# Research Reports on Mathematical and Computing Sciences

Binary Quadratic Optimization Problems That Are Difficult to Solve by Conic Relaxations

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July 2015, B–481

Department of Mathematical and Computing Sciences Tokyo Institute of Technology

series B: Operations Research

## B-481 Binary Quadratic Optimization Problems That Are Difficult to Solve by Conic Relaxations

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July 10, 2015

Abstract. Binary quadratic optimization problems (QOPs) have been an important class of optimization problems for their wide range of applications. Binary QOPs are known to be NP-hard, and the optimal values and solutions of binary QOPs have been approximated by conic relaxations, including semidefinite programming (SDP) relaxations and doubly nonnegative programming (DNN) relaxations. It is known that if the hierarchy of SDP relaxation by Lasserre is applied to binary QOPs, then the *n*th SDP with  $2^n - 1$  variables is guaranteed to attain the optimal value. For some 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 is effective, and (2) the hierarchy of SDP relaxation requires solving at least  $\lceil n/2 \rceil$ th SDP to attain the optimal value.

**Key words.** Binary integer quadratic program, the max-cut problem with equal weight, conic relaxations, a hierarchy of semidefinite relaxations, inexact optimal values.

AMS Classification. 90C20, 90C22, 90C26

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## 1 Introduction

Quadratic optimization problems (QOPs) can be written as  $QOP(\boldsymbol{Q}, A)$ :

$$\zeta(\boldsymbol{Q}, A) = \min\left\{\boldsymbol{x}^{T}\boldsymbol{Q}\boldsymbol{x} \mid \boldsymbol{x} = (x_{1}, \dots, x_{m})^{T} \in A\right\},$$
(1)

where the constraint set A, a subset of the *n*-dimensional Euclidean space  $\mathbb{R}^n$ , is described in terms of quadratic equalities and inequalities, and Q is in the space of  $n \times n$  real symmetric matrices  $\mathbb{S}^n$ .

Let

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

If we take  $A = B_0$  or  $A = B_1$ , then (1) becomes binary QOPs, which are the main subject of this paper. This class of binary QOPs includes the max-cut problem [4] as an important application. Both  $\text{QOP}(\boldsymbol{Q}, B_0)$  and  $\text{QOP}(\boldsymbol{Q}, B_1)$  are simple but yet known to be NP-hard.

For general QOPs, various linear conic relaxations have been proposed and studied extensively. In particular, semidefinite programming (SDP) relaxations are the most popular technique for computing lower bounds of their optimal values. The SDP relaxation provides a lower bound for (1), which 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 showed that the reformulated CPP problem is equivalent to the original QOP. Thus, the resulting CPP is the strongest conic relaxation in theory. It is, however, numerically intractable.

As a numerically tractable relaxation of their CPP reformulation of QOPs, a simplified doubly nonnegative programming (DNN) relaxation was proposed by Airma, Kim, and Kojima in [1]. They showed through numerical results on binary  $\text{QOP}(\boldsymbol{Q}, B_0)$  that the simplified DNN relaxation is stronger, but, it is still much more expensive than the standard SDP relaxation. More recently, Kim, Kojima and Toh [6] further applied the Lagrangian relaxation to the simplified DNN relaxation. A first-order method based on their Lagrangian-DNN relaxation was shown to work efficiently and effectively in computation with numerical results 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 equivalent to the optimal value in general, although they were shown to be effective in practice. On the other hand, if we view a QOP as a special case of a polynomial optimization problem (POP), then we can apply the hierarchy of SDP relaxations proposed for genreal POPs by Lasserre [7] to QOPs. In particular, when it is applied to binary QOPs, the *n*th SDP in the hierarchy (or the SDP with the relaxation order  $\omega = n$  in the terminology used in [10, 11]), 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 [10, 11]. This article provides numerical examples of binary QOPs with dimension  $n \in \{3, 4, ..., 11\}$  for which

- (i) neither the standard DNN relaxation nor the DNN relaxation derived from the CPP reformulation is effective,
- (ii) the hierarchy of SDP relaxation requires at least  $\omega = \lceil n/2 \rceil$ th SDP to attain the optimal value.

These problems are essentially equivalent to the max-cut problem of a graph with an odd number of nodes and equal weight. The numerical result for (ii) leads to a conjecture that there exists a  $Q \in \mathbb{S}^n$  for which (ii) holds if  $n \geq 3$ . The binary QOP examples given in this paper can be used for evaluating numerical methods for QOPs and for their further development.

In Section 2, we state our numerical examples of binary QOPs and numerical and theoretical results showing (i) and a numerical evidence for (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 even the hierarchy of SDP relaxation as their dimension increases. Section 3 includes the description of the SDP relaxation, the standard DNN relaxation, and the DNN relaxation derived from the CPP reformulation. In Section 4, we propose a conjecture and discuss its implication.

## 2 Main result

As an instance of binary QOPs, we consider  $\text{QOP}(\boldsymbol{E}, B_1)$ , where  $\boldsymbol{E}$  denotes the  $n \times n$  matrix with all elements 1. We can rewrite the objective quadratic function as  $\boldsymbol{x}^T \boldsymbol{E} \boldsymbol{x} = (\sum_{i=1}^n x_i)^2$ . It follows that the optimal value  $\zeta(\boldsymbol{E}, B_1)$  of  $\text{QOP}(\boldsymbol{E}, B_1)$  is 1 if the dimension n is odd and 0 otherwise. Since  $\boldsymbol{x}^T \boldsymbol{E} \boldsymbol{x} = 2 \sum_{1 \leq i < j \leq n} x_i x_j + n$  holds for every  $\boldsymbol{x} \in \{-1, 1\}^n$ ,  $\text{QOP}(\boldsymbol{E}, B_1)$  corresponds to the max-cut problem with equal weight.

Lasserre [8] showed that for every  $\boldsymbol{Q} \in \mathbb{S}^n$  the *n*th hierarchical SDP relaxation (or the SDP with the relaxation order  $\omega = n$ ) applied to  $\text{QOP}(\boldsymbol{Q}, B_1)$  always attains the optimal value  $\zeta(\boldsymbol{Q}, B_1)$ . We will see from numerical results that the hierarchy of SDP relaxation requires at least  $\omega = \lceil n/2 \rceil$  for the relaxation order to attain the optimal value  $\zeta(\boldsymbol{E}, B_1) = 1$  when dimension *n* is odd.

Let  $\boldsymbol{Q} \in \mathbb{R}^n$ . QOP $(\boldsymbol{Q}, B_1)$  can be converted to an equivalent binary QOP $(\boldsymbol{R}, B_0)$ , where  $\boldsymbol{R} = 4(\boldsymbol{Q} - \text{diag}(\boldsymbol{Q}\boldsymbol{e}))$  and  $\boldsymbol{e} = (1, 1, \dots, 1)^T \in \mathbb{R}^n$ . In fact, if an affine transformation  $\boldsymbol{x} = 2\boldsymbol{y} - \boldsymbol{e}$  is applied to QOP $(\boldsymbol{Q}, B_1)$ , then

$$oldsymbol{y} \in \{0,1\}^n$$
 if and only if  $oldsymbol{x} \in \{-1,1\}^n,$   
 $oldsymbol{x}^T oldsymbol{Q} oldsymbol{x} = 4oldsymbol{y}^T oldsymbol{Q} oldsymbol{y} - 4oldsymbol{e}^T oldsymbol{Q} oldsymbol{y} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{y} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{y} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{e} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{e} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} = oldsymbol{y}^T oldsymbol{R} oldsymbol{e} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} + oldsymbol{e}^T oldsymbol{R} oldsymbol{e} + oldsymbol{e}^T oldsymbol{Q} oldsymbol{e} + oldsymbol{e}^T oldsymbol{e} + oldsymbol{e}^T oldsymbol{e}^T oldsymbol{e} + oldsymbol{e}^T oldsymbol{e}^T oldsymbol{e} + oldsymbol{e}^T olds$ 

Here the last equality holds because  $e^T Q y = y^T \operatorname{diag}(Q e) y$  for every  $y \in \{0, 1\}^n$ . Therefore,  $\zeta(Q, B_1) = \zeta(R, B_0) + e^T Q e$ . Specifically, defining F = 4(E - nI), we see  $\zeta(E, B_1) = \zeta(F, B_0) + n^2$ .

As conic relaxation methods, we consider

- (s) a standard semidefinite programming (SDP) relaxation of  $QOP(\boldsymbol{E}, B_1)$ ,
- (d1) a standard doubly nonnegative (DNN) relaxation of  $QOP(\mathbf{F}, B_0)$ ,
- (d2) a DNN relaxation derived from the CPP reformulation of of  $QOP(\mathbf{F}, B_0)$  [1, 2],
- (h) the hierarchy of SDP relaxations of  $QOP(\boldsymbol{E}, B_1)$  proposed by Lasserre [7].

The lower bound for the optimal value of  $\text{QOP}(\mathbf{Q}, B)$  provided by each relaxation is denoted by  $\eta_s(\mathbf{Q})$ ,  $\eta_{d1}(\mathbf{Q})$ ,  $\eta_{d2}(\mathbf{Q})$  and  $\eta_h(\mathbf{Q}, \omega)$ , respectively. Here *B* stands for either  $B_1$  or  $B_0$ , and  $\omega$  denotes the relaxation order used in (h). Although we know that  $\eta_s(\mathbf{Q}) \leq \eta_{d1}(\mathbf{Q}) + \mathbf{e}^T \mathbf{Q} \mathbf{e} \leq \eta_{d2}(\mathbf{Q}) + \mathbf{e}^T \mathbf{Q} \mathbf{e}$  for any  $\mathbf{Q} \in \mathbb{S}^n$  by construction described in Section 3, (s) and (d1) are included since they are popular relaxations. We can additionally consider

(h') the hierarchy of SDP relaxations of  $QOP(\mathbf{F}, B_0)$ ,

but (h) and (h')'are known to be equivalent [12]. Some technical details of (s), (d1) and (d2) are given in Section 3. We refer to [7, 8] for (h).

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 3.0GHZ 8-core Intel Xeon E5 CPU and 64 GB memory.

Table 1 shows the numerical results on the relaxation methods (s), (d1) and (d2). SparseCoLO [3] was used to convert the DNN problems (d1) and (d2) into SDPs, and SeDuMi [9] to solve SDPs. All the lower bounds  $\eta_s(\mathbf{E})$ ),  $\eta_{d1}(\mathbf{F}) + n^2$  and  $\eta_{d2}(\mathbf{F}) + n^2$ obtained are nearly 0, which is the trivial lower bound for the optimal value  $\zeta(\mathbf{E}, B_1) = 1$ of QOP( $\mathbf{E}, B_1$ ). We also note that the values in Table 1 (and Table 2) must have involved some numerical error. For example,  $\eta_s(\mathbf{E}) \leq \eta_{d1}(\mathbf{F}) + n^2$  must have 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 the table, we see that all the methods (s), (d1), (d2) are not effective at all for QOP( $\mathbf{E}, B_1$ ) and QOP( $\mathbf{F}, B_0$ ) when n is odd. Theoretically,  $\eta_s(\mathbf{E}) = \eta_{d1}(\mathbf{F}) + n^2 = 0$  if  $n \geq 3$  is odd. This will be proved in Section 4.

n	$\zeta(oldsymbol{E})$	$\eta_s(oldsymbol{E})$	$\eta_{d1}(F) + n^2$	$\eta_{d2}(oldsymbol{F})+n^2$
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

Table 1: Numerical results on SDP and DNN relaxations

Table 2 shows 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 Glop-tiPoly [5] and SparsePOP [11] which implemented (h). SeDuMi [9] was used in the

both software packages for solving SDPs. GloptiPoly attempts to generate all optimal solutions when the optimal value is obtained. Although SparsePOP can only provide the optimal value of QOP( $\mathbf{E}, B_1$ ), it is faster than GloptiPoly and can process larger dimensional QOPs. In all cases of n = 3, 5, 7, 9, 11, the hierarchy of SDP relaxation can nearly attains the trivial lower bound 0 with relaxation order  $\lfloor n/2 \rfloor$ , and it attains the optimal value 1 with relaxation order  $\lceil n/2 \rceil$ . In case of n = 11, we notice that the lower bound  $\eta_h(11, \lceil 11/2 \rceil)$  attained by by SparsePOP displays a wider gap  $1 - 9.999785904e-01 \geq 2.14e-05$  compared to other cases. The reason is that SeDuMi, the SDP solver used in SparsePOP, stopped with a numerical error before attaining a given accuracy 1.0e-9.

	Opt	GloptiPoly		SparsePOP	
n	$\zeta(\boldsymbol{E},B_1)$	$\eta_h(\boldsymbol{E},\lfloor n/2 \rfloor)$	$\eta_h(\boldsymbol{E}, \lceil n/2 \rceil)$	$\eta_h(\boldsymbol{E},\lfloor n/2 \rfloor)$	$\eta_h(\boldsymbol{E}, \lceil n/2 \rceil) \; (\mathrm{sec})$
		(sec)	(sec)	(sec)	(sec)
3	1	-1.11e-11	+9.99999993e-01	-8.56e-12	+9.999999983e-01
		(0.1)	(0.1)	(0.1)	(0.1)
5	1	+8.39e-09	+1.00000002e+00	-2.78e-11	+9.999999987e-01
		(0.1)	(1.1)	(0.1)	(0.1)
7	1	+2.30e-07	+1.00000049e+00	-5.65e-09	+9.999999941e-01
		(11.8)	(678.1)	(0.5)	(6.1)
9	1	not tested	not tested	-7.93e-09	+9.999999332e-01
				(50.7)	(591.2)
11	1	not tested	not tested	-1.32e-09	+9.999785904e-01
				(11182.2)	(54716.8)

Table 2: Numerical results on the hierarchy of SDP relaxations [7].

**Remark.** Both GloptiPoly and SparsePOP are designed for general POPs, and their construction of SDP relaxation problems are not specialized for binary QOPs. We could considerably simplify SDP relaxation problems derived from binary QOPs to reduce their sizes, which would enable to process larger-scale QOPs. However, we note that the size of SDPs constructed still grows very rapidly as dimension n of binary QOPs and/or relaxation order  $\omega$  increases. Therefore, binary QOP( $\boldsymbol{E}, B_1$ ) that can be solved numerically by the hierarchy of SDP relaxation will be still limited to small-sized problems, probably  $n \leq 20$ . See Section 4 and [8].

#### 2.1 Even dimensional case

If n = 2, we can easily verify that  $\eta_s(\boldsymbol{E}, B_1) = \zeta(\boldsymbol{E}, B_1)$ . Suppose that n is even and not less that 4. Define the  $n \times n$  rank 1 matrix  $\boldsymbol{G} \in \mathbb{S}^n$  such that

$$\boldsymbol{G} = \left( egin{array}{cc} \boldsymbol{E} & \boldsymbol{0} \\ \boldsymbol{0}^T & \boldsymbol{0} \end{array} 
ight),$$

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  $\zeta(\boldsymbol{G}, B_1) = \zeta(\boldsymbol{E}, B_1)$ . If we define

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

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 Thus we may regard QOP( $\boldsymbol{G}, B_1$ ) and QOP( $\boldsymbol{H}, B_0$ ) in  $\mathbb{R}^n$  as binary QOPs obtained by introducing an additional dummy variable  $x_n$  to QOP( $\boldsymbol{E}, B_1$ ) and QOP( $\boldsymbol{F}, B_0$ ) in  $\mathbb{R}^{n-1}$ , respectively. We can easily 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, we can apply the discussions on binary QOP( $\boldsymbol{E}, B_1$ ) and QOP( $\boldsymbol{F}, B_0$ ) in the odd dimensional space  $\mathbb{R}^{n-1}$  to ones on binary QOP( $\boldsymbol{G}, B_1$ ) and QOP( $\boldsymbol{H}, B_0$ ) in the even dimensional space  $\mathbb{R}^n$ . We also note that  $\lfloor n/2 \rfloor = \lceil n/2 \rceil = \lceil (n-1)/2 \rceil$ .

#### 2.2 Full rank binary QOPs vs. rank-1 binary QOPs

From the fact that the coefficient matrix  $\boldsymbol{E}$  of the objective function of  $\text{QOP}(\boldsymbol{E}, B_1)$  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  $\text{QOP}(\boldsymbol{E}, B_1)$ by the relaxation methods (s), (d1), (d2) and (h).

We consider two types of coefficient matrices for  $\text{QOP}(\boldsymbol{Q}, B_1)$  to examine the role of the rank of Q. The first one is  $\boldsymbol{Q} \in \mathbb{S}^n$  with each component  $Q_{ij} \in \mathbb{R}$   $(1 \leq i \leq j)$ randomly chosen from (100, -100). In this case, the matrix  $\boldsymbol{Q}$  generated is of full rank almost surely. The second is a rank-1 matrix  $\boldsymbol{Q} = \boldsymbol{q}\boldsymbol{q}^T \in \mathbb{S}^n$  with each  $q_i \in \mathbb{R}$   $(1 \leq i \leq n)$ chosen from (10, -10).

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

## 2.3 A convex combination of $QOP(E, B_1)$ and $QOP(Q^1, B_1)$ with randomly generated full rank $Q^1$

Although the binary  $\text{QOP}(\boldsymbol{E}, B_1)$  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  $\lfloor n/2 \rfloor$ .

We note that not only the optimal value of  $\text{QOP}(\boldsymbol{Q}, B_1)$  but also its lower bounds obtained by the relaxation methods are continuous functions of  $\boldsymbol{Q}$ . Thus, if  $\boldsymbol{Q}$  is sufficiently close to  $\boldsymbol{E}$ ,  $\text{QOP}(\boldsymbol{Q}, B_1)$  remains difficult to solve by them. To see this, we now consider a convex combination  $\boldsymbol{Q}(\lambda)$  of  $\boldsymbol{E}$  and  $\boldsymbol{Q}^1 \in \mathbb{S}^n$  with each  $Q_{ij}^1$   $(1 \le i \le j \le 1)$ chosen randomly from interval (-1, 1) such that  $\boldsymbol{Q}(\lambda) = (1 - \lambda)\boldsymbol{E} + \lambda \boldsymbol{Q}^1$  for  $\lambda \in [0, 1]$ .

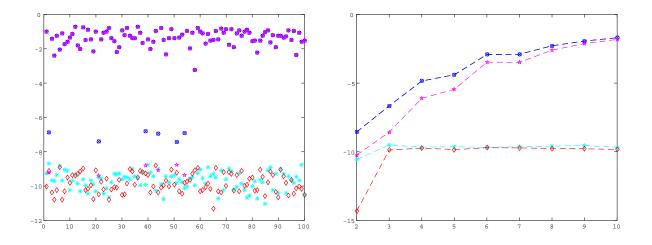


Figure 1: 100 QOP( $\boldsymbol{Q}, B_1$ )s with randomly generated full rank  $\boldsymbol{Q}$  solved by the standard DNN relaxation method  $\otimes$ , the DNN relaxation derived from the CPP reformulation  $\star$ , SparsePOP with  $\omega = 2 *$  and SparsePOP with  $\omega = 3 \diamond$ . The vertical axis stands for the relative accuracy  $\log_{10} ((\zeta - \eta) / \max\{|\zeta|, 1.0e-8\})$ , where  $\zeta$  is the optimal value of QOP( $\boldsymbol{Q}, B_1$ ) and  $\eta$  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 dimension n increases from n = 2 to n = 10.

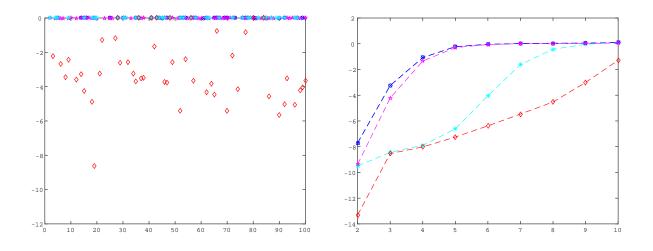


Figure 2: 100 QOP( $\boldsymbol{Q}, B_1$ )s with randomly generated rank-1  $\boldsymbol{Q}$  solved by the standard DNN relaxation method  $\otimes$ , the DNN relaxation derived from the CPP reformulation  $\star$ , SparsePOP with  $\omega = 2 *$  and SparsePOP with  $\omega = 3 \diamond$ . The vertical axis stands for the relative accuracy  $\log_{10} ((\zeta - \eta) / \max\{|\zeta|, 1.0e-8\})$ , where  $\zeta$  is the minimum value of QOP( $\boldsymbol{Q}, B_1$ ) and  $\eta$  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.

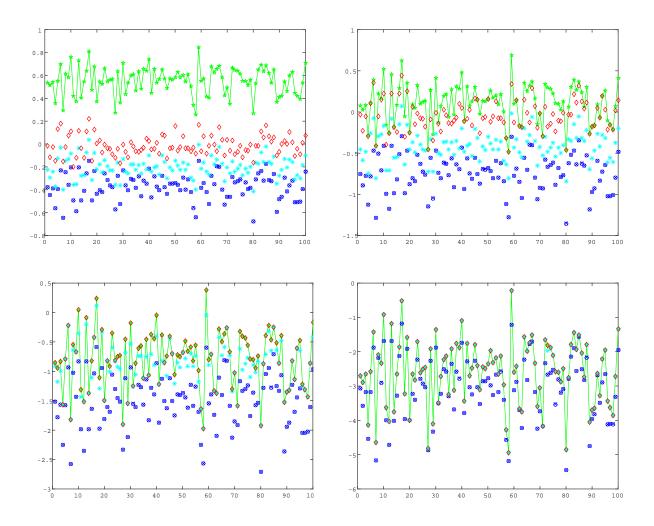


Figure 3: 100 QOP( $Q(\lambda), B_1$ )s with  $Q(\lambda) = (1-\lambda)E + \lambda Q^1$  solved by the standard DNN relaxation method  $\otimes$ , SparsePOP with  $\omega = 2 *$  and SparsePOP with  $\omega = 3 \diamond$ . Here  $Q^1$ is an 7 × 7 symmetric matrix with each  $Q_{ij}$  randomly chosen from the interval (-1, 1), 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  $\omega = 3 \diamond$ .

As  $\lambda$  increases, the difficulty of solving QOP( $Q(\lambda), B_1$ ) with an unknown optimal value and solution decreases, whose tendency is shown in Figure 3. When we take  $\lambda = 0.05$ , the optimal value (the green line) and the lower bounds obtained by the standard DNN relaxation method  $\otimes$ , SparsePOP with  $\omega = 2 *$  and SparsePOP with  $\omega = 3 \diamond$  exhibit a clear gap. As  $\lambda$  increases, the gap decreases, and SparsePOP with both  $\omega = 2 *$  and  $\omega = 3 \diamond$  attain the optimal value accurately when  $\lambda$  is near 0.4.

## 3 Some technical details

#### **3.1** SDP relaxation (s) of $QOP(Q, B_1)$

Let  $\boldsymbol{Q} \in \mathbb{S}^n$ . We rewrite  $\text{QOP}(\boldsymbol{Q}, B_1)$  as

minimize 
$$\boldsymbol{Q} \bullet \boldsymbol{x} \boldsymbol{x}^T$$
 subject to  $x_i^2 = 1 \ (i = 1, 2, \dots, m).$ 

We know that  $\boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n_+$  holds for every  $\boldsymbol{x} \in \mathbb{R}^n$ . Replacing  $\boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n_+$  by a single symmetric matrix variable  $\boldsymbol{X}$ , we obtain the standard SDP relaxation (s) of  $\text{QOP}(\boldsymbol{Q}, B_1)$ 

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

Here  $\boldsymbol{Q} \bullet \boldsymbol{X}$  denotes the inner product of  $\boldsymbol{Q}$  and  $\boldsymbol{X}$ ;  $\boldsymbol{Q} \bullet \boldsymbol{X} = \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} X_{ij}$ . If we add rank $(\boldsymbol{X}) = 1$  to the constraint, then the problem previously derived is known to be equivalent to  $\text{QOP}(\boldsymbol{Q}, B_1)$ .

Now suppose that  $n \ge 2$  and  $\mathbf{Q} = \mathbf{E} \in \mathbb{S}^n$ . Then we can easily verify that  $\mathbf{X} \in \mathbb{S}^n$  with components  $X_{ii} = 1$  (i = 1, 2, ..., n) and  $X_{ij} = X_{ji} = -1/(n-1)$   $(1 \le i < j \le n)$  is an optimal solution of QOP $(\mathbf{E}, B_1)$ , and that the optimal value is zero. This gives a theoretical proof for  $\eta_s(\mathbf{E}) = 0$ , which has been shown numerically in Table 1 for n = 3, 5, 7, 9, 11.

#### **3.2** DNN relaxation (d1) of $QOP(R, B_0)$

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

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

We note that  $\begin{pmatrix} 1 & \boldsymbol{y}^T \\ \boldsymbol{y} & \boldsymbol{Y} \end{pmatrix}$  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. Thus, replacing  $\boldsymbol{y}\boldsymbol{y}^T$  by a single symmetric matrix variable  $\boldsymbol{Y}$ , we obtain the standard DNN relaxation (d1) of QOP( $\boldsymbol{R}, B_0$ )

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

Let  $\boldsymbol{Q} \in \mathbb{S}^n$ . When we take  $\boldsymbol{R} = 4(\boldsymbol{Q} - \operatorname{diag}(\boldsymbol{Q}\boldsymbol{e})\boldsymbol{I})$ , then  $\operatorname{QOP}(\boldsymbol{Q}, B_1)$  and  $\operatorname{QOP}(\boldsymbol{R}, B_0)$ are equivalent as shown in Section 2. More precisely,  $\zeta(\boldsymbol{Q}, B_1) = \zeta(\boldsymbol{R}, B_0) + \boldsymbol{e}^T \boldsymbol{Q} \boldsymbol{e}$ . In this case,  $\eta_s(\boldsymbol{Q}) \leq \eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T \boldsymbol{Q} \boldsymbol{e} \leq \zeta(\boldsymbol{Q}, B_1)$  holds. Namely, the lower bound  $\eta_{d1}(\boldsymbol{R}) + \boldsymbol{e}^T \boldsymbol{Q} \boldsymbol{e}$ provided by the standard DNN relaxation (d1) of  $\operatorname{QOP}(\boldsymbol{R}, B_0)$  for the optimal value  $\zeta(\boldsymbol{Q}, B_1)$  of  $\operatorname{QOP}(\boldsymbol{Q}, B_1)$  is at least as tight as the lower bound  $\eta_s(\boldsymbol{Q})$  provided 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  $\boldsymbol{X} = 4\boldsymbol{Y} - 2\boldsymbol{e}\boldsymbol{y}^T - 2\boldsymbol{y}\boldsymbol{e}^T + \boldsymbol{e}\boldsymbol{e}^T$ . Then

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

Here the second equality follows from  $y_i = Y_{ii}$  (i = 1, 2, ..., n). Since  $\mathbf{Y} \succeq \mathbf{y} \mathbf{y}^T$ , we have that

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

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

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

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

Then we can verify that  $(\boldsymbol{y}, \boldsymbol{Y})$  is a feasible solution of  $\text{QOP}(\boldsymbol{F}, B_0)$ , *i.e.*, (d1) with  $\boldsymbol{R} = 4(\boldsymbol{E} - n^2 \boldsymbol{I})$ , and that the objective value  $-n^2$ . Hence  $\eta_{d2}(\boldsymbol{F}) + n^2 \leq 0$ . Since we already know that  $0 = \eta_s(\boldsymbol{E}) \leq \eta_{d2}(\boldsymbol{F}) + n^2$ , we obtain  $\eta_{d2}(\boldsymbol{F}) + n^2 = 0$ .

## 3.3 DNN relaxation (d2) derived from a CPP reformulation of $QOP(R, B_0)$

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

minimize 
$$\boldsymbol{y}^{T}\boldsymbol{R}\boldsymbol{y}$$
  
subject to  $y_{i}^{2} - y_{i} = 0 \ (i = 1, 2, ..., n),$   
 $u_{i}^{2} - u_{i} = 0 \ (i = 1, 2, ..., n), \ \boldsymbol{y} + \boldsymbol{u} = \boldsymbol{e},$   
 $\boldsymbol{y} \ge \boldsymbol{0}, \ \boldsymbol{u} \ge \boldsymbol{0}, \ \sum_{i=1}^{n} y_{i}u_{i} = 0.$ 

$$\left. \right\}$$

$$(2)$$

Here  $\boldsymbol{u} \in \mathbb{R}^n$  serves as a slack variable vector. The added constraints (2) are redundant for  $\text{QOP}(\boldsymbol{R}, B_0)$  itself, but they make its DNN relaxation, whose derivation is described in the subsequent discussion, stronger. In particular, the last three constraints in (2) forms a complementarity condition on  $\boldsymbol{y} \in \mathbb{R}^n$  and  $\boldsymbol{u} \in \mathbb{R}^n$ .

Let

$$A = (-e I I), H_1 = A^T A, H_2 = \begin{pmatrix} 0 & 0^T & 0^T \\ 0 & O & I \\ 0 & I & O \end{pmatrix}.$$

Then we can rewrite the problem above as

minimize 
$$\boldsymbol{R} \bullet \boldsymbol{y} \boldsymbol{y}^{T}$$
  
subject to  $y_{0} = 1, \ \boldsymbol{H}_{k} \bullet \begin{pmatrix} y_{0} \quad \boldsymbol{y}^{T} \quad \boldsymbol{u}^{T} \\ \boldsymbol{y} \quad \boldsymbol{y} \boldsymbol{y}^{T} \quad \boldsymbol{y} \boldsymbol{u}^{T} \\ \boldsymbol{u} \quad \boldsymbol{u} \boldsymbol{y}^{T} \quad \boldsymbol{u} \boldsymbol{u}^{T} \end{pmatrix} = 0 \ (k = 1, 2),$   
 $y_{0} = 1, \ \boldsymbol{y} \ge \boldsymbol{0}, \ \boldsymbol{u} \ge \boldsymbol{0},$   
 $y_{i}^{2} - y_{i} = 0 \ (i = 1, 2, \dots, n), \ u_{i}^{2} - u_{i} = 0 \ (i = 1, 2, \dots, n)$ 

We note that for every  $y_0 \ge 0$ ,  $y \ge 0$  and  $u \ge 0$ , the matrix  $\begin{pmatrix} y_0 & y^T & u^T \\ y & yy^T & yu^T \\ u & uy^T & uu^T \end{pmatrix}$  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  $\mathbb{N}^{1+2n}$ . Thus, as a conic relaxation of  $\text{QOP}(\mathbf{R}, B_0)$ , we obtain a linear conic optimization problem

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

Here K stands for either  $\mathbb{C}^{1+2n}$  (the CPP cone) or  $\mathbb{S}^{1+2n}_+ \cap \mathbb{N}^{1+2n}$  (the DNN cone). In the latter case, we have a DNN relaxation  $\mathrm{LCOP}(\mathbb{S}^{1+2n}_+ \cap \mathbb{N}^{1+2n})$  which corresponds to (d2).

If we remove the complementarity constraint  $\sum_{i=1}^{n} y_i u_i = 0$  in the previous discussion, the resulting LCOP(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 above construction of  $LCOP(\mathbb{C}^{1+2n})$  corresponds to the CPP reformulation of  $QOP(\mathbf{R}, B_0)$ , which was shown to be equivalent to  $QOP(\mathbf{R}, B_0)$  in a more general framework for a class of linearly constrained QOPs with continuous and binary variables, by Burer [2].

On the other hand, we can remove the 0-1 constraints  $y_i^2 - y_i = 0$ ,  $u_i^2 - u_i = 0$  (i = $1, 2, \ldots, n$  while keeping all the other constraints in (2) to obtain a CPP or DNN relaxation LCOP(K) without imposing 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  $QOP(\mathbf{R}, B_0)$  by Arima-Kim-Kojima [1]. The simplified CPP relaxation is equivalent to  $QOP(\mathbf{R}, B_0)$  too. See [1] for more details.

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

#### Relation between $QOP(Q, B_1)$ and $QOP(R, B_0)$ **3.4**

Let  $\boldsymbol{Q} \in \mathbb{S}^n$  be given. We have already seen that  $\text{QOP}(\boldsymbol{Q}, B_1)$  is equivalent to  $\text{QOP}(\boldsymbol{R}, B_0)$ with  $\mathbf{R} = 4(\mathbf{Q} - \text{diag}(\mathbf{Q}\mathbf{e})\mathbf{I}); \zeta(\mathbf{Q}, B_1) = \zeta(\mathbf{R}, B_0) + \mathbf{e}^T \mathbf{Q}\mathbf{e}$ . We note that if  $\mathbf{x} \in \mathbb{R}^n$  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. This means that the resulting  $QOP(\mathbf{R}, B_0)$  also

satisfies this symmetry; if  $\boldsymbol{y} \in \mathbb{R}^n$  is a feasible solution of  $\text{QOP}(\boldsymbol{R}, B_0)$  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  $\mathbf{R} \in \mathbb{S}^n$ . In general,  $\text{QOP}(\mathbf{R}, B_0)$  does not satisfy the aforementioned symmetry. Thus, we need an additional dimension (or an additional variable  $x_0$  as shown in the following) to convert  $\text{QOP}(\mathbf{R}, B_0)$  into an equivalent  $\text{QOP}(\mathbf{Q}, B_1)$ . In fact, define

$$oldsymbol{Q} = rac{1}{4} \left( egin{array}{cc} oldsymbol{e}^T oldsymbol{R} oldsymbol{e} & oldsymbol{e}^T oldsymbol{R} \ oldsymbol{R} oldsymbol{e} & oldsymbol{R} \end{array} 
ight).$$

Then it is easily verified that the QOP

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

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

## 4 Conjecture

Suppose that n is not less than 3. By Lasserre [8], we know that  $0 = \eta_h(\mathbf{Q}, 1) \leq \eta_h(\mathbf{Q}, \omega) \leq \eta_h(\mathbf{Q}, n) = 1$  for  $\mathbf{Q} \in \mathbb{S}^n$  and every  $\omega \geq 2$ . The numerical results shown in Table 2 and the discussions in Section 2.1 lead to a conjecture that

• there exists a  $\widetilde{\boldsymbol{Q}} \in \mathbb{S}^n$  such that  $\eta_h(\widetilde{\boldsymbol{Q}}, \omega) = 1$  if  $\omega \geq \lceil n/2 \rceil$  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 2.1.

We discuss some implications of this conjecture.

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

$$B_{0}(\omega) = \{ \boldsymbol{\alpha} \in B_{0} : \sum_{i=1}^{n} \alpha_{i} = \omega \},$$

$$C_{0}(\omega) = \{ \boldsymbol{\alpha} \in B_{0} : \sum_{i=1}^{n} \alpha_{i} \leq \omega \} = \bigcup_{\xi \leq \omega} B_{0}(\xi),$$

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

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

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

Here each  $\widehat{Q}_{\alpha}$  ( $\alpha \in B_1(2)$ ) corresponds to  $2Q_{ij}$  or  $Q_{ii}$  such that  $\overline{Q}_{\alpha} = 2Q_{ij}$  if  $\alpha_i = 1$ and  $\alpha_j = 1$  for some  $(1 \leq i < j \leq n)$  and  $\overline{Q}_{\alpha} = Q_{ii}$  if  $\alpha_i = 2$  for some  $(1 \leq i \leq n)$ .  $\widehat{\boldsymbol{M}}(\boldsymbol{y})$  denotes a moment matrix for QOP( $\boldsymbol{Q}, B_1$ ), which forms a  $\rho(\omega) \times \rho(\omega)$  symmetric matrix with each element corresponding 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  $y_0$  is fixed to 1, the number of independent variables involved in  $\widehat{\boldsymbol{M}}_{\omega}(\boldsymbol{y})$  amounts to  $\rho(2\omega) - 1$ . 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 involved in it determine the size of SDP<sub> $\omega$ </sub> to be solved for computing  $\eta_h(\boldsymbol{Q}, \omega)$ .

We now compare the size of  $\text{SDP}_n(\mathbf{Q})$  whose optimal value  $\eta_h(\mathbf{Q}, n)$  is guaranteed to attain  $\zeta(\mathbf{Q}, B_1)$  for all  $\mathbf{Q} \in \mathbb{S}^n$  and the size of  $\text{SDP}_{\lceil n \rceil}(\widetilde{\mathbf{Q}})$  involved in the conjecture. In the first  $\text{SDP}_n(\mathbf{Q})$ , 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 the second  $\text{SDP}_{\lceil n \rceil}(\widetilde{\mathbf{Q}})$ , these two numbers are:

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

Hence the size of  $\text{SDP}_{\lceil n/2 \rceil}$  for  $\eta_h(\tilde{\boldsymbol{Q}}, B_1, \lceil n/2 \rceil)$  is smaller than the size of  $\text{SDP}_n$  for  $\eta_h(\boldsymbol{Q}, B_1, n)$  although the number of independent variables involved them are identical.

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

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

If  $n \ge 4$  is even, then

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

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

Now define

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

which may be regarded as the worst case complexity to solve a class of binary QOPs,  $\{\text{QOP}(\boldsymbol{Q}, B_1) : \boldsymbol{Q} \in \mathbb{S}^n\}$  by the hierarchy of SDP relaxation method. If the conjecture above is true, then  $\lceil n/2 \rceil \leq \omega^*(n) \leq n$ . A more ambitious conjecture may be

• 
$$\omega^*(n) = \lceil n/2 \rceil$$
.

So far, we have not found any numerical counter example to this conjecture.

## 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. The binary QOP takes a very simple form in the sense that it does not involve any constraints other than requiring the variables binary. In connection with the difficulty of solving these simple binary QOPs, it is extremely interesting to mention that the randomized approximation algorithm using the standard SDP relaxation given by Goemans and Williamson [4] 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 SDP and DNN fail on the problem. Thus, any relaxation methods that can approximately solve them can be regarded to have an advantage over the other methods.

If the hierarchy of SDP relaxation is employed for the binary QOP instances, the minimum relaxation order to solve them within high accuracy was numerically found to be  $\omega = \lceil n/2 \rceil$ . Since the size of the SDP relaxation in the hierarchy grows very rapidly as  $\omega$  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.

## References

- N. Arima, S. Kim and M. Kojima. Simplified copositive and Lagrangian relaxations for linearly constrained quadratic optimization problems in continuous and binary variables. *Pacific Journal of Optimization* 10 437–451 (2014).
- [2] S. Burer. On the copositive representation of binary and continuous nonconvex quadratic programs. *Math. Program.* **120** 479–495 (2009).
- [3] K. Fujisawa, S. Kim, M. Kojima, Y. Okamoto and M. Yamashita. User's manual for SparseCoLO: conversion methods for SPARSE COnic-form Linear Optimization problems. Research Report B-453, Dept. of Math. and Comp. Sciecne, Tokyo Institute of Technology, Tokyo, Japan. February 2009.
- [4] M. X. Goemans and D. P. Williamson. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *Journal* of the Association for Computing Machinery 42 1115–1145 (1995).
- [5] D. Henrion, J. B. Lasserre. GloptiPoly: global optimization over polynomials with Matlab and SeDuMi. ACM Transactions on Mathematical Software 29 165–194 (2003).

- [6] S. Kim, M. Kojima and K. C. Toh. A Lagrangian-DNN relaxation: a fast method for computing tight lower bounds for a class of quadratic optimization problems. To appear in *Math. Program.*.
- [7] J. B. Lasserre. Global optimization with polynomials and the problems of moments. SIAM J. Optim. 11 796–817 (2001).
- [8] J. B. Lasserre. An explicit exact SDP relaxation for nonlinear 0-1 programs. Proceedings of the 8th International IPCO Conference on Integer Programming and Combinatorial Optimization, pages 293–303, Springer-Verlag London, UK (2001).
- [9] J. F. Strum. SeDuMi 1.02, a MATLAB toolbox for optimization over symmetric cones. Optim. Method Softw., 11 & 12, 625–653, 1999.
- [10] H. Waki, S. Kim, M. Kojima and M. Muramatsu. Sums of squares and semidefinite programming relaxations for polynomial optimization problems with structured sparsity. *SIAM J. Optim.* 17 218–242 (2006).
- [11] H. Waki, S. Kim, M. Kojima, M. Muramatsu and H. Sugimoto. SparsePOP : a sparse semidefinite programming relaxation of polynomial optimization problems. *ACM Transactions on Mathematical Software* **35** (2) 15 (2008).
- [12] H. Waki, M. Muramatsu and M. Kojima. Invariance under affine transformation in semidefinite programming relaxation for polynomial optimization problems. *Pacific Journal of Optimization* 5 297–312 (2009).