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Binary quadratic optimization problems that are difficult to solve by conic relaxations

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ABSTRACT

We study conic relaxations including semidefinite programming (SDP) relaxations and doubly nonnegative programming (DNN) relaxations to find the optimal values of binary QOPs. The main focus of the study is on how the relaxations perform with respect to the rank of the coefficient matrix in the objective of a binary QOP. More precisely, for a class of binary QOP instances, which include the max-cut problem of a graph with an odd number of nodes and equal weight, we show numerically that (1) neither the standard DNN relaxation nor the DNN relaxation derived from the completely positive formulation by Burer performs better than the standard SDP relaxation, and (2) Lasserre's hierarchy of SDP relaxations requires solving the SDP with the relaxation order at least $\lceil n/2 \rceil$ to attain the optimal value. The bound $\lceil n/2 \rceil$ for the max-cut problem of a graph with equal weight is consistent with Laurent's conjecture in 2003, which was proved recently by Fawzi, Saunderson and Parrilo in 2015.

1. Introduction

We consider quadratic optimization problems (QOPs):

$$\zeta(\boldsymbol{Q}, A) = \min \left\{ \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} \mid \boldsymbol{x} = (x_1, \ldots, x_m)^T \in A \right\}, \tag{1}$$

where $\boldsymbol{Q}$ is an $n \times n$ real symmetric matrix and $A \subset \mathbb{R}^n$ is the set of constraints described in terms of quadratic equalities and inequalities. Throughout the paper, we denote QOP (1) by QOP($\boldsymbol{Q}, A$).

Let

$$B_0 = \{0,1\}^n = \{\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n : x_i^2 - x_i = 0 \ (i = 1, 2, \ldots, n)\},$$
$$B_1 = \{-1,1\}^n = \{\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n : x_i^2 - 1 = 0 \ (i = 1, 2, \ldots, n)\}.$$

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Then, binary QOPs can be expressed as QOP($\boldsymbol{Q}, B_0$) and QOP($\boldsymbol{Q}, B_1$) by taking $A = B_0$ or $A = B_1$ in (1). This class of binary QOPs includes the max-cut problem [1] as an important application. Both QOP($\boldsymbol{Q}, B_0$) and QOP($\boldsymbol{Q}, B_1$) are known to be NP-hard.

For general QOPs, various linear conic relaxations have been proposed and extensively studied. Semidefinite programming (SDP) relaxations are regarded as popular techniques for computing lower bounds of the optimal values of QOPs. Lower bounds for (1) obtained by the SDP relaxations, however, may not be tight in many applications. For a stronger conic relaxation than the SDP relaxations, Burer [2] reformulated a class of linearly constrained QOPs with binary and continuous variables as completely positive programming (CPP) problems and proved that the reformulated CPP problem is equivalent to the original QOP. It is, however, numerically intractable.

As a numerically tractable relaxation of the CPP reformulation of QOPs, a simplified doubly nonnegative programming (DNN) relaxation was proposed by Arima, Kim, and Kojima in [3]. They showed through numerical results on binary QOP($\boldsymbol{Q}, B_0$) that the simplified DNN relaxation is stronger, but, it is still much more computationally costly than the standard SDP relaxation. More recently, Kim, Kojima and Toh [4] further applied the Lagrangian relaxation to the simplified DNN relaxation. They showed that a first-order method based on their Lagrangian-DNN relaxation performed efficiently and effectively in computation when it was tested on binary QOPs, quadratic multiple knapsack problems, maximum stable set problems, and quadratic assignment problems.

The lower bounds obtained by the simplified DNN relaxation and the Lagrangian-DNN relaxation for a given QOP are not equal to the optimal value in general, although they were shown to be effective in practice. On the other hand, if we consider a QOP as a special case of a polynomial optimization problem (POP), then we can apply the hierarchy of SDP relaxations proposed for general POPs by Lasserre [5] to QOPs. In particular, when it is applied to binary QOPs, the nth SDP in the hierarchy (or the SDP with the relaxation order $\omega = n$ in the terminology used in [6,7]), which involves $2^n - 1$ independent variables, attains the optimal value [8]. In practice, a small relaxation order (*e.g.*, $\omega \leq 4$) is usually sufficient to compute an accurate lower bound of the optimal value of a QOP [6,7].

For the problem of finding the cut polytope of the complete graph K_n with n nodes, Laurent in [9] conjectured that the lower bound for the number of iterations in Lasserre's semidefinite hierarchy is $\lceil n/2 \rceil$. As the size of the SDP relaxation in Lasserre's hierarchy increases exponentially with the relaxation order, the bound $\lceil n/2 \rceil$ in her work shows the amount of work required in solving the problem to optimality. The problem considered in [9] does not include any condition on the weights of K_n. Recently, Fawzi, Saunderson and Parrilo [10] proved the conjecture by applying their results on a finite abelian group to the binary QOPs. More recently, this result is extended to binary polynomial optimization problems in [11].

In this paper, we present numerical examples of binary QOPs with dimension $n \in \{3, 4, \ldots, 11\}$ for which

(i) neither the standard DNN relaxation nor the DNN relaxation derived from the CPP reformulation is effective in terms of obtaining tight bounds for the problems.
(ii) the hierarchy of SDP relaxation requires at least $\omega = \lceil n/2 \rceil$th SDP ($\lceil n/2 \rceil$-SDP) to attain the optimal value. Specifically, we show numerically that the rank of the coefficient matrix $\boldsymbol{Q}$ of the objective function plays an important role on ω.

While the DNN relaxations are expected to be stronger than the standard SDP relaxation, they do not provide tighter lower bounds for the binary QOP examples given in this paper. These problems turned out to be difficult to solve by the conic relaxations. If tighter bounds are obtained by a conic relaxation proposed for the problems, then the proposed relaxation can be regarded as a stronger relaxation than the DNN relaxations discussed in this paper. In this sense, the problems can be used to evaluate conic relaxation methods developed for binary QOPs.

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Table 1
Numerical results on SDP and DNN relaxations.

n	$\zeta(\boldsymbol{E})$	$\eta_s(\boldsymbol{E})$	$\eta_{d1}(\boldsymbol{F})+n^2$	$\eta_{d2}(\boldsymbol{F})+n^2$
3	1	+6.66e−16	−8.24e−10	−1.83e−09
5	1	+8.01e−09	−1.93e−09	−1.22e−08
7	1	+1.84e−14	−1.87e−08	−1.96e−09
9	1	+9.59e−09	−1.01e−08	−3.40e−08
11	1	+1.72e−12	−1.56e−08	−4.25e−09

In Section 2, we describe the SDP relaxation, the standard DNN relaxation, and the DNN relaxation derived from the CPP reformulation. In Section 3, we state our numerical results and numerical evidence for (i) and (ii). In addition, we provide two classes of binary QOPs which are difficult to solve by the standard DNN relaxation, the DNN relaxation derived from the CPP reformulation and the hierarchy of SDP relaxation as their dimension increases. In Section 4, we discuss the bound $\lceil n/2 \rceil$. Finally, we conclude in Section 5.

2. Preliminaries

2.1. SDP relaxation (s) of QOP($\boldsymbol{Q}, B_1$)

Let $\mathbb{S}^n$ be the space of $n \times n$ symmetric matrices and $\boldsymbol{Q} \in \mathbb{S}^n$. We rewrite QOP($\boldsymbol{Q}, B_1$) as

$$\text{minimize } \boldsymbol{Q} \bullet \boldsymbol{x}\boldsymbol{x}^T \quad \text{subject to } x_i^2 = 1 \ (i = 1, 2, \ldots, n).$$

Obviously, $\boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n_+$ holds for every $\boldsymbol{x} \in \mathbb{R}^n$. If $\boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n_+$ is replaced by a single symmetric matrix variable $\boldsymbol{X}$, the standard SDP relaxation (s) of QOP($\boldsymbol{Q}, B_1$) is obtained:

$$\text{(s)} : \text{minimize } \boldsymbol{Q} \bullet \boldsymbol{X} \quad \text{subject to } X_{ii} = 1 \ (i = 1, 2, \ldots, n), \ \boldsymbol{X} \in \mathbb{S}^n_+.$$

Here $\boldsymbol{Q} \bullet \boldsymbol{X}$ denotes the inner product of $\boldsymbol{Q}$ and $\boldsymbol{X}$; $\boldsymbol{Q} \bullet \boldsymbol{X} = \sum_{i=1}^n \sum_{j=1}^n Q_{ij} X_{ij}$. Problem ($s$) is equivalent to QOP($\boldsymbol{Q}, B_1$) if it includes the constraint rank($\boldsymbol{X}$) = 1.

Now suppose that $n \geq 2$ and $\boldsymbol{Q} = \boldsymbol{E} \in \mathbb{S}^n$, where $\boldsymbol{E}$ denotes the $n \times n$ matrix of all 1's. Then, it is easy to verify that $\boldsymbol{X} \in \mathbb{S}^n$ with $X_{ii} = 1$ $(i = 1, 2, \ldots, n)$ and $X_{ij} = X_{ji} = -1/(n-1)$ $(1 \leq i < j \leq n)$ is an optimal solution of (s), and that the optimal value is zero. This shows that the optimal value of (s) is 0, which will also be shown numerically in Table 1 for $n = 3, 5, 7, 9, 11$ in Section 3.

2.2. DNN relaxation (d1) of QOP($\boldsymbol{R}, B_0$)

Let $\boldsymbol{R} \in \mathbb{S}^n$. We write QOP($\boldsymbol{R}, B_0$) as

$$\text{minimize } \begin{pmatrix} 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{R} \end{pmatrix} \bullet \begin{pmatrix} 1 & \boldsymbol{y}^T \\ \boldsymbol{y} & \boldsymbol{y}\boldsymbol{y}^T \end{pmatrix} \quad \text{subject to } y_i^2 - y_i = 0 \ (i = 1, 2, \ldots, n).$$

Note that $\begin{pmatrix} 1 & \boldsymbol{y}^T \\ \boldsymbol{y} & \boldsymbol{y}\boldsymbol{y}^T \end{pmatrix}$ is contained in the intersection of $\mathbb{S}^{1+n}_+$ and the cone $\mathbb{N}^{1+n}$ of $(1+n) \times (1+n)$ nonnegative symmetric matrices. If $\boldsymbol{y}\boldsymbol{y}^T$ is replaced by a single symmetric matrix variable $\boldsymbol{Y}$, the following standard DNN relaxation (d1) of QOP($\boldsymbol{R}, B_0$) is obtained:

$$\text{(d1)} : \begin{array}{ll} \text{minimize} & \boldsymbol{R} \bullet \boldsymbol{Y} \\ \text{subject to} & y_i = Y_{ii} \ (i = 1, 2, \ldots, n), \ \begin{pmatrix} 1 & \boldsymbol{y}^T \\ \boldsymbol{y} & \boldsymbol{Y} \end{pmatrix} \in \mathbb{S}^{1+n}_+ \cap \mathbb{N}^{1+n}. \end{array}$$

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Let $\mathrm{diag}(\boldsymbol{v})$ be a diagonal matrix whose diagonal is $\boldsymbol{v} \in \mathbb{R}^n$. For every $\boldsymbol{Q} \in \mathbb{S}^n$, QOP$(\boldsymbol{Q}, B_1)$ can be converted to an equivalent binary QOP$(\boldsymbol{R}, B_0)$, where $\boldsymbol{R} = 4(\boldsymbol{Q} - \mathrm{diag}(\boldsymbol{Qe}))$ and $\boldsymbol{e} = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$. In fact, if an affine transformation $\boldsymbol{x} = 2\boldsymbol{y} - \boldsymbol{e}$ is applied to QOP$(\boldsymbol{Q}, B_1)$, then

$$\boldsymbol{y} \in \{0,1\}^n \quad \text{if and only if } \boldsymbol{x} \in \{-1,1\}^n,$$
$$\boldsymbol{x}^T\boldsymbol{Qx} = 4\boldsymbol{y}^T\boldsymbol{Qy} - 4\boldsymbol{e}^T\boldsymbol{Qy} + \boldsymbol{e}^T\boldsymbol{Qe} = \boldsymbol{y}^T\boldsymbol{Ry} + \boldsymbol{e}^T\boldsymbol{Qe} \quad \text{for every } \boldsymbol{y} \in \{0,1\}^n.$$

Here the last equality follows from $\boldsymbol{e}^T\boldsymbol{Qy} = \boldsymbol{y}^T\mathrm{diag}(\boldsymbol{Qe})\boldsymbol{y}$ for every $\boldsymbol{y} \in \{0,1\}^n$. Therefore, $\zeta(\boldsymbol{Q}, B_1) = \zeta(\boldsymbol{R}, B_0) + \boldsymbol{e}^T\boldsymbol{Qe}$. Specifically, if $\boldsymbol{F} = 4(\boldsymbol{E} - n\boldsymbol{I})$, then $\zeta(\boldsymbol{E}, B_1) = \zeta(\boldsymbol{F}, B_0) + n^2$.

Let $\eta_s(\boldsymbol{Q})$ and $\eta_{d1}(\boldsymbol{Q})$ denote the lower bounds for the optimal value of QOP$(\boldsymbol{Q}, B_1)$ obtained by the SDP relaxation (s) and DNN relaxation (d1), respectively. From $\zeta(\boldsymbol{Q}, B_1) = \zeta(\boldsymbol{R}, B_0) + \boldsymbol{e}^T\boldsymbol{Qe}$, we have that $\eta_s(\boldsymbol{Q}) \leq \eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T\boldsymbol{Qe} \leq \zeta(\boldsymbol{Q}, B_1)$. That is, the lower bound $\eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T\boldsymbol{Qe}$ obtained by the standard DNN relaxation (d1) of QOP$(\boldsymbol{R}, B_0)$ for the optimal value $\zeta(\boldsymbol{Q}, B_1)$ of QOP$(\boldsymbol{Q}, B_1)$ is at least as tight as the lower bound $\eta_s(\boldsymbol{Q})$ by the standard SDP relaxation (s). To see this, suppose that $\begin{pmatrix} 1 & \boldsymbol{y}^T \\ \boldsymbol{y} & \boldsymbol{Y} \end{pmatrix} \in \mathbb{S}^{1+n}$ is a feasible solution of (d1). Let $\boldsymbol{X} = 4\boldsymbol{Y} - 2\boldsymbol{ey}^T - 2\boldsymbol{ye}^T + \boldsymbol{ee}^T$. Then

$$\boldsymbol{Q} \bullet \boldsymbol{X} = 4\boldsymbol{Q} \bullet \boldsymbol{Y} - 4\boldsymbol{e}^T\boldsymbol{Qy} + \boldsymbol{e}^T\boldsymbol{Qe} = \boldsymbol{R} \bullet \boldsymbol{Y} + \boldsymbol{e}^T\boldsymbol{Qe}.$$

Here the last equality follows from $y_i = Y_{ii}$ $(i = 1, 2, \ldots, n)$. Using $\boldsymbol{Y} \succeq \boldsymbol{yy}^T$, we have that

$$\boldsymbol{X} \succeq 4\boldsymbol{yy}^T - 2\boldsymbol{ey}^T - 2\boldsymbol{ye}^T + \boldsymbol{ee}^T = (2\boldsymbol{y} - \boldsymbol{e})(2\boldsymbol{y} - \boldsymbol{e})^T \succeq \mathbf{O}.$$

From $y_i = Y_{ii}$ $(i = 1, 2, \ldots, n)$, $X_{ii} = 1$ $(i = 1, 2, \ldots, n)$ follows. Therefore, we have shown that $\boldsymbol{X}$ is a feasible solution of (s) with the objective value $\boldsymbol{R} \bullet \boldsymbol{Y} + \boldsymbol{e}^T\boldsymbol{Qe}$, which implies $\eta_s(\boldsymbol{Q}) \leq \eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T\boldsymbol{Qe}$.

2.3. DNN relaxation (d2) derived from a CPP reformulation of QOP$(\boldsymbol{R}, B_0)$

Let $\boldsymbol{R} \in \mathbb{S}^n$. To describe the DNN relaxation (d2) of QOP$(\boldsymbol{R}, B_0)$, we convert QOP$(\boldsymbol{R}, B_0)$ into

$$\begin{array}{lll} \text{minimize} & \boldsymbol{y}^T\boldsymbol{Ry} & \\ \text{subject to} & y_i^2 - y_i = 0 \ (i = 1, 2, \ldots, n), & (2) \\ & \left.\begin{array}{l} u_i^2 - u_i = 0 \ (i = 1, 2, \ldots, n), \ \boldsymbol{y} + \boldsymbol{u} = \boldsymbol{e}, \\ \boldsymbol{y} \geq \boldsymbol{0}, \ \boldsymbol{u} \geq \boldsymbol{0}, \ \displaystyle\sum_{i=1}^n y_i u_i = 0. \end{array}\right\} & (3) \end{array}$$

Here $\boldsymbol{u} \in \mathbb{R}^n$ serves as a vector of slack variables, (2) indicates the entire problem and the constraints in (3) are called as the added constraints. The added constraints (3) are redundant for QOP$(\boldsymbol{R}, B_0)$, but the DNN relaxation derived from QOP$(\boldsymbol{R}, B_0)$ with the added constraints is stronger than the DNN relaxation (d1). In particular, the last three constraints in (3) form a complementarity condition on $\boldsymbol{y} \in \mathbb{R}^n$ and $\boldsymbol{u} \in \mathbb{R}^n$.

We derive the DNN relaxation (d2). Let

$$\boldsymbol{A} = (-\boldsymbol{e} \ \boldsymbol{I} \ \boldsymbol{I}), \qquad \boldsymbol{H}_1 = \boldsymbol{A}^T\boldsymbol{A}, \qquad \boldsymbol{H}_2 = \begin{pmatrix} 0 & \boldsymbol{0}^T & \boldsymbol{0}^T \\ \boldsymbol{0} & \mathbf{O} & \boldsymbol{I} \\ \boldsymbol{0} & \boldsymbol{I} & \mathbf{O} \end{pmatrix}.$$

Then, we can rewrite (2) as

$$\begin{array}{ll} \text{minimize} & \boldsymbol{R} \bullet \boldsymbol{yy}^T \\ \text{subject to} & y_0 = 1, \ \boldsymbol{H}_k \bullet \begin{pmatrix} y_0 & \boldsymbol{y}^T & \boldsymbol{u}^T \\ \boldsymbol{y} & \boldsymbol{yy}^T & \boldsymbol{yu}^T \\ \boldsymbol{u} & \boldsymbol{uy}^T & \boldsymbol{uu}^T \end{pmatrix} = 0 \ (k = 1, 2), \end{array}$$

$$\begin{aligned}&y_0 = 1, \quad \boldsymbol{y} \geq \boldsymbol{0}, \ \boldsymbol{u} \geq \boldsymbol{0}, \\ &y_i^2 - y_i = 0 \quad (i = 1, 2, \ldots, n), \qquad u_i^2 - u_i = 0 \quad (i = 1, 2, \ldots, n).\end{aligned}$$

We note that for every $y_0 \geq 0$, $\boldsymbol{y} \geq \boldsymbol{0}$ and $\boldsymbol{u} \geq \boldsymbol{0}$, the matrix $\begin{pmatrix} y_0 & \boldsymbol{y}^T & \boldsymbol{u}^T \\ \boldsymbol{y} & \boldsymbol{y}\boldsymbol{y}^T & \boldsymbol{y}\boldsymbol{u}^T \\ \boldsymbol{u} & \boldsymbol{u}\boldsymbol{y}^T & \boldsymbol{u}\boldsymbol{u}^T \end{pmatrix}$ lies in the cone of $(1+2n) \times (1+2n)$ completely positive matrices $\mathbb{C}^{1+2n}$, which is included in the intersection of $\mathbb{S}_+^{1+2n}$ and $\mathbb{N}^{1+2n}$.

As a conic relaxation of QOP$(\boldsymbol{R}, B_0)$, we obtain a linear conic optimization problem:

$$\text{LCOP}(\mathbb{K}): \begin{cases} \text{minimize} & \boldsymbol{R} \bullet \boldsymbol{Y} \\ \text{subject to} & y_0 = 1, \quad \boldsymbol{H}_k \bullet \begin{pmatrix} y_0 & \boldsymbol{y}^T & \boldsymbol{u}^T \\ \boldsymbol{y} & \boldsymbol{Y} & \boldsymbol{W}^T \\ \boldsymbol{u} & \boldsymbol{W} & \boldsymbol{U} \end{pmatrix} = 0 \ (k = 1, 2), \\ & y_0 = 1, \quad Y_{ii} - y_i = 0 \ (i = 1, 2, \ldots, n), \\ & U_{ii} - u_i = 0 \quad (i = 1, 2, \ldots, n), \\ & \begin{pmatrix} y_0 & \boldsymbol{y}^T & \boldsymbol{u}^T \\ \boldsymbol{y} & \boldsymbol{Y} & \boldsymbol{W}^T \\ \boldsymbol{u} & \boldsymbol{W} & \boldsymbol{U} \end{pmatrix} \in \mathbb{K}, \end{cases}$$

where $\mathbb{K}$ stands for either $\mathbb{C}^{1+2n}$ (the CPP cone) or $\mathbb{S}_+^{1+2n} \cap \mathbb{N}^{1+2n}$ (the DNN cone). We denote the latter, a DNN relaxation LCOP$(\mathbb{S}_+^{1+2n} \cap \mathbb{N}^{1+2n})$, by (d2).

If the complementarity constraint $\sum_{i=1}^n y_i u_i = 0$ is removed in the previous discussion, the resulting LCOP$(\mathbb{K})$ does not involve the equality constraint $\boldsymbol{H}_2 \bullet \begin{pmatrix} y_0 & \boldsymbol{y}^T & \boldsymbol{u}^T \\ \boldsymbol{y} & \boldsymbol{Y} & \boldsymbol{W}^T \\ \boldsymbol{u} & \boldsymbol{W} & \boldsymbol{U} \end{pmatrix} = 0$. In this case, the previous construction of LCOP$(\mathbb{C}^{1+2n})$ corresponds to the CPP reformulation of QOP$(\boldsymbol{R}, B_0)$, which was shown to be equivalent to QOP$(\boldsymbol{R}, B_0)$ in a more general framework for a class of linearly constrained QOPs in continuous and binary variables by Burer [2].

On the other hand, if the 0-1 constraints $y_i^2 - y_i = 0$, $u_i^2 - u_i = 0$ $(i = 1, 2, \ldots, n)$ are removed from (2) and all the other constraints remain, then the resulting CPP or DNN relaxation LCOP$(\mathbb{K})$ do not include the constraints $Y_{ii} - y_i = 0$, $U_{ii} - u_i = 0$ $(i = 1, 2, \ldots, n)$. This construction corresponds to the simplified CPP and DNN relaxation of QOP$(\boldsymbol{R}, B_0)$ by Arima, Kim and Kojima in [3]. The simplified CPP relaxation is also equivalent to QOP$(\boldsymbol{R}, B_0)$. See [3] for more details.

If we take $\boldsymbol{R} = 4(\boldsymbol{Q} - \text{diag}(\boldsymbol{Q}\boldsymbol{e}))$, then the DNN relaxation (d2), which corresponds to LCOP$(\mathbb{S}_+^{1+2n} \cap \mathbb{N}^{1+2n})$, is the strongest relaxation of QOP$(\boldsymbol{Q}, B_1)$ among (s), (d1) and (d2); $\eta_s(\boldsymbol{Q}) \leq \eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T\boldsymbol{Q}\boldsymbol{e} \leq \eta_{d2}(\boldsymbol{R}) + \boldsymbol{e}^T\boldsymbol{Q}\boldsymbol{e} \leq \zeta(\boldsymbol{Q}, B_1)$, where $\eta_{d2}(\boldsymbol{R})$ denotes the lower bound for the optimal value of QOP$(\boldsymbol{R}, B_0)$ obtained by the DNN relaxation (d2).

Suppose that $n \geq 3$ is odd. Let $\boldsymbol{Q} = \boldsymbol{E} \in \mathbb{S}^n$, $\boldsymbol{R} = \boldsymbol{F} = 4(\boldsymbol{E} - n\boldsymbol{I})$, $\boldsymbol{y} = (1/2)\boldsymbol{e} \in \mathbb{R}^n$, and $\boldsymbol{Y}$ be a matrix in $\mathbb{S}^n$ defined by

$$Y_{ii} = y_i = 1/2 \quad (i = 1, 2, \ldots, n), \qquad Y_{ij} = Y_{ji} = (n-2)/(8\lfloor n/2 \rfloor) \quad (1 \leq i < j \leq n).$$

Then, we can verify that $(\boldsymbol{y}, \boldsymbol{Y})$ is a feasible solution of (d1) with $\boldsymbol{R} = 4(\boldsymbol{E} - n^2\boldsymbol{I})$, and that the objective value is $-n^2$. Hence $\eta_{d2}(\boldsymbol{F}) + n^2 \leq 0$. From the discussion in Sections 2.1 and 2.2, we know that $0 = \eta_s(\boldsymbol{E}) \leq \eta_{d2}(\boldsymbol{F}) + n^2$. Consequently, $\eta_{d2}(\boldsymbol{F}) + n^2 = 0$.

2.4. Relation between QOP$(\boldsymbol{Q}, B_1)$ and QOP$(\boldsymbol{R}, B_0)$

For a given $\boldsymbol{Q} \in \mathbb{S}^n$, we have seen that QOP$(\boldsymbol{Q}, B_1)$ is equivalent to QOP$(\boldsymbol{R}, B_0)$ with $\boldsymbol{R} = 4(\boldsymbol{Q} - \text{diag}(\boldsymbol{Q}\boldsymbol{e})\boldsymbol{I})$ and $\zeta(\boldsymbol{Q}, B_1) = \zeta(\boldsymbol{R}, B_0) + \boldsymbol{e}^T\boldsymbol{Q}\boldsymbol{e}$. We note that if $\boldsymbol{x} \in \mathbb{R}^n$ is a feasible solution of QOP$(\boldsymbol{Q}, B_1)$ with the objective value $\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x}$, then $-\boldsymbol{x}$ is a feasible solution with the same objective value. It means that the resulting QOP($\boldsymbol{R}, B_0$) also satisfies this symmetry. If $\boldsymbol{y} \in \mathbb{R}^n$ is a feasible solution of QOP($\boldsymbol{R}, B_0$) with the objective value $\boldsymbol{y}^T\boldsymbol{R}\boldsymbol{y}$, then $\boldsymbol{e} - \boldsymbol{y}$ is a feasible solution with the same objective value.

Now let $\boldsymbol{R} \in \mathbb{S}^n$. In general, QOP($\boldsymbol{R}, B_0$) does not satisfy the aforementioned symmetry. To convert QOP($\boldsymbol{R}, B_0$) into an equivalent QOP($\boldsymbol{Q}, B_1$), we need to increase the dimension of the problem or introduce an additional variable x_0 as shown in the following. Define

$$\boldsymbol{Q} = \frac{1}{4}\begin{pmatrix} \boldsymbol{e}^T\boldsymbol{R}\boldsymbol{e} & \boldsymbol{e}^T\boldsymbol{R} \\ \boldsymbol{R}\boldsymbol{e} & \boldsymbol{R} \end{pmatrix}.$$

Then, it is easy to verify that the QOP

$$\text{minimize } \boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} \quad \text{subject to } \boldsymbol{x} = (x_0, x_1, \dots, x_n) \in \{-1, 1\}^{1+n},\ x_0 = 1$$

is equivalent to QOP($\boldsymbol{R}, B_0$). Since this problem satisfies the symmetry, we can remove the constraint $x_0 = 1$, which results in QOP($\boldsymbol{Q}, B_1$) in $\mathbb{R}^{1+n}$.

3. Main result

We focus on solving QOP($\boldsymbol{Q}, B_1$) by varying the rank of $\boldsymbol{Q}$ from rank-1 $\boldsymbol{Q}$ to full rank $\boldsymbol{Q}$ and a convex combination of rank-1 and full rank $\boldsymbol{Q}$, using the conic relaxations mentioned in Section 2.

We first consider QOP($\boldsymbol{E}, B_1$) as an instance of binary QOPs. The objective quadratic function can be written as $\boldsymbol{x}^T\boldsymbol{E}\boldsymbol{x} = \left(\sum_{i=1}^n x_i\right)^2$. The optimal value $\zeta(\boldsymbol{E}, B_1)$ of QOP($\boldsymbol{E}, B_1$) is 1 if the dimension n is odd, and 0 otherwise. Since $\boldsymbol{x}^T\boldsymbol{E}\boldsymbol{x} = 2\sum_{1\le i<j\le n} x_i x_j + n$ holds for every $\boldsymbol{x} \in \{-1, 1\}^n$, QOP($\boldsymbol{E}, B_1$) corresponds to the max-cut problem with equal weight.

Lasserre in [8] showed that $\lceil n \rceil$-SDP in the hierarchy applied to QOP($\boldsymbol{Q}, B_1$) always attains the optimal value $\zeta(\boldsymbol{Q}, B_1)$ for every $\boldsymbol{Q} \in \mathbb{S}^n$, and $\lceil n \rceil$-SDP was reduced to $\lceil n/2 \rceil$-SDP in [9,10]. We will see from the numerical results in this section that it requires at least $\lceil n/2 \rceil$-SDP in the hierarchy to attain the optimal value $\zeta(\boldsymbol{E}, B_1) = 1$ when the dimension n is odd.

We consider the following conic relaxations discussed in Section 2.

- (s) the standard SDP relaxation of QOP($\boldsymbol{E}, B_1$),
- (d1) the standard DNN relaxation of QOP($\boldsymbol{F}, B_0$),
- (d2) the DNN relaxation derived from the CPP reformulation of QOP($\boldsymbol{F}, B_0$) [3,2],
- (h) the hierarchy of SDP relaxations of QOP($\boldsymbol{E}, B_1$) proposed by Lasserre [5].

The lower bound for the optimal value of QOP($\boldsymbol{Q}, B$) obtained by each relaxation is denoted by $\eta_s(\boldsymbol{Q})$, $\eta_{d1}(\boldsymbol{Q})$, $\eta_{d2}(\boldsymbol{Q})$ and $\eta_h(\boldsymbol{Q}, \omega)$, respectively. Here B stands for either B_1 or B_0, and ω denotes the relaxation order used in (h). Although it is known from the discussion in Section 2 that $\eta_s(\boldsymbol{Q}) \le \eta_{d1}(\boldsymbol{Q}) + \boldsymbol{e}^T\boldsymbol{Q}\boldsymbol{e} \le \eta_{d2}(\boldsymbol{Q}) + \boldsymbol{e}^T\boldsymbol{Q}\boldsymbol{e}$ for any $\boldsymbol{Q} \in \mathbb{S}^n$ by construction, (s) and (d1) are included to compare the tightness of the lower bounds. In addition, we could consider

- (h′) the hierarchy of SDP relaxations of QOP($\boldsymbol{F}, B_0$),

but (h) and (h′) are known to be equivalent [12]. For more details on (h), we refer to [5,8].

We report numerical results on the relaxation methods (s), (d1), (d2), and (h) applied to binary QOP($\boldsymbol{Q}, B_1$) and QOP($\boldsymbol{R}, B_0$), where $\boldsymbol{R} = 4(\boldsymbol{Q} - \text{diag}(\boldsymbol{Q}\boldsymbol{e}))$. All the experiments were performed in Matlab on a Mac Pro with 3.0 GHz 8-core Intel Xeon E5 CPU and 64 GB memory.

Table 1 shows the lower bounds obtained by the relaxation methods (s), (d1) and (d2). SparseCoLO [13] was used to convert the DNN problems (d1) and (d2) into SDPs, and SeDuMi [14] to solve SDPs. All the

Table 2
Numerical results on the hierarchy of SDP relaxations [5].

n	Opt	GloptiPoly		SparsePOP	
	$\zeta(\boldsymbol{E}, B_1)$	$\eta_h(\boldsymbol{E}, \lfloor n/2 \rfloor)$ (s)	$\eta_h(\boldsymbol{E}, \lceil n/2 \rceil)$ (s)	$\eta_h(\boldsymbol{E}, \lfloor n/2 \rfloor)$ (s)	$\eta_h(\boldsymbol{E}, \lceil n/2 \rceil)$ (s)
3	1	−1.11e−11 (0.1)	+9.999999993e−01 (0.1)	−8.56e−12 (0.1)	+9.999999983e−01 (0.1)
5	1	+8.39e−09 (0.1)	+1.000000002e+00 (1.1)	−2.78e−11 (0.1)	+9.999999987e−01 (0.1)
7	1	+2.30e−07 (11.8)	+1.000000049e+00 (678.1)	−5.65e−09 (0.5)	+9.999999941e−01 (6.1)
9	1	Not tested	Not tested	−7.93e−09 (50.7)	+9.999999332e−01 (591.2)
11	1	Not tested	Not tested	−1.32e−09 (11 182.2)	+9.999785904e−01 (54 716.8)

lower bounds $\eta_s(\boldsymbol{E})$, $\eta_{d1}(\boldsymbol{F}) + n^2$ and $\eta_{d2}(\boldsymbol{F}) + n^2$ are nearly 0, which is the trivial lower bound for the optimal value $\zeta(\boldsymbol{E}, B_1) = 1$ of QOP$(\boldsymbol{E}, B_1)$. We note that the values in Table 1 (and Table 2) must involve some numerical error. For example, $\eta_s(\boldsymbol{E}) \leq \eta_{d1}(\boldsymbol{F}) + n^2$ must hold theoretically since the lower bound provided by the standard DNN relaxation (d1) is at least as tight as the standard SDP relaxation (s). From Table 1, we see that all the methods (s), (d1), (d2) are not effective at all for QOP$(\boldsymbol{E}, B_1)$ and QOP$(\boldsymbol{F}, B_0)$ when n is odd. Theoretically, $\eta_s(\boldsymbol{E}) = \eta_{d1}(\boldsymbol{F}) + n^2 = 0$ if $n \geq 3$ is odd, as shown in Section 2.3.

In Table 2, we display the numerical results on the hierarchy of SDP relaxation (h) applied to QOP$(\boldsymbol{E}, B_1)$ with odd dimension $n = 3, 5, 7, 9, 11$. We used two software packages GloptiPoly [15] and SparsePOP [7] which implemented (h). SeDuMi [14] was used in the both software packages to solve the SDPs. GloptiPoly is designed to generate all optimal solutions when the optimal value is obtained. Although SparsePOP can only provide the optimal value of (h), it is faster and can deal with larger dimensional QOPs than GloptiPoly. In all cases of $n = 3, 5, 7, 9, 11$, the optimal value of the SDP relaxation of order $\lfloor n/2 \rfloor$ is close to the trivial bound 0, and the optimal value 1 is attained with relaxation order $\lceil n/2 \rceil$. For $n = 11$, we notice that the lower bound $\eta_h(11, \lceil 11/2 \rceil)$ obtained by SparsePOP displays a wider gap $1 - 9.999785904\text{e}-01 \geq 2.14\text{e}-05$ than the other cases. This is because SeDuMi, the SDP solver used in SparsePOP, stopped with numerical error before attaining the given accuracy 1.0e−9.

Remark. Both GloptiPoly and SparsePOP are designed to solve general POPs, thus their construction of SDP relaxation problems are not specialized for binary QOPs. We could considerably simplify SDP relaxation problems derived from binary QOPs to obtain smaller SDPs, which would enable us to solve large scale QOPs. However, the size of SDPs constructed this way still grows very rapidly as the dimension n of the binary QOP and the relaxation order ω increase. Therefore, binary QOP$(\boldsymbol{E}, B_1)$ that can be solved numerically by the hierarchy of SDP relaxation will still be limited to small-sized problems. See Section 4 and [8].

3.1. Even dimensional case

If $n = 2$, it is easy to see that $\eta_s(\boldsymbol{E}, B_1) = \zeta(\boldsymbol{E}, B_1)$. Let $\boldsymbol{X} = \begin{bmatrix} X_{11} & X_{12} \\ X_{12} & X_{22} \end{bmatrix} \in \mathbb{S}^2$. Then the standard SDP relaxation of (1) is

$$\min \boldsymbol{E} \bullet \boldsymbol{X} \quad \text{subject to } X_{11} = 1, X_{22} = 1, \boldsymbol{X} \succeq \mathbf{O}.$$

Clearly, $\boldsymbol{X}^* = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ is a feasible solution whose objective value $\boldsymbol{E} \bullet \boldsymbol{X}^*$ coincides with $\zeta(\boldsymbol{E}, B_1)$.

Suppose that $n \geq 4$ is even. Define the $n \times n$ rank-1 matrix $\boldsymbol{G} \in \mathbb{S}^n$ such that

$$\boldsymbol{G} = \begin{pmatrix} \boldsymbol{E} & \mathbf{0} \\ \mathbf{0}^T & 0 \end{pmatrix},$$

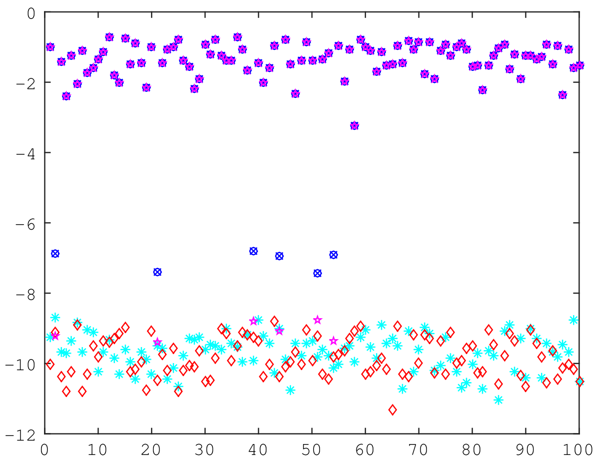

Fig. 1. 100 QOP($\boldsymbol{Q}, B_1$)s with randomly generated full rank $\boldsymbol{Q}$ solved by the standard DNN relaxation method ⊗, the DNN relaxation derived from the CPP reformulation ⋆, SparsePOP with $\omega = 2$ ∗ and SparsePOP with $\omega = 3$ ⋄. The vertical axis stands for the relative accuracy $\log_{10}((\zeta - \eta)/\max\{|\zeta|, 1.0\mathrm{e}-8\})$, where ζ is the optimal value of QOP($\boldsymbol{Q}, B_1$) and η the lower bound obtained by either of the relaxations mentioned above. The left figure shows for $n = 10$, and the right the change of the average relative accuracy over 100 QOP($\boldsymbol{E}, B_1$) (or QOP($\boldsymbol{F}, B_0$)) as the dimension n increases from $n = 2$ to $n = 10$.

where $\boldsymbol{E}$ denotes the $(n-1) \times (n-1)$-dimensional matrix of 1's. Obviously, QOP($\boldsymbol{G}, B_1$) in even number of variables $x_1, x_2, \ldots, x_n$ is equivalent to QOP($\boldsymbol{E}, B_1$) in odd number of variables $x_1, x_2, \ldots, x_{n-1}$ in the sense that $\zeta(\boldsymbol{G}, B_1) = \zeta(\boldsymbol{E}, B_1)$. If we define

$$\boldsymbol{H} = 4(\boldsymbol{G} - \mathrm{diag}(\boldsymbol{Ge})) = 4\begin{pmatrix} \boldsymbol{E} - (n-1)\boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0}^T & 0 \end{pmatrix},$$

then $\zeta(\boldsymbol{G}, B_1) = \zeta(\boldsymbol{H}, B_0) + (n-1)^2$. Hence $\zeta(\boldsymbol{H}, B_0) = \zeta(\boldsymbol{F}, B_0)$ holds. As a result, QOP($\boldsymbol{G}, B_1$) and QOP($\boldsymbol{H}, B_0$) in $\mathbb{R}^n$ can be regarded as binary QOPs obtained by introducing an additional variable x_n to QOP($\boldsymbol{E}, B_1$) and QOP($\boldsymbol{F}, B_0$) in $\mathbb{R}^{n-1}$, respectively. It is easy to verify that $\eta_s(\boldsymbol{G}) = \eta_s(\boldsymbol{E})$, $\eta_{d1}(\boldsymbol{H}) = \eta_{d1}(\boldsymbol{F})$, $\eta_{d2}(\boldsymbol{H}) = \eta_{d2}(\boldsymbol{F})$ and $\eta_h(\boldsymbol{G}, \omega) = \eta_h(\boldsymbol{E}, \omega)$ for every $\omega = 1, 2, \ldots$. Therefore, the discussions on binary QOP($\boldsymbol{E}, B_1$) and QOP($\boldsymbol{F}, B_0$) in the odd dimensional space $\mathbb{R}^{n-1}$ can be applied to ones on binary QOP($\boldsymbol{G}, B_1$) and QOP($\boldsymbol{H}, B_0$) in the even dimensional space $\mathbb{R}^n$. We note that $\lfloor n/2 \rfloor = \lceil n/2 \rceil = \lceil (n-1)/2 \rceil$.

3.2. Full rank binary QOPs vs. rank-1 binary QOPs

From the fact that the coefficient matrix $\boldsymbol{E}$ of the objective function of QOP($\boldsymbol{E}, B_1$) is of rank 1, it may be worthwhile to investigate that the rank of the coefficient matrix plays a role in failing to obtain a tight approximation to the true optimal value of QOP($\boldsymbol{E}, B_1$) by the relaxation methods (s), (d1), (d2) and (h).

We consider two types of coefficient matrices for QOP($\boldsymbol{Q}, B_1$) to examine whether the rank of $\boldsymbol{Q}$ affects the results of the conic relaxations. For the first type of $\boldsymbol{Q} \in \mathbb{S}^n$, each component $Q_{ij} \in \mathbb{R}$ $(1 \leq i \leq j)$ is randomly generated from $(100, -100)$. In this case, the matrix $\boldsymbol{Q}$ is of full rank, which can be checked in Matlab. For the second type, a rank-1 matrix $\boldsymbol{Q} = \boldsymbol{qq}^T \in \mathbb{S}^n$ is generated with each $q_i \in \mathbb{R}$ $(1 \leq i \leq n)$ chosen from $(10, -10)$.

Figs. 1 and 2 show numerical results on 100 cases of QOP($\boldsymbol{Q}, B_1$) with the two types of $\boldsymbol{Q}$'s. We observe that the two cases exhibit a clear difference. In the first case, 2-SDP in the hierarchy ∗ successfully generated tight lower bounds with respect to the relative accuracy $\log_{10}((\zeta - \eta)/\max\{|\zeta|, 1.0\mathrm{e}-8\})$. On the other hand, the quality of the lower bound obtained by 3-SDP in the hierarchy ⋄ deteriorates as the dimension n increases in the second case.

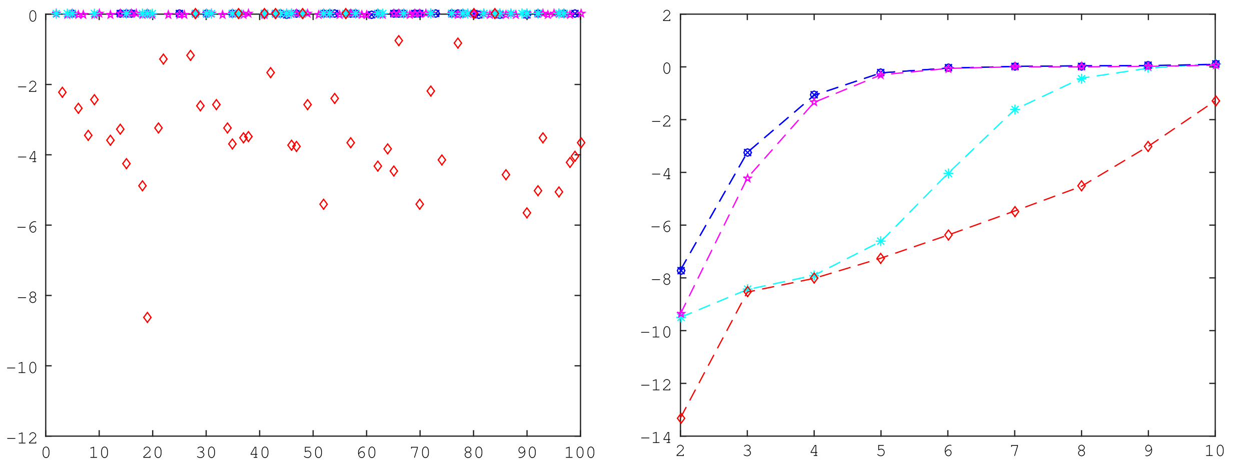

Fig. 2. 100 QOP($\boldsymbol{Q}, B_1$)s with randomly generated rank-1 $\boldsymbol{Q}$ solved by the standard DNN relaxation method ⊗, the DNN relaxation derived from the CPP reformulation ⋆, SparsePOP with $\omega = 2$ ∗ and SparsePOP with $\omega = 3$ ⋄. The vertical axis stands for the relative accuracy $\log_{10}((\zeta - \eta)/\max\{|\zeta|, 1.0\mathrm{e}-8\})$, where ζ is the minimum value of QOP($\boldsymbol{Q}, B_1$) and η the lower bound obtained by either of the relaxations mentioned above. The left figure displays for $n = 10$, and the right the change of the average relative accuracy over 100 BQOPs, as the dimension n increases from $n = 2$ to $n = 10$.

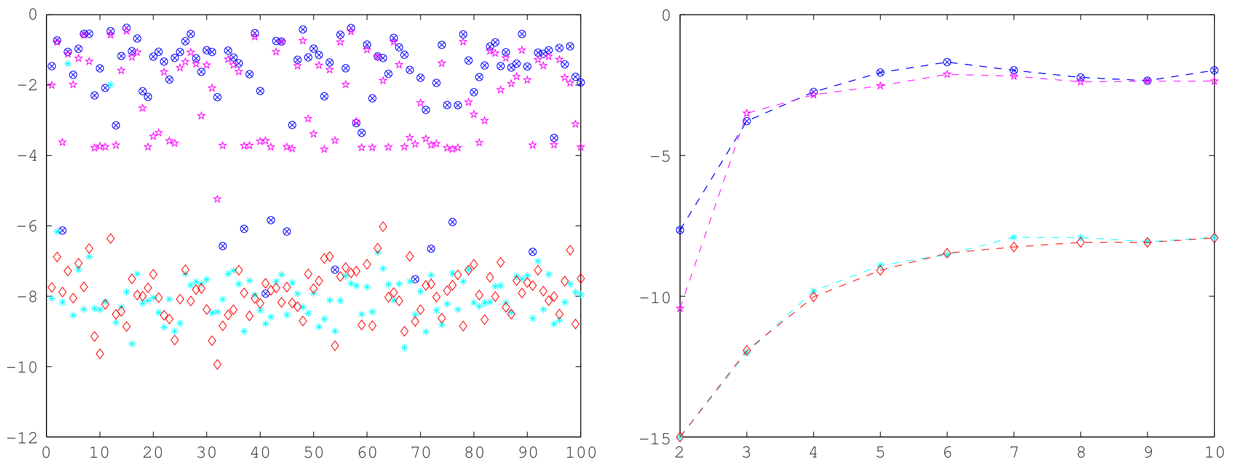

Fig. 3. 100 QOP($\boldsymbol{Q}, B_1$)s with randomly generated rank-2 $\boldsymbol{Q}$ solved by the standard DNN relaxation method ⊗, the DNN relaxation derived from the CPP reformulation ⋆, SparsePOP with $\omega = 2$ ∗ and SparsePOP with $\omega = 3$ ⋄. The meaning of the axes is the same as in the left figure in Fig. 1. The left figure shows for $n = 10$, and the right the change of the average relative accuracy over 100 QOP($\boldsymbol{E}, B_1$)s (or QOP($\boldsymbol{F}, B_0$)) as the dimension n increases from $n = 2$ to $n = 10$.

Since the relaxation methods are implemented with floating point double precision arithmetic, the rank of a matrix is determined based on a threshold value that decides whether a value should be treated as zero. In computation, the numerical rank of a matrix [16] becomes more meaningful than the theoretical rank. For instance, if rank-1 matrix $\boldsymbol{Q} = \boldsymbol{q}\boldsymbol{q}^T$ is slightly perturbed with a small number ϵ as $\overline{\boldsymbol{Q}} = \boldsymbol{Q} + \epsilon\boldsymbol{R}$, where $\boldsymbol{R} \in \mathbb{S}^n$ is a randomly generated matrix of rank n, then the rank of the perturbed matrix becomes n in theory. However, if ϵ is smaller than a given threshold value, the numerical rank of $\overline{\boldsymbol{Q}}$ remains as 1. Matlab provides "rank" command for the numerical rank with a threshold value.

We investigated the rank influence on obtaining the optimal value of QOP($\boldsymbol{Q}, B_1$). Figs. 3 and 4 show the results for $\boldsymbol{Q} \in \mathbb{S}^{10}$ of rank 2, 3 and 4. For the numerical experiments, we generated a symmetric matrix $\boldsymbol{P}$ where each element of $\boldsymbol{P}$ was randomly generated from $(100, -100)$ and obtained the eigen-decomposition as $\boldsymbol{P} = \sum_{i=1}^{n} \lambda_i \boldsymbol{q}_i \boldsymbol{q}_i^T$. Then, we chose $\boldsymbol{Q} = \sum_{i=1}^{r} \lambda_i \boldsymbol{q}_i \boldsymbol{q}_i^T$ by selecting λ_i's such that $\boldsymbol{Q}$ could not be positive

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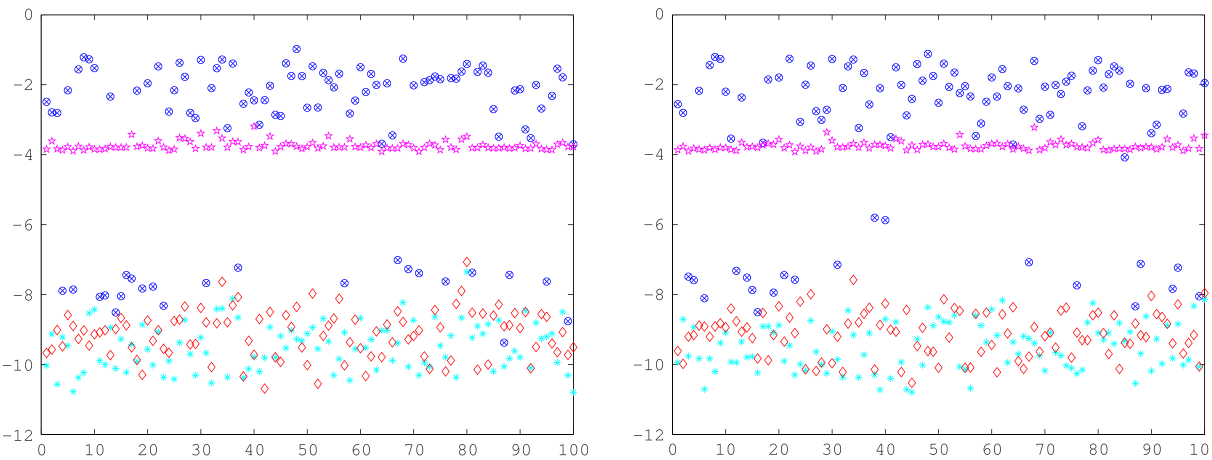

Fig. 4. 100 QOP($\boldsymbol{Q}$, B_1)s, where $\boldsymbol{Q}$ were randomly generated with $n = 10$ and $r = 3$ or 4, were solved by the standard DNN relaxation method ⊗, the DNN relaxation derived from the CPP reformulation ⋆, SparsePOP with $\omega = 2$ ∗ and SparsePOP with $\omega = 3$ ⋄. The meaning of the axes is the same as the left figure in Fig. 1. The left figure shows the results for $\boldsymbol{Q}$ of rank 3 and the right $\boldsymbol{Q}$ of rank 4.

definite, where r changes from 2 to 4. We observe that 2-SDP in the hierarchy ∗ and 3-SDP ⋄ generated tight lower bounds. The results obtained with $\boldsymbol{Q}$ of higher rank, from 5 to 9, were similar. Moreover, the results on QOP($\boldsymbol{Q}, B_1$) with positive and negative semidefinite $\boldsymbol{Q}$ of rank 2 to 9 were similar to those with $\boldsymbol{Q}$ of full rank. Thus, the numerical results show that QOP($\boldsymbol{Q}, B_1$) with rank-1 $\boldsymbol{Q}$ requires at least $\lceil n/2 \rceil$-SDP in the hierarchy, but QOP($\boldsymbol{Q}, B_1$) with $\boldsymbol{Q}$ of rank >1 can be solved by 2-SDP in the hierarchy.

3.3. A convex combination of QOP($\boldsymbol{E}, B_1$) and QOP($\boldsymbol{Q}^1, B_1$) with randomly generated $\boldsymbol{Q}^1$ of full rank

Although the binary QOP($\boldsymbol{E}, B_1$) with odd dimension is difficult to solve by the relaxation methods (s), (d1), (d2) and (h), it is certainly a trivial problem; the optimal value is 1 and each optimal solution $\boldsymbol{x}$ is characterized by the property that the number of $\{i : x_i = 1\}$ is either $\lfloor n/2 \rfloor$ or $\lceil n/2 \rceil$.

We note that not only the optimal value of QOP($\boldsymbol{Q}, B_1$) but also its lower bounds obtained by the relaxation methods are continuous functions of $\boldsymbol{Q}$. Thus, if $\boldsymbol{Q}$ is sufficiently close to $\boldsymbol{E}$, QOP($\boldsymbol{Q}, B_1$) remains difficult to solve by them. To see this, we now consider a convex combination $\boldsymbol{Q}(\lambda)$ of $\boldsymbol{E}$ and $\boldsymbol{Q}^1 \in \mathbb{S}^n$, where Q^1_{ij} $(1 \le i \le j \le n)$ is randomly chosen from $(-1, 1)$ and $\boldsymbol{Q}(\lambda) = (1-\lambda)\boldsymbol{E} + \lambda \boldsymbol{Q}^1$ for $\lambda \in [0, 1]$. The optimal value and optimal solution of QOP($\boldsymbol{Q}(\lambda), B_1$) are unknown. As λ increases, the difficulty of solving QOP($\boldsymbol{Q}(\lambda), B_1$) decreases as shown in Fig. 5. For $\lambda = 0.05$, the optimal value (the green line) and the lower bounds obtained by the standard DNN relaxation method ⊗, SparsePOP with $\omega = 2$ ∗ and SparsePOP with $\omega = 3$ ⋄ show a clear gap. As λ increases, the gap decreases. SparsePOP with both $\omega = 2$ ∗ and $\omega = 3$ ⋄ attains the optimal value accurately when λ is near 0.4.

4. $\lceil \frac{n}{2} \rceil$ bound

By the result in [8], we know that $\eta_h(\boldsymbol{Q}, \omega) \le \eta_h(\boldsymbol{Q}, \omega+1) \le \eta_h(\boldsymbol{Q}, n) = \zeta(\boldsymbol{Q}, B_1)$ for $\boldsymbol{Q} \in \mathbb{S}^n$ and every $\omega = 1, 2, \ldots, n-1$. From the numerical results shown in Table 2, the discussions in Section 3.1 and the results in [9–11], we have the following:

- there exists a $\widetilde{\boldsymbol{Q}} \in \mathbb{S}^n$ such that $\eta_h(\widetilde{\boldsymbol{Q}}, \omega) = \zeta(\boldsymbol{Q}, B_1) = 1$ if $\omega \ge \lceil n/2 \rceil$ and $\eta_h(\widetilde{\boldsymbol{Q}}, \omega) = 0$ otherwise; take $\widetilde{\boldsymbol{Q}} = \boldsymbol{E}$ if n is odd, and $\widetilde{\boldsymbol{Q}} = \boldsymbol{G}$ otherwise as shown in Section 3.1.

We discuss the implications of this result in this section.

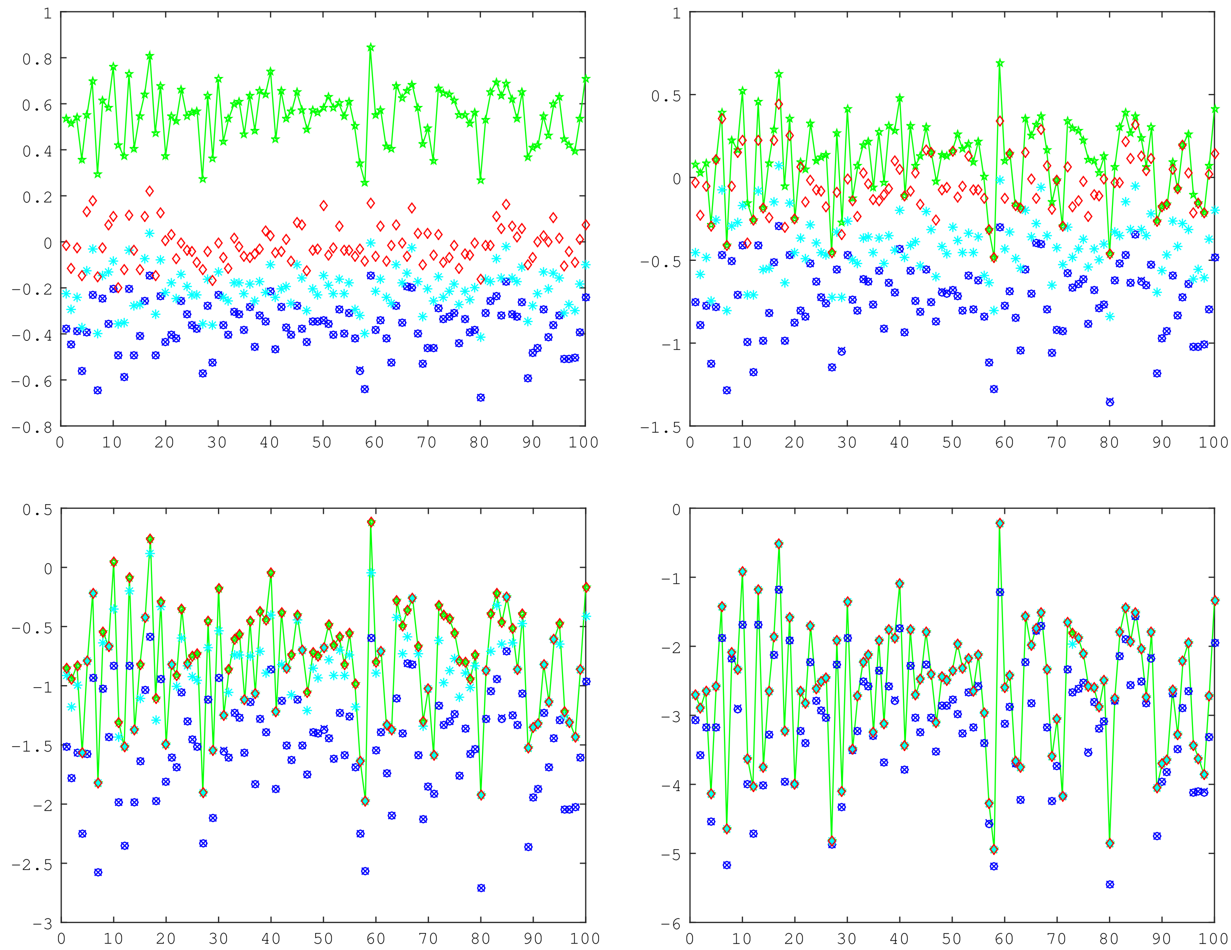

Fig. 5. 100 QOP($\boldsymbol{Q}(\lambda), B_1$)s with $\boldsymbol{Q}(\lambda) = (1-\lambda)\boldsymbol{E} + \lambda \boldsymbol{Q}^1$ solved by the standard DNN relaxation method $\otimes$, SparsePOP with $\omega = 2$ $*$ and SparsePOP with $\omega = 3$ $\diamond$. Here $\boldsymbol{Q}^1$ is a 7×7 symmetric matrix with each Q_{ij} randomly chosen from the interval $(-1, 1)$, $\boldsymbol{E}$ the 7×7 matrix of 1's, and $\lambda = 0.05,\ 0.10,\ 0.20$ and 0.40 (the upper left, the upper right, the bottom left, and the bottom right, respectively). The vertical axis stands for the minimum value of the QOP (the green), the lower bounds obtained by the standard DNN relaxation method $\otimes$, SparsePOP with $\omega = 2$ $*$ or SparsePOP with $\omega = 3$ $\diamond$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Recall that Laurent in [9] conjectured that the lower bound for the number of iterations in Lasserre's semidefinite hierarchies is $\lceil n/2 \rceil$ for the problem of finding the cut polytope of the complete graph K_n with n nodes, and that the conjecture was proved recently in [10]. The coefficient matrix $\boldsymbol{Q}$ of QOP($\boldsymbol{Q}, B_1$) corresponds to the weights of K_n in [9]. If the worst case complexity to solve a class of binary QOPs, $\{\mathrm{QOP}(\boldsymbol{Q}, B_1) : \boldsymbol{Q} \in \mathbb{S}^n\}$ by the hierarchy of SDP relaxation method is defined as

$$\omega^*(n) = \inf \left\{ \omega : \eta_h(\boldsymbol{Q}, \omega) = \zeta(\boldsymbol{Q}, B_1) \quad \text{for all } \boldsymbol{Q} \in \mathbb{S}^n \right\},$$

then the conjecture is described as $\omega^*(n) = \lceil n/2 \rceil$. Our discussion here is for $\widetilde{\boldsymbol{Q}}$ of QOP($\widetilde{\boldsymbol{Q}}, B_1$) instances that actually need the bound $\lceil \frac{n}{2} \rceil$, among all coefficient matrices.

For every $\omega = 1, 2, \ldots, n$, let

$$B_0(\omega) = \left\{ \boldsymbol{\alpha} \in B_0 : \sum_{i=1}^{n} \alpha_i = \omega \right\},$$

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$$C_0(\omega) = \left\{ \boldsymbol{\alpha} \in B_0 : \sum_{i=1}^n \alpha_i \leq \omega \right\} = \bigcup_{\xi \leq \omega} B_0(\xi),$$

$$\rho(\omega) = \text{the number of elements in } C_0(\omega) = \begin{cases} \displaystyle\sum_{k=0}^{\omega} \binom{n}{k} & \text{if } \omega < n, \\ 2^n & \text{otherwise.} \end{cases}$$

The hierarchy of SDP relaxation of QOP$(\boldsymbol{Q}, B_1)$ with the relaxation order ω is represented as

$$\mathrm{SDP}_\omega(\boldsymbol{Q}) : \ \eta_h(\boldsymbol{Q}, \omega) = \min \left\{ \sum_{\boldsymbol{\alpha} \in B_0(2)} \widehat{Q}_{\boldsymbol{\alpha}} y_{\boldsymbol{\alpha}} \ \middle| \ \widehat{\boldsymbol{M}}_\omega(\boldsymbol{y}) \succeq \mathbf{O} \right\}.$$

Here each $\widehat{Q}_{\boldsymbol{\alpha}}$ ($\boldsymbol{\alpha} \in B_0(2)$) corresponds to $2Q_{ij}$ or Q_{ii} such that $\widehat{Q}_{\boldsymbol{\alpha}} = 2Q_{ij}$ if $\alpha_i = 1$ and $\alpha_j = 1$ for some i, j ($1 \leq i < j \leq n$) and $\widehat{Q}_{\boldsymbol{\alpha}} = Q_{ii}$ if $\alpha_i = 2$ for some i ($1 \leq i \leq n$). $\widehat{\boldsymbol{M}}_\omega(\boldsymbol{y})$, a moment matrix for QOP$(\boldsymbol{Q}, B_1)$, is a $\rho(\omega) \times \rho(\omega)$ symmetric matrix whose element corresponds to a variable from the set $\{y_{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in C_0(2\omega)\}$ of variables. See [8] for more details. Since every variable of the set appears at least once in the moment matrix $\widehat{\boldsymbol{M}}_\omega(\boldsymbol{y})$ and $y_{\mathbf{0}}$ is fixed to 1, the number of independent variables involved in $\widehat{\boldsymbol{M}}_\omega(\boldsymbol{y})$ is $\rho(2\omega) - 1$. Thus the size $\rho(\omega)$ of the moment matrix $\widehat{\boldsymbol{M}}_\omega(\boldsymbol{y})$ and the number $\rho(2\omega) - 1$ of independent variables determine the size of SDP_ω to be solved for $\eta_h(\boldsymbol{Q}, \omega)$.

We now compare the size of $\mathrm{SDP}_{\lceil n/2 \rceil}(\widetilde{\boldsymbol{Q}})$ with that of $\mathrm{SDP}_n(\boldsymbol{Q})$ whose optimal value $\eta_h(\boldsymbol{Q}, n)$ is guaranteed to be $\zeta(\boldsymbol{Q}, B_1)$ for $\forall\ \boldsymbol{Q} \in \mathbb{S}^n$. In $\mathrm{SDP}_n(\boldsymbol{Q})$, the size of the moment matrix is $\rho(n) = 2^n$ and the number of independent variables is $\rho(2n) - 1 = 2^n - 1$. In $\mathrm{SDP}_{\lceil n/2 \rceil}(\widetilde{\boldsymbol{Q}})$, the two numbers are:

$$\rho(\lceil n/2 \rceil) = \sum_{k=0}^{\lceil n/2 \rceil} \binom{n}{k}, \qquad \rho(2\lceil n/2 \rceil) - 1 = 2^n - 1.$$

We observe that the size of $\mathrm{SDP}_{\lceil n/2 \rceil}$ for $\eta_h(\widetilde{\boldsymbol{Q}}, B_1, \lceil n/2 \rceil)$ is smaller than the size of SDP_n for $\eta_h(\boldsymbol{Q}, B_1, n)$, although the number of independent variables of $\mathrm{SDP}_{\lceil n/2 \rceil}$ is the same as that of SDP_n.

If $n \geq 3$ is odd, we see that

$$\begin{aligned} \rho(\lceil n/2 \rceil) &= \sum_{k=0}^{\lceil n/2 \rceil} \binom{n}{k} = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{k} + \binom{n}{\lceil n/2 \rceil} \\ &= \left(\sum_{k=0}^{n} \binom{n}{k} \right) /2 + \binom{n}{\lceil n/2 \rceil} = 2^{n-1} + \binom{n}{\lceil n/2 \rceil}. \end{aligned}$$

If $n \geq 4$ is even, then

$$\begin{aligned} \rho(\lceil n/2 \rceil) &= \sum_{k=0}^{\lceil n/2 \rceil} \binom{n}{k} = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{k} + \binom{n}{\lceil n/2 \rceil} /2 + \binom{n}{\lceil n/2 \rceil} /2 \\ &= \left(\sum_{k=0}^{n} \binom{n}{k} \right) /2 + \binom{n}{\lceil n/2 \rceil} /2 = 2^{n-1} + \binom{n}{\lceil n/2 \rceil} /2. \end{aligned}$$

In both cases, $2^{n-1} < \rho(\lceil n/2 \rceil) < 2^n$.

5. Concluding remarks

We have provided binary QOP instances that are difficult to solve by SDP and DNN relaxations. The instances are based on the max-cut problem of a graph with an odd number of nodes and equal weight. We

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have observed that the difficulty of solving the binary QOPs depends on the rank of the coefficient matrix of the objective of the binary QOP. The binary QOP takes a very simple form in the sense that it does not involve any other constraints than the ones requiring the variables binary. In connection with the difficulty of solving these binary QOPs, it is very interesting to mention that the randomized approximation algorithm using the standard SDP relaxation given by Goemans and Williamson [1] for the max-cut problem attains an optimal value of at least 0.87856 times the optimal value. Another problem known to be very difficult to solve is the quadratic assignment problem (QAP). The difficulty in this case rises from the size of the problem, too large to handle with available solution methods on a regular computer. Compared to the QAP, the size of the binary QOP instances presented in this paper is tiny, yet the SDP and DNN relaxations fail on the problems. Thus, any relaxation method that can approximately solve them can be regarded to have an advantage over the relaxation methods discussed in this paper.

If the hierarchy of SDP relaxation is employed for the binary QOP($\boldsymbol{Q}, B_1$), where $\boldsymbol{Q}$ is a $n \times n$ matrix of rank 1, the minimum relaxation order to solve them with high accuracy has been numerically confirmed to be $\omega = \lceil n/2 \rceil$. Since the size of the SDP relaxation in the hierarchy grows very rapidly as ω increases, the binary QOP instances with a moderate size cannot be solved by the hierarchy of SDP relaxation method. Therefore, the binary QOP instances presented in this paper can serve as challenging problems for developing conic relaxation methods in the future.

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