ON DUALITY GAP IN BINARY QUADRATIC PROGRAMMING*

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Abstract. We present in this paper new results on the duality gap between the binary quadratic optimization problem and its Lagrangian dual or semidefinite programming relaxation. We first derive a necessary and sufficient condition for the zero duality gap and discuss its relationship with the polynomial solvability of the primal problem. We then characterize the zeroness of the duality gap by the distance, δ, between $\{-1, 1\}^n$ and certain affine subspace C and show that the duality gap can be reduced by an amount proportional to δ^2. We finally establish the connection between the computation of δ and cell enumeration of hyperplane arrangement in discrete geometry and further identify two polynomially solvable cases of computing δ.

Key words. Binary quadratic programming; Lagrangian dual; semidefinite programming relaxation; cell enumeration of hyperplane arrangement.

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1. Introduction.

Consider the following quadratic binary optimization problem,

$$(P) \qquad \min_{x \in \{-1,1\}^n} f(x) = x^T Q x + 2c^T x,$$

where $Q \in \mathbb{R}^{n \times n}$ is symmetric and $c \in \mathbb{R}^n$.

There are many real-world applications of problem (P), for example, financial analysis [16], molecular conformation problem [18] and cellular radio channel assignment [9]. Many combinatorial optimization problems are special cases of (P), such as maximum cut problem (see e.g., [10, 12]). Specifically, by setting $c = 0$, problem (P) reduces to the form of maximum cut problem which has been proved to be NP-hard [11]. Thus, (P) is NP-hard in general. Polynomially solvable cases of (P) are investigated in [1, 7, 8, 19]. A systematic survey of the solution methods for solving (P) can be found in Chapter 10 of [14].

We investigate in this paper the Lagrangian relaxation and the dual problem of

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(P). Notice that (P) can be rewritten as

$$(P_c) \quad \min f(x) = x^T Qx + 2c^T x$$
$$\text{s.t.} \;\; x_i^2 - 1 = 0, \; i = 1, \ldots, n.$$

Dualizing each $x_i^2 - 1 = 0$ by a multiplier λ_i, we get the Lagrangian relaxation problem (L_λ):

$$\begin{aligned} d(\lambda) &= \inf_{x\in\mathbb{R}^n} L(x, \lambda) := f(x) + \sum_{i=1}^{n} \lambda_i(x_i^2 - 1) \\ &= \inf_{x\in\mathbb{R}^n} \{x^T (Q + \mathrm{diag}(\lambda))x + 2c^T x - e^T \lambda\}, \end{aligned} \tag{1.1}$$

where $e = (1, \ldots, 1)^T$ and $\mathrm{diag}(\lambda)$ denotes the diagonal matrix with λ_i being its ith diagonal element. The dual problem of (P_c) (or (P)) is

$$(D) \qquad \max_{\lambda\in\mathbb{R}^n} d(\lambda).$$

Let $v(\cdot)$ be the optimal value of problem $(\cdot)$. Obviously, the weak duality holds: $v(D) \le v(P)$. While a strict inequality holds, $(v(P) - v(D))$ measures the duality gap.

It is well known that (D) can be reduced to a semidefinite programming (SDP) problem (see [22]). Moreover, the Lagrangian bound $v(D)$ is equal to bounds generated by several other convex relaxation schemes (see [6, 13, 20, 21]). Malik *et al.* [15] investigated the gap between maximum cut problem, which is a special case of (P) where $c = 0$, and its semidefinite relaxation and showed that the gap can be reduced by computing a reduced-rank binary quadratic problem. Recently, Ben-Ameur and Neto [4] derived spectral bounds for maximum cut problem which are tighter than the well known Goemans and Williamson's SDP bound [12]. The spectral bounds in [4] invoke the eigenvalues of a matrix Q with modified diagonal entries and the distance from $\{-1, 1\}^n$ to some subspaces spanned by the eigenvectors of the modified Q.

The contribution of this paper is twofold. First, we characterize the duality gap by the distance δ between $\{-1, 1\}^n$ and set $C = \{x \in \mathbb{R}^n \mid (Q + \mathrm{diag}(\lambda^*))x = -c\}$, where λ^* is the optimal dual solution to (D). We show that the duality gap can be reduced by an amount $\xi_{r+1}\delta^2$, where ξ_{r+1} is the smallest positive eigenvalue of $Q + \mathrm{diag}(\lambda^*)$. This leads to an improved lower bound $\nu = v(D) + \xi_{r+1}\delta^2$ for (P) which is tighter than the Lagrangian bound or SDP bound of (P). Second, we establish the connection between the computation of δ and the cell enumerations of hyperplane arrangement in discrete geometry. It turns out δ can be computed in polynomial time for fixed r, where r is the rank of $Q + \mathrm{diag}(\lambda^*)$. In the special cases $r = 1$ and $r = n - 1$, we show that δ can be computed efficiently.

The paper is organized as follows. We investigate the basic duality properties of (P) in Section 2. Based on the optimality condition for zero duality gap, we characterize in Section 3 the duality gap by the distance δ. We then discuss the relations of the improved lower bound developed in this paper with the bound of [15] and the spectral bound of [4] for maximum cut problem, a special case of (P). In Section 4, we establish the connection between the computation of δ and the cell enumerations of hyperplane arrangement related to C. Finally, we conclude the paper in Section 5 with some further discussions.

2. Lagrangian Dual and Zero Duality Gap. In this section, we first introduce some basic properties of the Lagrangian dual problem (D). We then develop necessary and sufficient conditions for the zero duality gap between (P) and (D). Finally, we give a sufficient condition for the polynomial solvability of (P) based on a property of the optimal dual solution.

Using Shor's relaxation scheme, the dual problem (D) can be rewritten as a semidefinite programming problem:

$$
\begin{aligned}
(2.1) \qquad (D_s) \quad & \max \ -\tau - e^T\lambda \\
& \text{s.t.} \begin{pmatrix} Q + \mathrm{diag}(\lambda) & c \\ c^T & \tau \end{pmatrix} \succeq 0, \\
(2.2) \qquad & \tau \in \mathbb{R}, \ \lambda \in \mathbb{R}^n.
\end{aligned}
$$

Problem (D_s) is a semidefinite programming problem with $v(D_s) = v(D)$ and is polynomially solvable by interior point method (see [17, 24]). Obviously, (D) is equivalent to (D_s) in the sense that $v(D_s) = v(D)$ and λ^* is optimal to (D) if and only if (λ^*, τ^*) is optimal to (D_s), where $\tau^* = -v(D) - e^T\lambda^*$. It has been proved in [15] that the optimal solution to (D_s) is unique.

An alternative way to derive an SDP relaxation for (P) is lifting $x \in \mathbb{R}^n$ to $Y \in \mathcal{S}^n$. Note that $Y = xx^T$ for some $x \in \{-1, 1\}^n$ if and only if $Y = xx^T$ and $Y_{ii} = 1$, $i = 1, \ldots, n$. Relaxing $Y = xx^T$ to $Y \succeq xx^T$, we get the following SDP relaxation problem:

$$
\begin{aligned}
(P_s) \quad & \min \begin{pmatrix} Q & c \\ c^T & 0 \end{pmatrix} \bullet \begin{pmatrix} Y & x \\ x^T & 1 \end{pmatrix} \\
& \text{s.t. } Y_{ii} = 1, \ i = 1, \ldots, n, \\
& \begin{pmatrix} Y & x \\ x^T & 1 \end{pmatrix} \succeq 0,
\end{aligned}
$$

where $Y \in \mathcal{S}^n$. It can be shown that (P_s) is the conic dual of (D_s).

It is easy to see that the strict feasibility (Slater condition) of (D_s) and (P_s) always hold. By the conic duality theorem (see, e.g., Nesterov and Nemirovskii [17] or Ben-Tal [5]), the strict feasibility of (D_s) and (P_s) imply that (D_s) and (D_s) are solvable, $v(P_s) = v(D_s)$ and the complementary condition $X \bullet H(\lambda, \tau) = 0$ holds for any optimal solutions (Y, x) to (P_s) and (λ, τ) to (D_s), where we denote

$$X = \begin{pmatrix} Y & x \\ x^T & 1 \end{pmatrix}, \; H(\lambda, \tau) = \begin{pmatrix} Q + \mathrm{diag}(\lambda) & c \\ c^T & \tau \end{pmatrix}. \tag{2.3}$$

Since $X \succeq 0$ and $H(\lambda, \tau) \succeq 0$, $X \bullet H(\lambda, \tau) = 0$ is equivalent to $XH(\lambda, \tau) = 0$.

The KKT optimality conditions for (P_s) and (D_s) can then be described as follows.

Lemma 1. *Let (Y, x) and (λ, τ) be feasible solutions to (P_s) and (D_s), respectively. Then they are optimal if and only if*

$$XH(\lambda, \tau) = 0, \tag{2.4}$$

where X and $H(\lambda, \tau)$ are defined in (2.3).

By the definition of X and $H(\lambda, \tau)$, condition (2.4) is equivalent to

$$[Q + \mathrm{diag}(\lambda)]Y + cx^T = 0, \tag{2.5}$$

$$[Q + \mathrm{diag}(\lambda)]x + c = 0, \tag{2.6}$$

$$c^T Y + \tau x^T = 0, \tag{2.7}$$

$$c^T x + \tau = 0. \tag{2.8}$$

Lemma 2. ([3]) *For any $\lambda \in \mathbb{R}^n$, $d(\lambda) > -\infty$ with x solving (L_λ) if and only if*

(i) $Q + \mathrm{diag}(\lambda) \succeq 0$*;*

(ii) $[Q + \mathrm{diag}(\lambda)]x + c = 0$*.*

The following condition of saddle point type characterizes a zero duality gap between (P) and (D).

Lemma 3. *Let $x^* \in \{-1, 1\}^n$ and $\lambda^* \in \mathbb{R}^n$. Then, x^* solves (P), λ^* solves (D) and $v(P) = v(D)$ if and only if*

$$Q + \mathrm{diag}(\lambda^*) \succeq 0, \tag{2.9}$$

$$[Q + \mathrm{diag}(\lambda^*)]x^* + c = 0, \tag{2.10}$$

Proof. Suppose that conditions (2.9)-(2.10) hold for some $x^* \in \{-1, 1\}^n$ and $\lambda^* \in \mathbb{R}^n$. From conditions (i)-(ii) in Lemma 2, we know that x^* solves (L_{λ^*}) and

$$d(\lambda^*) = \min_{x \in \mathbb{R}^n} L(x, \lambda^*) = L(x^*, \lambda^*) = f(x^*) \geq v(P).$$

By the weak duality, λ^* solves (D) and $v(D) = v(P)$.

Conversely, if $x^* \in \{-1, 1\}^n$ and $\lambda^* \in \mathbb{R}^n$ solve (P) and (D), respectively, and $v(P) = v(D)$, then

$$L(x^*, \lambda^*) = f(x^*) + \sum_{i=1}^n \lambda_i^* [(x_i^*)^2 - 1] = f(x^*) = d(\lambda^*) = \min_{x \in \mathbb{R}^n} L(x, \lambda^*).$$

Thus, x^* solves (L_{λ^*}) and by Lemma 2, conditions (2.9)-(2.10) hold. □

Let λ^* be the optimal solution to (D). Let

$$Q^* = Q + \mathrm{diag}(\lambda^*), \tag{2.11}$$

$$C = \{x \in \mathbb{R}^n \mid Q^*x + c = 0\}. \tag{2.12}$$

PROPOSITION 1. *Let λ^* be an optimal solution to (D_s). Then $C \neq \emptyset$ and $v(P) = v(D)$ if and only if $C \cap \{-1,1\}^n \neq \emptyset$. Furthermore, any $x^* \in C \cap \{-1,1\}^n$ is an optimal solution to (P).*

Proof. Equation (2.6) implies that C is nonempty. The rest of the corollary follows directly from Lemma 3.□

PROPOSITION 2. *The duality gap $v(P) - v(D) = 0$ if and only if there exists an optimal solution (Y, x) to (P_s) satisfying $Y = xx^T$.*

Proof. The "if" part is obvious since (P_s) is relaxed from (P) by replacing $Y = xx^T$ with $Y \succeq xx^T$. Suppose that $v(P) - v(D) = 0$. Let $x \in \{-1,1\}^n$ and λ be optimal solutions to (P) and (D), respectively. By Lemma 3, the saddle point conditions (2.9)-(2.10) hold. Let $Y = xx^T$ and $\tau = -c^Tx$. Then, $Y_{ii} = x_i^2 = 1$ for $i = 1, \ldots, n$. Thus (Y, x) and (λ, τ) are respectively feasible to (P_s) and (D_s). Moreover, the complementarity condition (2.4) holds. Thus, by Lemma 1, (Y, x) is an optimal solution to (P_s) satisfying $Y = xx^T$. □

The following is a sufficient condition for the zero duality gap between (P) and (D).

PROPOSITION 3. *Assume that the optimal solution λ^* to (D) satisfies $Q^* \succ 0$. Then $x^* = -(Q^*)^{-1}c$ is the unique optimal solution to (P) and $v(P) = v(D)$. Moreover, (P) is polynomially solvable.*

Proof. Let (Y, x) be an optimal solution to (P_s). By Lemma 1, the complementarity conditions (2.5)-(2.8) hold. However, the equation in (2.6) has a unique solution $x = -(Q^*)^{-1}c$. Substituting it into (2.5), we obtain $Y = (Q^*)^{-1}cc^T(Q^*)^{-1} = xx^T$. Thus, $x_i^2 = Y_{ii} = 1$ for $i = 1, \ldots, n$, i.e., x is feasible to (P). It then follows from Lemma 3 that x is the unique solution to (P) and $v(P) - v(D) = 0$. □

3. Duality gap and improved bound. In this section, we discuss how to verify the zero duality gap between (P) and (D) when $Q^* = Q + \mathrm{diag}(\lambda^*)$ is *singular*. By characterizing the duality gap by the distance between $\{1,-1\}^n$ and set C defined in (2.12), we can either determine the zeroness of the duality gap or reduce the nonzero duality gap. A lower bound tighter than $v(D)$ is then obtained in cases where the duality gap is nonzero.

3.1. Duality gap and improved lower bound. Let λ^* be the optimal solution to (D_s). Assume that $\mathrm{rank}(Q^*) = n - r$ with $0 < r < n$. Let $0 = \xi_1 = \cdots = \xi_r <$

$\xi_{r+1} \le \cdots \le \xi_n$ be the eigenvalues of Q^*. Then, there exists an orthogonal matrix $U = (U_1, \ldots, U_n)$ such that

$$U^T Q^* U = \mathrm{diag}(0, \ldots, 0, \xi_{r+1}, \ldots, \xi_n). \tag{3.1}$$

It is easy to see that the null space of Q^* is spanned by $U_1, \ldots, U_r$.

LEMMA 4. *Let λ^* be the optimal solution to (D) and U be defined in (3.1). Then*

(i) $c^T U_i = 0$, *for* $i = 1, \ldots, r$;

(ii) $v(D) = -e^T\lambda^* - \sum_{i=r+1}^n (c^T U_i)^2/\xi_i$;

(iii) *For any $x \in \{-1, 1\}^n$, the objective value of (P) is given by*

$$f(x) = v(D) + \sum_{i=r+1}^n \xi_i (y_i + \frac{c^T U_i}{\xi_i})^2,$$

where $x = Uy$.

Proof. (i) Since $d(\lambda^*) > -\infty$, by Lemma 2, there exists x such that $Q^* x = -c$. By (3.1), for $i = 1, \ldots, r$, we have

$$\begin{aligned} -c^T U_i &= x^T Q^* U_i \\ &= x^T U \cdot \mathrm{diag}(0, \ldots, 0, \xi_{r+1}, \ldots, \xi_n) U^T U_i \\ &= x^T U \cdot \mathrm{diag}(0, \ldots, 0, \xi_{r+1}, \ldots, \xi_n) e_i \\ &= 0. \end{aligned}$$

(ii) By the definition of the dual problem, we have

$$\begin{aligned} v(D) = d(\lambda^*) &= \min_{x \in \mathbb{R}^n} [x^T Q^* x + 2c^T x - e^T \lambda^*] \\ &= \min_{y \in \mathbb{R}^n} [\sum_{i=r+1}^n \xi_i (y_i + \frac{c^T U_i}{\xi_i})^2 - e^T\lambda^* - \sum_{i=r+1}^n \frac{(c^T U_i)^2}{\xi_i}] \\ &= -e^T \lambda^* - \sum_{i=r+1}^n \frac{(c^T U_i)^2}{\xi_i}, \end{aligned}$$

where the relation $x = Uy$ is used in the above derivation.

(iii) Let $x = Uy$. For any $x \in \{-1, 1\}^n$, by (3.1) and part (ii), we have

$$\begin{aligned} f(x) &= x^T Q x + 2c^T x \\ &= x^T [Q + \mathrm{diag}(\lambda^*)] x + 2c^T x - e^T \lambda^* \\ &= y^T (U^T Q^* U) y + 2c^T U y - e^T \lambda^* \\ &= \sum_{i=r+1}^n \xi_i y_i^2 + 2c^T U y - e^T \lambda^* \\ &= \sum_{i=r+1}^n \xi_i \left(y_i + \frac{c^T U_i}{\xi_i} \right)^2 - e^T \lambda^* - \sum_{i=r+1}^n \frac{(c^T U_i)^2}{\xi_i} \\ &= v(D) + \sum_{i=r+1}^n \xi_i \left(y_i + \frac{c^T U_i}{\xi_i} \right)^2. \end{aligned}$$

□

Now, let's define the distance between $\{-1,1\}^n$ and $C = \{x \in \mathbb{R}^n \mid Q^* x = -c\}$:

$$\delta = \mathrm{dist}(\{-1,1\}^n, C) = \min\{\|x - z\| \mid x \in \{-1,1\}^n,\ z \in C\}. \tag{3.2}$$

Obviously, $\delta = 0$ if and only if there exists $x^* \in \{-1,1\}^n \cap C$. It then follows from Proposition 1 that $\delta = 0$ if and only if $v(P) = v(D)$. Moreover, any $x^* \in \{-1,1\}^n$ achieving the distance $\delta = 0$ is an optimal solution to (P).

THEOREM 1. *If $\delta > 0$, then an improved lower bound of the optimal value of (P) can be computed by*

$$\nu = v(D) + \xi_{r+1}\delta^2. \tag{3.3}$$

Proof. Let $Uw \in C$. By (3.1), $Q^* Uw = -c$ gives rise to

$$U \cdot \mathrm{diag}(0, \dots, 0, \xi_{r+1}, \dots, \xi_n) U^T U w = -c,$$

which in turn yields

$$\mathrm{diag}(0, \dots, 0, \xi_{r+1}, \dots, \xi_n) w = -U^T c,$$

Notice that $U_i^T c = 0$ by Lemma 2 (i). Thus, $z = Uw \in C$ if and only if

$$w_i \in \mathbb{R},\ i = 1, \dots, r,\ w_i = -\frac{c^T U_i}{\xi_i},\ i = r+1, \dots, n. \tag{3.4}$$

Using (3.4) and the orthogonality of U, we have

$$\begin{aligned}
\delta^2 &= \min\{\|x - z\|^2 \mid x \in \{-1,1\}^n,\ z \in C\} \\
&= \min\{\|Uy - Uw\|^2 \mid Uy \in \{-1,1\}^n,\ Uw \in C\} \\
&= \min\{\|y - w\|^2 \mid Uy \in \{-1,1\}^n,\ w_i \in \mathbb{R},\ i = 1, \dots, r,\ w_i = -\frac{c^T U_i}{\xi_i},\ i = r+1, \dots, n\} \\
&= \min\left\{ \sum_{i=1}^{r} \|y_i - w_i\|^2 + \sum_{i=r+1}^{n} (y_i + \frac{c^T U_i}{\xi_i})^2 \mid Uy \in \{-1,1\}^n,\ w_i \in \mathbb{R},\ i = 1, \dots, r \right\} \\
&= \min\left\{ \sum_{i=r+1}^{n} (y_i + \frac{c^T U_i}{\xi_i})^2 \mid Uy \in \{-1,1\}^n \right\}.
\end{aligned}$$

Thus, for any $x = Uy \in \{-1,1\}^n$, it holds

$$\delta^2 \le \sum_{i=r+1}^{n} (y_i + \frac{c^T U_i}{\xi_i})^2. \tag{3.5}$$

It then follows from Lemma 4 (iii) and (3.5) that, for any $x = Uy \in \{-1,1\}^n$,

$$\begin{aligned} f(x) &= v(D) + \sum_{i=r+1}^{n} \xi_i (y_i + \frac{c^T U_i}{\xi_i})^2 \\ &\geq v(D) + \xi_{r+1} \sum_{i=r+1}^{n} (y_i + \frac{c^T U_i}{\xi_i})^2 \\ &\geq v(D) + \xi_{r+1}\delta^2. \end{aligned}$$

Therefore, $\nu = v(D) + \xi_{r+1}\delta^2$ is an improved lower bound to $v(P)$. □

3.2. Relations between ν and other bounds for maximum cut problem. Next, we turn to discuss the relationships of the improved bound ν given in (3.3) with two other bounds in the literature for maximum cut problem, which is a special case of (P) with $c = 0$.

Malik et al. [15] considered the maximum cut problem in the following form:

$$f^* = \max_{\{-1,1\}^n} x^T Q x. \tag{3.6}$$

It is easy to see that the SDP relaxation of (3.6) is given by

$$\gamma^* = \min \sum_{i=1}^{n} \lambda_i \tag{3.7}$$

$$\text{s.t. } \operatorname{diag}(\lambda) - Q \succeq 0. \tag{3.8}$$

Let $(\operatorname{diag}(\lambda) - Q)$ have the following spectral decomposition:

$$\operatorname{diag}(\lambda^*) - Q = (V, V_+) \begin{pmatrix} 0_r & 0 \\ 0 & \Lambda_+ \end{pmatrix} \begin{pmatrix} V \\ V_+ \end{pmatrix}, \tag{3.9}$$

where $\Lambda_+ = \operatorname{diag}(\xi_{r+1}, \ldots, \xi_n)$ with $0 < \xi_{r+1} \leq \cdots \leq \xi_n$. By considering the following reduced rank problem:

$$\delta^* = \max_{\{-1,1\}^n} x^T V V^T x,$$

Malik et al. [15] proved that

$$\nu_m = \gamma^* - \xi_{r+1}(n - \delta^*) \tag{3.10}$$

is an improved upper bound of f^*.

Applying the improved bound ν defined in (3.3) to problem (3.6), we have the following upper bound for (3.6):

$$\nu_s = \gamma^* - \xi_{r+1}\delta^2, \tag{3.11}$$

where $\delta = \operatorname{dist}(\{-1,1\}^n, C)$ and $C = \{x \in \mathbb{R}^n \mid (\operatorname{diag}(\lambda^*) - Q)x = 0\}$.

PROPOSITION 4. *For the maximum cut problem (3.6), it holds $\nu_m = \nu_s$, where ν_m and ν_s are the improved bounds defined in (3.10) and (3.11), respectively.*

Proof. Since $c = 0$, we have the following from (3.9),

$$C = \{x \in \mathbb{R}^n \mid x = \sum_{i=1}^{r} z_i V_i,\ z \in \mathbb{R}^r\}.$$

Thus,

$$\begin{aligned}
\delta^2 &= \min\{\|x - y\|^2 \mid x \in \{-1,1\}^n, y \in C\} \\
&= \min\{\|x - \sum_{i=1}^{r} z_i V_i\|^2 \mid x \in \{-1,1\}^n,\ z \in \mathbb{R}^r\} \\
&= \min_{x\in\{-1,1\}^n} \min_{z\in\mathbb{R}^r} \|x - Vz\|^2 \\
&= \min_{x\in\{-1,1\}^n} \|x - VV^T x\|^2 \\
&= n - \max_{x\in\{-1,1\}^n} \|V^T x\|^2 \\
&= n - \delta^*,
\end{aligned}$$

where the fact that $V^T V = I_r$ is used. It then follows from (3.10) and (3.11) that $\nu_m = \nu_s$. □

Recently, Ben-Ameur and Neto [4] derived some spectral bounds for maximum cut problem in the following form:

$$\begin{aligned}
(3.12) \qquad w^* = \max\ & f(x) = \frac{1}{4}\sum_{i,j=1}^{n} w_{ij}(1 - x_i x_j) = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} - \frac{1}{4}x^T W x \\
\text{s.t. } & x \in \{-1,1\}^n,
\end{aligned}$$

which has the following equivalent form,

$$\begin{aligned}
(3.13) \qquad \tilde{w} = \min\ & \frac{1}{2}x^T W x \\
\text{s.t. } & x \in \{-1,1\}^n,
\end{aligned}$$

while the SDP relaxation of (3.13) is given by

$$\begin{aligned}
(3.14) \qquad \tilde{\delta} = \min\ & \sum_{i=1}^{n} \lambda_i \\
\text{s.t. } & W + 2\text{diag}(\lambda) \succeq 0.
\end{aligned}$$

Obviously, $w^* = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} - \frac{1}{2}\tilde{w}$. Let λ^* be the optimal solution to (3.14) and $W^* = W + 2\text{diag}(\lambda^*) \succeq 0$ have the following spectral decomposition:

$$(3.15) \qquad W^* = U\text{diag}(\xi_1, \cdots, \xi_n)U^T,$$

where $\xi_1, \xi_2, \ldots, \xi_n$ are the eigenvalues of W^* with a nondecreasing ranking order. Ben-Ameur and Neto [4] introduced a family of distance measures,

$$d_k = \text{dist}(\{-1,1\}^n, \text{span}(U_1,\ldots,U_k)), \quad k = 1,\ldots,n, \tag{3.16}$$

which yields, especially, $d_n = 0$ and

$$d_1 = \text{dist}(\{-1,1\}^n, U_1) = \sqrt{n - \|U_1\|_1^2}, \tag{3.17}$$

where $\|a\|_1 = \sum_{i=1}^n |a_i|$ for $a \in \mathbb{R}^n$. Let

$$\nu_1 = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} + \frac{1}{4}\sum_{i=1}^n w_{ii} - \frac{1}{4}\xi_1 n, \tag{3.18}$$

$$\nu_2 = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} + \frac{1}{4}\sum_{i=1}^n w_{ii} - \frac{1}{4}\xi_1 n - \frac{1}{4}(\xi_2 - \xi_1)(n - \|U_1\|_1^2), \tag{3.19}$$

$$\nu_3 = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} + \frac{1}{4}\sum_{i=1}^n w_{ii} - \frac{1}{4}\xi_1 n - \frac{1}{4}\sum_{i=1}^{n-1} d_i^2(\xi_{i+1} - \xi_i). \tag{3.20}$$

Ben-Ameur and Neto [4] showed that ν_i $(i = 1,2,3)$ are all upper bounds of w^*, while ν_1 is exactly the SDP bound of (3.12), namely,

$$\nu_1 = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} - \frac{1}{2}\tilde{\delta}.$$

Applying the improved bound ν defined in (3.3) to problem (3.13), we obtain the following upper bound for the maximum cut problem (3.12):

$$\nu_4 = \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} - \frac{1}{2}\tilde{\delta} - \frac{1}{4}\xi_{r+1}\delta^2 = \nu_1 - \frac{1}{4}\xi_{r+1}\delta^2, \tag{3.21}$$

where $\delta = \text{dist}(\{-1,1\}^n, C)$ and $C = \{x \in \mathbb{R}^n \mid W^* x = 0\}$. Let $\text{rank}(W^*) = n - r$. Notice that $1 \le r \le n-1$ (see [15]). Using (3.15), we have $C = \text{span}(U_1,\ldots,U_r)$, which gives rise to $\delta = d_r$ with d_r being defined in (3.16). If $r = 1$, then $\delta = d_1 = \sqrt{n - \|U_1\|_1^2}$. Thus, from (3.17), (3.18) and (3.19), we have $\nu_4 = \nu_2$. If $r \ge 2$, then $\nu_2 = \nu_1 \ge \nu_4$. Notice that $d_1 \ge d_2 \ge \cdots \ge d_{n-1} \ge 0$ and $\xi_1 = \cdots = \xi_r = 0$. It follows from (3.20) and (3.21) that

$$\begin{aligned}
\nu_3 &= \frac{1}{2}\sum_{1\le i<j\le n} w_{ij} + \frac{1}{4}\sum_{i=1}^n w_{ii} - \frac{1}{4}\xi_1 n - \frac{1}{4}\sum_{i=1}^{n-1} d_i^2(\xi_{i+1} - \xi_i) \\
&= \nu_1 - \frac{1}{4}\sum_{i=1}^{n-1} d_i^2(\xi_{i+1} - \xi_i) \\
&= \nu_1 - \frac{1}{4}\xi_{r+1} d_r^2 - \frac{1}{4}\sum_{i=r+1}^{n-1} d_i^2(\xi_{i+1} - \xi_i) \\
&= \nu_4 - \frac{1}{4}\sum_{i=r+1}^{n-1} d_i^2(\xi_{i+1} - \xi_i).
\end{aligned}$$

In particular, when $r = n-1$, we have $\nu_3 = \nu_4$. The above discussion leads to the following result:

Proposition 5. *Let* $\mathrm{rank}(W^*) = n - r$. *Then*

(i) $\nu_2 = \nu_4$ *when* $r = 1$ *and* $\nu_2 > \nu_4$ *when* $r > 1$;

(ii) $\nu_3 = \nu_4$ *when* $r = n-1$ *and* $\nu_3 = \nu_4 - \frac{1}{4}\sum_{i=r+1}^{n-1} d_i^2(\xi_{i+1} - \xi_i) \le \nu_4$ *when* $r < n-1$.

The above result indicates that for maximum cut problem, the improved bound ν_4 is tighter than ν_2, while it is dominated by ν_3. We notice, however, that computing ν_3 requires more computational efforts than ν_4 since the additional distances $d_{r+2}, \ldots, d_{n-1}$ have to be computed. It was shown in [4] that computing d_{n-1} is NP-hard.

4. Computation of δ. In this section, we discuss the issue of how to compute the distance δ. We first establish the relation between the computation of δ and the cell enumeration of hyperplane arrangement in discrete geometry. Two special cases, $r = 1$ and $r = n-1$, will be then discussed.

4.1. Computation of δ and cell enumeration. Notice that set C can be expressed as

$$C = \{x \in \mathbb{R}^n \mid x = x^0 + \sum_{k=1}^{r} z_k U_k,\ z \in \mathbb{R}^r\}, \tag{4.1}$$

where $Q^* x^0 = -c$ and $U_1, \ldots, U_r$ are defined in decomposition (3.1). By (3.1) and Lemma 4 (i), a special choice of solution x^0 is given by

$$x^0 = Uw, \text{ where } w_i = 0,\ i = 1, \ldots, r,\ w_i = -\frac{U_i^T c}{\xi_i}, i = r+1, \ldots, n.$$

For any $x \in C$ with $x_i \neq 0$ for $i = 1, \ldots, n$, its distance to $\{-1,1\}^n$ is entirely determined by the sign of x_i for $i = 1, \ldots, n$. More precisely, $\mathrm{dist}(x, \{-1,1\}^n) = \mathrm{dist}(x, w)$, where $w = \mathrm{sign}(x)$ is the sign vector of x defined by

$$w_i = \mathrm{sign}(x_i) = \begin{cases} 1, & \text{if } x_i > 0 \\ -1, & \text{if } x_i < 0 \end{cases}$$

for $i = 1, \ldots, n$. Let

$$P = \{x \in C \mid x_i \neq 0,\ i = 1, \ldots, n\}.$$

For any $x \in P$, define

$$T_x = \{y \in P \mid \mathrm{sign}(y) = \mathrm{sign}(x)\}. \tag{4.2}$$

Then, $w = \mathrm{sign}(x)$ is the point of $\{-1,1\}^n$ that achieves the minimum distance from T_x to $\{-1,1\}^n$. It is easy to see that $C = \mathrm{cl}(\cup_{x \in P} T_x)$ and there is only a finite number of distinct T_x's for all $x \in P$. If we are able to find all such distinct T_x's, then the distance between $\{-1,1\}^n$ and C must be achieved in $\{-1,1\}^n$ at one of the sign vectors of T_x's.

Suppose that we have found all the distinct T_x's for $x \in P$, listed as $T_1, \ldots, T_p$. Moreover, suppose that an interior point π^i of T_i is obtained for each T_i. Let $V = (U_1, \ldots, U_r)$. Using (4.1) and the projection theorem, we have

$$\begin{aligned} \delta &= \mathrm{dist}(\{-1,1\}^n, C) \\ &= \min_{i=1,\ldots,p} \mathrm{dist}(\mathrm{sign}(\pi^i), C) \\ &= \min_{i=1,\ldots,p} \|(VV^T - I)(\mathrm{sign}(\pi^i) - x^0)\|. \end{aligned} \tag{4.3}$$

We now turn to discuss how to find all the distinct T_x's for $x \in C$. Let

$$g_j(z) = x_j^0 + \sum_{i=1}^{r} V_{ij} z_i,$$

where V_{ij} is the jth element of V_i, $j = 1, \ldots, n$. Setting $x_j = 0$ ($j = 1, \ldots, n$) in (4.1) gives rise to n hyperplanes in $\mathbb{R}^r$:

$$h_j = \{z \in \mathbb{R}^r \mid g_j(z) = 0\},\ i = 1, \cdots, n. \tag{4.4}$$

These n hyperplanes partition C into a number of r-dimensional convex polyhedral sets. All faces of these partitioned convex polyhedral sets define an *arrangement* of C. Each r-dimensional convex polyhedral set from this partition is called a *cell* of the hyperplane arrangement (see, e.g., [2][23]). Define

$$\begin{aligned} h_j^+ &= \{z \in \mathbb{R}^r \mid g_j(z) > 0\},\ i = 1, \cdots, n, \\ h_j^- &= \{z \in \mathbb{R}^r \mid g_j(z) < 0\},\ i = 1, \cdots, n. \end{aligned}$$

Let φ be a cell generated from the hyperplane arrangement defined by (4.4) and π be an interior point of φ. Associate the cell φ with a sign vector $\chi(\varphi) \in \{-1,1\}^n$ defined by

$$\chi(\varphi)_j = \begin{cases} 1, & \text{if } \pi \in h_j^+, \\ -1, & \text{if } \pi \in h_j^-. \end{cases}$$

Since the sign vector of a cell is invariant for any interior point of φ, we can represent a cell φ by its sign vector $\chi(\varphi)$.

A key observation is that there is a one-to-one mapping between the cells of the hyperplane arrangement defined by (4.4) and the sets T_x defined in (4.2). More precisely, each sign vector of a cell is the sign vector of a set T_x and vice versa. Therefore, the distance δ can be calculated via formulation (4.3) by enumerating all the cells of the hyperplane arrangement defined by (4.4).

It has been known that the number of cells generated from the hyperplane arrangement specified by (4.4) is $O(n^r)$ (see, e.g., [25]). Therefore, for fixed r, the distance δ can be computed in polynomial time. Efficient search methods for enumerating all the cells of a hyperplane arrangement were proposed in [2][23].

EXAMPLE 1. Consider the following 10-dimensional instance of (P),

$$Q = \begin{pmatrix} 0 & 3 & 6 & -3 & 6 & 3 & -5 & -4 & 8 & -1 \\ 3 & 0 & -6 & -10 & -3 & 8 & -6 & 8 & 5 & 7 \\ 6 & -6 & 0 & -7 & 7 & 7 & 4 & 9 & 2 & -4 \\ -3 & -10 & -7 & 0 & 9 & 8 & 6 & 9 & -6 & -5 \\ 6 & -3 & 7 & 9 & 0 & -4 & -5 & 4 & -3 & 1 \\ 3 & 8 & 7 & 8 & -4 & 0 & -4 & -10 & -8 & -5 \\ -5 & -6 & 4 & 6 & -5 & -4 & 0 & 9 & -10 & 6 \\ -4 & 8 & 9 & 9 & 4 & -10 & 9 & 0 & -1 & 4 \\ 8 & 5 & 2 & -6 & -3 & -8 & -10 & -1 & 0 & 6 \\ -1 & 7 & -4 & -5 & 1 & -5 & 6 & 4 & 6 & 0 \end{pmatrix}, \quad c = \begin{pmatrix} -5 \\ -4 \\ -5 \\ 4 \\ 2 \\ 2 \\ -4 \\ -3 \\ 3 \\ 4 \end{pmatrix}.$$

By solving the SDP relaxation (D_2) for this example, we obtain the optimal dual solution $\lambda^* = (5.0114, 14.7031, 19.8221, 20.8034, 13.6508, 23.0041, 10.1066, 12.8147, 15.6921, 7.9364)^T$ with $v(D) = -298.6424$. It can be verified that $r = 10 - \text{rank}(Q^*) = 2$ and $U^T Q^* U = \text{diag}(\xi)$, where $\xi = (0, 0, 6.0529, 16.1134, 25.0209, 36.9903, 38.1915, 48.6065, 55.4609, 60.6526)^T$. By equation (4.1), we can express any $x \in C = \{x \in \mathbb{R}^{10} \mid Q^* x = -c\}$ as follows,

$$\begin{cases} x_1 = 0.8987 + 0.1121 z_1 - 0.4837 z_2, \;\; x_2 = 0.3559 + 0.2092 z_1 + 0.4303 z_2 \\ x_3 = 0.0263 - 0.3542 z_1 + 0.1941 z_2, \;\; x_4 = -0.0172 + 0.3674 z_1 + 0.1393 z_2 \\ x_5 = -0.1760 - 0.3287 z_1 + 0.2002 z_2, \;\; x_6 = -0.2340 - 0.3043 z_1 - 0.1514 z_2, \\ x_7 = 0.4983 - 0.3651 z_1 + 0.3394 z_2, \;\; x_8 = -0.0229 - 0.3129 z_1 - 0.4873 z_2, \\ x_9 = -0.2056 - 0.3229 z_1 + 0.1931 z_2, \;\; x_{10} = -0.5186 + 0.3836 z_1 - 0.2662 z_2, \end{cases}$$

where $z_1, z_2 \in \mathbb{R}$. Each pair of two of the above equations gives rise to 4 candidate points in Γ. It can be verified there are 56 different points in Γ among the scanned $2^2 \times 10 \times 9/2 = 180$ candidate points. Using formulation (4.3), we can calculate the distance $\delta = 0.6618$. Thus, by Theorem 1 (ii), a tighter lower bound is given by

$$\bar{\nu} = v(D) + \xi_{r+1}\delta^2 = -298.6424 + 0.5 \times 0.6618^2 \times 6.0529 = -295.9914.$$

Since $v(P) = -290$, the duality gap is $v(P) - v(D) = 8.6424$. Therefore, the ratio of reduction in the duality gap is $\frac{\bar{\nu} - V(D)}{V(P) - V(D)} = 30.68\%$ for this example.

4.2. The case $r = 1$**.** When $r = 1$, C is a one-dimensional line in $\mathbb{R}^n$ with the following expression,

$$C = \{x \in \mathbb{R}^n \mid x = x^0 + zU_1, \; z \in \mathbb{R}\}.$$

For each j with $U_{1j} \neq 0$, the sign of x_j changes at point $\alpha_j = -x_j^0/U_{1j}$. It is possible that some α_js take the same value. Rank all different α_j's in the following ascending order,

$$\alpha_{j_1} < \alpha_{j_2} < \cdots < \alpha_{j_{p-1}}.$$

We see that $p \leq n+1$. Let $\alpha_{j_0} = -\infty$ and $\alpha_{j_p} = +\infty$. Then C is partitioned into p intervals $C^i = (\alpha_{j_{i-1}}, \alpha_{j_i})$, $i = 1, \ldots, p$. An interior point π^i of C^i can be taken as follows,

$$\begin{cases} \pi^1 = x^0 + (\alpha_{j_1} - 1)U_1, \ \pi^p = x^0 + (\alpha_{j_{p-1}} + 1)U_1, \\ \pi^i = x^0 + \frac{1}{2}(\alpha_{j_{i-1}} + \alpha_{j_i})U_1, \quad i = 2, \ldots, p-1. \end{cases} \tag{4.5}$$

Using (4.3), we have

$$\delta = \min_{i=1,\ldots,p} \|(U_1U_1^T - I)(\text{sign}(\pi^i - x^0)\|, \tag{4.6}$$

where π^i $(i = 1, \cdots, p)$ are calculated by (4.5).

PROPOSITION 6. *If $r = 1$, then δ can be computed in polynomial time.*

Proof. Since $p \leq n+1$, the conclusion follows from (4.6). □

EXAMPLE 2. Consider an instance with

$$Q = \begin{pmatrix} 0 & -7 & -10 & 4 \\ -7 & 0 & -1 & -2 \\ -10 & -1 & 0 & -6 \\ 4 & -2 & -6 & 0 \end{pmatrix}, \ c = \begin{pmatrix} -1 \\ 3 \\ 1 \\ -5 \end{pmatrix}$$

For this example, the optimal solution to (D_s) is $\lambda^* = (7.4223, 4.7188, 7.0063, 3.5195)^T$ with $v(D) = v(D_2) = -50.1242$, and the vector of the eigenvalues of $Q^* = Q + 2\text{diag}(\lambda^*)$ is $\xi = (0, 4.9716, 12.1793, 28.1830)^T$. Thus, $r = n - \text{rank}(Q^*) = 4 - 3 = 1$. Using (4.6), we can compute the distance $\delta = 0.6042$, which leads to a nonzero duality gap. By Theorem 1, an improved lower is given by

$$\bar{\nu} = v(D) + \times 4.9716 \times 0.6042^2 = -48.3092.$$

As $v(P) = -48$ in this example, the ratio of reduction in duality gap is $\frac{\bar{\nu} - v(D)}{v(P) - v(D)} = 85.44\%$.

4.3. The Case $r = n - 1$. Suppose that $r = n - 1$. Then, set C is an $(n-1)$-dimensional hyperplane in $\mathbb{R}^n$ and there exist a and $b \in \mathbb{R}^n$ with $a \neq 0$ such that

$$C = \{x \in \mathbb{R}^n \mid a^T x = b\}.$$

LEMMA 5. *Let $P = \{x \in \mathbb{R}^n \mid Dx \le c\}$, where D is an $s \times n$ matrix. Assume that i) P is bounded and ii) either $P \subseteq C^+ = \{x \in \mathbb{R}^n \mid a^T x \ge b\}$ or $P \subseteq C^- = \{x \in \mathbb{R}^n \mid a^T x \le b\}$. Then there exist an extreme point $\bar{x}$ of P and a point $\bar{y} \in C$ such that*

$$\|\bar{x} - \bar{y}\| = \mathrm{dist}(P, C) = \min\{\|x - y\| \mid x \in P,\ y \in C\}.$$

Proof. By the assumption, if $P \cap C \neq \emptyset$, then b is the optimal value of the linear program $\min\{a^T x \mid x \in P\}$ or $\max\{a^T x \mid x \in P\}$. So there is an extreme point $\bar{x}$ of P that achieves this optimal value, i.e., $a^T \bar{x} = b$. Hence, the lemma holds by taking $\bar{y} = \bar{x}$. Next, we suppose that $P \cap C = \emptyset$. By the definition of $\mathrm{dist}(P, C)$, there exist $\hat{x} \in P$ and $\hat{y} \in C$ such that

$$\frac{1}{2}\|\hat{x} - \hat{y}\|^2 = \min\{\frac{1}{2}\|x - y\|^2 \mid x \in P,\ y \in C\}.$$

By the KKT conditions, there exists $\gamma \in \mathbb{R}^s$ and $\mu \in \mathbb{R}$ such that

$$\hat{x} - \hat{y} + D^T \gamma = 0, \tag{4.7}$$

$$-(\hat{x} - \hat{y}) + \mu a = 0, \tag{4.8}$$

$$\gamma^T (D\hat{x} - c) = 0, \tag{4.9}$$

$$D\hat{x} \le c,\ a^T \hat{y} = b,\ \gamma \ge 0. \tag{4.10}$$

Since $P \cap C = \emptyset$, we have $\hat{x} \neq \hat{y}$, which in turn implies $\mu \neq 0$ from (4.8). Using (4.7)-(4.10), for any $x \in P$, we have

$$(\hat{y} - \hat{x})^T (x - \hat{x}) = \gamma^T D(x - \hat{x}) = \gamma^T (Dx - c) \le 0. \tag{4.11}$$

Combining (4.8) and (4.11), we obtain $\mu a^T \hat{x} \le \mu a^T x$ for all $x \in P$. Therefore, $\hat{x}$ is an optimal solution to the linear program: $\min\{\mu a^T x \mid x \in P\}$. Thus, there exists an extreme point $\bar{x}$ of P such that $a^T \bar{x} = a^T \hat{x}$. Let $\bar{y}$ be the projection of $\bar{x}$ on C. Then, there exists $\sigma \neq 0$ such that $\bar{x} - \bar{y} = \sigma a$. Since both $\bar{y}$ and $\hat{y} \in C$, it holds $a^T (\bar{y} - \hat{y}) = 0$. It then follows that $\sigma \|a\|^2 = a^T (\bar{x} - \bar{y}) = a^T (\hat{x} - \hat{y}) = \mu \|a\|^2$. Thus, $\sigma = \mu$ and hence $\|\bar{x} - \bar{y}\| = \|\hat{x} - \hat{y}\| = \mathrm{dist}(P, C)$. □

PROPOSITION 7. *Assume that $r = n - 1$ and C is of the expression $C = \{x \in \mathbb{R}^n \mid a^T x = b\}$. If either $\sum_{i=1}^n |a_i| \le b$ or $-\sum_{i=1}^n |a_i| \ge b$, then $\delta = \mathrm{dist}(\{-1, 1\}^n, C)$ can be computed in polynomial time.*

Proof. By assumption, we have $\max\{a^T x \mid x \in [-1, 1]^n\} \le b$ or $\min\{a^T x \mid x \in [-1, 1]^n\} \ge b$. Applying Lemma 5 with $P = [-1, 1]^n$, we have $\delta = \mathrm{dist}(\{-1, 1\}^n, C) = \mathrm{dist}([-1, 1]^n, C)$. The computation of $\mathrm{dist}([-1, 1]^n, C)$ is equivalent to the following convex quadratic program:

$$\min\ \|x - y\|^2$$

$$\text{s.t.} \quad -1 \le x_i \le 1, \; i = 1, \dots, n,$$
$$a^T y = b,$$

which is polynomially solvable. □

We notice from Proposition 7 that the condition that $[-1,1]^n$ lies in one of the two half-spaces formed by hyperplane C is indispensable for establishing the polynomial solvability of δ. In general case of $r = n-1$, computing δ is still NP-hard as $\delta = d_{n-1}$ (cf. (3.16)) when $c = 0$ and computing d_{n-1} is NP-hard (see [4]).

5. Conclusion and discussions. We have presented new results in this paper on the duality gap between the binary quadratic optimization problem and its Lagrangian dual. Furthermore, we have gained new insights into the polynomial solvability of certain subclasses of problem (P) by investigating the duality gap. Facilitated by the derived optimality conditions, we have characterized the duality gap by the distance δ between $\{-1,1\}^n$ and C and have showed that an improved lower bound can be obtained if the distance is nonzero. We have also discussed the relations of the improved bound with other two bounds in the literature for maximum cut problem. It worths pointing out that our approach can be easily extended to deal with binary quadratic programming problem with linear constraints.

A key issue in utilizing the improved bound proposed in this paper is the computation of δ. We have established the connection between the computation of δ and the cell enumeration of hyperplane arrangement. As the total number of the cells grows in $O(n^r)$, calculating the distance δ by enumerating all the cells is computationally expensive when r is large. Nevertheless, an improved lower bound of $v(P)$ can be still obtained if a positive lower bound of δ can be estimated. In fact, for any $0 < \underline{\delta} \le \delta$, it follows from (3.3) that

$$\tilde{v} = v(D) + \xi_{r+1}\underline{\delta}^2 \tag{5.1}$$

is still a lower bound of $v(P)$. A simple way for estimating the lower bound of δ is to consider the origin-centered sphere $S_0 = \{x \in \mathbb{R}^n \mid \|x\| \le \sqrt{n}\}$. Since $\{-1,1\}^n \subset [-1,1]^n \subset S_0$, we have $0 \le \underline{\delta}_1 = \|x^0\| - \sqrt{n} \le \delta$ when $S_0 \cap C = \emptyset$. Furthermore, since $\underline{\delta}_1 \le \underline{\delta}_2 = \text{dist}([-1,1]^n, C) \le \delta$ when $[-1,1]^n \cap C = \emptyset$, solving convex quadratic programming problem

$$\begin{aligned} \underline{\delta}_2 = &\min \ \|x - Vz - x^0\|^2 \\ &\text{s.t.} \ \ 0 \le x_i \le 1, \; i = 1, \dots, n, \\ &\qquad z \in \mathbb{R}^r \end{aligned}$$

provides an improved lower bound for δ.

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