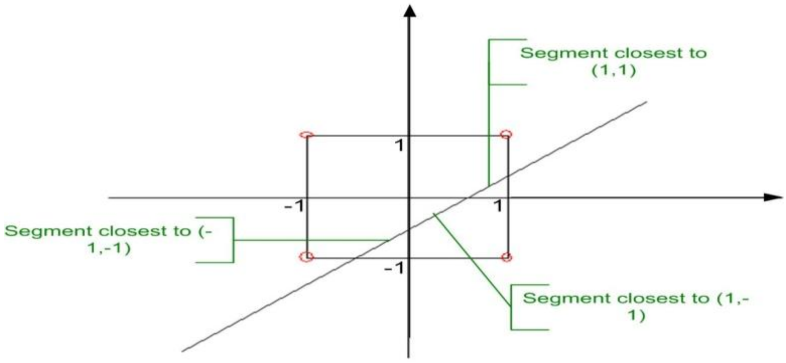

Fig.1 Dividing a line to segments by the distance to points in $\{-1,1\}^2$

In Figure 1, we would like to find the closest point in $\{-1,1\}^2$ to a line in the plane. We can divide the line into segments according to there distance to the points in $\{-1,1\}^2$. Then by enumerating these segments, we can find the closest point in $\{-1,1\}^2$ to the line. Armed with this example, let us look at a general case. Given an affine space H, we want to know $dist(\{-1,1\}^n, H\}$. This can be done by identifying the closest point in $\{-1,1\}^n$ to H. We can express H by

$$H = \{x \in \mathbb{R}^n : x = x^0 + \sum_{i=1}^{r} z_i u^i ; z \in \mathbb{R}^r\} = lin(u^1, \dots, u^r) + x^0$$

where $x^0 = (x_1^0, \dots, x_n^0) \in \mathbb{R}^n$, $u^i = (u_1^i, \dots, u_n^i) \in \mathbb{R}^n, i = 1, \dots, r$. To any point $x' = (x_1', \dots, x_n')$ in H, the closest point in $\{-1,1\}^n$ is $sign(x')$. Thus if we look at the cells cut out by the following n hyperplanes in $\mathbb{R}^r$:

$$x^0 + \sum_{i=1}^{r} z_i u^i = \mathbf{0} \quad (1)$$

then any point $x' = x^0 + \sum_{i=1}^{r} z_i u^i$ generated from the z in the same cell in $\mathbb{R}^r$ will have a common closest point in $\{-1,1\}^n$. It has been known that the number of cells cut out by Equation (1) is bounded by $O(n^r)$ (see [5] and [14]). Let us index the cells by $C^1, \dots C^N$, then each cell corresponds to a closest point in $\{-1,1\}^n$, denoted by $c^1, \dots, c^N$. By reverse enumeration technique in [1], [6] and [11], those cells and the corresponding closest points can be enumerated in time $O(n^r)$. Obviously the closest point in $\{-1,1\}^n$ to H must be among $\{c^1, \dots, c^N\}$, which can be found during the enumeration.

We index the points in the set $\{-1,1\}^n$ by $y^1, y^2, \dots, y^{2^n}$ such that $dist(y^1, H) \le dist(y^2, H) \le \dots \le dist(y^{2^n}, H)$. By above discussion, we can identify y^1, but can we identify y^2, y^3 and so on? We are going to propose an algorithm to find $y^2, y^3, \dots$. progressively. Here let us define the k-th neighborhood of a point $y = (y_1, \dots, y_n) \in \{-1,1\}^n$ by

$$N(y,k) \triangleq \{x \in \{-1,1\}^n : \|y - x\|_2^2 = 4k\}$$

which contains points in $\{-1,1\}^n$ that differ from y by exactly k coordinates. And for an index set $I \subset \{1, \dots, n\}$, we define the tail combination set of y by

$$Tail(y, I) \triangleq \{x \in \{-1,1\}^n : x_i = y_i, \forall i \in \{1, \dots, n\} \setminus I\}$$

which contains points in $\{-1,1\}^n$ that are of the same value with y in the coordinates in $\{1, \dots, n\} \setminus I$.

Before we introduce the algorithm, we need the following lemma.

Lemma1. *Let $w^j \in N(c^i, 1)$ denotes the point that defers from c^i in the j-th coordinate. Let $I \subset \{1, \dots, n\}$and $T \subset Tail(c^i, I)$. Suppose the set $O = \{c^i\} \cup \{w^j, j \in I\} \cup T$ has been removed from $\{-1,1\}^n$. Then for any point $a \in C^i$, the closest point in $\{-1,1\}^n \setminus O$ to it must lies in $G^i \triangleq ((N(c^i, 1) \cup Tail(c^i, I)) \setminus O$.*

Proof. Any point $x \in \{-1,1\}^n \setminus G^i$ must differ from c^i in at least one coordinate in $\{1, \dots, n) \setminus I$. Thus $dist(a, N(c^i, 1) \setminus \{w^j, j \in I\}) \le dist(a, x)$.

The algorithm to obtain from the binary set the 2nd closest point and 3rd closest point and so on to an affine space is given as follows.

Algorithm 1(**Arrangement by Distance**)

(1) *Let $j = 1$. Conduct reverse enumeration to find $C^1, \dots C^N$and $c^1, \dots, c^N$. Let $G^i = \{c^i\}P = \{c^1, \dots, c^N\}$, $O = \{\}(empty)$. Then*

$$y_1 = \underset{c \in P}{argmin} dist(c, H).$$

(2) *Remove $y_j$from P. If P is empty, stop.*
Add $y_j$into O.
For each cell C^i, update G^i as stated in Lemma 1.
Update $P = \cup_{i=1}^{N} G^i$.

$$y_j = \underset{c \in P}{argmin} dist(c, H).$$

(3) *Go to (2).*

The set O contains the set of identified points. For every iteration j, we update the set P such that for any point in the affine space H, its closest point in $\{-1,1\}^n \setminus O$ is included in P. Thus the algorithm is valid.

3. Improved Bounds for Binary Quadratic Problems without the Linear Term

In this section we consider $(BQP0)$, the binary quadratic problems without the linear term. We will review the improved bounds for $(BQP0)$ in [3] and [9].Let the spectral decomposition of Q be:

$$Q = [u^1, \dots, u^n] Diag(\xi_1, \dots, \xi_n) [u^1, \dots, u^n]^T$$

where $\xi_1 \le \xi_2 \le \dots \le \xi_n$ are the eigenvalues of Q and $u^1, \dots, u^n$ are the corresponding orthonormal eigenvectors. For any point $a \in \{-1,1\}^n$, we denote the distance between it and the linear space spanned by $u^1, u^2, \dots, u^j$ by $dist(a, lin(u^1, \dots, u^j))$. We can decompose $a = \alpha_1 u_1 + \dots + \alpha_n u_n$. Then we have:

$$a^T a = n = \alpha_1^2 + \alpha_2^2 + \ldots + \alpha_n^2$$

and

$$\begin{aligned} dist(a, lin(u_1, \ldots, u_j)) &= \left\| x - [u^1, \ldots, u^j][u^1, \ldots, u^j]^T x \right\|_2 \\ &= \left\| [u^1, \ldots, u^n]^T (x - [u^1, \ldots, u^j][u^1, \ldots, u^j]^T x) \right\|_2 \\ &= \left\| (\alpha_1, \ldots, \alpha_n)^T - (\alpha_1, \ldots, \alpha_j, 0, \ldots, 0)^T \right\|_2 \\ &= \sqrt{\alpha_{j+1}^2 + \ldots + \alpha_n^2}. \end{aligned}$$

We define $d_j \triangleq dist(\{-1,1\}^n, lin(u^1, \ldots, u^j)) = \min_{a \in \{-1,1\}^n} dist(a, lin(u^1, \ldots, u^j))$. Thus for any $a \in \{-1,1\}^n$, we have $dist^2(a, lin(u^1, \ldots, u^j)) = \alpha_{j+1}^2 + \ldots + \alpha_n^2 \geq d_j^2$.

Theorem 1 ([3]) $v(BQP0) \geq \xi_1 n + \sum_{j=1}^{n-1} d_j^2 (\xi_{j+1} - \xi_j)$.

Proof. Let a be the optimal solution to $(BQP0)$. Decompose $a = \alpha_1 u_1 + \ldots + \alpha_n u_n$.Then

$$\begin{aligned} v(BQP0) &= a^T Q a (2) \\ &= a^T [u^1, \ldots, u^n] Diag(\xi_1, \ldots, \xi_n) [u^1, \ldots, u^n]^T a \\ &= \xi_1 \alpha_1^2 + \xi_2 \alpha_2^2 + \ldots + \xi_n \alpha_n^2 \\ &= \xi_1 (\alpha_1^2 + \alpha_2^2 + \ldots + \alpha_n^2) \\ &+ (\xi_2 - \xi_1)(\alpha_2^2 + \ldots + \alpha_n^2) \\ &+ (\xi_3 - \xi_2)(\alpha_3^2 + \ldots + \alpha_n^2) \\ &+ \ldots \\ &+ (\xi_n - \xi_{n-1}) \alpha_n^2 \\ &\geq \xi_1 n + \sum_{j=1}^{n-1} d_j^2 (\xi_{j+1} - \xi_j). \end{aligned}$$

As a special case to (Ds), there is a dual SDP relaxation for $(BQP0)$ and will return the optimal dual solution λ^* such that $Q^* \triangleq Q + Diag(\lambda^*) \succcurlyeq 0$ and the optimal dual objective value will be $-e^T \lambda^*$. Suppose Q^* has spectral decomposition:

$$Q^* = [u'^1, \ldots, u'^n] Diag(0, \ldots, 0, \xi'_{r+1}, \ldots, \xi'_n) [u'^1, \ldots, u'^n]^T$$

where $0 = \xi'_1 = \ldots = \xi'_r < \xi'_{r+1} \ldots \leq \xi'_n$ are the eigenvalues of Q and $u^1, \ldots, u^n$ are the corresponding orthonormal eigenvectors. And define $d'_j \triangleq dist(\{-1,1\}^n, lin(u'^1, \ldots, u'^j))$. Then similar to Equation (2), let a be the optimal solution to $(BQP0)$ and we have:

$$\begin{aligned} v(BQP0) &= a^T Q^* a - e^T \lambda^* (3) \\ &\geq -e^T \lambda^* + \sum_{j=r}^{n-1} d_j'^2 (\xi'_{j+1} - \xi'_j). \end{aligned}$$

By truncating part of the sum in the above inequality, we have the bound stated in [9]:

$$v(BQP0) \geq -e^T \lambda^* + d_r'^2 \xi'_{r+1}. (4)$$

Both d_r and d'_r are the distance of $\{-1,1\}^n$ to an affine space, thus for fixed r, they can be computed via reverse enumeration technique as discussed in Section 2.

4. Improved Bounds for Binary Quadratic Problems with the Linear Term

Sun et al. [12] generalized the bound in Equation (4)for (BQP). In this section we will generalize the spectral bounds in [3] for $(BQP0)$ to (BQP) and prove the bound in [12] as a special case. Solve (Ds) and we will get an unique optimal dual SDP solution λ^* for (BQP). The existence and uniqueness of the λ^* is addressed in [9]. Let $Q^* \triangleq Q + 2Diag(\lambda^*)$, then $v(Ds)$ can be expressed as:

$$v(Ds) = \min\{f^*(x) \triangleq \frac{1}{2} x^T Q^* x + c^T x - e^T \lambda^*\}.$$

and the derivative of $f^*(x)$ is $Q^* x + c$. Thus c must lie in the range space of Q^*, otherwise there will be no stationary point in $f^*(x)$. Decompose Q^* to be:

$$Q^* = [u^1, \ldots, u^n] Diag(0, \ldots, 0, \xi_{r+1}, \ldots, \xi_n) [u^1, \ldots, u^n]^T$$

where $0 = \xi_1 = \ldots = \xi_r < \xi_{r+1} \leq \ldots \leq \xi_n$ are the eigenvalues of Q^* and $u^1, \ldots, u^n$ are the corresponding orthonormal eigenvectors. And define

$$R = [u^{r+1}, \ldots, u^n] Diag(\frac{1}{\xi_{r+1}}, \ldots, \frac{1}{\xi_n}) [u^{r+1}, \ldots, u^n]^T$$

Lemma 2. $f^*(x) = \frac{1}{2}(Q^* x + c)^T R (Q^* x + c) - e^T \lambda^* - \frac{1}{2} c^T R c$.

Proof.

$$
\begin{aligned}
f^*(x) &= \frac{1}{2}(Q^*x+c)^T R(Q^*x+c) - e^T\lambda^* - \frac{1}{2}c^T Rc \\
&= \frac{1}{2}x^T Q^* R Q^* x + c^T R Q^* x - e^T\lambda^* \\
&= \frac{1}{2}x^T [u^{r+1},\dots,u^n] Diag(\xi_{r+1},\dots,\xi_n)[u^{r+1},\dots,u^n]^T \\
&\times [u^{r+1},\dots,u^n] Diag(\frac{1}{\xi_{r+1}},\dots,\frac{1}{\xi_n})[u^{r+1},\dots,u^n]^T \\
&\times [u^{r+1},\dots,u^n] Diag(\xi_{r+1},\dots,\xi_n)[u^{r+1},\dots,u^n]^T x \\
&+ c^T [u^{r+1},\dots,u^n] Diag(\frac{1}{\xi_{r+1}},\dots,\frac{1}{\xi_n})[u^{r+1},\dots,u^n]^T \\
&\times [u^{r+1},\dots,u^n] Diag(\xi_{r+1},\dots,\xi_n)[u^{r+1},\dots,u^n]^T x \\
&- e^T\lambda^* \\
&= \frac{1}{2}x^T Q^* x + c^T [u^{r+1},\dots,u^n][u^{r+1},\dots,u^n]^T x - e^T\lambda^* \\
&= \frac{1}{2}x^T Q^* x + c^T x - e^T\lambda^*
\end{aligned}
$$

The last equality is due to the fact that $c^T[u^{r+1},\dots,u^n][u^{r+1},\dots,u^n]^T = c^T$, which results from that fact that c lies in the range space of Q^*. Thus $c = [u^{r+1},\dots,u^n]y$ for some y and this $y = [u^{r+1},\dots,u^n]^T c$.

Because R is positive semidefinite, we can get that

$$v(Ds) = \min\{\frac{1}{2}(Q^*x+c)^T R(Q^*x+c) - e^T\lambda^* - \frac{1}{2}c^T Rc\} = -e^T\lambda^* - \frac{1}{2}c^T Rc.$$

and the minimum is attained at the set $S^* \triangleq \{x \in \mathbb{R}^n : Q^*x = -c\}$. Choose any point $x^0 \in S^*$ and fix it, we can write $S^* = lin(u^1,\dots,u^r) + x^0$. For any point $a \in \{-1,1\}^n$, we denote the distance between a and the affine space

$$\{x \in \mathbb{R}^n : x = x^0 + \sum_{i=1}^{j} z_i u^i; z \in \mathbb{R}^j\} = lin(u^1,\dots,u^j) + x^0$$

by $dist(a, lin(u^1,\dots,u^j) + x^0)$. We can decompose $a - x^0 = \alpha_1 u^1 + \dots + \alpha_n u^n$. Then we have:

$$
\begin{aligned}
dist(a, lin(u_1,\dots,u_j) + x^0) &= \left\|[u^{j+1},\dots,u^n][u^{j+1},\dots,u^n]^T(a-x^0)\right\|_2 \\
&= \left\|(\alpha_{j+1}u^{j+1} + \dots + \alpha_n u^n)\right\|_2 \\
&= \left\|[u^1,\dots,u^n]^T(\alpha_{j+1}u^{j+1} + \dots + \alpha_n u^n)\right\|_2 \\
&= \left\|(0,\dots,0,\alpha_{j+1},\dots,\alpha_n)\right\|_2 \\
&= \sqrt{\alpha_{j+1}^2 + \dots + \alpha_n^2}.
\end{aligned}
$$

We define $d_j \triangleq dist(\{-1,1\}^n, lin(u^1,\dots,u^j) + x^0) = \min_{a\in\{-1,1\}^n} dist(a, lin(u^1,\dots,u^j) + x^0)$. Thus for any $a \in \{-1,1\}^n$, we have $dist^2(a, lin(u^1,\dots,u^j) + x^0) = \alpha_{j+1}^2 + \dots + \alpha_n^2 \geq d_j^2$.

Theorem 2 $v(BQP) \geq v(Ds) + \frac{1}{2}\sum_{j=r}^{n-1}(\xi_{j+1} - \xi_j)d_j^2$.

Proof. Let $a \in \{-1,1\}^n$ be the optimal solution to (BQP). Decompose $a - x^0 = \alpha_1 u^1 + \dots + \alpha_n u^n$. We have

$$
\begin{aligned}
f^*(a) &= \frac{1}{2}(Q^*(a - x^0 + x^0) + c)^T R(Q^*(a - x^0 + x^0) + c) - e^T\lambda^* - \frac{1}{2}c^T Rc \quad \mathbf{(5)} \\
&= \frac{1}{2}(a-x^0)^T Q^*(a-x^0) - e^T\lambda^* - \frac{1}{2}c^T Rc \text{ (Because } Q^*x^0 + c = 0) \\
&= v(Ds) + \frac{1}{2}(a-x^0)^T Q^*(a-x^0) \\
&= v(Ds) + \frac{1}{2}(\xi_{r+1}\alpha_{r+1}^2 + \dots + \xi_n\alpha_n^2) \\
&= v(Ds) + \frac{1}{2}\xi_{r+1}(\alpha_{r+1}^2 + \dots + \alpha_n^2) \\
&+ \frac{1}{2}(\xi_{r+2} - \xi_{r+1})(\alpha_{r+2}^2 + \dots + \alpha_n^2) \\
&+ \dots \\
&+ \frac{1}{2}(\xi_n - \xi_{n+1})(\alpha_n^2) \\
&\geq v(Ds) + \frac{1}{2}\sum_{j=r}^{n-1}(\xi_{j+1} - \xi_j)d_j^2.
\end{aligned}
$$

Truncating the sum in the right hand side of Theorem 2, we have the bound developed by Sun et al. [12]:

$$v(BQP) \geq v(Ds) + \frac{1}{2}\xi_{r+1}d_r^2 = v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(\{-1,1\}^n, S^*). \quad \mathbf{(6)}$$

The above bound can be understood geometrically. We have the following lemma.

Lemma 3 *The contour of* $f^*(x) = v(Ds) + \frac{1}{2}\xi_{r+1}d_r^2$ *is the maximum contour of* $f^*(x)$ *contained by the set* $\{x \in \mathbb{R}^n: dist(x, S^*) \leq d_r\}$.

Proof. For any point a such that $f^*(a) \leq v(Ds) + \frac{1}{2}\xi_{r+1}d_r^2$, decompose $a - x^0 = \alpha_1 u^1 + \ldots + \alpha_n u^n$. We have

$$\begin{aligned} f^*(a) &= \frac{1}{2}(Q^*(a - x^0 + x^0) + c)^T R(Q^*(a - x^0 + x^0) + c) - e^T\lambda^* - \frac{1}{2}c^T Rc \\ &= v(Ds) + \frac{1}{2}(\xi_{r+1}\alpha_{r+1}^2 + \ldots + \xi_n\alpha_n^2) \\ &\leq v(Ds) + \frac{1}{2}\xi_{r+1}d_r^2 \end{aligned}$$

Thus $\xi_{r+1}\alpha_{r+1}^2 + \ldots + \xi_n\alpha_n^2 \leq \xi_{r+1}d_r^2$, implying that $dist^2(x, S^*) = \alpha_{r+1}^2 + \ldots + \alpha_n^2 \leq d_r^2$. Then equality is attained by choosing a such that $\alpha_{r+1} = d_r$ and $\alpha_{r+2} = \ldots = \alpha_n = 0$.

The situation can be viewed in the following graph.

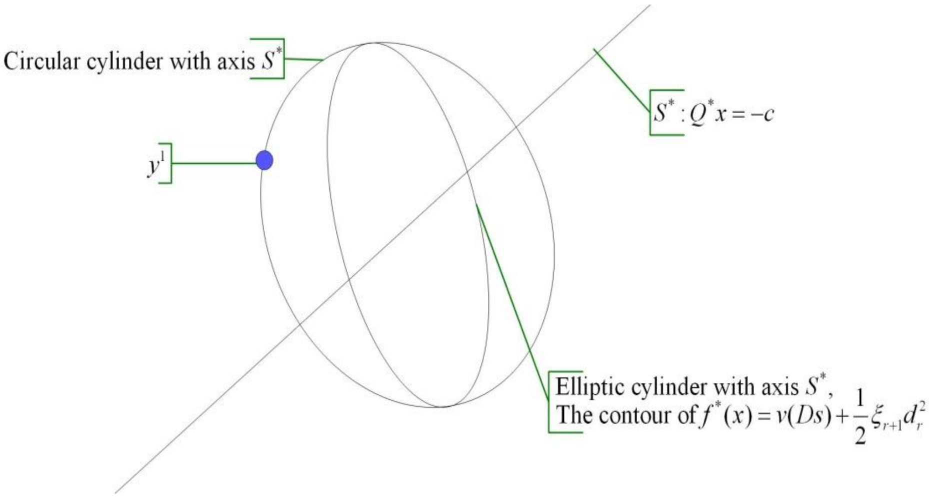

Fig.2 Geometrical interpretation of the improved bound by Equation (6)

As can be seen from Figure 2, there is no point of $\{-1,1\}^n$ inside the contour of $f^*(x) = v(Ds) + \frac{1}{2}\xi_{r+1}d_r^2$, which forms a lower bound for (BQP). Since d_r is the distance of $\{-1,1\}^n$ to an affine space, for fixed r, they can be computed in polynomial time via reverse enumeration technique as discussed in Section 2.

5. A Sequence of Improved Bounds

In this section, we are going to develop a sequence of improved bounds for (BQP) based on Algorithm 1 developed in Section 2. We use the notations developed in Section 4. The sequence of bounds will start on the bound by Sun et al. [12] in Equation (6).

Index the points in the set $\{-1,1\}^n$ by $y^1, y^2, \ldots, y^{2^n}$ such that $dist(y^1, S^*) \leq dist(y^2, S^*) \leq \ldots \leq dist(y^{2^n}, S^*)$. By Algorithm 1 we can find them progressively from y^1. Recall that the objective function $f(x) = \frac{1}{2}x^T Qx + c^T x$ agrees with $f^*(x)$ on the set $\{-1,1\}^n$.

Lemma 4 *For any* $i \geq 1$, *if* $b_i \triangleq v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(y^i, S^*) < \min_{y \in \{y^1,\ldots,y^i\}} f(y)$, *then* b_i *is a lower bound to* (BQP), *otherwise the optimal solution to* (BQP) *is* $x^* = arg \min_{y \in \{y^1,\ldots,y^i\}} f(y)$.

Proof. If $b_i < \min_{y \in \{y^1,\ldots,y^i\}} f(y)$, for any $j > i$, from Equations (5), we have $f(y^j) \geq v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(y^j, S^*) \geq v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(y^i, S^*) = b_i$. Thus for any $y \in \{-1,1\}^n$, $f(y) > b_i$.

If $b_i \geq \min_{y \in \{y^1,\ldots,y^i\}} f(y)$, if $x^* \notin \{y^1, \ldots, y^i\}$, then $f(x^*) < \min_{y \in \{y^1,\ldots,y^i\}} f(y) \leq b_i$. But $f(x^*) \geq v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(x^*, S^*) \geq b_i$. We have a contradiction, thus $x^* \in \{y^1, \ldots, y^i\}$.

Armed with Lemma 4 and Algorithm 1, we are ready to state the algorithm for a sequence of improved bounds.

Algorithm2 (**Sequence of Bounds**)

(1) $i = 1; P = \{\};$

(2) *Return* y^i *from Algorithm1;*

$P = P \cup \{y^i\};$

If $v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(y^i, S^*) < \min_{y \in P} f(y),$

$b_i \triangleq v(Ds) + \frac{1}{2}\xi_{r+1}dist^2(y^i, S^*);$

$i = i + 1;$

Go to (2);

else

$$x^* = \arg\min_{y \in P} f(y)$$

Stop;

EndIf

Algorithm 2 must terminate because the set $\{-1,1\}^n$ is finite. If the total iteration is k, then we have the sequence of bounds $b_1 \leq \ldots \leq b_{k-1} \leq v(BQP)$.

6. Conclusion

In this paper, we have generalized the spectral bounds in the literature to the general binary quadratic programming problem. By applying the reverse enumeration technique, we have further developed an algorithm to obtained from the binary set the 2nd closest point and 3rd closest point and so on to an affine space and proposed a sequence of improved SDP bounds for the binary quadratic programming problem. Since the state-of-the-art solution for solving this problem accurately is based on branch-and-bound frameworks, our results can help developing more efficient exact algorithms to solve the binary quadratic programming problem.

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