Theoretical and computational study of several linearisation techniques for Binary Quadratic Problems

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Abstract

We perform a theoretical and computational study of the classical Linearisation Techniques (LT) and we propose a new LT for Binary Quadratic Problems (BQPs). We discuss the relations between the Linear Programming (LP) relaxations of the considered LT for generic BQPs. We prove that for a specific class of BQP all the LTs have the same LP relaxation value. We also compare the LT computational performance for four different BQPs from the literature. We consider the Unconstrained BQP and the Maximum Cut of edge-weighted graphs and, in order to measure the effects of constraints on the computational performance, we also consider the quadratic extension of two classical combinatorial optimization problems, i.e., the Knapsack and Stable Set problems.

keywords: Linearisation Techniques, Binary Quadratic Problems, Max Cut Problem, Quadratic Knapsack Problem, Quadratic Stable Set Problem.

1. Introduction

A widely used technique for solving Binary Quadratic Problems (BQPs) is by formulating them as Mixed Integer Linear Programs (MILPs). The main advantage of these linear reformulations is the use of generic MILP solvers, which keep improving their computational performance (see for example Lodi [19]). Several Linearisation Techniques (LTs) have been proposed in the literature, the seminal works of this stream of research are Fortet [9] and Glover and Woolsey [12], both based on introducing additional binary variables. Other LTs have been proposed based only on introducing additional continuous variables; in this stream of research we cite the following works: Glover and Woolsey [13], Glover [11], and Sherali and Smith [24]. All these LTs are presented in detail in Section 2 and compared in Section 3, which is devoted to computational results. The LT of Chaovalitwongse et al. [6] is deeply related to the LT of Sherali and Smith and, for this reason, these two techniques will be discussed together. A further LT is presented by Adams and Sherali [2], this approach is generalized to design the reformulation–linearisation technique (RLT) in Sherali and Adams [23]. Recently, other interesting LTs have been introduced in Gueye and Michelon [14] and Hansen and Meyer [15]. In [14], the authors propose a framework for unconstrained BQP based on two steps: in the first step the objective function is decomposed with a clique covering heuristic algorithm, while in the second step, valid inequalities are added to the model to get a better dual bound. In [15], a new family of LTs with a linear number of additional variables and constraints is presented. These LTs are based on a polyform representation of the objective function. The authors show that the best LT among the ones proposed is as tight as the LT of Glover and Woolsey [13] and it requires the solution of an auxiliary LP with a quadratic number of additional variables and constraints.

Paper Contribution. A first contribution of this paper is an overview of the strength of the Linear Programming (LP) relaxations of several LTs. Our analysis points out new interconnections between the classical LTs and an alternative LT, called Extended Linear Formulation (ELF). This new LT has been inspired by the ideas proposed in Jaumard et al. [17], where a reformulation specifically conceived for the Quadratic Stable Set Problem (QSSP) is proposed. For generic BQPs, the LT proposed by Glover and Woolsey in [13] and ELF are stronger than the LTs proposed by Glover in [11] and Sherali and Smith in [24]. The first two LTs require a quadratic number of additional variables and constraints, while the third and the forth require only a linear number.

A new theoretical result presented is the equivalence between the LP-relaxation value of all the LTs introduced for a specific class of BQPs. This class is rather generic and it contains the BQP formulation of the Max-Cut Problem.

An additional contribution of this paper is an extensive computational comparison of the LTs for four different classes of problem with and without linear constraints. In particular, we tested the Unconstrained BQP, the Max Cut Problem and the quadratic extensions of the Knapsack and the Stable Set problems.

2. Linearisation techniques for Binary Quadratic Problems

A generic Binary Quadratic Problem (BQP), with n variables and p constraints, can be formulated using the following quadratic formulation:

$$\min \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j + \sum_{i=1}^{n} L_i x_i : x \in K, \quad x \in \{0,1\}^n \right\} ,$$

where $Q \in \mathbb{R}^{n \times n}$, $L \in \mathbb{R}^n$, $K = \{x \in \mathbb{R}^n : Ax \geq b\}$, $A \in \mathbb{R}^{p \times n}$ and $b \in \mathbb{R}^p$. Q is a generic symmetric matrix, not restricted to being convex. Without loss of generality, we may assume $Q_{ii} = 0$, since we may incorporate those elements in the linear terms L_i (for a given binary variable x we have $x^2 = x$). In the following, we define as the Linear Programming (LP) Relaxation of a formulation, the same formulation where the constraints $x \in \{0,1\}^n$ are substituted by $x \in [0,1]^n$. In the next sections, we describe several alternatives for LTs for BQPs present in the literature and then we introduce the new Extended Linear Formulation (ELF).

2.1 Glover-Woolsey Linear Formulation

The standard method for linearising the quadratic terms is the one introduced by Glover and Woolsey and described in [13]. This linear formulation, called $\text{GW}_{[13]}$, reads as follows.

$$
\begin{aligned}
\mathrm{GW}_{[13]}: \quad & \min \sum_{i=1}^{n}\sum_{j=i+1}^{n} 2Q_{ij}y_{ij} + \sum_{i=1}^{n} L_i x_i \\
& y_{ij} \le x_i && i,j = 1,\dots,n,\ \ i<j && (1)\\
& y_{ij} \le x_j && i,j = 1,\dots,n,\ \ i<j && (2)\\
& y_{ij} \ge x_i + x_j - 1 && i,j = 1,\dots,n,\ \ i<j && (3)\\
& y_{ij} \ge 0 && i,j = 1,\dots,n,\ \ i<j && (4)\\
& x \in K \\
& x \in \{0,1\}^n \,.
\end{aligned}
$$

A new variable y_{ij} takes the place of the product between the original variables x_i and x_j in the objective function. We recall that GW$_{[13]}$ increases the size of the problem by adding $n(n-1)/2$ variables and $4n(n-1)/2$ constraints. These constraints enforce $y_{ij} = x_i x_j$ for all couples of binary variables x_i and x_j.

A constraint is redundant for a formulation if its removal does not change the set of optimal solutions of its LP-relaxation. Accordingly, the number of constraints of GW$_{[13]}$ can be reduced as follows:

Proposition 1. *Inequalities* (1) *and* (2)*, corresponding to non-negative entries of* Q*, and inequalities* (3) *and* (4)*, corresponding to non-positive entries of* Q*, are redundant for* GW$_{[13]}$.

Proof. See for example Forrester and Greenberg [8]. □

GW$_{[13]}$ can be strengthened by applying the so-called Reformulation Linearisation Technique (RLT) presented in Sherali and Adams [23]. The RLT is a procedure divided into two steps: the reformulation step creates additional nonlinear constraints by multiplying the constraints in K by product factors of the binary variables x and their complements $(1-x)$, and subsequently enforces the identity $x^2 = x$. The linearisation step then substitutes a continuous variable for each distinct product of variables. Hence, GW$_{[13]}$ can be viewed as first level RLT applied only on the bound constraints $0 \le x \le 1$. An alternative way to improve the strength of GW$_{[13]}$ is to include the so-called triangle and cycle inequalities (see for example [14] or [20]). In our analysis we do not consider these enhancements since we are interested in the basic version of GW$_{[13]}$.

2.2 Glover Linear Formulation

In this section we introduce the linearisation described in Glover [11]. This linear formulation, called G$_{[11]}$, reads as follows.

$$\begin{aligned}
\mathrm{G}_{[11]}: \quad & \min \sum_{i=1}^{n} w_i + \sum_{i=1}^{n} L_i x_i \\
& w_i \le Q_i^+ x_i && i = 1, \ldots, n && (5)\\
& w_i \ge Q_i^- x_i && i = 1, \ldots, n && (6)\\
& w_i \le \sum_{j=1}^{n} Q_{ij} x_j - Q_i^- (1 - x_i) && i = 1, \ldots, n && (7)\\
& w_i \ge \sum_{j=1}^{n} Q_{ij} x_j - Q_i^+ (1 - x_i) && i = 1, \ldots, n && (8)\\
& x \in K \\
& x \in \{0,1\}^n \ ,
\end{aligned}$$

where Q_i^+ and Q_i^- are suitable upper and lower bounds on the expression $\sum_{j=1}^{n} Q_{ij} x_j$, respectively. The main idea behind this linearisation is the introduction of the additional set of variables w_i representing the quantity $\sum_{j=1}^{n} Q_{ij} x_j$ if $x_i = 1$, or taking a value of 0 otherwise. Formulation $\mathrm{G}_{[11]}$ has the big advantage of using less variables and constraints than $\mathrm{GW}_{[13]}$. On the other hand, it requires the introduction of the so-called "big-M" constraints, leading to a weaker LP-relaxation.

An important point concerns the computation of Q_i^- and Q_i^+. In Glover [11], the author suggests to impose:

$$Q_i^- = \sum_{j=1}^{n} \min\{0, Q_{ij}\}, \quad Q_i^+ = \sum_{j=1}^{n} \max\{0, Q_{ij}\} \ . \tag{9}$$

Subsequently, in several works (see for example Adams et al. [1] and Wang et al. [25]) this approach has been improved by taking into account the feasible region K and hence computing the values for Q_i^- and Q_i^+ with more accuracy. This can be done as follows:

$$Q_i^- = \min_{x \in K} \sum_{j=1}^{n} Q_{ij} x_j, \quad Q_i^+ = \max_{x \in K} \sum_{j=1}^{n} Q_{ij} x_j. \tag{10}$$

It is easy to check that equations (9) and equations (10) coincide when $K = \emptyset$. From now on, when we refer to $\mathrm{G}_{[11]}$ we imply the version with Q_i^- and Q_i^+ defined in (9), since computing equations (10) may require the solution of an optimization problem which depends on the structure of K. Regardless of the method used for computing Q_i^- and Q_i^+, $\mathrm{G}_{[11]}$ increases the size of the problem by adding only n variables and $4n$ constraints.

However, since we are minimizing and the coefficients of the w variables are positive, it is possible to reduce the number of constraints:

Proposition 2. *Inequalities* (5) *and* (7) *are redundant for* $\mathrm{G}_{[11]}$.

Proof. See Adams et al. [1]. □

2.3 Sherali-Smith Linear Formulation

The third method linearises the quadratic terms using the techniques described in Sherali and Smith [24]. This linear formulation, called $\text{SS}_{[24]}$, reads as follows:

$$
\begin{aligned}
\text{SS}_{[24]}: \quad \min \ & \sum_{i=1}^{n} s_i + \sum_{i=1}^{n} (L_i + Q_i^-) x_i \\
& y_i = \sum_{j=1}^{n} Q_{ij} x_j - s_i - Q_i^- && i = 1, \ldots, n && (11) \\
& y_i \leq (Q_i^+ - Q_i^-)(1 - x_i) && i = 1, \ldots, n && (12) \\
& s_i \leq (Q_i^+ - Q_i^-) x_i && i = 1, \ldots, n && (13) \\
& y_i \geq 0 && i = 1, \ldots, n && (14) \\
& s_i \geq 0 && i = 1, \ldots, n && (15) \\
& x \in K \\
& x \in \{0, 1\}^n \ ,
\end{aligned}
$$

where Q_i^+ and Q_i^- are defined as in (9) or in (10). Since the latter case requires the computation of an additional optimization problem, we use (9) as for $\text{G}_{[11]}$. In Sherali and Smith [24], the authors introduce three formulations, called BP, $\bar{\text{BP}}$ and BP-strong. However, in absence of quadratic constraints, they are all equivalent and they can be written as $\text{SS}_{[24]}$. The idea behind $\text{SS}_{[24]}$ is similar to the one behind $\text{G}_{[11]}$, i.e., the introduction of additional variables representing the sum $\sum_{j=1}^{n} Q_{ij} - Q_i^-$ and using big-M constraints. $\text{SS}_{[24]}$ increases the size of the problem by adding $2n$ variables, $4n$ inequalities and n equations. More precisely, variables y can be projected out using equations (11), thus resulting in only n additional variables and $4n$ inequalities (12)-(15).

Formulation $\text{SS}_{[24]}$ is a strengthening of a precedent formulation proposed by Chaovalitwongse et al. [6] called $\text{CPP}_{[6]}$ which uses instead the following weaker (see Sherali and Smith [24]) definition of Q_i^+ and Q_i^-:

$$
Q_i^+ = \max_i \sum_{j=1}^{n} |Q_{ij}|, \quad Q_i^- = -\max_i \sum_{j=1}^{n} |Q_{ij}|.
$$

Like for $\text{G}_{[11]}$, also for $\text{SS}_{[24]}$ (and analogously for $\text{CPP}_{[6]}$) some constraints can be eliminated:

Proposition 3. *Inequalities* (13) *and* (14)*, are redundant for* $\text{SS}_{[24]}$.

Proof. See Sherali and Smith [24]. □

2.4 Extended Linear Formulation

We now introduce a new linearisation, called Extended Linear Formulation (ELF).

$$
\begin{aligned}
\text{ELF}: \quad \min \ & \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij} + \sum_{i=1}^{n} L_i x_i - \sum_{i=1}^{n}\sum_{j=i+1}^{n} 2Q_{ij}(z_{ij}^i + z_{ij}^j) \\
& z_{ij}^i + z_{ij}^j \le 1 \qquad i,j = 1,\dots,n, \ \ i<j \qquad (16)\\
& x_i + z_{ij}^i \le 1 \qquad i,j = 1,\dots,n, \ \ i<j \qquad (17)\\
& x_j + z_{ij}^j \le 1 \qquad i,j = 1,\dots,n, \ \ i<j \qquad (18)\\
& x_i + z_{ij}^i + z_{ij}^j \ge 1 \quad i,j = 1,\dots,n, \ \ i<j \qquad (19)\\
& x_j + z_{ij}^i + z_{ij}^j \ge 1 \quad i,j = 1,\dots,n, \ \ i<j \qquad (20)\\
& x \in K \\
& x \in \{0,1\}^n \,.
\end{aligned}
$$

This linearisation increases the size of the problem by adding $n(n-1)$ variables and $5n(n-1)$ constraints. A pair of new variables z_{ij}^i and z_{ij}^j is used instead of the product of variables x_i and x_j. These new variables modify the objective function and appear in the new set of constraints. The total sum of the quadratic costs is paid in the objective function ($\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}$) and then the correct value is reconstructed with the use of the z variables ($\sum_{i=1}^{n}\sum_{j=i+1}^{n} 2Q_{ij}(z_{ij}^i + z_{ij}^j)$). The values of the z variables are set according to the values of the x variables thanks to constraints (16)-(20), i.e., if $x_i = x_j = 1$ then $z_{ij}^i = z_{ij}^j = 0$, on the other hand, if one or both variables x_i and x_j have a value of 0, then we have $z_{ij}^i + z_{ij}^j = 1$, which implies the correctness of the formulation.

Finally, the following Proposition allows the reduction of the number of constraints also for ELF:

Proposition 4. *Inequalities* (19) *and* (20)*, corresponding to non-negative entries of Q, and inequalities* (16)*,* (17) *and* (18)*, corresponding to non-positive entries of Q are redundant for ELF.*

Proof. Let $(\tilde{x}, \tilde{z}^i, \tilde{z}^j)$ be an optimal solution of the LP-relaxation of ELF satisfying all inequalities except one of the constraints (19) associated to an entry $Q_{kl} \ge 0$. Let $x_k + z_{kl}^i + z_{kl}^j \ge 1$ be the violated inequality. And w.l.o.g, we assume that $\tilde{z}_{kl}^j \ge 0$, since the other constraints impose: $0 \le z_{kl}^i + z_{kl}^j \le 1$. We can increase the value of $\tilde{z}_{kl}^i$ to $\tilde{z}_{kl}^i + \Delta$ with $\Delta = \min\{1 - \tilde{z}_{kl}^i - \tilde{z}_{kl}^j, 1 - \tilde{x}_k - \tilde{z}_{kl}^i\}$. The constraint is violated hence $\tilde{x}_k + \tilde{z}_{kl}^i + \tilde{z}_{kl}^j < 1$, this implies: (i) $0 < 1 - \tilde{z}_{kl}^i - \tilde{z}_{kl}^j$, since $0 \le \tilde{x}_k$ and $\tilde{x}_k < 1 - \tilde{z}_{kl}^i - \tilde{z}_{kl}^j$; (ii) $0 < 1 - \tilde{x}_k - \tilde{z}_{kl}^i$, since $\tilde{x}_k + \tilde{z}_{kl}^i < 1$ and $\tilde{z}_{kl}^j \ge 0$; and therefore, Δ is positive. By observing that Δ corresponds to the minimum between the slacks of constraints (16) and (17) associated to k and l, the new solution is feasible by construction. The objective function value decreases by $-\Delta Q_{kj}$ This contradicts the fact of being optimal and violating one of the constraints (19). The same holds for constraints (20).

Similar considerations can be done for inequalities (16), (17) and (18) when $Q_{kl} \le 0$. Hence, eliminating from ELF the inequalities (19) and (20), corresponding to a couple of indices k and l with non-negative Q_{kl} or the inequalities (16), (17) and (18), corresponding to a couple of indices k and l with non-positive Q_{kl}, does not change the set of optimal solutions of the LP-relaxation of ELF (i.e., they are redundant). □

Formulations	Variables	Constraints	
		Original	Reduced
GW[13]	$n(n-1)/2$	$2n(n-1)$	$n(n-1)$
G[11],CPP[6], SS[24]	n	$4n$	$2n$
ELF	$n(n-1)$	$5n(n-1)$	$\approx \frac{5}{2}n(n-1)$

Table 1: Number of additional variables and constraints used in each LT.

Constraints (16), (17) and (18) provide upper bounds on the variables z, while constraints (19) and (20) provide lower bounds. Hence, according to the sign of the coefficients of the matrix Q and the sense of the objective function, some of them are redundant.

2.5 Formulation Summary

In Table 1, we report the number of additional variables and constraints needed by each LT. The columns concerning the constraints are subdivided in two parts: the table column – Original – report the number of inequalities needed by each formulation while the table column – Reduced – report the number of non redundant constraints needed by each formulation (see Propositions 1, 2, 3 and 4). In the following, this reduction of the formulation dimensions will be referred to as `Constraint-Redundancy` elimination. As far as GW[13], G[11], CPP[6] and SS[24] are concerned, regardless of the sign of the entries of Q, the `Constraint - Redundancy` elimination allows to reduce by one half the number of additional constraints. For ELF the situation is slightly different because the number of non redundant constraints depends on the sign of Q and it is hence included in the interval $[2n(n-1), 3n(n-1)]$, for this reason we reported the average value of $\frac{5}{2}n(n-1)$. As explained in Adams et al. [1], the number of constraints of G[11] can be further reduced to n via a variable transformation.

2.5.1 Formulation strength

In this section, we present a comparison of the strength of the LT discussed in the previous sections.

The strong connection between G[11] and SS[24] is given by the following proposition:

Proposition 5. *The polyhedra defined by the LP-relaxations of* G[11] *and* SS[24] *are isomorphic under a linear transformation that keeps the values of the x variables unchanged and the relation between the s and the w variables is the following:*

$$s_i = w_i - Q_i^- x_i \qquad i = 1, \dots, n.$$

Proof. As first step, it is possible to apply to SS[24] the variable substitution $s_i = w_i - Q_i^- x_i$ and subsequently equations (11) can be used to substitute variables y into the remaining constraints, thus obtaining exactly G[11]. By applying to G[11] the variable substitution $w_i = s_i + Q_i^- x_i$, we obtain SS[24]. □

A direct consequence of Proposition 5 is that the optimal LP-relaxation values of $\text{G}_{[11]}$ and $\text{SS}_{[24]}$ are identical.

The following proposition shows that ELF is an extended formulation of $\text{GW}_{[13]}$:

Proposition 6. *The polyhedra defined by the LP-relaxations of* $\text{GW}_{[13]}$ *and* ELF *are isomorphic under a linear transformation that keeps the values of the x variables unchanged and the relations between the z and the y variables are the following:*

$$z_{ij}^i = 1 - x_i, \quad z_{ij}^j = x_i - y_{ij} \qquad i, j = 1, \ldots, n, i < j.$$

Proof. Let $(\bar{x}, \bar{y})$ be a feasible solution to the LP-relaxation of $\text{GW}_{[13]}$. We consider the following solution $(\tilde{x}, \tilde{z}^i, \tilde{z}^j)$ of the LP-relaxation of ELF: $\tilde{x}_i = \bar{x}_i$, $\tilde{z}_{ij}^i = 1 - \bar{x}_i$, $\tilde{z}_{ij}^j = \bar{x}_i - \bar{y}_{ij}$. It is easy to check that it is feasible and it has the same value. Now let $(\tilde{x}, \tilde{z}^i, \tilde{z}^j)$ be a feasible solution to the LP-relaxation of ELF. We consider the following solution $(\bar{x}, \bar{y})$ of the LP-relaxation of $\text{GW}_{[13]}$: $\bar{x}_i = \tilde{x}_i$, $\bar{y}_{ij} = 1 - \tilde{z}_{ij}^i - \tilde{z}_{ij}^j$. Again, it is easy to check that it is feasible and it has the same value. This implies that for every feasible solution of the LP-relaxation of $\text{GW}_{[13]}$ there exists one feasible solution of the LP-relaxation of ELF of the same value and vice versa, proving the statement. □

Also in this case, a direct consequence of Proposition 6 is that the LP-relaxation values of $\text{GW}_{[13]}$ and ELF are identical. The new linearisation ELF can be seen as an extended formulation (see e.g., [7]) of GW in the sense that the projection on the (x,y)-space of the polytope defined by (16)-(20), and constraints $y_{ij} = 1 - z_{ij}^i - z_{ij}^j$ $(i, j = 1, \ldots, n,\ i < j)$, is equal to the polytope defined by (1)-(4) and by $x \in [0, 1]^n$. Moreover, Proposition 6 also implies that every valid inequality for $\text{GW}_{[13]}$ is also valid for ELF.

We recall that in the following analysis we use formulas (9), which imply:

$$\sum_{j=1}^{n} Q_{ij} = Q_i^+ + Q_i^-.$$

To the best of our knowledge, no formal proof concerning the relation between the LP relaxations of $\text{GW}_{[13]}$ and $\text{G}_{[11]}$ has been given in the literature. For sake of completeness, we present the following Proposition, that will be useful in the rest of the section:

Proposition 7. *The LP-relaxation of $GW_{[13]}$ is stronger than the LP relaxation of $G_{[11]}$.*

Proof. Let $(\tilde{x}, \tilde{y})$ be a feasible solution of the LP-relaxation of $\text{GW}_{[13]}$, we consider the solution $(\bar{x}, \bar{w})$ obtained from $(\tilde{x}, \tilde{y})$ as follows:

$$\bar{x}_i = \tilde{x}_i \qquad \bar{w}_i = \sum_{j=1}^{n} Q_{ij} \tilde{y}_{ij} \qquad i = 1, \ldots, n;$$

both solutions have by construction the same objective function value. We now show that the solution $(\bar{x}, \bar{w})$ is feasible for the LP-relaxation of $\text{G}_{[11]}$. We notice that, for each $i = 1, \ldots, n$, we have:

$$\bar{w}_i = \sum_{j=1}^{n} Q_{ij}\tilde{y}_{ij} = \sum_{\substack{j=1\dots,n:\\ Q_{ij}<0}} Q_{ij}\tilde{y}_{ij} + \sum_{\substack{j=1\dots,n:\\ Q_{ij}\geq 0}} Q_{ij}\tilde{y}_{ij} \geq \sum_{\substack{j=1\dots,n:\\ Q_{ij}<0}} Q_{ij}\tilde{y}_{ij} \geq \sum_{\substack{j=1\dots,n:\\ Q_{ij}<0}} Q_{ij}\tilde{x}_i = Q_i^-\tilde{x}_i$$

where the last inequality derives from $\tilde{y}_{ij} \leq \tilde{x}_i$. Analogously, for each $i = 1, \dots, n$, we have:

$$\begin{aligned}\bar{w}_i &= \sum_{j=1}^{n} Q_{ij}\tilde{y}_{ij} = \sum_{\substack{j=1\dots,n:\\ Q_{ij}<0}} Q_{ij}\tilde{y}_{ij} + \sum_{\substack{j=1\dots,n:\\ Q_{ij}\geq 0}} Q_{ij}\tilde{y}_{ij} \geq \\ &\geq \sum_{\substack{j=1\dots,n:\\ Q_{ij}<0}} Q_{ij}\tilde{x}_j + \sum_{\substack{j=1\dots,n:\\ Q_{ij}\geq 0}} Q_{ij}\tilde{x}_i + \sum_{\substack{j=1\dots,n:\\ Q_{ij}\geq 0}} Q_{ij}\tilde{x}_j - \sum_{\substack{j=1\dots,n:\\ Q_{ij}\geq 0}} Q_{ij} = \\ &= \sum_{j=1}^{n} Q_{ij}\tilde{x}_j - Q_i^+(1-\tilde{x}_i)\end{aligned}$$

where the first inequalities derive from $\tilde{y}_{ij} \leq \tilde{x}_i$ and $\tilde{y}_{ij} \geq \tilde{x}_i + \tilde{x}_j - 1$. The two sequences of inequalities show that the solution $(\bar{x}, \bar{y})$ respects inequalities (6) and (8). Finally, we provide an instance where the optimal value of the LP-relaxation of GW[13] is greater than the optimal value of the LP-relaxation of G[11]. Consider the following instance with $K = \emptyset$, $n = 3$ and $L = \begin{bmatrix} 1 & -1 & 8 \end{bmatrix}$; $Q = \begin{bmatrix} 0 & -1 & 1 \\ -1 & 0 & -5 \\ 1 & -5 & 0 \end{bmatrix}$. The optimal solution of the LP-relaxation of GW[13] is $\tilde{x}_1 = 0$, $\tilde{x}_2 = 1$, $\tilde{x}_3 = 1$, $\tilde{y}_{12} = 0$, $\tilde{y}_{13} = 0$, $\tilde{y}_{23} = 1$ and the optimal solution value is -3. On the other hand, the optimal solution of the LP-relaxation of G[11] is $\bar{x}_1 = 0.\overline{54}$, $\bar{x}_2 = 1$, $\bar{x}_3 = 0.\overline{90}$, $\bar{w}_1 = -0.\overline{54}$, $\bar{w}_2 = -5.\overline{09}$, $\bar{w}_3 = -4.\overline{54}$ and the optimal solution value is $-3.\overline{36}$. □

We now introduce two lemmas that are used to show a new property of the LP-relaxation of GW[13] and G[11]. Both lemmas use the following Proposition:

Proposition 8. *In case of $K = \emptyset$, given a feasible vector $\bar{x}$ for GW[13] (resp. G[11]), the optimal values of the $\bar{y}$ (resp. $\bar{w}$) are:*

$$\bar{y}_{ij} = \begin{cases} \max\{0, \bar{x}_i + \bar{x}_i - 1\} & \text{if } Q_{ij} \geq 0 \\ \min\{\bar{x}_i, \bar{x}_j\} & \text{if } Q_{ij} < 0 \end{cases} \qquad i, j = 1, \dots, n,$$

$$\bar{w}_i = \max\left\{Q_i^-\bar{x}_i, \sum_{j=1}^{n} Q_{ij}\bar{x}_j - Q_i^+(1-\bar{x}_i)\right\} \qquad i = 1, \dots, n.$$

Proof. The statement is a direct consequence of the sign of the y and w variables in the respective objective functions and of the fact that there are no additional constraints, except for the ones linking the x variables to the y and w variables respectively. □

Lemma 1. *If $K = \emptyset$, let $(\tilde{x}, \tilde{y})$ and $(\bar{x}, \bar{w})$ be two optimal solutions of the LP-relaxations of GW[13] and G[11] respectively. If $\tilde{x}_i = \bar{x}_i = \frac{1}{2}$ for all $i = 1, \dots, n$, both solutions have the same objective function value equal to $\frac{1}{2}\sum_{i=1}^{n}(Q_i^- + L_i)$.*

Proof. It is sufficient to compute the objective function value of both solutions. If $Q_{ij} \geq 0$, we have $\tilde{y}_{ij} = \max\{0, \tilde{x}_i + \tilde{x}_i - 1\} = \max\{0, 0\} = 0$. If $Q_{ij} < 0$, we have $\tilde{y}_{ij} = \min\{\tilde{x}_i, \tilde{x}_j\} = \min\left\{\frac{1}{2}, \frac{1}{2}\right\} = \frac{1}{2}$. The objective function value of GW$_{[13]}$ is hence the following:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\tilde{y}_{ij} + \sum_{i=1}^{n} L_i\tilde{x}_i = \frac{1}{2}\sum_{\substack{i,j=1\dots,n:\\ Q_{ij}<0}} Q_{ij} + \frac{1}{2}\sum_{i=1}^{n} L_i = \frac{1}{2}\sum_{i=1}^{n}(Q_i^- + L_i);$$

Moreover, we have $\bar{w}_i = \max\{Q_i^- x_i, \sum_{j=1}^n Q_{ij}\bar{x}_j - Q_i^+(1-\bar{x}_i)\}$, leading to the following objective function value of G$_{[11]}$:

$$\begin{aligned}\sum_{i=1}^{n}\bar{w}_i + \sum_{i=1}^{n} L_i\bar{x}_i &= \sum_{i=1}^{n}\max\left\{Q_i^-\bar{x}_i, \sum_{j=1}^{n} Q_{ij}\bar{x}_j - Q_i^+(1-\bar{x}_i)\right\} + \sum_{i=1}^{n} L_i\bar{x}_i \\ &= \sum_{i=1}^{n}\max\left\{\frac{1}{2}Q_i^-, \frac{1}{2}\sum_{j=1}^{n}(Q_{ij} - Q_i^+)\right\} + \frac{1}{2}\sum_{i=1}^{n} L_i \\ &= \sum_{i=1}^{n}\max\left\{\frac{1}{2}Q_i^-, \frac{1}{2}Q_i^-\right\} + \frac{1}{2}\sum_{i=1}^{n} L_i = \frac{1}{2}\sum_{i=1}^{n}(Q_i^- + L_i).\end{aligned}$$

□

Lemma 2. *If $K = \emptyset$ and $L_i = -\sum_{j=1}^n Q_{ij}$ $(i = 1, 2, \dots, n)$, an optimal solution of the LP-relaxation of GW$_{[13]}$ is the following:*

$$\begin{aligned}\bar{x}_i &= \frac{1}{2}, & i = 1, \dots, n, \\ \bar{y}_{ij} &= \begin{cases} 0 & \textit{if } Q_{ij} \geq 0; \\ \frac{1}{2} & \textit{if } Q_{ij} < 0 \end{cases} & i, j = 1, \dots, n.\end{aligned}$$

Proof. The objective function is separable, hence, we measure the impact of changing one single variable at a time. We consider the solutions $\hat{x} = \bar{x} \pm \epsilon e_{\hat{i}}$ with $\hat{i} = 1, \dots, n$ and $\epsilon \geq 0$, where $e_{\hat{i}}$ is an n-dimensional vector with value 1 in the $\hat{i}$-th component and 0 otherwise.
We consider first the case $\hat{x} = \bar{x} + \epsilon e_{\hat{i}}$. Proposition 8 implies that the $\hat{y}$ variable corresponding to $\hat{x} = \bar{x} + \epsilon e_{\hat{i}}$ is equal to $\bar{y}$, except for $i = \hat{i}$, where we have:

$$\hat{y}_{\hat{i}j} = \begin{cases} \epsilon & \text{if } Q_{\hat{i}j} \geq 0 \\ \frac{1}{2} & \text{if } Q_{\hat{i}j} < 0 \end{cases} \qquad j = 1, \dots, n.$$

If we consider the objective function value of the LP-relaxation of GW$_{[13]}$ we obtain, for a given

$\hat{i}$:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\hat{y}_{ij} + \sum_{i=1}^{n} L_i\hat{x}_i = \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\hat{y}_{ij} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\hat{x}_i =$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} + \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}\geq 0}} Q_{\hat{i}j} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\bar{x}_i - \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}\geq 0}} Q_{\hat{i}j} - \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}<0}} Q_{\hat{i}j} =$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\bar{x}_i - \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}<0}} Q_{\hat{i}j} \geq \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} + \sum_{i=1}^{n} L_i\bar{x}_i.$$

Secondly, if we consider the solution $\hat{x} = x - \epsilon e_{\hat{i}}$, it also differs from $\bar{x}$ when $i = \hat{i}$, where we have:

$$\bar{y}_{\hat{i}j} = \begin{cases} 0 & \text{if } Q_{\hat{i}j} \geq 0 \\ \dfrac{1}{2} - \epsilon & \text{if } Q_{\hat{i}j} < 0 \end{cases} \quad i, j = 1, \dots, n.$$

This leads to

$$\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\hat{y}_{ij} + \sum_{i=1}^{n} L_i\hat{x}_i = \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\hat{y}_{ij} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\hat{x}_i =$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} - \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}<0}} Q_{\hat{i}j} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\bar{x}_i + \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}\geq 0}} Q_{\hat{i}j} + \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}<0}} Q_{\hat{i}j} =$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} - \sum_{i=1}^{n}(\sum_{j=1}^{n} Q_{ij})\bar{x}_i + \epsilon \sum_{\substack{j=1\dots,n\,:\\ Q_{\hat{i}j}\geq 0}} Q_{\hat{i}j} \geq \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}\bar{y}_{ij} + \sum_{i=1}^{n} L_i\bar{x}_i.$$

In both cases, the objective function value of $(\hat{x}, \hat{y})$ is greater than the one of $(\bar{x}, \bar{y})$, proving that $(\bar{x}, \bar{y})$ is optimal. □

The following theorem introduces an interesting class of BQP instances, where all the LT considered in this paper are equivalent in terms of LP-relaxation:

Theorem 1. *If $K = \emptyset$ and $L_i = -\sum_{j=1}^{n} Q_{ij} (i = 1, 2, \dots, n)$, the optimal solution values of the LP-relaxation of GW$_{[13]}$ and G$_{[11]}$ coincide and they are both equal to $\frac{1}{2}\sum_{i=1}^{n}(Q_i^- + L_i)$. Moreover, let $(\bar{x}, \bar{w})$ and $(\tilde{x}, \tilde{y})$ be the optimal solutions of their LP-relaxations, we have $\bar{x}_i = \tilde{x}_i = \frac{1}{2}$ $(i = 1, \dots, n)$ and $\tilde{y}$ and $\bar{w}$ are defined accordingly to Proposition 8.*

Proof. If $L_i = -\sum_{j=1}^{n} Q_{ij}$, we can apply Lemma 2 to identify the optimal solution of the LP-relaxation of GW$_{[13]}$ and its value. We can hence use Lemma 1 to show that there exists an optimal solution to G$_{[11]}$ with $\bar{x} = \tilde{x}$ and with the same objective function value. Finally, we notice that, G$_{[11]}$ can not be stronger than GW$_{[13]}$ (Proposition 7), for this reason, we have that the solution with $\bar{x} = \tilde{x} = \frac{1}{2}$ is also an optimal solution to G$_{[11]}$. □

LP of $\text{GW}_{[13]}$	$\Rightarrow (Prop.\ 7)$	LP of $\text{G}_{[11]}$		
$\Updownarrow (Prop.\ 6)$		$\Updownarrow (Prop.\ 5)$		
LP of ELF		LP of $\text{SS}_{[24]}$	$\Rightarrow$ (see [24])	LP of $\text{CPP}_{[6]}$

Table 2: Summary of the relations between the strength of the LP-relaxations.

An important class of instances, satisfying Theorem 1, corresponds to BQP reformulation of the Max Cut problem (see Section 3.1).

Finally, in Table 2, we summarize the relations between the different LP-relaxations of the formulations studied. The relation "A $\Leftrightarrow$ B" stands for "A and B have the same LP-relaxation value" and "A $\Rightarrow$ B" stands for "A has a stronger LP-relaxation value than B". For each relation, we report the reference where it is proved.

3. Computational experiments

In this section, we assess the computational performances of the LTs discussed in this paper, i.e., $\text{GW}_{[13]}$, $\text{G}_{[11]}$, $\text{SS}_{[24]}$ and the new ELF. Preliminary experiments showed that the LP-relaxation of $\text{CPP}_{[6]}$ is extremely weak on all the test-beds, this is due to the fact of having large big-M values compared to the ones of $\text{SS}_{[24]}$. Since this formulation is computationally dominated by $\text{SS}_{[24]}$, it is dropped from the comparison tests.

The first part of our tests is based on the Unconstrained BQP and on the Maximum Cut Problem. The second part of our tests is based on quadratic instances with linear constraints, more precisely we consider the Quadratic Knapsack Problem and the Quadratic Stable Set Problem. In our computational comparison we decided not to use any problem dependent valid inequalities, since our goal is to compare the formulations in their basic versions.

All the experiments have been performed on a computer with a 3.40 Ghz 8-core Intel Core i7-3770 processor and 16Gb RAM, running a 64 bits Linux operating system. We use `CPLEX` 12.7.0 [16] as MILP solver ran single-threaded with default parameter settings. The tests have been performed with the `Constraint-Redundancy` elimination activated. It is worth mentioning that, thanks to preliminary experiments, we observed a substantial worsening (up to several orders of magnitude) of the overall computing time of `CPLEX` when this intuitive adjustment of the LTs is not applied.

MILP solvers implement different branch-and-cut algorithms and they all heuristically separate generic cuts in order to improve the quality of the dual bounds. In addition, the solvers perform several variable-and-constraint reduction techniques which are based on the specific formulation to solve. These aspects must be taken into account when analyzing the computational performance of different LTs. For example a more aggressive strategy of a solver applied to a specific LT (rather than to another one) may influence the computational behavior. Unfortunately these distortions generated by the specific implementations of the solvers are impossible to eliminate. In other words, the computational analysis of the next section is dependent on the choice of `CPLEX` 12.7.0 and the conclusions may be slightly different in case an other solver is used (or simply other settings of parameters). Nevertheless our experiments give an overall assessment of the relative computational performance of the different LTs for four different classes of problems and using one of the state-of-the-art MILP solvers.

3.1 Unconstrained Problems

Problem description. Our first aim is to investigate the strength of the different formulations without the influence of additional constraints ($K = \emptyset$). For this reason, we adopt the Biq Mac library (see Wiegele [26]) as a case study. The Biq Mac library is a collection of instances widely used in the literature, see for example Rendl et al. [22] or, more recently, Krislock et al. [18]. It is composed of two families of problems: the first one is the *Unconstrained BQP* (UBQP):

$$\min \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j + \sum_{i=1}^{n} L_i x_i : x \in \{0,1\}^n \right\} ,$$

where Q is a symmetric matrix of order n. The second family is the *Max Cut* (MC) problem. The MC consists of finding a maximum weighted bipartition of a graph G of n vertices (see for example Rendl et al. [22]) and it can be formulated as follows:

$$\max \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{Q}_{ij} x_i x_j : x \in \{-1,1\}^n \right\} ,$$

where $\tilde{Q}$ is the Laplacian matrix of the graph G. It is well known that the UBQP and the MC are equivalent (see Caprara [4] or Krislock et al. [18]).

The Biq Mac library used for the experiments is divided into five classes: `beasley`, `gka`, and `be` are UBQP instances, while `rudy`, `ising` are MC instances. The classes altogether form a test bed of 343 instances. Some are randomly generated instances and others come from a statistical physics application. In each class, the instances differ in terms of size n, density of the matrix Q and L (for further details on the instance features, we refer the reader to Wiegele [26]).

In our experiments we used the UBQP formulation of the MC problem obtained with the following transformation. Let w_{ij} ($i, j = 1, \dots, n$, $w_{ij} = w_{ji}$) be the set of weights associated to a given graph G, the UBQP for the MC on G has the following objective function (see [4]):

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} [x_i(1-x_j) + x_j(1-x_i)] = -\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i x_j + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(x_i + x_j) =$$
$$-\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i x_j + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_j = -\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i x_j + \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i \ .$$

The last term of the chain of equations shows that all UBQP instances arising from MC instances have $L_i = -\sum_{j=1}^{n} Q_{ij}$ and hence belong to the class of instances of Theorem 1.

Tables description. In Table 3 and Table 4 we report the results concerning the whole Biq Mac Library. Both tables are divided into 5 horizontal blocks, one for each class of instances (`be`,

	n	#	LP times				LP iterations				LP gaps			
			GW$_{[13]}$	ELF	G$_{[11]}$	SS$_{[24]}$	GW$_{[13]}$	ELF	G$_{[11]}$	SS$_{[24]}$	GW$_{[13]}$	ELF	G$_{[11]}$	SS$_{[24]}$
be	*100*	*10*	0.07	0.31	0.01	0.01	4292.1	8831.0	210.5	100.0	73.6	73.6	73.6	73.6
	120	*20*	0.05	0.22	0.01	0.01	3451.2	7033.0	259.7	122.4	63.6	63.6	63.7	63.7
	150	*20*	0.27	0.48	0.02	0.01	4899.6	10985.4	328.2	151.5	69.1	69.1	69.1	69.1
	200	*20*	0.82	1.50	0.04	0.02	8669.5	19494.1	437.4	200.6	79.1	79.1	79.1	79.1
	250	*10*	0.07	0.11	0.04	0.03	2798.4	5856.1	569.6	291.5	42.6	42.6	43.7	43.7
beasley	*50*	*10*	0.00	0.00	0.00	0.00	120.9	234.2	82.0	63.4	0.1	0.1	10.2	10.2
	100	*10*	0.01	0.01	0.00	0.00	676.1	1034.4	218.0	136.5	12.9	12.9	22.9	22.9
	250	*10*	0.07	0.12	0.05	0.03	2822.2	5943.2	598.8	278.8	44.3	44.3	44.9	44.9
	500	*10*	0.64	1.11	0.32	0.19	10543.1	22787.4	1184.8	504.1	87.4	87.4	87.4	87.4
gka	*20*	*1*	0.00	0.00	0.00	0.00	28.0	408.0	20.0	21.0	66.0	66.0	67.3	67.3
	30	*3*	0.00	0.00	0.00	0.00	171.7	561.3	54.3	34.7	40.3	40.3	43.1	43.1
	40	*2*	0.00	0.02	0.00	0.00	337.5	1382.5	62.5	41.0	60.4	60.4	61.2	61.2
	50	*4*	0.00	0.01	0.00	0.00	312.3	1143.0	84.0	58.5	34.3	34.3	39.4	39.4
	60	*3*	0.00	0.01	0.00	0.00	328.7	1738.3	91.3	71.3	38.3	38.3	41.7	41.7
	70	*3*	0.01	0.02	0.00	0.00	390.3	2252.0	122.7	81.7	40.1	40.1	45.8	45.8
	80	*3*	0.00	0.02	0.00	0.00	465.7	2779.0	133.0	98.0	35.1	35.1	43.1	43.1
	90	*2*	0.01	0.04	0.00	0.00	341.0	4443.0	131.5	108.5	45.7	45.7	52.7	52.7
	100	*13*	0.02	0.10	0.00	0.00	1925.1	4654.2	203.5	109.3	50.7	50.7	53.3	53.3
	125	*1*	0.03	0.15	0.01	0.01	182.0	15366.0	118.0	121.0	92.2	92.2	92.7	92.7
	200	*5*	0.27	0.60	0.03	0.02	4898.2	10759.0	431.6	209.6	58.9	58.9	59.7	59.7
	500	*5*	32.52	64.78	0.55	0.35	50312.4	114504.4	1153.4	500.4	92.8	92.8	92.8	92.8
ising	*100*	*9*	0.03	0.07	0.01	0.00	3437.1	6506.9	203.7	101.1	20.4	20.4	20.4	20.4
	125	*3*	0.01	0.01	0.00	0.00	510.0	842.7	261.7	127.3	27.2	27.2	27.2	27.2
	150	*6*	0.13	0.29	0.02	0.01	10253.0	19422.7	306.8	150.0	19.2	19.2	19.2	19.2
	200	*6*	0.24	0.57	0.03	0.02	15686.3	29183.7	409.2	200.0	18.8	18.8	18.8	18.8
	216	*3*	0.01	0.02	0.01	0.01	777.0	1438.3	456.3	217.7	29.1	29.1	29.1	29.1
	225	*3*	0.00	0.02	0.01	0.01	633.0	1082.7	462.0	234.7	16.9	16.9	16.9	16.9
	250	*6*	0.32	0.95	0.05	0.04	20947.0	39318.8	512.5	250.0	19.9	19.9	19.9	19.9
	300	*6*	0.56	1.15	0.08	0.07	26308.3	49666.8	616.3	300.0	19.5	19.5	19.5	19.5
	343	*3*	0.02	0.04	0.03	0.02	1233.3	2283.3	722.7	346.3	29.7	29.7	29.7	29.7
	400	*3*	0.02	0.04	0.02	0.02	1117.0	1936.7	817.0	415.7	17.9	17.9	17.9	17.9
rudy	*60*	*10*	0.00	0.02	0.00	0.00	618.9	2334.2	63.2	63.2	40.1	40.1	40.1	40.1
	80	*30*	0.01	0.06	0.00	0.00	1372.1	3478.5	136.2	81.0	59.0	59.0	59.0	59.0
	100	*90*	0.02	0.10	0.00	0.00	1916.5	5402.2	161.7	102.6	56.6	56.6	56.6	56.6

Table 3: Computational comparison of the LP-relaxations of the LTs for Biq Mac instances

	n	#	MILP times								MILP branching nodes				exit gaps			
			$GW_{[13]}$		ELF		$G_{[11]}$		$SS_{[24]}$		$GW_{[13]}$	ELF	$G_{[11]}$	$SS_{[24]}$	$GW_{[13]}$	ELF	$G_{[11]}$	$SS_{[24]}$
be	*100*	*10*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	903	159877	489570	294827	**33.8**	64.7	50.0	51.1
	120	*20*	1730.6	**1**	tl	0	tl	0	tl	0	4400	368818	286643	218557	**20.5**	50.4	40.0	40.8
	150	*20*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	1667	234478	229528	162299	**33.2**	60.2	47.3	50.5
	200	*20*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	266	117224	129028	207618	57.2	69.0	**54.7**	62.1
	250	*10*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	4032	433728	41637	42396	**8.5**	32.7	25.5	25.3
beasley	*50*	*10*	**0.0**	**10**	0.0	**10**	0.0	**10**	0.0	**10**	0	0	74	1	**0.0**	**0.0**	**0.0**	0.0
	100	*10*	0.3	**10**	**0.2**	**10**	11.2	**10**	7.2	**10**	5	142	1637	1440	**0.0**	0.0	**0.0**	0.0
	250	*10*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	3642	484278	41674	47243	**10.1**	35.4	27.4	27.5
	500	*10*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	0	75038	6188	86809	81.7	58.9	**54.4**	59.2
gka	*20*	*1*	**0.0**	**1**	0.0	**1**	0.0	**1**	0.0	**1**	0	21	44	43	**0.0**	**0.0**	**0.0**	**0.0**
	30	*3*	**0.0**	**3**	0.0	**3**	0.1	**3**	0.1	**3**	0	33	247	109	**0.0**	**0.0**	**0.0**	**0.0**
	40	*2*	0.7	**2**	**0.4**	**2**	1.8	**2**	1.8	**2**	0	363	2222	1324	**0.0**	**0.0**	**0.0**	**0.0**
	50	*4*	**0.6**	**4**	1.0	**4**	10.2	**4**	8.7	**4**	2	771	4607	3771	**0.0**	**0.0**	**0.0**	0.0
	60	*3*	**0.5**	**3**	0.5	**3**	5.2	**3**	4.6	**3**	9	375	1153	1460	**0.0**	**0.0**	**0.0**	0.0
	70	*3*	0.8	**3**	**0.6**	**3**	7.1	**3**	7.7	**3**	12	266	1927	1731	**0.0**	**0.0**	**0.0**	**0.0**
	80	*3*	**0.5**	**3**	0.5	**3**	4.9	**3**	3.9	**3**	12	160	1466	887	**0.0**	**0.0**	**0.0**	0.0
	90	*2*	**0.5**	**2**	1.0	**2**	1.6	**2**	1.1	**2**	30	141	784	532	**0.0**	**0.0**	**0.0**	**0.0**
	100	*13*	987.5	**6**	1241.4	4	1242.1	4	1241.5	4	2848	332199	264265	208236	**9.9**	30.1	24.6	25.4
	125	*1*	**3.8**	**1**	6.9	**1**	5.0	**1**	7.6	**1**	176	529	3170	2827	**0.0**	**0.0**	**0.0**	**0.0**
	200	*5*	1465.3	**1**	tl	0	tl	0	tl	0	1079	211712	118335	114323	**24.9**	50.1	39.9	44.9
	500	*5*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	0	19242	5329	130956	90.1	86.3	**75.3**	78.0
ising	*100*	*9*	74.2	**9**	**65.6**	**9**	1644.5	1	1699.4	1	5679	10918	1943960	3449968	0.0	**0.0**	7.6	7.5
	125	*3*	**1.6**	**3**	17.9	**3**	tl	0	tl	0	38	27326	3487383	4886222	**0.0**	0.0	15.2	16.4
	150	*6*	902.3	**4**	1045.3	3	tl	0	tl	0	16394	55880	370536	1059850	**1.0**	1.3	13.3	12.5
	200	*6*	1697.4	**1**	tl	0	tl	0	tl	0	30829	98811	265229	647454	4.5	**4.3**	14.8	14.0
	216	*3*	**13.6**	**3**	tl	0	tl	0	tl	0	595	1896661	3025926	2521665	**0.0**	7.3	23.9	23.0
	225	*3*	**0.8**	**3**	4.9	**3**	tl	0	tl	0	57	6695	3973997	3392715	**0.0**	0.0	11.9	11.8
	250	*6*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	28752	66611	202984	413173	7.8	**7.6**	17.1	16.3
	300	*6*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	27969	58156	161895	282489	**8.3**	8.9	17.2	16.3
	343	*3*	**140.4**	**3**	tl	0	tl	0	tl	0	2496	1124983	1645263	1550100	**0.0**	15.2	27.0	25.6
	400	*3*	**2.4**	**3**	900.7	**3**	tl	0	tl	0	162	594238	1580827	1505487	**0.0**	0.0	14.1	13.3
rudy	*60*	*10*	tl	**0**	tl	**0**	tl	**0**	tl	**0**	44880	1897854	3508202	1294517	**3.8**	19.8	17.0	17.4
	80	*30*	1197.4	**10**	1209.3	**10**	tl	0	tl	0	4691	503775	1005699	717697	**21.2**	35.1	33.4	33.0
	100	*90*	1223.8	**30**	1561.2	20	tl	0	tl	0	3897	676430	784450	533997	**22.7**	37.5	35.3	33.7

Table 4: Computational comparison of the different formulations for solving Biq Mac instances to proven optimality

beasly, gka, ising and rudy). In each line we group together the results relative to instances of the same size (same values of n). The first two columns of both tables report the size of the subclasses of instances and their cardinality (i.e., the number of instances of a specific subclass).

In Table 3 we report the results concerning the computational behavior for solving the LP-relaxation of the LTs considered. The table provides the following information:

- *LP times*. The average time required by CPLEX to solve the LP-relaxation to proven optimality.
- *LP iterations*. The average number of simplex iterations need by CPLEX to solve the LP-relaxation.
- *LP gaps*. The average gap (in percentage) between the optimal value of the LP-relaxation and the optimal solution value (or best know incumbent solution).

In Table 4 we report the results concerning the computational behavior for solving the test problems with the different LTs to proven optimality. The table provides the following information:

- *MILP times*. The average computational time required by CPLEX to solve the problem to proved optimality and the number of instances solved within the time-limit of 1800 seconds (we report tl and 0 in case all the instances of a specific subclass and formulation reach the time limit). In each line, the most efficient LT is reported in bold text, i.e., the one with shorter computing time or larger number of instances solved respectively.
- *MILP branching nodes*. The average number of nodes explored by CPLEX in the Branch-and-Bound tree.
- *MILP exit gaps*. The average percentage exit gap between the upper and the lower bounds computed by CPLEX in case the time limit is reached (0.0 is reported otherwise). The LT with the lowest open gap is reported in bold text.

Tables discussion. Table 3 shows, as expected, that the four LTs considered present the same LP-relaxation values for the MC instances. On the other hand, the situation for the Biq instances is different: $\text{GW}_{[13]}$ and ELF are characterized by stronger LP-relaxation values (the difference is less clear for the be and beasley class of instances). As far as LP times and iterations are concerned, $\text{GW}_{[13]}$ and ELF take a higher number of iterations and longer computing times than $\text{G}_{[11]}$ and $\text{SS}_{[24]}$. This figure can be explained by the higher number of additional variables and constraints. Since for the MC instances all the LP-relaxation bounds are equivalent, $\text{SS}_{[24]}$ is the more effective option to compute it.
Concerning Table 4, the formulations with the best computational behavior for the Biq Mac instances are $\text{GW}_{[13]}$ and ELF. These formulations clearly outperform $\text{G}_{[11]}$ and $\text{SS}_{[24]}$ concerning both the average computing time and the total number of instances solved. For the Biq instances, this is due to the fact of having stronger LP-relaxation values which allows a better computational convergence. For the Mac instances, where the LP-relaxation values coincides, the different behavior can be explained by the better performance of $\text{GW}_{[13]}$ and ELF during the branching scheme and by the efficacy of the generic cuts generated by CPLEX. In case the time limit is reached, ELF explores a higher number of branching nodes than $\text{GW}_{[13]}$ but the average exit gaps are higher. This figure is due to the different policy of CPLEX in separating cuts at the root node, i.e., for

$GW_{[13]}$, CPLEX spends a large amount of time in improving the root node bound, while for ELF CPLEX starts immediately to branch.

3.2 Constrained Problems

In the remaining part of this computational section we introduce and discuss the other two test problems considered, i.e., the Quadratic Stable Set Problem and the Quadratic Knapsack Problem. These two problems are used to measure the behaviour of the different LTs discussed in this paper in presence of constraints.

3.2.1 Quadratic Stable Set Problem

Problem description. We recall that a stable set is a subset of fully disconnected vertices. Following the notation of Section 2, we present the problem in minimization form. The formal definition of the Quadratic Stable Set Problem (QSSP) is the following: given an undirected graph $G = (V, E)$, with $V = \{v_1, \ldots, v_n\}$ the set of vertices and E the set of edges, a vector of linear cost $L \in \mathbb{R}^n$ on the vertices and a symmetric matrix of quadratic costs $Q \in \mathbb{R}^{n\times n}$ on couples of vertices, the QSSP searches for a stable set of G with minimum cost. In other words, if vertices i and j are in the solution, not only the linear costs are collected but also an additional quadratic cost equal to Q_{ij} is considered.

The mathematical formulation of the QSSP reads as follows:

$$\min \left\{ \sum_{i=1}^{n} \sum_{j=i+1}^{n} 2Q_{ij}x_i x_j + \sum_{i=1}^{n} L_i x_i : x_i + x_j \le 1, \forall (v_i, v_j) \in E, x \in \{0,1\}^n \right\}$$

This quadratic counterpart of the Linear Stable Set Problem has not received much attention in the literature (for further details on the QSSP we refer the interested reader to Furini and Traversi [10]). As test-bed we used 16 instances introduced in [10], based on random graphs a number of vertices $n = 150$, density $\mu \in \{50\%, 75\%\}$, and a percentage of negative quadratic costs $\nu \in \{25\%, 50\%, 75\%\}$. We used 2 instances for each class using different random seeds.
In the following paragraph we discuss the special case of QSSP with $\nu = 0\%$

A relevant special case. As observed in Jaumard et al. [17], the QSSP with only non-negative costs, i.e., $Q_{ij} \ge 0, v_i, v_j \in V$, can be viewed as a weighted Stable Set Problem (SSP) on an extended graph $\tilde{G} = (\tilde{V}, \tilde{E})$, where $\tilde{V} = V \cup V_1 \cup V_2$, $\tilde{E} = E \cup E_1 \cup E_2 \cup E_{12}$ and

$$\begin{aligned}
V_1 &= \{v_{ij}^i : v_i, v_j \in V, Q_{ij} > 0\}, \\
V_2 &= \{v_{ij}^j : v_i, v_j \in V, Q_{ij} > 0\}, \\
E_1 &= \{(v_i, v_{ij}^i), v_i \in V, v_{ij}^i \in V_1 : Q_{ij} > 0\}, \\
E_2 &= \{(v_{ij}^j, v_j), v_j \in V, v_{ij}^j \in V_2 : Q_{ij} > 0\}, \\
E_{12} &= \{(v_{ij}^i, v_{ij}^j), v_{ij}^i \in V_1, v_{ij}^j \in V_2 : Q_{ij} > 0\}.
\end{aligned}$$

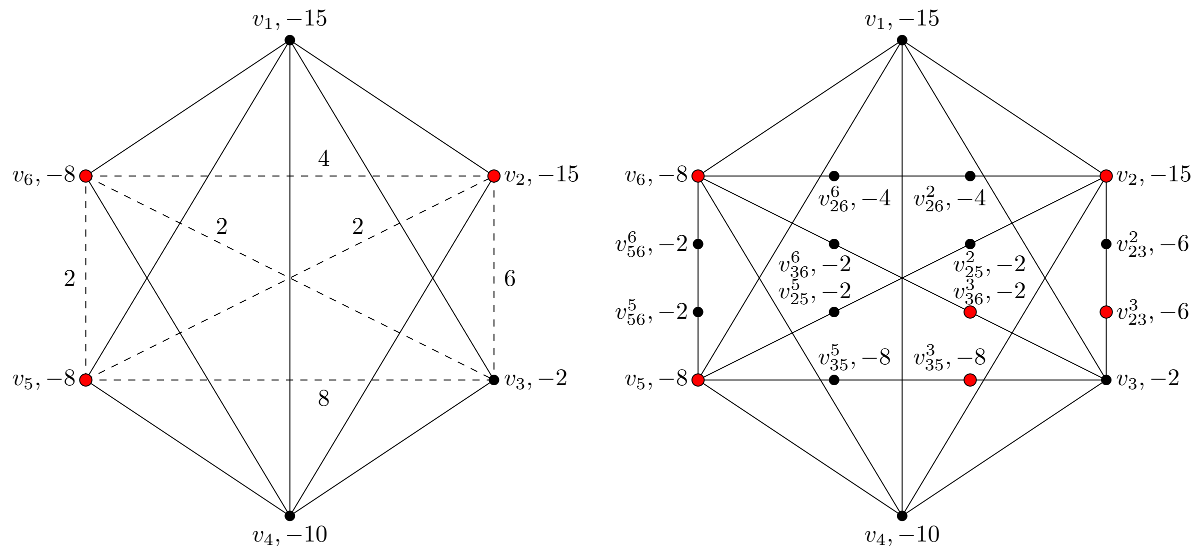

Figure 1: Example: a graph G (left) and the corresponding extended graph $\tilde{G}$ (right).

The cost of nodes $v_{ij}^i \in V_1$ and $v_{ij}^j \in V_2$ are equal to $-Q_{ij}$, replacing in this way the initial quadratic costs Q. The optimal solution value of QSSP on G is then equal to the optimal solution value of the weighted SSP on $\tilde{G}$ plus the constant $\sum_{i=1}^n \sum_{j=1}^n Q_{ij}$.

An example of the extended graph is given in Figure 1. On the left part of the figure we report a graph $G = (V, E)$ with 6 vertices and 9 edges and the following costs:

$$Q = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 1 & 2 \\ 0 & 3 & 0 & 0 & 4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 4 & 0 & 0 & 1 \\ 0 & 2 & 1 & 0 & 1 & 0 \end{bmatrix}; L = \begin{bmatrix} -15 & -15 & -2 & -10 & -8 & -8 \end{bmatrix}.$$

The dashed lines represent a positive entry Q_{ij}. On the right part of the figure we report the corresponding extended graph $\tilde{G} = (\tilde{V}, \tilde{E})$ with 18 vertices and 25 edges. In both graph, the optimal solutions are represented by the vertices in red. The cost of the stable set $\{v_2, v_5, v_6\}$ in G is equal to -23, while the cost of the stable set $\{v_2, v_5, v_6, v_{23}^3; v_{35}^3, v_{36}^3\}$ in $\tilde{G}$ is equal to -47. Finally, the constant part is equal to 24.

In other words, for the QSSP with $Q_{ij} \geq 0$, ELF introduces only the sets of constraints (16), (17) and (18) and, hence, it is equivalent to the standard ILP formulation with edge constraints for the Weighted Stable Set Problem on the extended graph $\tilde{G}$.

Table description. In Table 5 we report the results concerning the computational behaviour of the four LTs studied on the QSSP benchmark. In each line, we group together the average results relative to instances with same values of μ and ν. Each entry of the table provides the aggregated results on 2 instances ($\# = 2$ on the table). We provide, for each LT, the following information:

- *MILP times*. The average computational time required by `CPLEX` to solve the problem to proved optimality.

n	μ	ν	#	MILP times				MILP branching nodes			
				GW[13]	ELF	G[11]	SS[24]	GW[13]	ELF	G[11]	SS[24]
150	*50*	*25*	2	139.68	340.94	216.82	334.01	1613.50	3143.00	198666.50	126996.00
		50	2	1216.65	540.30	291.52	366.40	3915.50	10166.50	337011.00	171489.00
		75	2	1490.78	626.17	314.91	362.90	14382.00	15674.50	394338.50	169204.00
	75	*25*	2	37.59	52.26	19.29	44.41	149.50	139.00	6277.00	7910.00
		50	2	85.14	84.61	20.70	44.03	260.50	264.00	9651.00	7731.50
		75	2	98.99	119.84	23.99	43.58	832.50	835.50	13440.50	10856.00

n	μ	ν	#	LP times				LP gaps			
				GW[13]	ELF	G[11]	SS[24]	GW[13]	ELF	G[11]	SS[24]
150	*50*	*25*	2	0.05	0.49	0.07	0.08	98.14	98.14	99.08	99.08
		50	2	0.06	0.86	0.02	0.06	98.06	98.06	99.01	99.01
		75	2	0.07	1.28	0.01	0.02	98.00	98.00	98.98	98.98
	75	*25*	2	0.01	0.41	0.01	0.12	97.47	97.47	99.41	99.41
		50	2	0.01	0.59	0.01	0.08	97.68	97.68	99.42	99.42
		75	2	0.01	0.05	0.01	0.03	98.41	98.41	99.59	99.59

Table 5: Computational comparison of the different formulations for solving QSSP instances

- *MILP branching nodes*. The average number of nodes in the Branch-and-Bound tree explored by `CPLEX`.
- *LP times*. The average time required by `CPLEX` to solve the LP-relaxation to proven optimality.
- *LP gaps*. The average percentage gap between the optimal value of the LP-relaxation and the optimal solution.

Table discussion. The formulations with the best computational behavior for the QSSP instances are G[11] and SS[24] on average. ELF presents on average a better computing time of GW[13] The number of MILP branching nodes of ELF is slightly greater than GW[13]. G[11] and SS[24] are characterized by a higher number of nodes. This fact is not surprising since those formulations have a weaker LP-relaxation compared to GW[13] and ELF. However, the weakness of G[11] and SS[24] is counterbalanced by their smaller size in terms of variables and constraints (See Table 1) which leads to a faster node solution time. Finally, it is interesting to notice that the more difficult instances are the one with density $\mu = 50\%$ and percentage of negative costs $\nu \in \{50\%, 75\%\}$.

3.2.2 Quadratic Knapsack Problem

Problem description. The Quadratic Knapsack Problem (QKP) consists in maximizing a quadratic function with positive coefficients subject to a linear capacity constraint. The mathematical formulation reads as follows:

$$\max \left\{ \sum_{i=1}^{n} \sum_{j=i+1}^{n} 2Q_{ij} x_i x_j + \sum_{i=1}^{n} L_i x_i : \sum_{i=1}^{n} c_i x_i \leq C, x \in \{0,1\}^n \right\} ,$$

n	δ	#	MILP times				MILP branching nodes			
			GW[13]	ELF	G[11]	SS[24]	GW[13]	ELF	G[11]	SS[24]
100	*25*	*10*	0.54	0.51	0.98	0.86	188.50	188.10	1004.80	717.60
	50	*10*	4.40	4.06	2.76	2.78	438.50	405.10	2303.50	1978.10
	75	*10*	39.39	42.23	19.96	59.65	3122.20	4212.70	9549.00	18980.50
	100	*10*	113.82	145.09	5.87	6.73	5098.44	4918.67	7570.89	5816.89
			LP times				LP gaps			
n	δ	#	GW[13]	ELF	G[11]	SS[24]	GW[13]	ELF	G[11]	SS[24]
100	*25*	*10*	0.03	0.03	0.00	0.00	1.71	1.71	12.41	12.41
	50	*10*	0.08	0.11	0.00	0.00	1.51	1.51	11.15	11.15
	75	*10*	0.15	0.27	0.00	0.01	4.48	4.48	13.53	13.53
	100	*10*	0.37	0.50	0.01	0.00	1.19	1.19	11.93	11.93

Table 6: Computational comparison of the different formulations for solving QKP instances

where c_i $(i = 1, \dots, n)$ are integer non negative coefficients representing the size of the items and C is the capacity of the knapsack. In addition to the classical knapsack, where only linear profits L_i are considered, here we maximize also the profits associated to couples of objects (their profit is represented by Q_{ij}). For further information on the problem, see Caprara et al. [5] and Pisinger [21]. In our computational tests we used randomly generated instances taken from Billionnet and Soutif [3] with $n = 100$ and density $\delta = 25\%, 50\%, 75\%, 100\%$, i.e., δ is the number of non-zero coefficients of the objective function divided by $n(n-1)/2$.

Table description. In Table 6 we report the results concerning the computational behaviour for solving the test problems to proven optimality. Table 6 presents the same information of Table 5. Each line presents the aggregated results concerning 10 instances with same same size and δ.

Table discussion. It is interesting to notice that, when the density δ is high, the number of MILP branching nodes is comparable for all the formulations considered. Apart from this feature, the computational behaviour for the QKP of the formulations studied is in line with the one obtained for the QSSP, showing that $G_{[11]}$ and $SS_{[24]}$ are the formulations with the better computational behaviour.

4. Conclusions

In this paper we compared several LTs for Binary Quadratic Problems present in the literature, called here $GW_{[13]}$, $G_{[11]}$ and $SS_{[24]}$ with a new formulation called ELF. We showed the equivalence of the LP-relaxation values of $G_{[11]}$, $SS_{[24]}$, $GW_{[13]}$ and ELF when dealing with a specific class of Unconstrained Binary Quadratic Problems. Among the formulations studied, $GW_{[13]}$ and ELF provide the better performances in practice when applied to unconstrained problems while $G_{[11]}$ and, to a lesser extent, $SS_{[24]}$ perform better on the special classes of constrained problems that have been tested in the paper. Whether this observation generalizes to other types of constrained problems is an interesting question that may be worth further investigations. The new proposed formulation ELF performs relatively well in all classes of instances. Even if $GW_{[13]}$ and ELF present the same LP-relaxation, their behaviour in practice can be different according to the problem considered: $GW_{[13]}$ is slightly preferable over ELF when dealing with Biq Mac instances, while the contrary happens when solving QSSP instances. For the two considered problems with constraints, the trade off between the strength of the LP-relaxation and the speed in the solution of the MILP branching nodes plays in favour of $G_{[11]}$ and $SS_{[24]}$. Finally, we recall that the selection of the best LT depends also on the current performance and engineering of the MILP solvers.

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