

**New formulations and relaxations
for mixed-binary quadratic optimization**

LIU Jia, LRI, Université Paris Sud

joint work with

**I.M. Bomze, J. Cheng, P.J.C. Dickinson and
A. Lisser**

PGMO days 2016

09 November 2016

Mixed-binary QPs, key condition

Consider (for indefinite Q and $\{c, a_i, b\} \subset \mathbb{R}^n$)

$$\left. \begin{aligned} z^* = \min \quad & x^\top Qx + 2c^\top x \\ \text{s. t.} \quad & a_i^\top x = b_i \quad \text{for } i \in [1:m] \\ & x \in \mathbb{R}_+^n \\ & x_j \in \{0, 1\} \quad \text{for } j \in B, \end{aligned} \right\} (P)$$

B ... binary variables

$[1:n] \setminus B$... continuous variables

$A = [a_1^\top, \dots, a_m^\top]^\top$ $m \times n$ constraint matrix.

Polyhedron $Z = \{x \in \mathbb{R}_+^n : Ax = b\}$ contains feasible set.

Assume Burer's *key condition*: Z gives linear relaxation,

$$x \in Z \quad \Rightarrow \quad x_j \in [0, 1] \text{ for all } j \in B. \quad (K)$$

Burer's reformulation: enter copositivity

Linearizing by squaring equalities like RLT: put $X_{ij} = x_i x_j$.

If (K) holds, then (P) is equivalent to the *copositive problem*

$$\begin{array}{ll}
 \min & \langle Q, X \rangle + 2c^\top x \\
 \text{s. t.} & a_i^\top x = b_i \quad \text{for } i \in [1:m] \\
 & \langle a_i a_i^\top, X \rangle = b_i^2 \quad \text{for } i \in [1:m] \\
 & X_{jj} = x_j \quad \text{for } j \in B \\
 & \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1},
 \end{array} \quad \left. \vphantom{\begin{array}{l} \min \\ \text{s. t.} \end{array}} \right\} (B)$$

where $\langle Q, X \rangle = \text{trace}(QX)$ and

$$\mathcal{CP}^n = \text{conv} \{ xx^\top : x \in \mathbb{R}_+^n \}$$

is the *cp cone*. Its dual is the *copositive cone*

$$[\mathcal{CP}^n]^* = \{ C = C^\top \text{ } n \times n\text{-matrix} : x^\top C x \geq 0 \text{ if } x \in \mathbb{R}_+^n \} .$$

Counting variables/constraints

Original formulation: $2m + |B|$ constraints,
symmetric matrix variable of order $n + 1$ (one entry fixed).

Aggregation [Arima/Kim/Kojima '14]:

$$\left. \begin{array}{l} \min \quad \langle Q, X \rangle + 2c^\top x \\ \text{s. t.} \quad \sum_{i=1}^m (a_i^\top X a_i - 2b_i a_i^\top x + b_i^2) = 0, \\ \quad \quad \sum_{j \in B} (X_{jj} - x_j) = 0, \\ \quad \quad \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1}, \end{array} \right\} (A)$$

gives equivalent reformulation with only two constraints.

Doubly NonNegative relaxation

In both formulations, cone constraint can be relaxed

– *DNN-relaxation*:

replace $\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1}$ with $\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}$.

Motivation: any cp matrix is psd and has no negative entries.

$$(B) \rightarrow (DB), \quad (A) \rightarrow (DA)$$

Leads to SDP with $\binom{n}{2}$ additional nonnegativity constraints, for both formulations: (DB) and (DA) .

Exploiting linear constraints

Idea: use equality constraints to reduce order of matrix variable:
choose $x_0 \in Z$ (only need $Ax_0 = b$) and linearly independent

$$\{a_{m+1}, \dots, a_n\} \subset \{a_1, \dots, a_m\}^\perp$$

and form

$$B = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ x_0 & a_{m+1} & a_{m+2} & \cdots & a_n \end{bmatrix}.$$

Have

$$Az = \zeta b \quad \Leftrightarrow \quad \begin{bmatrix} \zeta \\ z \end{bmatrix} = By \quad \text{for some } y \in \mathbb{R}^{n+1-m}.$$

Reduced equivalent formulation

[Burer]: (DB) is equivalent to

$$\left. \begin{array}{l} \min \quad \langle Q, X \rangle + 2c^\top x \\ \text{s. t.} \quad \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} = BYB^\top, \\ \quad \quad X_{jj} = x_j, \text{ for } j \in B, \\ \quad \quad \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{N}^{n+1}, Y \in \mathcal{S}_+^{n+1-m}. \end{array} \right\} (DR)$$

... has smaller psd Y but additional equalities.

Same holds for original reformulation (R) of (B) where

$$\begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1} \text{ replaces weaker } \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{N}^{n+1}, Y \in \mathcal{S}_+^{n+1-m}.$$

Motivation

We shall prove the equivalence of problems (B) , (A) and (R) and similar results for the relaxations, from which, we aim at finding new reformulations.

- Reformulations of linear constraints
- Reformulations of binary constraints

From the combinations of the reformulations of different constraints, we find new reformulations of (B) .

Linear constraints: aggregation and facial reduction

We shall consider the following four linear subspaces in \mathcal{S}^{n+1} :

$$\mathcal{L}_1 = \left\{ \begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}^{n+1} : \exists Y \in \mathcal{S}^{n+1-m} \text{ s.t. } BYB^\top = \begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \right\},$$

$$\mathcal{L}_2 = \left\{ \begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}^{n+1} : \begin{array}{l} a_i^\top x = b_i x_0 \quad \text{for } i \in [1:m], \\ a_i^\top X = b_i x^\top \quad \text{for } i \in [1:m] \end{array} \right\},$$

$$\mathcal{L}_3 = \left\{ \begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}^{n+1} : \begin{array}{l} a_i^\top x = b_i x_0 \quad \text{for } i \in [1:m], \\ a_i^\top X a_i = b_i^2 x_0 \quad \text{for } i \in [1:m] \end{array} \right\},$$

$$\mathcal{L}_4 = \left\{ \begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}^{n+1} : \sum_{i=1}^m (a_i^\top X a_i - 2b_i a_i^\top x + b_i^2 x_0) = 0 \right\}.$$

Equivalence when intersecting with psd cone

Notice that $\mathcal{L}_1 = \mathbf{B}\mathcal{S}^{n+1-m}\mathbf{B}^\top$.

We will now show that in fact when intersecting with the positive semidefinite cone these four cones coincide.

Theorem 1. *We have*

$$(a) \quad \mathcal{L}_1 = \mathcal{L}_2 \subseteq \mathcal{L}_3 \subseteq \mathcal{L}_4,$$

$$(b) \quad \mathcal{L}_1 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_2 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_3 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_4 \cap \mathcal{S}_+^{n+1}$$

$$(c) \quad \mathcal{L}_1 \cap \mathcal{S}_+^{n+1} = \mathbf{B}\mathcal{S}_+^{n+1-m}\mathbf{B}^\top.$$

Binary constraints: aggregation

We further look at what can be done with the constraints related to the binary constraints. We consider the following cones:

$$\mathcal{B}_1 = \left\{ \begin{pmatrix} x_0 & \mathbf{x}^\top \\ \mathbf{x} & \mathbf{X} \end{pmatrix} \in \mathcal{S}^{n+1} : X_{jj} = x_j \quad \text{for } j \in B \right\},$$
$$\mathcal{B}_2 = \left\{ \begin{pmatrix} x_0 & \mathbf{x}^\top \\ \mathbf{x} & \mathbf{X} \end{pmatrix} \in \mathcal{S}^{n+1} : \sum_{j \in B} (X_{jj} - x_j) = 0 \right\}.$$

Equivalence when intersecting with psd cone and linear constrained set

We shall show the following results:

Lemma 2. *Let $i \in [1:4]$ and $\begin{pmatrix} x_0 & x^\top \\ x & X \end{pmatrix} \in \mathcal{L}_i \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}$. Then $X_{jk} \leq x_k$ for all $k \in [1:n]$, $j \in B$.*

Theorem 3. *For all $i, j \in [1:4]$ we have*

$$\begin{aligned} \mathcal{B}_1 \cap \mathcal{L}_i \cap \mathcal{CP}^{n+1} &= \mathcal{B}_2 \cap \mathcal{L}_j \cap \mathcal{CP}^{n+1}, \\ \mathcal{B}_1 \cap \mathcal{L}_i \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} &= \mathcal{B}_2 \cap \mathcal{L}_j \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}. \end{aligned}$$

Reformulations of (B)

From the equivalences between \mathcal{L}_i , $i, j \in [1:4]$, and \mathcal{B}_k , $k = 1, 2$, we have

$$(B) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_1 \cap \mathcal{L}_3 \cap \mathcal{CP}^{n+1} \right\}$$

$$(A) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_4 \cap \mathcal{CP}^{n+1} \right\}$$

$$(R) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_1 \cap \mathcal{L}_1 \cap \mathcal{CP}^{n+1} \right\}$$

$$(B) \Leftrightarrow (A) \Leftrightarrow (R)$$

Reformulations of (DB)

$$(DB) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_1 \cap \mathcal{L}_3 \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} \right\}$$

means no merging

$$(DA) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_4 \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} \right\}$$

means merging both linear and binary constraints

$$(DR) \Leftrightarrow \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_1 \cap (\mathcal{B}\mathcal{S}_+^{n+1-m}\mathcal{B}^\top) \cap \mathcal{N}^{n+1} \right\}$$

means reduced psd without merging binary constraints

$$(DB) \Leftrightarrow (DA) \Leftrightarrow (DR)$$

Merging only linear constraints

Merging only linear constraints leads a new reformulations of
 (DB): $\min\{\langle Q, X \rangle + 2c^\top x : \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_1 \cap \mathcal{L}_4 \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}\}$, i.e.

$$\begin{aligned}
 & \min \quad \langle Q, X \rangle + 2c^\top x \\
 & \text{s. t.} \quad \sum_{i=1}^m (a_i^\top X a_i - 2b_i a_i^\top x + b_i^2) = 0 \\
 & \quad \quad X_{jj} = x_j \quad \text{for } j \in B, \\
 & \quad \quad \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{N}^{n+1} \cap \mathcal{S}_+^{n+1}.
 \end{aligned} \tag{DML}$$

Meanwhile, it is a reformulation of (B) when

$$\mathcal{CP}^{n+1} \text{ replaces } \mathcal{N}^{n+1} \cap \mathcal{S}_+^{n+1}.$$

Merging only binary constraints

Merging only binary constraints also leads to new reformulations of (DB): $\min\{\langle Q, X \rangle + 2c^\top x : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_3 \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}\},$

$$\begin{aligned}
 & \min \quad \langle Q, X \rangle + 2c^\top x \\
 & \text{s. t.} \quad a_i^\top x = b_i && \text{for } i \in [1:m] \\
 & \quad \langle a_i a_i^\top, X \rangle = b_i^2 && \text{for } i \in [1:m] \\
 & \quad \sum_{j \in B} (X_{jj} - x_j) = 0 \\
 & \quad \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}.
 \end{aligned} \tag{DMB}$$

Meanwhile, it is a reformulation of (B) when

$$CP^{n+1} \text{ replaces } \mathcal{N}^{n+1} \cap \mathcal{S}_+^{n+1}.$$

Merging strategy for reduced problem

Merging binary constraints of (R) , we have a reformulation of

$$(R): \min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_1 \cap \mathcal{CP}^{n+1} \right\}$$

$$\begin{aligned} \min \quad & \langle Q, X \rangle + 2c^\top x \\ \text{s. t.} \quad & \sum_{j \in B} (X_{jj} - x_j) = 0 \\ & BYB^\top = \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \\ & \begin{pmatrix} \mathbf{1} & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1}, Y \in \mathcal{S}^{n+1-m}. \end{aligned} \tag{MR}$$

Reformulation of (DR)

Replacing $\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP}^{n+1}$, $Y \in \mathcal{S}^{n+1-m}$ in (DR) by $\begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{N}^{n+1}$, $Y \in \mathcal{S}_+^{n+1-m}$ gives a reformulation of (DR) .

$$\min \left\{ \langle Q, X \rangle + 2c^\top x : \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{B}_2 \cap (\mathcal{B}\mathcal{S}_+^{n+1-m}\mathcal{B}^\top) \cap \mathcal{N}^{n+1} \right\} \quad (DMR)$$

$$(DB) \Leftrightarrow (DA) \Leftrightarrow (DR)$$

$$\Leftrightarrow (DML) \Leftrightarrow (DMB) \Leftrightarrow (DMR)$$

An example

Consider a multidimensional quadratic knapsack problems

$$\begin{aligned} \max \quad & x^\top Qx \\ \text{s. t.} \quad & \tilde{a}_i^\top x \leq b_i \quad \text{for } i \in [1:m] \\ & x \in \{0, 1\}^n. \end{aligned} \tag{1}$$

Adding slack variables to remove the inequality constraints

$$\begin{aligned} \max \quad & x^\top Qx \\ \text{s. t.} \quad & \tilde{a}_i^\top x + v_i = b_i \quad \text{for } i \in [1:m] \\ & x \in \{0, 1\}^n \\ & v \in \mathbb{R}_+^m. \end{aligned} \tag{2}$$

Add m slack variables!

Reformulation to satisfy condition (K)

Adding slack variables to guarantee the variables are restricted in $[0, 1]$.

$$\begin{aligned} \max \quad & x^\top Qx \\ \text{s. t.} \quad & \tilde{a}_i^\top x + v_i = b_i \quad \text{for } i \in [1:m] \\ & x_j + z_j = 1 \quad \text{for } j \in [1:n] \\ & x \in \{0, 1\}^n \\ & v \in \mathbb{R}_+^m, z \in \mathbb{R}_+^n, x \in \mathbb{R}_+^n. \end{aligned} \tag{3}$$

Numerical results

A MQKP with 2 knapsacks and 5 goods.

	Statistics of solution status					
	<i>(DB)</i>	<i>(DML)</i>	<i>(DMB)</i>	<i>(DA)</i>	<i>(DR)</i>	<i>(DMR)</i>
SDPT3	25.0888	26.5766*	25.0888	28.744*	25.0888	25.0888
SeDuMi	25.0888	26.5767*	25.0888	28.744*	25.0888	25.0888
Mosek	25.0888	NaN**	25.0888	NaN**	25.0888	25.0888
Sdpnalt	NaN**	NaN**	NaN**	NaN**	25.0888	25.0888

*: Inaccurate solved, the algorithm converge only to a near optimal or dual feasible solution.

** : Failed, the sdp problem is unsolvable by solvers

When the problem is precisely solved, all sdp relaxation problems have the same optimal value.

Statistics of solution status

We choose 4 different sizes and run 100 groups of sdp problems with different parameters under the same size.

		<i>(DB)</i>	<i>(DML)</i>	<i>(DMB)</i>	<i>(DA)</i>	<i>(DR)</i>	<i>(DMR)</i>
6*10	'Solved'	12	0	10	0	100	100
	'Inacc./Solved'	88	100	90	100	0	0
	'Failed'	0	0	0	0	0	0
10*10	'Solved'	0	0	0	0	99	98
	'Inacc./Solved'	100	100	98	100	1	2
	'Failed'	0	0	2	0	0	0
15*10	'Solved'	0	0	0	0	100	100
	'Inacc./Solved'	6	100	13	100	0	0
	'Failed'	94	0	87	0	0	0
30*5	'Solved'	0	0	0	0	41	99
	'Inacc./Solved'	85	100	90	100	59	1
	'Failed'	15	0	10	0	0	0

Average solution times

		<i>(DB)</i>	<i>(DML)</i>	<i>(DMB)</i>	<i>(DA)</i>	<i>(DR)</i>	<i>(DMR)</i>
6*10	'Solved'	1.01	-	1.06	-	0.28	0.28
	'Inacc./Solved'	1.07	1.20	1.09	1.16	-	-
	'Failed'	-	-	-	-	-	-
10*10	'Solved'	-	-	-	-	0.40	0.40
	'Inacc./Solved'	2.51	3.01	2.62	3.04	0.45	0.43
	'Failed'	-	-	1.08	-	-	-
15*10	'Solved'	-	-	-	-	0.73	0.73
	'Inacc./Solved'	4.84	9.48	6.64	9.27	-	-
	'Failed'	2.59	-	2.65	-	-	-
30*5	'Solved'	-	-	-	-	5.72	5.07
	'Inacc./Solved'	217.35	380.23	234.98	324.25	5.75	5.31
	'Failed'	65.21	-	71.12	-	-	-

Results are derived with Sedumi.

Conclusions

- The sdp problems have no feasible points in the interior of the semi-definite cone. Still hard to solve! further improvement!
- Most of the reduced sdp problems can be solve precisely, while the non-reduced sdp problems can not.
- The CPU time of reduced sdp problems are much less.
- Compared the reduced sdp problem with no merging, the reduced sdp problem with merging is more tractable.

Selected references in chronological order

- [Shor '87] Quadratic optimization problems, *Izv. Akad. Nauk SSSR Tekhn. Kibernet.* **22**, 128–139.
- [Hotho *et al.*'06] Information retrieval in folksonomies: Search and ranking, in *The Semantic Web: Research and Applications*, 411-426. Springer, Heidelberg.
- [Burer '09] On the copositive representation of binary and continuous non-convex quadratic programs, *Math. Programming* **120**, 479–495.
- [Saha *et al.*'10] Dense Subgraphs with Restrictions and Applications to Gene Annotation Graphs, in *Research in Computational Molecular Biology*, 456–472, Springer, Berlin.
- [Bhaskara *et al.*'12] On quadratic programming with a ratio objective, in *Proc.ICALP'12*, 109-120. Springer, Berlin.

Selected references, continued

- [Dickinson/Gijben '14] On the computational complexity of membership problems for the completely positive cone and its dual, *Comput. Optim. Appl.* **57**, 403–415.
- [B. '15] Copositive relaxation beats Lagrangian dual bounds in quadratically and linearly constrained QPs, *SIAM J. Optimization* **25**, 1249–1275.
- [Amaral/B.'15] Copositivity-based approximations for mixed-integer fractional quadratic optimization, *Pacific J. Optimization* **11**, 225–238.
- [Peña/Vera/Zuluaga '15] Completely positive reformulations for polynomial optimization, *Math. Programming B* **151**, 405–431.
- [B. '16] Copositivity for second-order optimality conditions in general smooth optimization problems, *Optimization*, to appear.

Thank you!