Quadratization and convexification in polynomial binary optimization

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Abstract

In this paper, we discuss several reformulations and solution approaches for the problem of minimizing a polynomial in binary variables (P). We review and integrate different literature streams to describe a methodology consisting of three distinct phases, together with several possible variants for each phase. The first phase determines a recursive decomposition of each monomial of interest into pairs of submonomials, down to the initial variables. The decomposition gives rise to a so-called *quadratization scheme*. The second phase builds a *quadratic reformulation* of (P) from a given quadratization scheme, by associating a new auxiliary variable with each submonomial that appears in the scheme. A quadratic reformulation of (P) is obtained by enforcing relations between the auxiliary variables and the monomials that they represent, either through linear constraints or through penalty terms in the objective function. The resulting quadratic problem (QP) is non-convex in general and is still difficult to solve. At this stage we introduce the third phase of the resolution process, which consists in *convexifying* (QP). We consider different types of convexification methods, including complete linearization or quadratic convex reformulations. Theoretical properties of the different phases are recalled from the literature or are further clarified. Finally, we present some experimental results to illustrate the discussion.

1 Introduction

We consider the *Polynomial Unconstrained Binary Programming* (P) problem

$$\text{(P)} \quad \begin{cases} \min \quad f(x) \triangleq \sum_{M \in \mathcal{M}} a_M \prod_{i \in M} x_i & (1) \\ \text{s. t.} \quad x_i \in \{0,1\} \qquad \forall i \in [n] & (2) \end{cases}$$

where the objective function $f(x)$ is a polynomial defined on binary variables $x \in \{0,1\}^n$. We denote the set of variable indices by $[n] = \{1, ..., n\}$. Without loss of generality, we can assume

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that $f(x)$ is a multilinear polynomial since $x_i^2 = x_i$ for any binary variable $x_i \in \{0,1\}$, for $i \in [n]$. Hence, $f(x)$ consists of a sum of *monomials* $\prod_{i \in M} x_i$ weighted by non-zero coefficients $a_M \in \mathbb{Q}$, for $M \in \mathcal{M} \subseteq 2^{[n]}$. For the sake of simplicity, we will also use the word *monomial* to refer to a subset of indices $M \subseteq 2^{[n]}$. The *degree of a monomial* M is $|M|$, and the *degree of the polynomial* f is defined as $d_f = \max_{M \in \mathcal{M}} |M|$.

Problem (P) is a very general model that allows the formulation of many well-known problems in optimization. When $d_f = 2$, the problem becomes a quadratic unconstrained binary optimization (QUBO) problem. This important special case encompasses classical combinatorial optimization problems such as maximum cut or stable set problems; it has recently been identified as playing a central role in quantum computing (see for example [10, 14, 27, 44]). When $d_f \geq 3$, (P) can be used to formulate many classical problems such as uncapacitated facility location in operations research, 3-SAT and maximum satisfiability in computer science, or applications in different fields such as the construction of binary sequences with low aperiodic correlation, a very challenging problem in signal design theory, or the restoration of blurred images in computer vision; see, e.g., [4, 10, 14, 8, 25, 34, 35], as well as Section 6.1 and Section 6.2 hereunder.

Since (P) generalizes unconstrained binary quadratic optimization, it is NP-hard for any fixed $d_f \geq 2$ [26]. Practical difficulties arise from the non-convexity of f and from the integrality of the variables. Various approaches have been proposed to handle these difficulties. They will be briefly reviewed in Section 2.

In this paper, we focus on a class of methods based on quadratic reformulations of problem (P), which are subsequently solved via convexification techniques. These methods have their roots in a seminal paper by Rosenberg [46] and have been more recently revived by several researchers (see, e.g., [3, 8, 13]; more references will be provided in subsequent sections).

We propose to look at the generic approach as consisting of three phases, and we describe several alternative techniques for each phase. *Phase I* consists in determining a recursive decomposition of each monomial into a product of two sub-monomials, where each sub-monomial is again decomposed into a product of two, and so forth down to the initial variables. This decomposition is called a *quadratization scheme*. *Phase II* consists in building a *quadratic reformulation*, that is, a quadratic problem equivalent to (P), from any given quadratization scheme. For this purpose, each element of the given quadratization scheme is associated with an auxiliary variable that models a submonomial. The basic idea is then to enforce relations between auxiliary variables and the product that they represent, which can be done using either linear constraints as in [24], or quadratic penalties in the objective function as in [3, 46]. The resulting quadratic problem is non-convex in general and still difficult to solve. At this stage we consider *Phase III* of the resolution process, or *convexification* phase, which consists in computing a new formulation equivalent to the quadratic problem obtained in Phase II, but this time with a convex continuous relaxation. We consider two types of convexification approaches. In the first one, we simply produce a standard linearization of the quadratic problem obtained in Phase II. In the second type, we compute an equivalent formulation which is quadratic and convex using semi-definite programming [5, 21]. Both approaches can be applied to any unconstrained quadratic binary optimization problem, whether it is a quadratic reformulation of a polynomial problem of type (P) or not. However, in the particular case at hand, where we deal with a quadratic reformulation of a higher-degree problem, we can also use the recent `PQCR` [21] method which improves the convex reformulation.

Our contribution. Research on quadratic reformulations of (P) has frequently examined one or two of the phases in isolation, e.g., by focusing on the choice of the quadratic reformulation obtained from Phases I and II, and then relying on generic solvers to handle Phase III [13, 45], or conversely, by picking a simple quadratic reformulation, and then focusing on the choice of the convexification method in Phase III [21]. The aim of the present paper is to revisit the three-phase approach from a more holistic perspective. It aims at examining the joint impact of the phases, from quadratic reformulation to convexification. On the theoretical side, we provide a unified framework for several definitions of quadratic reformulations that were previously introduced independently in the literature. We also clarify some basic properties of these reformulations and relationships among them. We discuss which quadratic reformulations can be meaningfully combined with the convexification methods presented in [5, 21]. From a computational perspective, we conduct a set of experiments which illustrate the difficulty of choosing the best combination of a quadratic reformulation with a convexification technique, as this choice may depend on the type of instances considered.

Outline of the paper. Section 2 provides a brief literature review and lays out the fundamental concepts required to formally describe the three-phase approach considered in this paper. Sections 3, 4 and 5 respectively discuss Phases I, II and III in detail. Section 6 presents the results of computational tests aimed at experimentally comparing different combinations of quadratic reformulations and convexification methods, and Section 7 concludes the paper.

2 Literature review and basic concepts

Let us briefly review some of the literature on algorithms for polynomial unconstrained binary programming. Most such algorithms simply apply branch-and-bound to an appropriate linear reformulation of (P), such as the *standard linearization* based on pioneering work published in [24, 29, 48, 49]. The basic idea behind standard linearization is to introduce an auxiliary variable y_M for every monomial $M \in \mathcal{M}$, and to force the equality $y_M = \prod_{i \in M} x_i$ by means of linear constraints. More precisely, the standard linearization of (P) is the mixed integer linear programming problem

$$
\text{(SL)} \quad \left\{ \begin{array}{lll}
\min & \displaystyle\sum_{i=1}^{n} a_i x_i + \sum_{M \in \mathcal{M}: |M| \geq 2} a_M y_M & \\
\text{s. t.} & & \\
& y_M \leq x_i & M \in \mathcal{M} : |M| \geq 2,\ i \in M \qquad (3) \\
& y_M \geq \displaystyle\sum_{i \in M} x_i - (|M| - 1) & M \in \mathcal{M} : |M| \geq 2 \qquad (4) \\
& y_M \geq 0 & M \in \mathcal{M} : |M| \geq 2 \qquad (5) \\
& x \in \{0,1\}^n & \qquad (6)
\end{array} \right.
$$

It is easy to check that the inequalities (3), (4), (5) imply $y_M = \prod_{i \in M} x_i$ when x is a binary vector. Therefore, problem (SL) is equivalent to (P).

The standard linearization of (P) has been studied by many researchers. When $f(x)$ consists of a single monomial or has a specific acyclic structure [11, 20], its continuous relaxation is exact (i.e., its extreme points are binary). For the general case, several recent publications present valid

inequalities for the convex hull of the feasible binary solutions, see, e.g., [15, 18, 17, 19, 22]. In [13], Buchheim and Rinaldi established a polyhedral description based on a quadratic reformulation of (P). They also proved the equivalence between separation algorithms for (SL) and for the cut polytope. Compact linearizations requiring a smaller number of additional variables than (SL) have been introduced in [28, 29] and in other papers.

Other approaches to (P) can be found in the literature. Some of them rely on specialized combinatorial pseudo-Boolean methods (see, e.g., [10, 14]), like the dynamic programming *Basic Algorithm* discussed in [30, 31], or a related dynamic programming algorithm proposed in [16]. Algorithms for the more general class of mixed-integer nonlinear programs can also be applied to (P) (see, e.g., [1, 12, 36, 37, 41, 47]). Although these algorithms were not originally tailored for binary programming, they can handle (P) by imposing $x_i^2 = x_i$ for $i \in [n]$. We do not discuss these approaches in more detail, as they are not directly related to our work.

On the other hand, as mentioned in the Introduction, another stream of literature centers around quadratic reformulations of problem (P). More precisely, the first two phases of the algorithms that we consider aim at reformulating (P) as an equivalent quadratic problem of the form

$$\text{(QP)} \quad \begin{cases} \min & G(z) \triangleq z^T Q z + c^T z \\ \text{s. t.} & A_i z = b_i \quad \forall i \in [l] \\ & z^T Q_i z + c_i^T z = b_i \quad \forall i \in [q] \\ & z \in \{0,1\}^{n+m}. \end{cases}$$

The dimension of the binary vector z is $n + m$: the first n components of z correspond to the *original* variables $x \in \{0,1\}^n$ of problem (P) and the last m components correspond to a vector of *auxiliary* variables $y \in \{0,1\}^m$ which are introduced to define the quadratic reformulation. The correspondence between auxiliary and original variables is enforced by using either linear constraints $A_i z = b_i$, for $i \in [l]$, or quadratic constraints $z^T Q_i z + c_i^T z = b_i$, for $i \in [q]$, or penalties in the quadratic objective function (in which case l or q may be 0), or both penalties and constraints. In the special case of a (QP) formulation with $l = q = 0$, the problem becomes a quadratic unconstrained binary optimization (QUBO) problem.

We now formally define the concept of quadratic reformulation.

Definition 1 (**Quadratic reformulation of a polynomial optimization problem**)**.** (QP) is a *quadratic reformulation* of (P) if and only if, for every optimal solution $\hat{z} = (\hat{x}, \hat{y}) \in \{0,1\}^{n+m}$ of (QP), $\hat{x}$ is an optimal solution of (P).

In the quadratic reformulations to be discussed in this paper, it will always be the case that (P) and (QP) have the same optimal value, i.e., $f(\hat{x}) = G(\hat{z})$, although this condition is not strictly required in Definition 1.

The following related definition was previously introduced in several papers; see [2, 3, 9]. It applies to any *pseudo-Boolean function*, that is, to any real-valued function $f(x)$ defined on $x \in \{0,1\}^n$.

Definition 2 (**Quadratization of a pseudo-Boolean function**)**.** Given a pseudo-Boolean function $f(x)$ on $\{0,1\}^n$, a function $h(z) = h(x,y)$ is a *quadratization* of $f(x)$ if h is a quadratic polynomial depending on the original variables $x \in \{0,1\}^n$ and on a set of auxiliary variables $y \in \{0,1\}^m$ such that

$$f(x) = \min\{h(x,y) : y \in \{0,1\}^m\} \quad \forall x \in \{0,1\}^n.$$

Clearly, when $h(z)$ is a quadratization of the pseudo-Boolean function $f(x)$, then the problem: $\min\{h(z) : z \in \{0,1\}^{n+m}\}$ is a straightforward unconstrained quadratic reformulation of the polynomial optimization problem (P). This type of reformulation will be of special interest in the sequel, as the quadratic reformulations that we consider are closely related to quadratizations of the objective function.

Common goals for finding good quadratic reformulations in the literature have been: introducing as few auxiliary variables as possible in order to limit the dimension of the reformulated problem, or introducing a small number of (non-submodular) positive quadratic terms in the objective function, as this is often a good property for computational performance [3, 7, 25, 34, 45]. Other goals have been to define quadratic reformulations for particular classes of functions, such as symmetric functions [2, 7].

In this paper, we restrict our attention to quadratic reformulations resulting from the application of Phases I and II, that is, quadratic reformulations constructed on the basis of a quadratization scheme. Such quadratic reformulations have been previously considered in the literature and presented in various ways [3, 13, 21, 25, 46]. In the next sections, we provide a unified presentation of these methods and clarify the relations between them.

3 Phase I: Construction of quadratization schemes

Let us consider the first phase of the construction of a convex reformulation of (P), which consists in the elaboration of a *quadratization scheme*. The goal is to determine a valid decomposition of the monomials of the objective function f that will allow us to produce a quadratic reformulation in Phase II. Concretely, each monomial is recursively decomposed into exactly two products, down to the initial variables. Then, each element of the decomposition will be substituted by an auxiliary variable in the quadratic reformulation phase, thus reducing the degree of f. We further link this definition with related concepts existing in the literature.

3.1 Definition of quadratization schemes

We start with the definition of a scheme for a single monomial.

Definition 3 (**Quadratization scheme of a monomial**)**.** A *quadratization scheme* for a monomial M, where $|M| \geq 3$, is a directed acyclic graph $G_M = (V_M, A_M)$ with the following properties:

i) $V_M \subseteq 2^M$, i.e., each vertex in V_M is a subset of M;

ii) $M \in V_M$; M is the *root* of G_M: it has indegree 0, and all other vertices have nonzero indegree;

iii) $\{i\} \in V_M$ for all $i \in M$; the vertices $\{i\}$, $i \in M$, are the *leaves* of G_M: they have outdegree 0;

iv) when a vertex $E \in V_M$ is not a leaf of G_M, its outdegree is 2, and

- the arcs leaving E are denoted as $(E, l_M(E)) \in A_M$ and $(E, r_M(E)) \in A_M$; $l_M(E)$ and $r_M(E)$ are the *left child* and *right child* of E, respectively;
- $l_M(E)$ and $r_M(E)$ define a nontrivial decomposition of E into two subsets: $0 < |l_M(E)| < |E|$, $0 < |r_M(E)| < |E|$, and $E = l_M(E) \cup r_M(E)$.

For simplicity, we assume that each subset of M can appear at most once as a vertex in V_M, although this assumption could be lifted at the expense of heavier notations. In the sequel, it will be useful to have a distinct notation for the set $\mathcal{E}_M \triangleq \{E \in V_M : |E| \geq 2, E \neq M\}$ which contains all vertices of G_M except the root M and the leaves $\{i\}$, $i \in M$. As a matter of terminology, remember that a *hypergraph* $\mathcal{H}$ on a ground set V is a set of subsets of V, that is, a set $\mathcal{H} \subseteq 2^V$. The elements of $\mathcal{H}$ are the *edges* of the hypergraph. So, V_M and $\mathcal{E}_M$ are hypergraphs on M.

We look at l_M and r_M as applications on $\mathcal{E}_M \cup \{M\}$, and we sometimes find it convenient to extend them to V_M by defining $l_M(\{i\}) = r_M(\{i\}) = \emptyset$ for all $i \in M$. Also, note that the quadratization scheme $G_M = (V_M, A_M)$ is equivalently defined by the triplet (V_M, l_M, r_M) or by the triplet $(\mathcal{E}_M, l_M, r_M)$; we will use either of these notations.

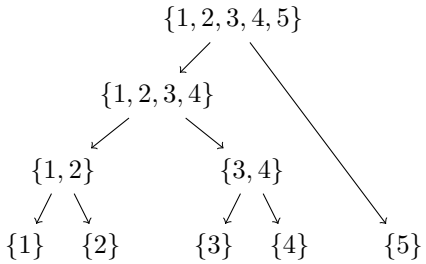
To illustrate the definitions, let us give three examples of quadratization schemes for a degree 5 monomial.

Example 1. Consider the monomial $M = \{1, 2, 3, 4, 5\}$.

We define (V_M^1, l_M^1, r_M^1), a first quadratization scheme of M, by $V_M^1 = \Big\{\{1\},\{2\},\{3\},\{4\},\{5\},\{1,2\},\{3,4\},\{1,2,3,4\},\{1,2,3,4,5\}\Big\}$ with

- $l_M^1(\{1,2\}) = \{1\}$, $r_M^1(\{1,2\}) = \{2\}$
- $l_M^1(\{3,4\}) = \{3\}$, $r_M^1(\{3,4\}) = \{4\}$
- $l_M^1(\{1,2,3,4\}) = \{1,2\}$, $r_M^1(\{1,2,3,4\}) = \{3,4\}$
- $l_M^1(\{1,2,3,4,5\}) = \{1,2,3,4\}$, $r_M^1(\{1,2,3,4,5\}) = \{5\}$

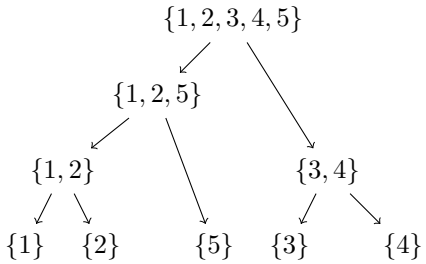
and $\mathcal{E}_M^1 = \Big\{\{1,2\},\{3,4\},\{1,2,3,4\}\Big\}$.



Next, we define (V_M^2, l_M^2, r_M^2), a second quadratization scheme of M, by $V_M^2 = \Big\{\{1\},\{2\},\{3\},\{4\},\{5\},\{1,2\},\{3,4\},\{1,2,5\},\{1,2,3,4,5\}\Big\}$ with

- $l_M^2(\{1,2\}) = \{1\}$, $r_M^2(\{1,2\}) = \{2\}$
- $l_M^2(\{3,4\}) = \{3\}$, $r_M^2(\{3,4\}) = \{4\}$
- $l_M^2(\{1,2,5\}) = \{1,2\}$, $r_M^2(\{1,2,5\}) = \{5\}$
- $l_M^2(\{1,2,3,4,5\}) = \{1,2,5\}$, $r_M^2(\{1,2,3,4,5\}) = \{3,4\}$

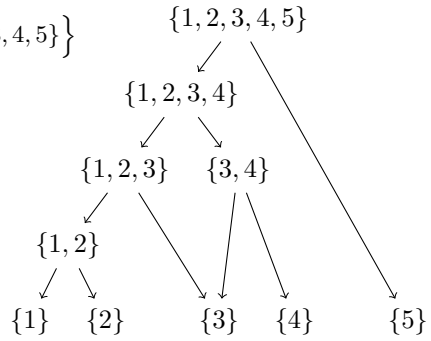
and $\mathcal{E}_M^2 = \Big\{\{1,2\},\{3,4\},\{1,2,5\}\Big\}$.



Finally, a third quadratization scheme (V_M^3, l_M^3, r_M^3) is given by $V_M^3 = \Big\{\{1\},\{2\},\{3\},\{4\},\{5\},\{1,2\},\{3,4\},\{1,2,3\},\{1,2,3,4\},\{1,2,3,4,5\}\Big\}$ with

- $l_M^3(\{1,2\}) = \{1\}$, $r_M^3(\{1,2\}) = \{2\}$
- $l_M^3(\{3,4\}) = \{3\}$, $r_M^3(\{3,4\}) = \{4\}$
- $l_M^3(\{1,2,3\}) = \{1,2\}$, $r_M^3(\{1,2,3\}) = \{3\}$
- $l_M^3(\{1,2,3,4\}) = \{1,2,3\}$, $r_M^3(\{1,2,3,4\}) = \{3,4\}$
- $l_M^3(\{1,2,3,4,5\}) = \{1,2,3,4\}$, $r_M^3(\{1,2,3,4,5\}) = \{5\}$

and $\mathcal{E}_M^3 = \Big\{\{1,2\},\{3,4\},\{1,2,3\},\{1,2,3,4\}\Big\}$.



As illustrated by Example 1, a quadratization scheme provides a decomposition of monomials into pairs of subsets, which are themselves decomposed into pairs, and so forth, until singletons are obtained. Reading a scheme bottom-up, starting from the leaves, suggests how pairs of original or auxiliary variables can be recursively substituted by new ones. We will return to this interpretation in more detail in Section 4.

In Definition 3, we did not assume that $l_M(E) \cap r_M(E) = \emptyset$ for every $E \in V_M$, $|E| \geq 2$. When this additional property holds, we say that the scheme is *disjoint*. For instance, the first two schemes in Example 1 are disjoint, the third one is not.

Let us call G_M a *rooted binary tree* if every vertex of G_M other than the root has indegree equal to 1.

Proposition 4. *A quadratization scheme is disjoint if and only if it is a rooted binary tree.*

Proof. If $l_M(E) \cap r_M(E) \neq \emptyset$ holds for some E, say, $i \in l_M(E) \cap r_M(E)$, then there is a directed path from $l_M(E)$ to $\{i\}$ and from $r_M(E)$ to $\{i\}$. These two paths meet in a first vertex which therefore has indegree at least 2, and hence G_M is not a tree.

Conversely, assume that G_M is not a rooted binary tree, meaning that there is a vertex $E \in V_M$ with indegree larger than 1. So, there exist two distinct paths from the root M to E. Let $F \in V_M$ be a vertex where these two paths diverge; say, $l_M(F)$ is on the first path and $r_M(F)$ is on the second one. Since E is a descendant of both $l_M(F)$ and $r_M(F)$, it follows that $E \subseteq l_M(F) \cap r_M(F)$, and the scheme is not disjoint. □

We now characterize the size of a quadratization scheme.

Proposition 5 (**Size of a quadratization scheme**). *Every quadratization scheme for a monomial M satisfies:*

(a) $|V_M| \geq 2|M| - 1$ *and* $|\mathcal{E}_M| \geq |M| - 2$.

(b) If the scheme is disjoint, $|V_M| = 2|M| - 1$ *and* $|\mathcal{E}_M| = |M| - 2$.

Let us now turn to the case of a generic polynomial function f, as in Equation (1). Since a polynomial is defined by a set of monomials $\mathcal{M}$ (together with their coefficients), we define a quadratization scheme for a set of monomials or equivalently, for a hypergraph $\mathcal{M}$.

Definition 6 (**Quadratization scheme for a set of monomials**). A *quadratization scheme* for a hypergraph $\mathcal{M} \subseteq 2^{[n]}$ is a collection of quadratization schemes $\mathcal{S} = \left\{G_M = (V_M, A_M) : M \in \mathcal{M}\right\}$, where each G_M is a quadratization scheme for the corresponding monomial $M \in \mathcal{M}$.

Observe that a same subset $E \subseteq [n]$ can appear in several of the schemes G_M. Therefore, the collection of sets $(E : E \in V_M, M \in \mathcal{M})$ is a multiset, or a hypergraph with repeated edges. Nevertheless, we find it convenient to look at $\mathcal{S}$ as a collection of vertex disjoint digraphs, as illustrated in Example 2 hereunder. Moreover, we denote as $\mathcal{E}$ the hypergraph (without repeated edges)

$$\mathcal{E} \triangleq \bigcup_{M \in \mathcal{M}} \mathcal{E}_M = \bigcup_{M \in \mathcal{M}} (V_M \setminus (\{M\} \cup \bigcup_{i \in M} \{i\})). \tag{7}$$

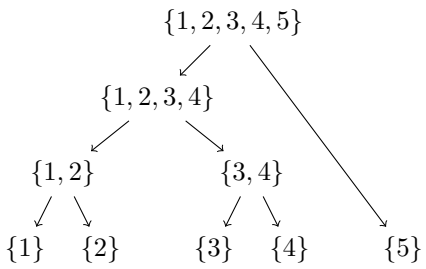
Note that even though $M \notin \mathcal{E}_M$, $\mathcal{M} \cap \mathcal{E}$ might be nonempty if a monomial $M \in \mathcal{M}$ appears in the quadratization scheme of another monomial, that is, if $M \in \mathcal{E}_{M'}$ for $M' \in \mathcal{M}, M' \neq M$.

Example 2. Let $f(x) = a_1 x_1 x_2 x_3 x_4 x_5 + a_2 x_1 x_2 x_3 x_4$ be a polyomial containing two monomials, $\mathcal{M} = \{M_1 = \{1, 2, 3, 4, 5\}, M_2 = \{1, 2, 3, 4\}\}$, and $n = 5$. A quadratization scheme $\mathcal{S} = \left\{G_{M_1}, G_{M_2}\right\}$ for $\mathcal{M}$ can be defined as follows:

$V_{M_1} = \Big\{\{1\},\{2\},\{3\},\{4\},\{5\},\{1,2\},\{3,4\},\{1,2,3,4\},\{1,2,3,4,5\}\Big\}$

- $l_{M_1}(\{1,2\}) = \{1\}$, $r_{M_1}(\{1,2\}) = \{2\}$
- $l_{M_1}(\{3,4\}) = \{3\}$, $r_{M_1}(\{3,4\}) = \{4\}$
- $l_{M_1}(\{1,2,3,4\}) = \{1,2\}$, $r_{M_1}(\{1,2,3,4\}) = \{3,4\}$
- $l_{M_1}(\{1,2,3,4,5\}) = \{1,2,3,4\}$, $r_{M_1}(\{1,2,3,4,5\}) = \{5\}$

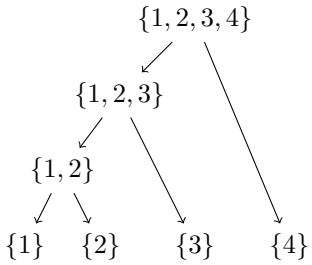
and $\mathcal{E}_{M_1} = \Big\{\{1,2\},\{3,4\},\{1,2,3,4\}\Big\}$.



$V_{M_2} = \Big\{\{1\},\{2\},\{3\},\{4\},\{1,2\},\{1,2,3\},\{1,2,3,4\}\Big\}$

- $l_{M_2}(\{1,2\}) = \{1\}$, $r_{M_2}(\{1,2\}) = \{2\}$
- $l_{M_2}(\{1,2,3\}) = \{1,2\}$, $r_{M_2}(\{1,2,3\}) = \{3\}$
- $l_{M_2}(\{1,2,3,4\}) = \{1,2,3\}$, $r_{M_2}(\{1,2,3,4\}) = \{4\}$

and $\mathcal{E}_{M_2} = \Big\{\{1,2\},\{1,2,3\}\Big\}$.



The hypergraph $\mathcal{E}$ without repeated edges is $\mathcal{E} = \Big\{\{1,2\},\{3,4\},\{1,2,3\},\{1,2,3,4\}\Big\}$.

3.2 Related concepts

Definitions closely related to Definitions 3 and 6 have been previously introduced in the literature. In particular, *pairwise covers* of the hypergraph associated with a polynomial have been considered by Anthony et al. [3], and the concept of *reducibility* of a set of monomials has been introduced by Buchheim and Rinaldi in [13]. Let us briefly discuss and clarify the relations.

Definition 7. When $\mathcal{M}$, $\mathcal{H}$ are two hypergraphs, we say that $\mathcal{H}$ is a *pairwise cover* of $\mathcal{M}$ if, for every set $M \in \mathcal{M}$ with $|M| \geq 2$, there are two sets $l(M), r(M) \in \mathcal{H}$ such that $0 < |l(M)| < |M|$, $0 < |r(M)| < |M|$ and $l(M) \cup r(M) = M$.

The original definition in [3] is restricted to $|M| \geq 3$, but the adaptation is harmless and is more coherent with the present paper.

Example 3. Consider again the hypergraph $\mathcal{M} = \{M_1 = \{1,2,3,4,5\}, M_2 = \{1,2,3,4\}\}$ of Example 2. Then, $\mathcal{H} = \{\{4\},\{5\},\{1,2,3\},\{1,2,3,4\}\}$ is a pairwise cover of $\mathcal{M}$ with $l(\{1,2,3,4,5\}) = \{1,2,3,4\}$, $r(\{1,2,3,4,5\}) = \{5\}$, $l(\{1,2,3,4\}) = \{1,2,3\}$, and $r(\{1,2,3,4\}) = \{4\}$.

The definition of pairwise covers is obviously related to the definition of quadratization schemes and in fact, in Example 3, the decomposition of the monomials M_1, M_2 is the same as in the quadratization scheme of Example 2. A main difference, however, is that the definition of pairwise covers does not require a left-right decomposition of each subset $S \in \mathcal{H}$: the condition only applies to subsets $M \in \mathcal{M}$. In other words, pairwise covers only relate to the first level of quadratization schemes, just under the root monomials.

The exact relation between pairwise covers and quadratization schemes is clarified by the next result.

Proposition 8. *If* $\mathcal{S} = \left\{(V_M, A_M) : M \in \mathcal{M}\right\}$ *is a quadratization scheme for* $\mathcal{M}$*, then* $\mathcal{H} = \bigcup_{M\in\mathcal{M}}\{l_M(M), r_M(M)\}$ *is a pairwise cover of* $\mathcal{M}$*. Conversely, if* $\mathcal{H}$ *is a pairwise cover of* $\mathcal{M}$ *such that* $\mathcal{H} \subseteq \mathcal{M}$*, then* $\mathcal{M}$ *has a quadratization scheme* $\mathcal{S} = \left\{(V_M, A_M) : M \in \mathcal{M}\right\}$ *such that* $\bigcup_{M\in\mathcal{M}} V_M \subseteq \mathcal{H}$*.*

Proof. The first claim is obvious. For the second one, assume that $\mathcal{H}$ is a pairwise cover of $\mathcal{M}$ such that $\mathcal{H} \subseteq \mathcal{M}$. For each monomial $M \in \mathcal{M}$, define V_M and A_M inductively as follows:

1. $M \in V_M$;
2. $(M, l(M)) \in A_M$ and $(M, r(M)) \in A_M$;
3. if $(E_1, E_2) \in A_M$, then $E_2 \in V_M$, and if $|E_2| \geq 2$, then $(E_2, l(E_2)) \in A_M$, $(E_2, r(E_2)) \in A_M$.

Then, (V_M, A_M) is a quadratization scheme for M and $V_M \subseteq \mathcal{H}$. □

Remark 1. The quadratization scheme defined for $\mathcal{M}$ in the previous proof has the property that, for all $M, M', M'' \in \mathcal{M}$, $l_{M'}(M) = l_{M''}(M) = l(M)$, and $r_{M'}(M) = r_{M''}(M) = r(M)$: in other words, the left-right decomposition of each set M is unique in the scheme, as opposed to what is illustrated in Example 2 where the set $\{1, 2, 3, 4\}$ is decomposed in two different ways. This shows that quadratization schemes, as we have introduced them in Definition 3 and Definition 6, offer more flexibility than decompositions based on pairwise covers.

The second statement in Proposition 8 explains why Anthony et al. [3] restrict their attention to special types of pairwise covers. More precisely, Theorem 4 in [3] establishes constructively that, if $\mathcal{H}$ is a pairwise cover of $\mathcal{M}$ such that $\mathcal{H} \subseteq \mathcal{M}$, then the function $f(x) = \sum_{M\in\mathcal{M}} a_M \prod_{i\in M} x_i$ has a quadratization (recall Definition 2) using at most $|\mathcal{H}|$ auxiliary variables. Even though this is not explicitly mentioned in [3], it is easy to check that the existence of a pairwise cover $\mathcal{H}$ such that $\mathcal{H} \subseteq \mathcal{M}$ is equivalent to the condition that $\mathcal{M}$ is a pairwise cover of itself (say, a *pairwise self-cover*). Therefore, as a consequence of Theorem 4 in [3], we can state that if $\mathcal{M}$ is a pairwise self-cover, then $f(x)$ has a quadratization using at most $|\mathcal{M}|$ auxiliary variables. Given a function f, the pairwise cover quadratization methods to be described in subsequent sections will concentrate on extending $\mathcal{M}$ (that is, on adding monomials with coefficient zero in f) until $\mathcal{M}$ becomes a pairwise self-cover and hence, until a quadratization scheme becomes available by virtue of Proposition 8. Anthony et al. [3] observed that such a pairwise self-cover can be constructed in polynomial time.

In a different framework, Buchheim and Rinaldi [13] had previously proposed a heuristic procedure in order to extend $\mathcal{M}$ to a pairwise self-cover (which they call a *reducible set* of monomials). They used these notions to provide a quadratic reformulation of problem (P), and to show that a complete description of the standard linearization polytope of (P) can be derived from a complete polyhedral description of the quadratic reformulation.

4 Phase II: Building quadratic reformulations

We now present an adaptation of several approaches of the literature for reformulating problem (P) into an equivalent quadratic optimization problem, in the sense of Definition 1. Different types of reformulations that do not rely on quadratization schemes have been proposed, for instance,

in [2, 3, 7, 9, 23, 25, 34]. In this paper, however, we restrict our attention to reformulations derived from an arbitrary quadratization scheme $\mathcal{S}$.

To do this, the basic idea is to introduce a set of $|\mathcal{E}|$ *auxiliary variables*, where $\mathcal{E}$ is defined by equation (7), so that each additional variable corresponds to an "intermediate" vertex in one of the graphs G_M. Let $z \in \{0,1\}^N$, where $N = n + |\mathcal{E}|$, the first n components of z correspond to the vector of *original variables* x, and the last $|\mathcal{E}|$ components correspond to the auxiliary variables. If the equalities $z_E = z_{l_M(E)} z_{r_M(E)}$ hold for all $E \in \mathcal{E}_M$, then it follows from the definition of quadratization schemes that $z_E = \prod_{i \in E} z_i$ also holds for all $E \in \mathcal{E}_M$. When this is the case, we say that z defines a *consistent assignment* of values to the variables, or simply, that z is *consistent*. It follows that, given a scheme $\mathcal{S}$, we can reformulate (P) as the equivalent quadratically constrained quadratic programming problem ($\texttt{QCQP}^{\mathcal{S}}$):

$$(\texttt{QCQP}^{\mathcal{S}}) \begin{cases} \min\limits_{z \in \{0,1\}^N} \quad g(z) \triangleq \sum\limits_{\substack{M \in \mathcal{M}: \\ |M| \leq 2}} a_M \prod\limits_{i \in M} z_i + \sum\limits_{\substack{M \in \mathcal{M}: \\ |M| \geq 3}} a_M z_{l_M(M)} z_{r_M(M)} & (8) \\ \text{s.t.} \\ \quad z_E = z_{l_M(E)} z_{r_M(E)} \qquad \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M. & (9) \end{cases}$$

Both the objective function and the constraints of ($\texttt{QCQP}^{\mathcal{S}}$) are usually non-convex. In this section, we focus on rewriting the quadratic constraints (9) and we show that they can be enforced either using linear inequalities or using penalties in the objective function. Doing so, we accordingly obtain either a linearly constrained quadratic problem, or an unconstrained quadratic problem. The resulting problems are still non-convex, in general, but now the non-convexity can only arise from the quadratic objective function and from the integrality of the variables, not from the additional constraints.

4.1 A quadratic reformulation based on standard linearizations

Similarly to the standard linearization of the objective function, the quadratic equations (9) can be reformulated by a set of linear constraints. This leads to the following quadratic reformulation ($\texttt{FOR}^{\mathcal{S}}$) (for Fortet [24]) of ($\texttt{QCQP}^{\mathcal{S}}$) and of (P):

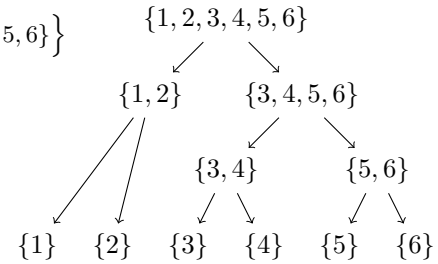
$$(\texttt{FOR}^{\mathcal{S}}) \begin{cases} \min\limits_{z \in \{0,1\}^N} \quad g(z) \\ \text{s.t.} \\ \quad z_E \leq z_{l_M(E)},\ z_E \leq z_{r_M(E)} \qquad \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M & (10) \\ \quad z_E \geq z_{l_M(E)} + z_{r_M(E)} - 1,\ z_E \geq 0 \quad \forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M & (11) \end{cases}$$

where $g(z)$ is defined by Equation (8).

Example 4. Let $f(x) = -6.5x_1x_2x_3x_4x_5x_6 - 5.6x_1x_2x_3$, with $\mathcal{M} = \{M_1 = \{1,2,3,4,5,6\}, M_2 = \{1,2,3\}\}$, and $n = 6$. Consider the quadratization scheme $\mathcal{S} = \left\{G_{M_1}, G_{M_2}\right\}$, where:

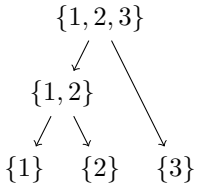
$V_{M_1} =$
$\Big\{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\},\{1,2\},\{3,4\},\{5,6\},\{3,4,5,6\},\{1,2,3,4,5,6\}\Big\}$

- $l_{M_1}(\{1,2\}) = \{1\}$, $r_{M_1}(\{1,2\}) = \{2\}$
- $l_{M_1}(\{3,4\}) = \{3\}$, $r_{M_1}(\{3,4\}) = \{4\}$
- $l_{M_1}(\{5,6\}) = \{5\}$, $r_{M_1}(\{5,6\}) = \{6\}$
- $l_{M_1}(\{3,4,5,6\}) = \{3,4\}$, $r_{M_1}(\{3,4,5,6\}) = \{5,6\}$
- $l_{M_1}(M_1) = \{1,2\}$, $r_{M_1}(M_1) = \{3,4,5,6\}$



$V_{M_2} = \Big\{\{1\},\{2\},\{3\},\{1,2\},\{1,2,3\}\Big\}$

- $l_{M_2}(\{1,2\}) = \{1\}$, $r_{M_2}(\{1,2\}) = \{2\}$
- $l_{M_2}(M_2) = \{1,2\}$, $r_{M_2}(M_2) = \{3\}$



with $\mathcal{E}_{M_1} = \Big\{\{1,2\},\{3,4\},\{5,6\},\{3,4,5,6\}\Big\}$, $\mathcal{E}_{M_2} = \Big\{\{1,2\}\Big\}$, and $\mathcal{E} = \Big\{\{1,2\},\{3,4\},\{5,6\},\{3,4,5,6\}\Big\}$.

Standard linearization consists in performing the following substitutions $z_{\{1,2\}} = z_1 z_2$, $z_{\{3,4\}} = z_3 z_4$, $z_{\{5,6\}} = z_5 z_6$, $z_{\{3,4,5,6\}} = z_{\{3,4\}} z_{\{5,6\}}$ in $f(x)$ and adding the appropriate set of constraints. The final linearly constrained quadratic reformulation is:

$$(\texttt{FOR}^{\mathcal{S}})\begin{cases} \min\limits_{z\in\{0,1\}^{10}} g(z) = -6.5 z_{\{1,2\}} z_{\{3,4,5,6\}} - 5.6 z_{\{1,2\}} z_3 \\ \text{s.t. } z_{\{1,2\}} \le z_1,\ z_{\{1,2\}} \le z_2,\ z_{\{1,2\}} \ge z_1 + z_2 - 1,\ z_{\{1,2\}} \ge 0 \\ \quad z_{\{3,4\}} \le z_3,\ z_{\{3,4\}} \le z_4,\ z_{\{3,4\}} \ge z_3 + z_4 - 1,\ z_{\{3,4\}} \ge 0 \\ \quad z_{\{5,6\}} \le z_5,\ z_{\{5,6\}} \le z_6,\ z_{\{5,6\}} \ge z_5 + z_6 - 1,\ z_{\{5,6\}} \ge 0 \\ \quad z_{\{3,4,5,6\}} \le z_{\{3,4\}},\ z_{\{3,4,5,6\}} \le z_{\{5,6\}},\ z_{\{3,4,5,6\}} \ge z_{\{3,4\}} + z_{\{5,6\}} - 1,\ z_{\{3,4,5,6\}} \ge 0 \end{cases}$$

4.2 A quadratic reformulation based on Rosenberg's method

We first provide an explicit quadratic reformulation of (P) by applying the central idea of Rosenberg's method [46]. The original algorithm is iterative and produces a quadratic reformulation by selecting a pair of (original or auxiliary) variables say, z_i, z_j, and by substituting a new variable $z_{i,j}$ for the product $z_i z_j$ in the objective function. The equality $z_{i,j} = z_i z_j$ is enforced by adding to the function a quadratic penalty term of the form $p_{i,j}(3z_{i,j} - 2z_i z_{i,j} - 2z_j z_{i,j} + z_i z_j)$ with a large enough multiplier $p_{i,j}$ (it suffices to set $p_{i,j}$ equal to the sum of the absolute values of the coefficients of the terms containing the product $z_i z_j$; see, e.g., [14]). This step is repeated until the penalized objective function becomes quadratic.

The procedure can be interpreted as implicitly defining a quadratic scheme $\mathcal{S}$ bottom-up, starting from the leaves. In order to integrate it in our framework, we can actually translate it to produce an explicit reformulation of (P) based on $(\texttt{QCQP}^{\mathcal{S}})$. Given a scheme $\mathcal{S}$, for each monomial M and $E \in \mathcal{E}_M$, let us introduce the penalty functions

$$q^R_M(E) \triangleq 3z_E - 2z_{l_M(E)} z_E - 2z_{r_M(E)} z_E + z_{l_M(E)} z_{r_M(E)} \tag{12}$$

which possess the following (easily verified) properties: for all binary values of z_E, $z_{l_M(E)}$, $z_{r_M(E)}$,

$$q_M^R(E) \geq 0, \tag{13}$$

$$z_E = z_{l_M(E)} z_{r_M(E)} \iff q_M^R(E) = 0. \tag{14}$$

If we repeatedly apply Rosenberg's approach to reduce the degree of M according to the quadratization scheme $\mathcal{S}$, we eventually find that the monomial $a_M \prod_{i \in M} x_i$ can be substituted in the objective function by

$$\rho_M(z) \triangleq a_M z_{l_M(M)} z_{r_M(M)} + |a_M| \sum_{E \in \mathcal{E}_M} q_M^R(E). \tag{15}$$

If we now apply the scheme $\mathcal{S}$ to the complete set of monomials $\mathcal{M}$ (i.e., to the function $f(x)$) and if we recall the definition of the function $g(z)$ in equation (8), we can transform the objective function into the quadratic function:

$$g^R(z) \triangleq \sum_{\substack{M \in \mathcal{M}: \\ |M| \leq 2}} a_M \prod_{i \in M} z_i + \sum_{\substack{M \in \mathcal{M}: \\ |M| \geq 3}} \rho_M(z) \tag{16}$$

$$= g(z) + \sum_{\substack{M \in \mathcal{M}: \\ |M| \geq 3}} |a_M| \sum_{E \in \mathcal{E}_M} q_M^R(E). \tag{17}$$

The resulting unconstrained quadratic reformulation of ($\texttt{QCQP}^{\mathcal{S}}$) and of (P) is the following problem:

$$(\texttt{ROS}^{\mathcal{S}}) \left\{ \min_{z \in \{0,1\}^N} g^R(z). \right.$$

For the sake of completeness, let us formally establish the correctness of the transformation (remember Definition 2).

Theorem 9. *For every quadratization scheme $\mathcal{S} = \{G_M = (V_M, l_M, r_M) : M \in \mathcal{M}\}$, the function $g^R(z)$ is a quadratization of $f(x)$ and ($\texttt{ROS}^{\mathcal{S}}$) is a quadratic reformulation of (P).*

Proof. Consider any binary minimizer of $g^R(z)$, say z^*, and let $x_i^* = z_i^*$ for $i \in [n]$. If z^* is consistent, then in view of Equation (14), $g^R(z^*) = f(x^*)$ as required for a quadratization.

On the other hand, if z^* is not consistent, then there is $M \in \mathcal{M}$ and $E \in \mathcal{E}_M$ such that $z_E^* \neq z_{l_M(E)}^* z_{r_M(E)}^*$. We say that z^* is inconsistent for this monomial M. In view of Equations (13)-(14), for any such M,

$$\rho_M(z^*) \geq a_M z_{l_M(M)}^* z_{r_M(M)}^* + |a_M| \geq \max(a_M, 0).$$

Next, define z^+ to be consistent with x^*, that is, let $z_S^+ = \prod_{i \in S} z_i^* = \prod_{i \in S} x_i^*$ for all subsets $S \in \bigcup_{\substack{M \in \mathcal{M}: \\ |M| \geq 3}} V_M$. For any monomial M, if z^* is consistent for M, then $\rho_M(z^+) = \rho_M(z^*)$. On the other hand, if z^* is inconsistent for M, then there are two cases:

1. if $\prod_{i \in M} x_i^* = 1$, then $\rho_M(z^+) = a_M z_{l_M(M)}^+ z_{r_M(M)}^+ = a_M \leq \max(a_M, 0) \leq \rho_M(z^*)$;

2. if $\prod_{i\in M} x_i^* = 0$, then $\rho_M(z^+) = a_M z^+_{l_M(M)} z^+_{r_M(M)} = 0 \leq \max(a_M, 0) \leq \rho_M(z^*)$.

It easily follows from these inequalities that $g^R(z^+) \leq g^R(z^*)$. Thus, $g^R(z)$ has a minimizer which is consistent (namely, z^+), and we conclude that $g^R(z)$ is a quadratization of $f(x)$ as in the first part of the proof. This implies, in turn, that ($\texttt{ROS}^{\mathcal{S}}$) is a quadratic reformulation of (P). □

Remark 2. For the record, it may be interesting to notice that in his original paper, Rosenberg [46] did not use the penalty multipliers $|a_M|$ that we use in ($\texttt{ROS}^{\mathcal{S}}$), but introduced a different, more flexible way to compute valid multipliers. As a result, the reformulation $g(z)$ produced by his original method does not necessarily yield a quadratization, contrary to what was suggested a bit hastily, for example in [3, 9].

Remark 3. The number of auxiliary variables in $g^R(z)$ is equal to the size of $\mathcal{E}$ in the quadratization scheme. Since Anthony et al. [3] observed that there exist quadratization schemes of size $O(2^{\frac{n}{2}})$, it follows that every pseudo-Boolean function has a quadratization involving $O(2^{\frac{n}{2}})$ auxiliary variables. This reasoning provides an alternative, easier proof of Theorem 4 in [3].

Remark 4. The function $g^R(z)$ can be rewritten as

$$g^R(z) = g(z) + \sum_{E\in\mathcal{E}} \Big(\sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3 \text{ and } E\in\mathcal{E}_M}} |a_M| q^R_M(E) \Big).$$

If each monomial has a unique decomposition in $\mathcal{S}$, that is, if $l_M(E) = l_{M'}(E) = l(E)$ and $r_M(E) = r_{M'}(E) = r(E)$ for all M, M' such that $E \in \mathcal{E}_M \cap \mathcal{E}_{M'}$, then this simply becomes

$$g^R(z) = g(z) + \sum_{E\in\mathcal{E}} \Big(\sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3 \text{ and } E\in\mathcal{E}_M}} |a_M| \Big) (3z_E - 2z_{l(E)}z_E - 2z_{r(E)}z_E + z_{l(E)}z_{r(E)}).$$

Here, the coefficient of the penalty function associated with variable z_E in ($\texttt{ROS}^{\mathcal{S}}$) is the sum of the absolute values of the coefficients of the terms of f whose decomposition involves E. This case arises, in particular, when $\mathcal{S}$ arises from a pairwise cover as explained in Proposition 8 (see Remark 1).

Example 5 (Example 4 continued)**.** To illustrate Remark 4, consider again the objective function $f(x) = -6.5x_1x_2x_3x_4x_5x_6 - 5.6x_1x_2x_3$, and the quadratization scheme $\mathcal{S}$. To build the penalized objective function we add a penalty function to $g(z)$ for each $E \in \mathcal{E}$:

- $P_{\{1,2\}}(3z_{\{1,2\}} - 2z_1z_{\{1,2\}} - 2z_2z_{\{1,2\}} + z_1z_2)$ with $P_{\{1,2\}} = \sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3, \{1,2\}\in\mathcal{E}_M}} |a_M| = 6.5 + 5.6 = 12.1$
- $P_{\{3,4\}}(3z_{\{3,4\}} - 2z_3z_{\{3,4\}} - 2z_4z_{\{3,4\}} + z_3z_4)$ with $P_{\{3,4\}} = \sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3, \{3,4\}\in\mathcal{E}_M}} |a_M| = 6.5$
- $P_{\{5,6\}}(3z_{\{5,6\}} - 2z_5z_{\{5,6\}} - 2z_6z_{\{5,6\}} + z_5z_6)$ with $P_{\{5,6\}} = \sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3, \{5,6\}\in\mathcal{E}_M}} |a_M| = 6.5$
- $P_{\{3,4,5,6\}}(3z_{\{3,4,5,6\}} - 2z_{\{3,4\}}z_{\{3,4,5,6\}} - 2z_{\{5,6\}}z_{\{3,4,5,6\}} + z_{\{3,4\}}z_{\{5,6\}})$ with $P_{\{3,4,5,6\}} = \sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3,\\ \{3,4,5,6\}\in\mathcal{E}_M}} |a_M| = 6.5$

We obtain as final quadratic reformulation:

$$(\texttt{ROS}^{\mathcal{S}})\begin{cases}\min\limits_{z\in\{0,1\}^{10}} & -6.5z_{\{1,2\}}z_{\{3,4,5,6\}} - 5.6z_{\{1,2\}}z_3 + 12.1(3z_{\{1,2\}} - 2z_1z_{\{1,2\}} - 2z_2z_{\{1,2\}} + z_1z_2)\\ & +6.5(3z_{\{3,4\}} - 2z_3z_{\{3,4\}} - 2z_4z_{\{3,4\}} + z_3z_4) + 6.5(3z_{\{5,6\}} - 2z_5z_{\{5,6\}} - 2z_6z_{\{5,6\}} + z_5z_6)\\ & +6.5(3z_{\{3,4,5,6\}} - 2z_{\{3,4\}}z_{\{3,4,5,6\}} - 2z_{\{5,6\}}z_{\{3,4,5,6\}} + z_{\{3,4\}}z_{\{5,6\}})\end{cases}$$

4.3 A quadratic reformulation based on ABCG quadratization

We call ABCG a quadratization procedure due to Anthony et al. [3] . Given a scheme $\mathcal{S}$, for each monomial M and $E \in \mathcal{E}_M$, let

$$q_M^A(E) \triangleq \big(2|E| - 1 - 2\sum_{j\in E} z_j\big)z_E + z_{l_M(E)}z_{r_M(E)}. \tag{18}$$

Let again $g(z)$ be given by Equation (8), and define

$$g^A(z) \triangleq g(z) + \sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3}} \sum_{E\in\mathcal{E}_M} \beta_M(E)\, q_M^A(E) \tag{19}$$

where the coefficients $\beta_M(E)$ are given by the following "top-down" recursion in the graph G_M:

- if $E \in \{l_M(M), r_M(M)\}$, then
$$\beta_M(E) = |a_M|; \tag{20}$$
- if $E \in \mathcal{E}_M \setminus \{l_M(M), r_M(M)\}$, then
$$\beta_M(E) = \sum_{\substack{S\in\mathcal{E}_M:\\ E\in\{l_M(S), r_M(S)\}}} \beta_M(S). \tag{21}$$

The recursive definition (20)-(21) has a simple graphical interpretation: for all $M \in \mathcal{M}$ and $E \in \mathcal{E}_M$, $\beta_M(E)$ is equal to $|a_M|\pi_{M,E}$, where $\pi_{M,E}$ is the number of directed paths from the root M to vertex E in the quadratization scheme G_M. In particular, $\beta_M(E) \geq |a_M| \geq 0$.

The quadratic expression $q_M^A(E)$ plays a similar role for ABCG as the quadratic expressions $q_M^R(E)$ in Equation (12) for Rosenberg's procedure. However, contrary to $q_M^R(E)$, there is no guarantee that $q_M^A(E)$ is nonnegative for all assignments of values to the variables. One can easily establish the following property which will prove sufficient for our purpose: for all binary values of $z_j, z_E, z_{l_M(E)}, z_{r_M(E)}$,

$$\text{if } z_E = z_{l_M(E)}z_{r_M(E)} \text{ and } z_E = \prod_{j\in E} z_j \text{ then } q_M^A(E) = 0. \tag{22}$$

Anthony et al. [3] proved that $g^A(z)$ is a quadratization of the original function $f(x)$ when the scheme $\mathcal{S} = \{G_M = (V_M, l_M, r_M) : M \in \mathcal{M}\}$ is associated with a pairwise cover. For the sake of completeness, we formally establish the next, more general statement, where $(\texttt{ABCG}^{\mathcal{S}})$ denotes the unconstrained quadratic minimization problem

$$(\texttt{ABCG}^{\mathcal{S}})\begin{cases}\min\limits_{z\in\{0,1\}^N} & g^A(z)\end{cases}$$

where $g^A(z)$ is defined by Equation (19).

Theorem 10. *For every quadratization scheme $\mathcal{S} = \{G_M = (V_M, l_M, r_M) : M \in \mathcal{M}\}$, the function $g^A(z)$ is a quadratization of $f(x)$ and ($\texttt{ABCG}^{\mathcal{S}}$) is a quadratic reformulation of (P).*

Proof. It suffices to prove that $g^A(z)$ is a quadratization of $f(x)$. As in the proof of Theorem 9, consider any binary minimizer of g^A, say z^*, and let $x_i^* = z_i^*$ for $i \in [n]$. If z^* is consistent with x^*, then in view of Equation (22), $g^A(z^*) = g(z^*) = f(x^*)$ as required from a quadratization.

We are now going to show that we can actually assume without loss of generality that z^* is consistent. Let us rewrite $g^A(z)$ in the form

$$g^A(z) = \sum_{\substack{M \in \mathcal{M}: \\ |M| \leq 2}} a_M \prod_{i \in M} z_i + \sum_{\substack{M \in \mathcal{M}: \\ |M| \geq 3}} \alpha_M(z) \tag{23}$$

where

$$\alpha_M(z) \triangleq a_M z_{l_M(M)} z_{r_M(M)} + \sum_{E \in \mathcal{E}_M} \beta_M(E) \left((2|E| - 1 - 2\sum_{j \in E} z_j) z_E + z_{l_M(E)} z_{r_M(E)} \right). \tag{24}$$

Consider now any variable z_E which appears in $g^A(z)$ with $|E| \geq 2$, $E \in \mathcal{E}_M$ for some $M \in \mathcal{M}$. (Note that E may actually appear in several schemes G_M, but this will not affect the reasoning hereunder.) We would like to identify the multiplier of z_E in $\alpha_M(z)$. Let us distinguish two cases.

Case 1: E appears in the decomposition of M, that is, $E \in \{l_M(M), r_M(M)\}$. Assume without loss of generality that $E = l_M(M)$. Then, in (24), z_E is multiplied by

$$c_{M,E}(z) = a_M z_{r_M(M)} + \beta_M(E)(2|E| - 1 - 2\sum_{j \in E} z_j),$$

where the second term results from the decomposition of E in G_M. Consider again two subcases.

1.1. If $\prod_{j \in E} z_j^* = 1$, or equivalently $\sum_{j \in E} z_j^* = |E|$, then by definition (20):

$$c_{M,E}(z^*) = a_M z^*_{r_M(M)} - \beta_M(E) = a_M z^*_{r_M(M)} - |a_M| \leq 0.$$

Since z^* is a minimizer of g^A, we can assume that $z_E^* = 1$, meaning that z_E^* is consistent with the value of $\prod_{j \in E} z_j^*$. (As already observed, E may appear in the quadratization scheme of several monomials M, but as we will see below, the conclusion $c_{M,E}(z) \leq 0$ will hold in all cases.)

1.2. If $\prod_{j \in E} z_j^* = 0$, then $2|E| - 1 - 2\sum_{j \in E} z_j^* \geq 1$. From this and from definition (20), it follows that

$$c_{M,E}(z^*) \geq a_M z^*_{r_M(M)} + \beta_M(E) = a_M z^*_{r_M(M)} + |a_M| \geq 0.$$

So, in this case, we can safely assume that $z_E^* = 0 = \prod_{j \in E} z_j^*$.

Let us now turn to the second case.

Case 2: E appears in the decomposition of one or several sets $S \in \mathcal{E}_M$, $S \neq M$. For notational simplicity and without loss of generality, let us assume that for all such sets S, there holds $E = l_M(S)$. Then, in (24), z_E is multiplied by

$$c_{M,E}(z) = \beta_M(E)(2|E| - 1 - 2\sum_{j \in E} z_j) + \sum_{\substack{S \in \mathcal{E}_M: \\ E \in \{l_M(S), r_M(S)\}}} \beta_M(S) z_{r_M(S)}.$$

2.1. If $\prod_{j\in E} z_j^* = 1$, then in view of definition (21),

$$c_{M,E}(z^*) = -\beta_M(E) + \sum_{\substack{S\in\mathcal{E}_M:\\ E\in\{l_M(S),r_M(S)\}}} \beta_M(S) z^*_{r_M(S)} \le -\beta_M(E) + \sum_{\substack{S\in\mathcal{E}_M:\\ E\in\{l_M(S),r_M(S)\}}} \beta_M(S) = 0.$$

Since z^* is a minimizer of g^A, we can assume that $z^*_E = 1 = \prod_{j\in E} z^*_j$.

2.2. If $\prod_{j\in E} z_j^* = 0$, then

$$c_{M,E}(z^*) \ge \beta_M(E) + \sum_{\substack{S\in\mathcal{E}_M:\\ E\in\{l_M(S),r_M(S)\}}} \beta_M(S) z^*_{r_M(S)} \ge 0.$$

So, in this case, we can safely assume that $z^*_E = 0 = \prod_{j\in E} z^*_j$.

In all cases, we conclude that z^* can be assumed to be consistent. Hence, as argued in the first part of the proof, $g^A(z^*) = f(x^*)$ and $g^A(z)$ is a quadratization of $f(x)$. □

As observed earlier, $\beta_M(E)$ is equal to $|a_M|\pi_{M,E}$, where $\pi_{M,E}$ is the number of directed paths from the root M to vertex E in the quadratization scheme G_M. As a consequence, we immediately obtain the following simplified form of Theorem 10 for disjoint schemes (compare with Remark 4):

Proposition 11. *For every disjoint quadratization scheme $\mathcal{S} = \{G_M = (V_M, l_M, r_M) : M \in \mathcal{M}\}$, the function*

$$g^A(z) = g(z) + \sum_{E\in\mathcal{E}} \Big(\sum_{\substack{M\in\mathcal{M}:\\ |M|\ge 3 \text{ and } E\in\mathcal{E}_M}} |a_M| \Big)\, q^A_M(E).$$

is a quadratization of $f(x)$.

Proof. When $\mathcal{S}$ is disjoint, every vertex $E \neq M$ has indegree 1 in G_M (see Proposition 4). Hence $\pi_{M,E} = 1$ and $\beta_M(E) = |a_M|$. □

Remark 5. Proposition 11 shows that in the disjoint case, the penalty coefficients are the same in Rosenberg's procedure and in ABCG. However this is not the case for the penalty *functions* $q^R_M(E)$ and $q^A_M(E)$, which can be different as illustrated by the next example.

Example 6 (Example 4 continued)**.** Consider again the function $f(x) = -6.5x_1x_2x_3x_4x_5x_6 - 5.6x_1x_2x_3$, and the quadratization scheme $\mathcal{S}$. We construct the penalty function term by term for every $M \in \mathcal{M}$ with $|M| \ge 3$ and every $E \in \mathcal{E}_M$.

Since the quadratization scheme $\mathcal{S}$ is disjoint, we have that for $M_1 = \{1,2,3,4,5,6\}$, $\beta_{M_1}(E) = |a_{M_1}| = 6.5$ for every $E \in \mathcal{E}_{M_1}$ and for $M_2 = \{1,2,3\}$, $\beta_{M_2}(E) = |a_{M_2}| = 5.6$ for every $E \in \mathcal{E}_{M_2}$.

For $M_1 = \{1,2,3,4,5,6\}$, the sets $E \in \mathcal{E}_{M_1}$ and their corresponding penalty terms are

- $E = \{3,4,5,6\}$. The penalty term is
  $6.5\left(7z_{\{3,4,5,6\}} - 2z_3z_{\{3,4,5,6\}} - 2z_4z_{\{3,4,5,6\}} - 2z_5z_{\{3,4,5,6\}} - 2z_6z_{\{3,4,5,6\}} + z_{\{3,4\}}z_{\{5,6\}}\right).$
- $E = \{1,2\}$. The penalty term is $6.5\left(3z_{\{1,2\}} - 2z_1z_{\{1,2\}} - 2z_2z_{\{1,2\}} + z_1z_2\right).$
- $E = \{3,4\}$. The penalty term is $6.5\left(3z_{\{3,4\}} - 2z_3z_{\{3,4\}} - 2z_4z_{\{3,4\}} + z_3z_4\right).$

- $E = \{5, 6\}$. The penalty term is $6.5\left(3z_{\{5,6\}} - 2z_5 z_{\{5,6\}} - 2z_6 z_{\{5,6\}} + z_5 z_6\right)$.

For $M_2 = \{1, 2, 3\}$, there is only one set $E \in \mathcal{E}_{M_2}$:

- $E = \{1, 2\}$. The penalty term is $5.6\left(3z_{\{1,2\}} - 2z_1 z_{\{1,2\}} - 2z_2 z_{\{1,2\}} + z_1 z_2\right)$.

We finally obtain the quadratic reformulation:

$$(\texttt{ABCG}^{\mathcal{S}}) \begin{cases} \min\limits_{z\in\{0,1\}^{10}} & -6.5z_{\{1,2\}}z_{\{3,4,5,6\}} - 5.6z_{\{1,2\}}z_3 + 12.1(3z_{\{1,2\}} - 2z_1 z_{\{1,2\}} - 2z_2 z_{\{1,2\}} + z_1 z_2) \\ & +6.5(3z_{\{3,4\}} - 2z_3 z_{\{3,4\}} - 2z_4 z_{\{3,4\}} + z_3 z_4) + 6.5(3z_{\{5,6\}} - 2z_5 z_{\{5,6\}} - 2z_6 z_{\{5,6\}} + z_5 z_6) \\ & +6.5(7z_{\{3,4,5,6\}} - 2z_3 z_{\{3,4,5,6\}} - 2z_4 z_{\{3,4,5,6\}} - 2z_5 z_{\{3,4,5,6\}} - 2z_6 z_{\{3,4,5,6\}} + z_{\{3,4\}} z_{\{5,6\}}). \end{cases}$$

Observe the difference between functions $g^R(z)$ and $g^A(z)$ for this example. In Rosenberg's procedure, the penalties for a variable z_E involve the direct successors of monomial E, while in ABCG they involve the leaves of the quadratization scheme (i.e., the initial variables). Compare, for example, the penalties associated with $z_{\{3,4,5,6\}}$ in Example 5 and in the current Example 6.

5 Phase III: Convexifying the quadratic reformulation

In the previous section, from a given quadratization scheme $\mathcal{S}$, we have built three quadratic formulations equivalent to (P), all of them sharing the same set of N binary variables z: a linearly constrained binary quadratic problem ($\texttt{FOR}^{\mathcal{S}}$), and two unconstrained binary quadratic programs ($\texttt{ROS}^{\mathcal{S}}$) and ($\texttt{ABCG}^{\mathcal{S}}$). In these three formulations, the objective function is non-convex. So, to solve these optimization problems, a convexification step would be typically required. We propose in this section a linearization and a convexification method for each of these three problems, and we compare them from the point of view of the bounds obtained by continuous relaxation.

5.1 Linearization of the objective function

In this section, we propose to linearize the three quadratic reformulations. For this purpose, the basic idea is to apply once again the standard linearization described in Section 4 to the nonlinear terms of the quadratic functions $g(z)$, $g^R(z)$, or $g^A(z)$ (this is also implemented in commercial solvers like CPLEX [33] or Gurobi [43]). We thus obtain three linear reformulations of (P). We then compare the continuous relaxation bounds of these linear problems.

Linearization of ($\texttt{FOR}^{\mathcal{S}}$). To linearize problem ($\texttt{FOR}^{\mathcal{S}}$), we first introduce a new variable $Z_{\{i_1\},\{i_2\}}$ for each monomial $M = \{i_1, i_2\} \in \mathcal{M}$ of degree 2. Then, we introduce a variable $Z_{l_M(M),r_M(M)}$ to represent the product $z_{l_M(M)}z_{r_M(M)}$ in ($\texttt{FOR}^{\mathcal{S}}$) for each monomial $M \in \mathcal{M}$ of degree at least three. This variable also represents the monomial M itself. We obtain the following 0-1 linear programming reformulation of ($\texttt{FOR}^{\mathcal{S}}$) and therefore of (P):

$$
(\texttt{FOR-L}^{\mathcal{S}})\begin{cases}
\min \quad g_L(z,Z) \triangleq \sum_{i=1}^{n} a_i z_i + \sum_{\substack{M\in\mathcal{M}\\ M=\{i_1,i_2\}}} a_M Z_{\{i_1\},\{i_2\}} + \sum_{\substack{M\in\mathcal{M}\\ |M|\geq 3}} a_M Z_{l_M(M),r_M(M)} & (25)\\
\text{s.t. } (10)-(11) & \\
\quad Z_{\{i_1\},\{i_2\}} \leq z_{i_1},\ Z_{\{i_1\},\{i_2\}} \leq z_{i_2},\ Z_{\{i_1\},\{i_2\}} \geq z_{i_1}+z_{i_2}-1 \quad \forall M\in\mathcal{M}: M=\{i_1,i_2\} & (26)\\
\quad Z_{l_M(M),r_M(M)} \leq z_{l_M(M)},\ Z_{l_M(M),r_M(M)} \leq z_{r_M(M)} \quad \forall M\in\mathcal{M}: |M|\geq 3 & (27)\\
\quad Z_{l_M(M),r_M(M)} \geq z_{l_M(M)} + z_{r_M(M)} - 1 \qquad \forall M\in\mathcal{M}: |M|\geq 3 & (28)\\
\quad z\in\{0,1\}^N, \quad 0\leq Z\leq 1, &
\end{cases}
$$

where the shorthand notation $0 \leq Z \leq 1$ means that each component of Z is between 0 and 1.

The number of auxiliary variables in ($\texttt{FOR-L}^{\mathcal{S}}$) is equal to $|\mathcal{M}| + |\mathcal{E}|$. In contrast with this, the standard linearization (SL) introduced in Section 2 contains $|\mathcal{M}|$ auxiliary variables, and is independent of any quadratization scheme. We can compare the value of the LP bounds provided by these two linearizations when $\mathcal{S}$ is a *disjoint* quadratization scheme.

Proposition 12. *For every disjoint quadratization scheme $\mathcal{S}$, the LP bound provided by the continuous relaxation of ($\texttt{FOR-L}^{\mathcal{S}}$) is at least as good as the LP bound provided by the continuous relaxation of (SL).*

Proof. Let (z^*, Z^*) be an optimal solution of the relaxation of ($\texttt{FOR-L}^{\mathcal{S}}$). We build the following point $(\tilde{x}, \tilde{y})$: $\tilde{x}_i = z_i^*$ for $i = 1, ..., n$, $\tilde{y}_{\{i_1,i_2\}} = Z^*_{\{i_1\},\{i_2\}}$ for every degree-2 monomial $\{i_1, i_2\} \in \mathcal{M}$, and $\tilde{y}_M = Z^*_{l_M(M),r_M(M)}$ for every monomial $M \in \mathcal{M}$ with $|M| \geq 3$.

Let us check that $(\tilde{x}, \tilde{y})$ is a feasible solution of (SL). For any degree-2 monomial $M = \{i_1, i_2\}$, Constraints (3) and (4) follow from (26). Moreover, Constraints (10)-(11) iteratively enforce $z^*_E \leq z^*_i$ and $z^*_E \geq \sum_{i\in E} z^*_i - (|E| - 1)$ for all $E \in \mathcal{E}$ and all $i \in E$. Therefore, for any monomial M with $|M| \geq 3$, Constraints (3) follow from (10)-(11),(27), and $M = l_M(M) \cup r_M(M)$. To verify Constraints (4), note that it follows from (28) that:

$$
\tilde{y}_M \geq z^*_{l_M(M)} + z^*_{r_M(M)} - 1 \geq \sum_{i\in l_M(M)} z^*_i - (|l_M(M)| - 1) + \sum_{i\in r_M(M)} z^*_i - (|r_M(M)| - 1) - 1
$$

and the last expression is equal to $\sum_{i\in M} \tilde{x}_i - (|M| - 1)$ as $l_M(M), r_M(M)$ form a partition of M.

Finally, solution $(\tilde{x}, \tilde{y})$ has the same objective value in (SL) as (z^*, Z^*) in ($\texttt{FOR-L}^{\mathcal{S}}$). We conclude that the optimal value of ($\texttt{FOR-L}^{\mathcal{S}}$) is smaller than or equal to that of (SL).

□

Linearization of ($\texttt{ROS}^{\mathcal{S}}$). Now, we introduce the linearization of problem ($\texttt{ROS}^{\mathcal{S}}$). Observe that the penalty functions of the Rosenberg procedure are composed of quadratic terms that do not appear in ($\texttt{FOR}^{\mathcal{S}}$). Therefore, the linearization of problems ($\texttt{ROS}^{\mathcal{S}}$) requires more auxiliary variables than ($\texttt{FOR-L}^{\mathcal{S}}$): in addition to the Z variables already in ($\texttt{FOR-L}^{\mathcal{S}}$), the products $z_E z_{l_M(E)}$, $z_E z_{r_M(E)}$ and $z_{l_M(E)} z_{r_M(E)}$ are respectively linearized by new auxiliary variables that we denote by $Z_{E,l_M(E)}$, $Z_{E,r_M(E)}$ and $Z_{l_M(E),r_M(E)}$, $\forall E \in \mathcal{E}, \forall M \in \mathcal{M} : E \in \mathcal{E}_M$. (Nevertheless, in order to simplify the presentation, we use the same letter Z to denote the vector of auxiliary variables in ($\texttt{ROS-L}^{\mathcal{S}}$) and in ($\texttt{FOR-L}^{\mathcal{S}}$).) We build the following mixed-integer linear problem equivalent to ($\texttt{ROS}^{\mathcal{S}}$) and to (P):

$$
(\texttt{ROS-L}^{\mathcal{S}})\begin{cases}
\min \quad g_{LR}(z,Z) \triangleq g_L(z,Z) + \displaystyle\sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3}} \sum_{E\in\mathcal{E}_M} |a_M|\Big(3z_E - 2Z_{E,l_M(E)} - 2Z_{E,r_M(E)} + Z_{l_M(E),r_M(E)}\Big) & \\
\text{s.t. } (26)-(28) & \\
\quad Z_{E,l_M(E)} \leq z_{l_M(E)},\ Z_{E,l_M(E)} \leq z_E \quad \forall E\in\mathcal{E}, \forall M\in\mathcal{M}: E\in\mathcal{E}_M. & (29)\\
\quad Z_{E,r_M(E)} \leq z_{r_M(E)},\ Z_{E,r_M(E)} \leq z_E \quad \forall E\in\mathcal{E}, \forall M\in\mathcal{M}: E\in\mathcal{E}_M & (30)\\
\quad Z_{l_M(E),r_M(E)} \geq z_{l_M(E)} + z_{r_M(E)} - 1 \quad \forall E\in\mathcal{E}, \forall M\in\mathcal{M}: E\in\mathcal{E}_M & (31)\\
\quad z_E \leq z_{l_M(E)},\ z_E \leq z_{r_M(E)} \qquad \forall E\in\mathcal{E}, \forall M\in\mathcal{M}: E\in\mathcal{E}_M & (32)\\
\quad z\in\{0,1\}^N \quad 0\leq Z\leq 1. &
\end{cases}
$$

The function $g_L(z,Z)$ in the objective function is given by Equation (25). Constraints (29) are enough to enforce the equality $Z_{E,l_M(E)} = z_E z_{l_M(E)}$ in any optimal solution because variable $Z_{E,l_M(E)}$ appears in the objective function with a negative coefficient, and nowhere else. The same holds for Constraints (30) which enforce the equality $Z_{E,r_M(E)} = z_E z_{r_M(E)}$. Constraints (31) enforce the equality $Z_{l_M(E),r_M(E)} = z_{l_M(E)} z_{r_M(E)}$ in any optimal solution as this variable has a positive coefficient in the objective function whenever $|E| \geq 3$. This property may not hold, however, when E is a degree-2 monomial and $Z_{l_M(E),r_M(E)}$ also appears with a negative coefficient in $g_L(z,Z)$. But in this case, Constraints (31) are redundant with (26), which impose the required equalities. Constraints (32) are valid inequalities that follow from the fact that in any optimal solution $\tilde{z}$ of $(\texttt{ROS}^{\mathcal{S}})$ and therefore of $(\texttt{ROS-L}^{\mathcal{S}})$, $\tilde{z}_E$ must be equal to the product $\tilde{z}_{l_M(E)}\tilde{z}_{r_M(E)}$.

We next show that the addition of Constraints (32) allows us to significantly reduce the size of $(\texttt{ROS-L}^{\mathcal{S}})$ (the letter C in $(\texttt{ROS-C}^{\mathcal{S}})$ refers to a *compact* reformulation):

Proposition 13. *Let $(\textit{ROS-C}^{\mathcal{S}})$ be the following problem:*

$$
(\textit{ROS-C}^{\mathcal{S}})\begin{cases}
\min \quad g'_{LR}(z,Z) \triangleq g_L(z,Z) + \displaystyle\sum_{\substack{M\in\mathcal{M}:E\in\mathcal{E}_M\\ |M|\geq 3}} |a_M|(Z_{l_M(E),r_M(E)} - z_E) & \\
\textit{s.t. } (26)-(28),\ (31),\ (32) & \\
\quad z\in\{0,1\}^N \quad 0\leq Z\leq 1. &
\end{cases}
$$

Problems $(\textit{ROS-L}^{\mathcal{S}})$ and $(\textit{ROS-C}^{\mathcal{S}})$ have the same optimal value. The same property holds for their LP relaxations.

Proof. In an optimal solution of $(\texttt{ROS-L}^{\mathcal{S}})$, $Z_{E,l_M(E)}$ is as large as possible, therefore it is equal to $\min(z_E, z_{l_M(E)})$ which is in turn equal to z_E by Constraints (32). The same reasoning applies for variable $Z_{E,r_M(E)}$ which is equal to z_E in any optimal solution. One can therefore fix both $Z_{E,l_M(E)}$ and $Z_{E,r_M(E)}$ to z_E in $(\texttt{ROS-L}^{\mathcal{S}})$ and straightforwardly get $(\texttt{ROS-C}^{\mathcal{S}})$. Integrality plays no role in this argument, so the same conclusion holds for the linear relaxations of $(\texttt{ROS-L}^{\mathcal{S}})$ and $(\texttt{ROS-C}^{\mathcal{S}})$. □

The compact problem $(\texttt{ROS-C}^{\mathcal{S}})$ has the same variables as $(\texttt{FOR-L}^{\mathcal{S}})$ and additional variables $Z_{l_M(E),r_M(E)}$. We now compare the LP bounds of linearizations $(\texttt{FOR-L}^{\mathcal{S}})$ and $(\texttt{ROS-C}^{\mathcal{S}})$.

Proposition 14. *For every quadratization scheme $\mathcal{S}$, the LP bound provided by the continuous relaxation of $(\textit{FOR-L}^{\mathcal{S}})$ is at least as good as the LP bound provided by the continuous relaxation of $(\textit{ROS-C}^{\mathcal{S}})$.*

Proof. Let (z^*, Z^*) be an optimal solution of the relaxation of $(\texttt{FOR-L}^{\mathcal{S}})$. Let us build a solution $(\tilde{z}, \tilde{Z})$ of the relaxation of $(\texttt{ROS-C}^{\mathcal{S}})$. We set $\tilde{z} = z^*$ and $\tilde{Z} = Z^*$ for the components of Z that are common to both problems. We also set $\tilde{Z}_{l_M(E),r_M(E)} = z^*_E$. One can easily check that $(\tilde{z}, \tilde{Z})$ is a feasible solution of the linear relaxation of $(\texttt{ROS-C}^{\mathcal{S}})$ with the same value as (z^*, Z^*) in the linear relaxation of $(\texttt{FOR-L}^{\mathcal{S}})$. □

Linearization of $(\texttt{ABCG}^{\mathcal{S}})$. Let us now turn to the ABCG procedure. We need the Z variables present in $(\texttt{FOR-L}^{\mathcal{S}})$, variables $Z_{l_M(E),r_M(E)}$ already used in $(\texttt{ROS-L}^{\mathcal{S}})$, and we add a new variable denoted by $Z_{E,\{j\}}$ for each product $z_j z_E$, for all $M \in \mathcal{M}$, $E \in \mathcal{E}_M$ and $j \in E$. We build the following mixed-integer linear problem equivalent to $(\texttt{ABCG}^{\mathcal{S}})$ and to (P):

$$(\texttt{ABCG-L}^{\mathcal{S}}) \begin{cases} \min \quad g_{LA}(z,Z) \triangleq g_L(z,Z) + \displaystyle\sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3}} \sum_{E\in\mathcal{E}_M} \beta_M(E)\Big((2|E|-1)z_E - 2\sum_{j\in E} Z_{E,\{j\}} + Z_{l_M(E),r_M(E)}\Big) \\ \text{s.t. } (26)-(28),\ (31),\ (32) \\ \quad Z_{E,\{j\}} \leq z_j,\ Z_{E,\{j\}} \leq z_E \qquad \forall E \in \mathcal{E}, \forall j \in E \\ \quad z \in \{0,1\}^N \quad 0 \leq Z \leq 1. \end{cases} \tag{33}$$

Here again, variables $Z_{E,\{j\}}$ are weighted by negative coefficients in $g_{LA}(z,Z)$, so Constraints (33) are enough to linearize $z_j z_E$ by $Z_{E,\{j\}}$. For the same reasons as in $(\texttt{ROS-L}^{\mathcal{S}})$, Constraints (32) are valid inequalities in $(\texttt{ABCG-L}^{\mathcal{S}})$. We now show that variables $Z_{E,\{j\}}$ can be fixed and Constraints (33) can be dropped to obtain a compact reformulation of $(\texttt{ABCG-L}^{\mathcal{S}})$.

Proposition 15. *Let* $(\textit{ABCG-C}^{\mathcal{S}})$ *be the following problem:*

$$(\textit{ABCG-C}^{\mathcal{S}}) \begin{cases} \min \quad g'_{LA}(z,Z) \triangleq g_L(z,Z) + \displaystyle\sum_{\substack{M\in\mathcal{M}:\\ |M|\geq 3}} \sum_{E\in\mathcal{E}_M} \beta_M(E)(Z_{l_M(E),r_M(E)} - z_E) \\ \textit{s.t. } (26)-(28),\ (31),\ (32) \\ \quad z \in \{0,1\}^N \quad 0 \leq Z \leq 1 \end{cases}$$

Problems $(\textit{ABCG-L}^{\mathcal{S}})$ *and* $(\textit{ABCG-C}^{\mathcal{S}})$ *have the same optimal value. The same property holds for their LP relaxations.*

Proof. The proof is similar to the proof of Proposition 13. It is enough to observe that, in an optimal solution of $(\texttt{ABCG-L}^{\mathcal{S}})$, $Z_{E,\{j\}}$ is as large as possible and is therefore equal to $\min(z_E, z_j)$. Constraints (32) can be applied iteratively starting from z_E until reaching the leaf $\{j\}$. Hence, $\min(z_E, z_j) = z_E$ and $Z_{E,\{j\}} = z_E$. It follows that $(2|E|-1)z_E - 2\displaystyle\sum_{j\in E} Z_{E,\{j\}} = -z_E$. □

The following proposition states that the LP bounds of linearizations $(\texttt{FOR-L}^{\mathcal{S}})$ and $(\texttt{ABCG-C}^{\mathcal{S}})$ compare similarly to above.

Proposition 16. *For every quadratization scheme* $\mathcal{S}$*, the LP bound provided by the continuous relaxation of* $(\textit{FOR-L}^{\mathcal{S}})$ *is at least as good as the LP bound provided by the continuous relaxation of* $(\textit{ABCG-C}^{\mathcal{S}})$.

Proof. Identical to the proof of Proposition 14. □

Finally, we can observe that the compact mixed integer linear programs (ROS-C$^{\mathcal{S}}$) and (ABCG-C$^{\mathcal{S}}$) differ only by the penalty coefficient in their objective functions. As proved in Proposition 11, these coefficients are identical when the quadratization scheme is disjoint. This observation is recorded in the following statement.

Corollary 17. *When $\beta_M(E) = |a_M|$ for all $M \in \mathcal{M}$, $E \in \mathcal{E}_M$, problems (ROS-C$^{\mathcal{S}}$) and (ABCG-C$^{\mathcal{S}}$) are identical. This happens in particular when the quadratization scheme $\mathcal{S}$ is disjoint.*

As a conclusion of this section, we can assert that the linearized forms of (ROS$^{\mathcal{S}}$) and (ABCG$^{\mathcal{S}}$) are weaker than (FOR$^{\mathcal{S}}$), in terms of quality of the bounds they deliver. In fact, an important difference between the quadratic reformulation (FOR$^{\mathcal{S}}$) and the penalized quadratic programs (ROS$^{\mathcal{S}}$) and (ABCG$^{\mathcal{S}}$) is that in (FOR$^{\mathcal{S}}$), due to Constraints (10)-(11), the equivalence with (P) holds at each binary point, while for problems (ROS$^{\mathcal{S}}$) and (ABCG$^{\mathcal{S}}$), it only holds at the optimum. For the latter two formulations, the link between the variables z_E and the products $z_{l_M(E)}z_{r_M(E)}$ is somehow lost. (If we reestablish this relation by imposing the equality $z_E = z_{l_M(E)}z_{r_M(E)}$ in their linearized versions, then the penalties vanish in (ROS-C$^{\mathcal{S}}$) and (ABCG-C$^{\mathcal{S}}$), which both simply reduce to (FOR-L$^{\mathcal{S}}$).)

5.2 Quadratic convex reformulations

In this section, we apply convexification techniques to the quadratic formulations (FOR$^{\mathcal{S}}$), (ROS$^{\mathcal{S}}$) and (ABCG$^{\mathcal{S}}$) described in Section 4. The general idea is to replace the functions $g(z)$, $g^R(z)$ and $g^A(z)$ by equivalent quadratic convex functions. This provides an alternative approach to the linearization step described in Section 5.1.

For simplicity, we detail the method for problem (FOR$^{\mathcal{S}}$). As $z^2 = z$ when z is binary, the function $g(z)$ can be considered as a pure quadratic form. From now, we write its Hessian matrix representation as

$$g(z) = \frac{1}{2} z^T Q z$$

where Q is a symmetric matrix of order N.

One common method to get a quadratic convex reformulation of (FOR$^{\mathcal{S}}$) is then to use λ_{min}, that is, the smallest eigenvalue of Q, and to replace $g(z)$ by

$$g_{\lambda_{min}}(z) \triangleq \frac{1}{2}\left(z^T Q z - \lambda_{min} \sum_{E \in \mathcal{E}} (z_E^2 - z_E)\right).$$

The equality $g(z) = g_{\lambda_{min}}(z)$ holds when each z_E is a binary variable. The Hessian matrix of this equivalent form of the objective function is $Q - \lambda_{min} I_N$, where I_N is the identity matrix of order N. Since $Q - \lambda_{min} I_N$ is positive semidefinite, the function $g_{\lambda_{min}}(z)$ is convex. Thus, the continuous relaxation of the reformulated problem is a convex quadratic problem which can be solved by branch-and-bound. Different improvements of this basic convexification method are presented hereunder.

5.2.1 Convexification for quadratic problems: the QCR method

QCR is a quadratic convex reformulation method proposed by Billionnet and Elloumi [5]. It is an improvement of the smallest eigenvalue method based on two key ideas. First, it considers

a parameterized non-uniform diagonal convexification. Second, it uses semidefinite programming to determine the parameters that maximize the optimal value of the continuous relaxation of the resulting problem.

QCR method applied to (FOR$^{\mathcal{S}}$). We can rewrite (FOR$^{\mathcal{S}}$) as the following equivalent quadratic problem, parameterized by any vector $\alpha \in \mathbb{R}^N$:

$$(\texttt{FOR-Q}^{\mathcal{S}}_{\alpha}) \begin{cases} \min & g_\alpha(z) \triangleq g(z) + \displaystyle\sum_{E \in \mathcal{E} \cup [n]} \alpha_E (z_E^2 - z_E) \\ \text{s.t.} & (10) - (11) \\ & z \in \{0,1\}^N. \end{cases}$$

Here again, it is clear that $g_\alpha(z) = g(z)$ for any $z \in \{0,1\}^N$. Since there exist many values of the parameter vector $\alpha \in \mathbb{R}^N$ that make $g_\alpha(z)$ convex, we next try to determine a value of α that makes $g_\alpha(z)$ convex while maximizing the continuous relaxation value of (FOR-Q$^{\mathcal{S}}_{\alpha}$). For this purpose, we compute the dual optimal solution of the following semi-definite relaxation of (FOR$^{\mathcal{S}}$):

$$(SDP) \begin{cases} \min & g_L(z, Z) & & \\ \text{s.t.} & (10) - (11) & & \\ & Z_{E,E} - z_E = 0 & E \in \mathcal{E} \cup [n] & (34) \\ & \begin{pmatrix} 1 & z^T \\ z & Z \end{pmatrix} \succeq 0 & & (35) \\ & z \in \mathbb{R}^N,\ Z \in \mathbb{S}_N & & (36) \end{cases}$$

where $\mathbb{S}_N$ is the set of symmetric matrices of order N, and the Z variables are introduced in the same spirit as in the linear reformulations of Section 5.1 in order to replace the product of two z variables. Constraints (35) are the Shor relaxation of the equality $Z = zz^T$. It is proven in [5] that an optimal α^* can be deduced from the optimal dual variables associated to Constraints (34). The continuous relaxation of (FOR-Q$^{\mathcal{S}}_{\alpha^*}$) ((FOR-Q$*^{\mathcal{S}}$) for short) is a quadratic convex problem leading to the highest possible dual bound in this framework. It is also proven in [5] that it has the same optimal value as problem (SDP).

QCR method applied to (ROS$^{\mathcal{S}}$). We can similarly apply the QCR method to convexify problem (ROS$^{\mathcal{S}}$). The main difference with the previous case (beside the fact that the objective functions are different) is that (ROS$^{\mathcal{S}}$) is unconstrained. Therefore, Constraints (10)-(11) are not present, which means that (ROS$^{\mathcal{S}}$) is reformulated as the following problem:

$$(\texttt{ROS-Q}*^{\mathcal{S}}) \begin{cases} \min & g^R(z) + \displaystyle\sum_{E \in \mathcal{E} \cup [n]} \mu_E^* (z_E^2 - z_E) \\ \text{s.t.} & z \in \{0,1\}^N \end{cases}$$

where the optimal parameters μ_E^* are the optimal dual variables of Constraints (34) in the semidefinite program:

$$(SDP_R)\begin{cases}\min & g_{LR}(z,Z)\\ \text{s.t.} & (34)-(36).\end{cases}$$

QCR method applied to (ABCG$^{\mathcal{S}}$). Finally, the application of method QCR to (ABCG$^{\mathcal{S}}$) consists in solving the following quadratic convex problem:

$$(\texttt{ABCG-Q*}^{\mathcal{S}})\begin{cases}\min & g^A(z)+\sum\limits_{E\in\mathcal{E}\cup[n]}\nu_E^*(z_E^2-z_E)\\ \text{s.t.} & z\in\{0,1\}^N\end{cases}$$

where the optimal parameters ν_E^* are the optimal dual variables of Constraints (34) in the semidefinite program:

$$(SDP_A)\begin{cases}\min & g_{LA}(z,Z)\\ \text{s.t.} & (34)-(36).\end{cases}$$

5.2.2 Convexification for polynomial problems: the PQCR method

We now describe a more elaborate convex quadratic reformulation approach called PQCR [21], which is more specifically adapted to binary polynomial optimization problems and takes more deeply advantage of the specific quadratization scheme. This method has an initial step that can be viewed as yielding a quadratization scheme $\mathcal{S}$ together with the associated reformulation by the quadratic problem with linear constraints (FOR$^{\mathcal{S}}$). Next, it applies a convexification step to (FOR$^{\mathcal{S}}$), based on a stronger SDP relaxation than QCR. We next detail this convexification step, following the presentation given in [21].

We start by introducing three sets of quadratic forms that, in addition to the forms $z_E^2-z_E$, vanish on the feasible domain of (FOR$^{\mathcal{S}}$) (i.e., when z is binary and Constraints (10)-(11) are satisfied):

$$\begin{cases} z_E - z_{l_M(E)}z_{r_M(E)} = 0 & \forall E\in\mathcal{E},\forall M\in\mathcal{M}: E\in\mathcal{E}_M \quad (37)\\ z_{E_1} - z_{E_1}z_{E_2} = 0 & \forall E_1,E_2\in\mathcal{E}\cup[n]:\ E_2\subset E_1 \quad (38)\\ z_{E_1}z_{E_2} - z_{E_3}z_{E_4} = 0 & \forall E_1,..,E_4\in\mathcal{E}\cup[n]:\ E_1\cup E_2 = E_3\cup E_4. \quad (39)\end{cases}$$

With each of these equations, we associate a real scalar multiplier, say δ_E for Constraints (37), β_{E_1,E_2} for Constraints (38), and $\lambda_{E_1,E_2,E_3,E_4}$ for Constraints (39). We next add to $g_\alpha(z)$ the quadratic forms in (37)–(39) multiplied by their associated coefficient. This yields the following parameterized function:

$$g_{\alpha,\delta,\beta,\lambda}(z) \triangleq g_\alpha(z) + \sum_{\substack{E\in\mathcal{E},M\in\mathcal{M}:\\ E\in\mathcal{E}_M}}\delta_E^M(z_E - z_{l_M(E)}z_{r_M(E)}) + \sum_{\substack{E_1,E_2\in\mathcal{E}\cup[n]:\\ E_2\subset E_1}}\beta_{E_1,E_2}(z_{E_1}-z_{E_1}z_{E_2}) + \sum_{\substack{E_1,..,E_4\in\mathcal{E}\cup[n]:\\ E_1\cup E_2=E_3\cup E_4}}\lambda_{E_1,E_2,E_3,E_4}(z_{E_1}z_{E_2}-z_{E_3}z_{E_4}).$$

Function $g_{\alpha,\delta,\beta,\lambda}(z)$ has the same value as $g(z)$ for any binary z satisfying the standard inequalities (10)-(11). Moreover, there exist parameters α, β, δ and λ such that $g_{\alpha,\delta,\beta,\lambda}$ is a convex function (take, for instance, $\alpha = -\lambda_{min}$ and $\beta = \delta = \lambda = 0$).

Replacing g by this new objective function, we obtain the following family of convex mixed-integer quadratic equivalent formulations of ($\texttt{FOR}^{\mathcal{S}}$):

$$(\texttt{PQCR}^{\mathcal{S}}_{\alpha,\delta,\beta,\lambda}) \begin{cases} \min g_{\alpha,\delta,\beta,\lambda}(z) \\ \text{s.t.} \quad (10)-(11) \\ \qquad z \in \{0,1\}^N. \end{cases}$$

It is proved in [21, 38] that optimal parameters $(\alpha^*, \delta^*, \beta^*, \lambda^*)$ that make $g_{\alpha,\delta,\beta,\lambda}$ convex and maximize the continuous relaxation bound of ($\texttt{PQCR}^{\mathcal{S}}_{\alpha,\delta,\beta,\lambda}$) can be deduced from the dual solution of the following semidefinite program (SDP'):

$$(SDP') \begin{cases} \min \quad g_L(z,Z) & & \\ \text{s.t.} \quad (34)-(36) & & \\ \quad z_E - Z_{l_M(E),r_M(E)} = 0 & E \in \mathcal{E}, M \in \mathcal{M} : E \in \mathcal{E}_M & (40) \\ \quad z_{E_1} - Z_{E_1,E_2} = 0 & E_1, E_2 \in \mathcal{E} \cup [n] : \ E_2 \subset E_1 & (41) \\ \quad Z_{E_1,E_2} - Z_{E_3,E_4} = 0 & E_1,..,E_4 \in \mathcal{E} \cup [n] : \ E_1 \cup E_2 = E_3 \cup E_4 \ . & (42) \end{cases}$$

It is interesting to note that, as proved in [38], Constraints (10)-(11) become redundant when adding Constraints (40)-(42). However, (SDP') has many more constraints than (SDP). The optimal parameters $(\alpha^*, \delta^*, \beta^*, \lambda^*)$ can be obtained as optimal values of the dual variables respectively associated with Constraints (34), (40), (41), and (42). Here again the continuous relaxation bound of ($\texttt{PQCR}^{\mathcal{S}}_{\alpha^*,\delta^*,\beta^*,\lambda^*}$) (($\texttt{PQCR*}^{\mathcal{S}}$) for short) is as tight as the semidefinite programming bound.

6 Computational comparison of quadratization schemes

In this section, we compare the performance of different combinations of quadratization schemes, quadratic reformulations and convexification techniques in terms of CPU time and root node gap of the branch-and-bound algorithm on two families of instances of polynomial binary optimization problems like (P). More precisely, for the three steps of our solution methods, we consider four quadratization schemes to be described hereafter, the three quadratic reformulations introduced in Section 4, and the three convexification methods presented in Section 5. We also compare the different approaches with the standard linearization (SL) presented in Section 2. We summarize in Table 1 the methods that we have tested. We did not consider the PQCR convexification applied to penalty-based quadratic reformulations, as it only works if the linearization inequalities are explicitly added to the constraint set.

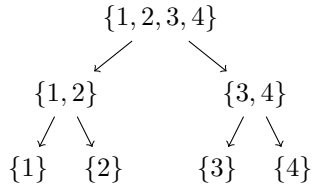
Quadratization Scheme $\mathcal{S}$	Quadratic reformulation	Convexification		
		Linearization	QCR	PQCR
-	-	(SL)	–	–
QA, QB, QC, QD	(FOR$^{\mathcal{S}}$)	(FOR-L$^{\mathcal{S}}$)	(FOR-Q*$^{\mathcal{S}}$)	(PQCR*$^{\mathcal{S}}$)
	(ROS$^{\mathcal{S}}$)	(ROS-L$^{\mathcal{S}}$) (ROS-C$^{\mathcal{S}}$)	(ROS-Q*$^{\mathcal{S}}$)	×
	(ABCG$^{\mathcal{S}}$)	(ABCG-L$^{\mathcal{S}}$) (ABCG-C$^{\mathcal{S}}$)	(ABCG-Q*$^{\mathcal{S}}$)	×

Table 1: Methods considered in our experiments with associated phases.

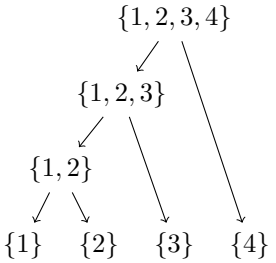
Let us now describe the four specific quadratization schemes that we consider. The case of monomials of degree 2 is trivial, so we focus on the longer ones.

- QA [21, 38] is a "lexicographic" quadratization scheme. To obtain it, we start by sorting the monomials in non increasing order of their degrees, and we sort the monomials of the same degree in lexicographic order. Then, in this order, iteratively: *(i)* Select the first product of variables x_ix_j that appears in the next monomial of degree at least 3. *(ii)* For any monomial M containing i and j, set $l_M(M) = \{i, j\}$ and $r_M(M) = M \setminus \{i, j\}$. *(iii)* Add $l_M(M)$ and $r_M(M)$ to the sorted monomial set.
- QB (Heuristic 2 in Chapter 7 of [45]) is similar to QA. The difference is that in step *(i)*, we first consider the products x_ix_j which appear most frequently in $f(x)$.
- QC: Recursively split any monomial $M = \{1, \dots, d\}$ with $d \geq 3$ into $l_M(M) = \{1, \dots, d-1\}$ and $r_M(M) = \{d\}$.
- QD: Recursively split any monomial $M = \{1, \dots, d\}$ with $d \geq 3$ into $l_M(M) = \{1, \dots, d-1\}$ and $r_M(M) = \{2, \dots, d\}$. This is our only quadratization scheme with non-disjoint subsets l_M and r_M.

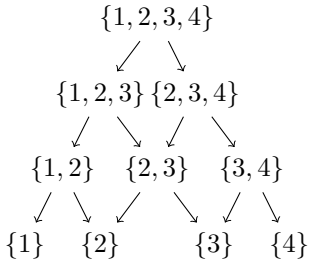
One can easily check that these quadratization schemes fulfill Definition 1. We illustrate them in Figure 4 for the monomial $x_1x_2x_3x_4$.



(a) Quadratization schemes `QA` and `QB`



(b) Quadratization scheme `QC`



(c) Quadratization scheme `QD`

Figure 4: Illustration of the quadratization schemes `QA`, `QB`, `QC`, `QD`

Experimental environment

Our experiments were carried out on a server with 2 CPU Intel Xeon each of them having 16 cores and 32 threads of 2.3 GHz and $8 * 16$ GB of RAM using a Linux operating system. For convexifications (`FOR-Q`$^{\mathcal{S}}_{\alpha^*}$), (`ROS-Q*`$^{\mathcal{S}}$), (`ABCG-Q*`$^{\mathcal{S}}$), we used the solver `Mosek` [42] to solve the semi-definite programs (SDP), (SDP_R), and (SDP_A). For algorithm `PQCR`, the quadratisation schemes considered in our experiments lead to a very large number of Constraints (42). This raises two experimental difficulties: generating all the Constraints (42) is very costly in CPU time, and in addition no standard solver is able to directly handle the resulting (SDP') problem. To overcome this difficulty, we solved (SDP') heuristically, and in particular we considered only the subset of Constraints (42) where at least one of E_1 or E_2, and one of E_3 or E_4 correspond to an original variable x_i. Then we used the solver `Mosek` together with the Conic Bundle library [32] to solve (SDP') heuristically within a lagrangian duality framework as described in [6]. Finally, to solve the convex (linear or quadratic) reformulations, we used the solver `Gurobi` [43]. We set the total time limit to 3 hours.

6.1 The *Low Auto-correlation Binary Sequence* problem

The first class of instances that we consider is associated with the *Low Auto-correlation Binary Sequence* problem. The problem is to find binary sequences with low off-peak auto-correlations. It has various practical applications in communication engineering or theoretical physics [4]. More formally, let $B = (b_1, \ldots, b_n)$ be a sequence with $b_i \in \{-1, 1\}$, and for a given $k = 1, \ldots, n-1$,

define the auto-correlation

$$C_k(B) = \sum_{i=1}^{n-k} b_i b_{i+k}.$$

Given two integers n_0 and n, with $n_0 \leq n$ the problem is to find a sequence B of length n that minimizes the degree-4 polynomial

$$E_{n_0}(B) = \sum_{k=1}^{n_0-1} C_k^2(B).$$

In order to apply our methods, we convert the variables from $\{-1, 1\}$ to $\{0, 1\}$ using the standard transformation $x = \frac{b+1}{2}$. The problem admits a lot of symmetries. In particular the correlations C_k are identical for a sequence B and its complement. We exploit this symmetry by fixing to 0 the variable that appears the most.

We present in Table 2 the characteristics of the considered instances, where each instance is labeled `b.n.`$\mathtt{n_0}$ (column *Instance*) and $|\mathcal{M}|$ is the number of monomial of the objective function. These instances were introduced by [39] and can be found on the MINLPLib [40] website. For each quadratization (`QA`, `QB`, `QC`, and `QD`), we display $|\mathcal{E}|$, the number of auxiliary variables, and $|(SDP')|$, the number of constraints that we incorporated in (SDP') in method `PQCR`. As mentioned above, $|(SDP')|$ only accounts for a subset of Constraints (42), which means that the root node gap of `PQCR` could in principle be significantly improved by generating more constraints. As an illustration, the real number of constraints of (SDP') for instance `b.25.6` is 1525 for `QA`, 1071 for `QB`, 41944, for `QC`, and 53595 for `QD`.

We can observe in Table 2 that the number of intermediate monomials appearing in the quadratization schemes, namely, $|\mathcal{E}|$, is always smaller than the number of original monomials $|\mathcal{M}|$. This is particularly true for the quadratization schemes `QA` and `QB` which, for each original monomial of degree 4, only add auxiliary intermediate monomials of degree two. They therefore add at most $n(n-1)/2$ monomials, regardless of the number of original monomials. This also implies that the convexification methods of Table 1 (which all have $n+|\mathcal{E}|$ variables) will have a significantly smaller number of variables than the linearization methods (which use at least $|\mathcal{M}| + |\mathcal{E}|$ variables). The same observation holds for Table 3 in Section 6.2.

Instance	$\|\mathcal{M}\|$	$\|\mathcal{E}\|$				$\|(SDP')\|$			
		QA	QB	QC	QD	QA	QB	QC	QD
b.20.5	207	44	25	68	86	498	163	750	1034
b.20.10	833	103	118	245	320	2477	3152	5395	7966
b.20.15	1494	144	157	447	625	4652	5271	13603	22299
b.25.6	407	79	69	144	169	1187	873	2102	2619
b.25.13	1782	180	202	540	717	5900	7234	15942	24347
b.25.19	3040	240	258	934	1312	10088	11200	37170	61312
b.25.25	3677	264	294	1140	1665	12012	14136	50532	87621
b.30.4	223	51	33	73	76	433	189	631	658
b.30.8	926	143	141	324	401	3125	2923	6574	8997
b.30.15	2944	265	299	924	1228	10497	13009	32702	50120
b.35.4	263	61	38	88	91	523	214	766	793
b.35.9	1381	198	197	493	616	5064	4819	11423	15928
b.40.5	447	104	45	168	206	1278	263	1970	2634
b.45.5	507	119	50	193	236	1473	288	2275	3034
b.50.6	882	179	144	344	394	2887	1848	5302	6444
b.55.6	977	199	159	384	439	3227	2043	5942	7209
b.60.8	2036	323	291	774	941	7625	6073	16684	22437

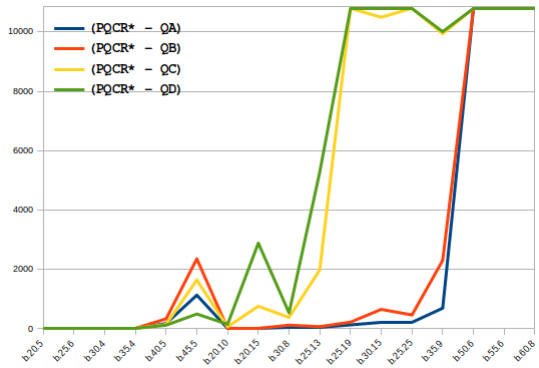
Table 2: Characteristics of the auto-correlation instances

We present in Figures 5-7 a comparison of the CPU times and of the initial gaps observed for the auto-correlation instances. In Figures 5 and 6, for a given quadratic reformulation and a given convexification, we compare the quadratization schemes (QA, QB, QC, and QD). (We do not report the results for methods (ROS-Q$*^{\mathcal{S}}$) and (ABCG-Q$*^{\mathcal{S}}$), since they solve only one instance out of 17 within the time limit.) The x-axis represents the instances and the y-axis the CPU times in seconds or the initial gaps $= 100 * \frac{|\text{LB}-\text{S}|}{\text{S}}$, with LB the continuous relaxation value of the method, and S the value of the best known solution. Note that the scale of the vertical axis for the initial gap differs significantly from figure to figure.

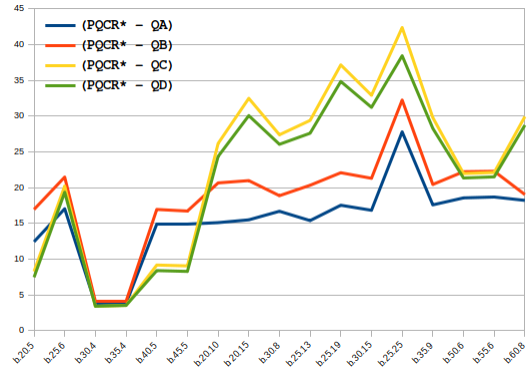
We observe that the CPU times (Figures 5a and 5c resp.) and the initial gaps (Figures 5b and 5d resp.) of the convexification methods based on quadratic convex reformulation ((PQCR$*^{\mathcal{S}}$) and (FOR-Q$*^{\mathcal{S}}$) resp.) are impacted by the choice of the quadratization. Note that the solution time of (SDP') is included in the total time, and is on average about 25 seconds for QA and QB, 500 for QC, and 1450 for QD. On the other side, the impact of the quadratization scheme on the linearization methods is much smaller. It barely affects the CPU time, as shown in Figures 6a and 6c. For (FOR-L$^{\mathcal{S}}$), the initial gap is very large but quite stable, and even identical for the quadratizations QA, QC, and QD. For (ROS-C$^{\mathcal{S}}$), however, the choice of the quadratization has a real impact on the initial gaps, with a factor of about 2 between the gaps of the quadratization schemes QC and QD.

The quadratization scheme that is globally most efficient, irrespective of the methods, is QA. For this reason, we compare the performance of the different methods when QA is applied; see Figure 7. More precisely, we compare the CPU time (Figure 7a) and the initial gaps (Figure 7b) for the three best performing methods: (PQCR$*^{\text{QA}}$), (ROS-C$^{\text{QA}}$) and (FOR-L$^{\text{QA}}$) with the performance of the standard linearization (SL). We observe that (PQCR$*^{\text{QA}}$) outperforms the other methods in terms of both CPU time and initial gaps. The linearizations (FOR-L$^{\text{QA}}$) and (ROS-C$^{\text{QA}}$) have about the same CPU times, while the initial gaps with (FOR-L$^{\text{QA}}$) are almost twice as small as those with (ROS-C$^{\text{QA}}$).

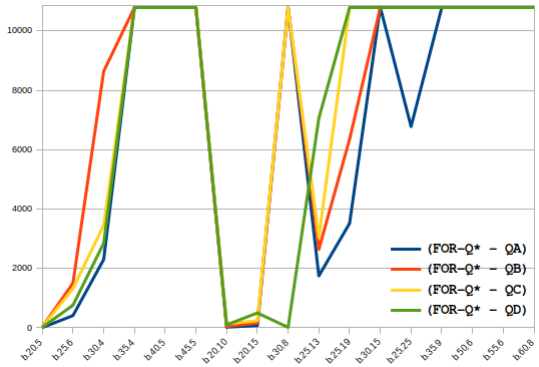
Finally, for the standard linearization (SL), we observe that despite an initial gap comparable to that of (FOR-L^{QA}), it is the slowest formulation. Figure 7d displays a comparison of the initial gaps of all the considered methods; we observe that the quadratic reformulation and convexification steps have a clear impact on these gaps. Finally, Figure 7c illustrates the improvement in computing time brought by the compact linearization (ROS-C^{QA}) when compared to the linearization (ROS-L^{QA}) (which is identical to (ABCG-L^{QA})). We observe that it performs comparably to the linearization (FOR-L^{QA}).



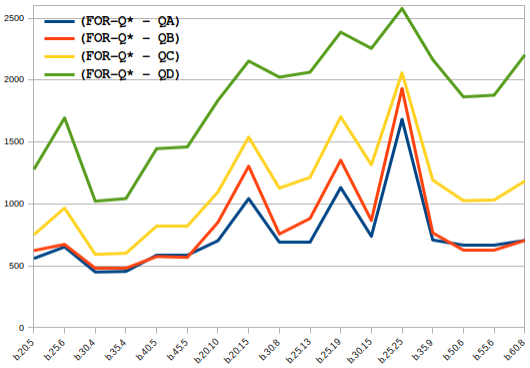
(a) CPU times: (PQCR*$^{\mathcal{S}}$) with QA, QB, QC and QD



(b) Initial gaps: (PQCR*$^{\mathcal{S}}$) with QA, QB, QC and QD

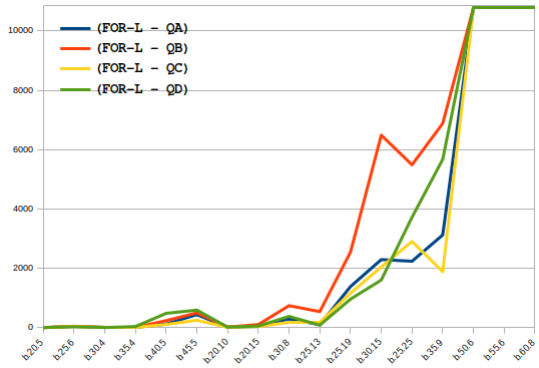


(c) CPU times: (FOR-Q*$^{\mathcal{S}}$) with QA, QB, QC and QD

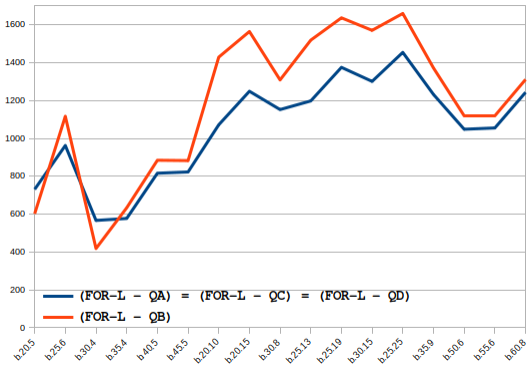


(d) Initial gaps: (FOR-Q*$^{\mathcal{S}}$) with QA, QB, QC and QD

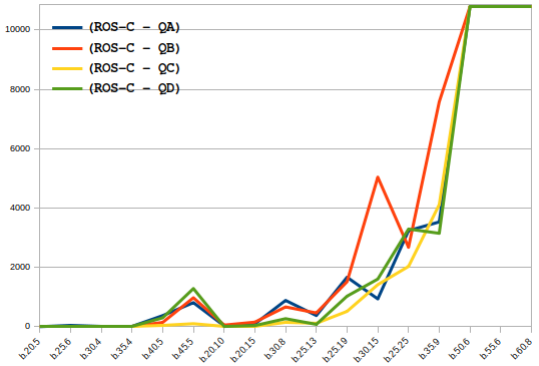
Figure 5: Auto-correlation: CPU times and initial gaps for QCR and PQCR applied to (FOR$^{\mathcal{S}}$).



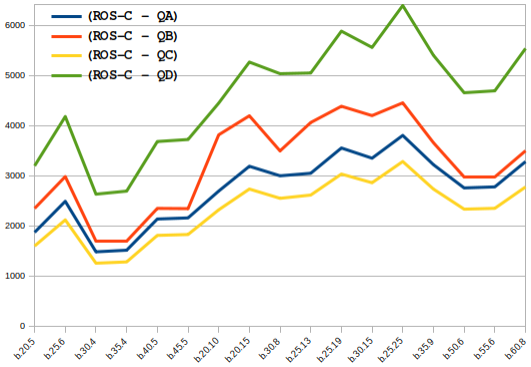
(a) CPU times: (FOR-L$^{\mathcal{S}}$) with QA, QB, QC and QD



(b) Initial gaps: (FOR-L$^{\mathcal{S}}$) with QA, QB, QC and QD

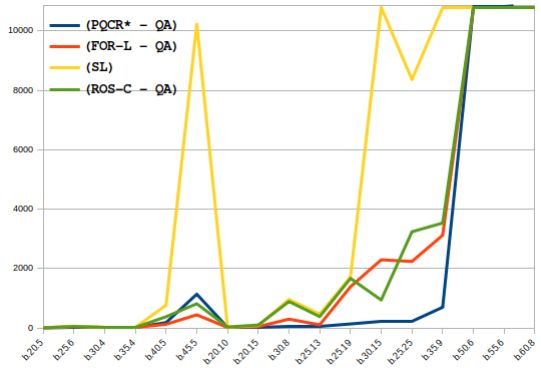


(c) CPU times: (ROS-C$^{\mathcal{S}}$) with QA, QB, QC and QD

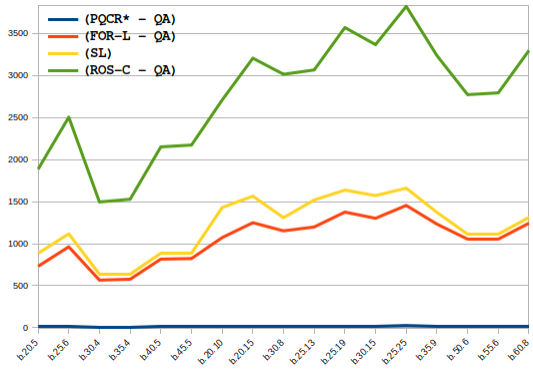


(d) Initial gaps: (ROS-C$^{\mathcal{S}}$) with QA, QB, QC and QD

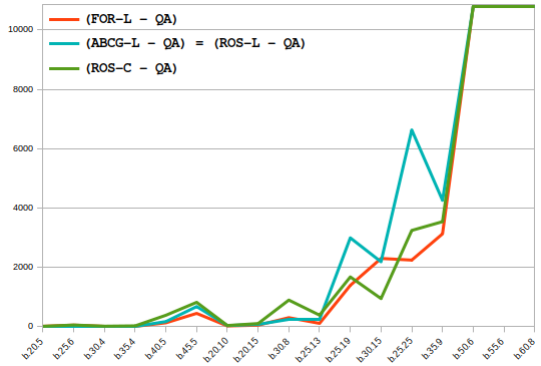
Figure 6: Auto correlation: CPU times and initial gaps for the linearizations.



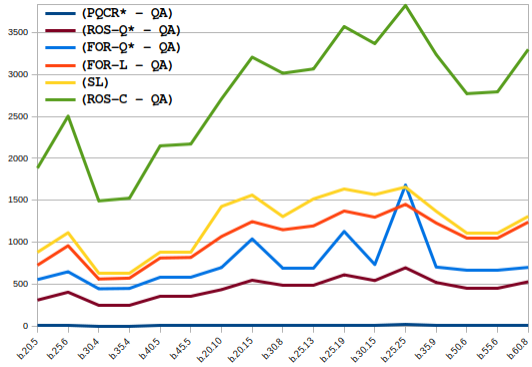
(a) CPU times: best performing methods with `QA`



(b) Initial gaps: best performing methods with `QA`



(c) CPU times for linearizations with `QA`



(d) Initial gaps for all methods with `QA`

Figure 7: Auto-correlation: CPU times and initial gaps with quadratization scheme `QA`

6.2 The image restoration problem

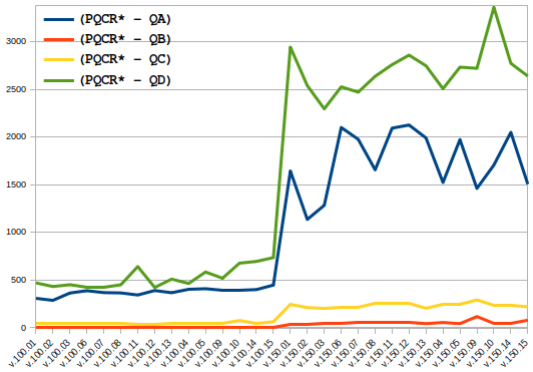
A second set of instances stems from the *image restoration* problem [8, 25, 34, 35]. The goal is here to reconstruct an original sharp base image from a blurred image. An image is a rectangle containing $n = l \times h$ (black or white) pixels. This rectangle is modeled as a binary matrix of the same dimension. The problem can be written as the minimization of a degree-4 polynomial of binary variables where each variable represents a pixel. The coefficients of the monomials are indicative of how likely a configuration is to appear in the sharp base image. The size of the considered instances is $l \times h = 10 \times 10$ and $l \times h = 10 \times 15$, or in the polynomial formulation $n = 100$ and 150, with a number of monomials equal to $|\mathcal{M}| = 668$ and 1033, respectively. In our experiments, 15 instances of each size are considered, for a total of 30 instances. Note that the 15 instances of the same size have identical monomials with different coefficients. The name of each image restoration instance describes its characteristics `v.n.r`: `n` is the number of binary variables and `r` is the index of the instance with the same characteristics. We report in Table 3 the number of auxiliary variables $|\mathcal{E}|$, and $|(SDP')|$, the number of constraints of (SDP') considered for these instances. Here again, we only generate a subset of Constraints (42). These instances have a larger number of initial variables, but are much sparser than the low auto-correlation instances.

instance	$\|\mathcal{M}\|$	$\|\mathcal{E}\|$				$\|(SDP')\|$			
		QA	QB	QC	QD	QA	QB	QC	QD
v.100.r	668	252	159	324	423	2990	1317	3446	4687
v.150.r	1033	392	249	504	653	4730	2097	5436	7317

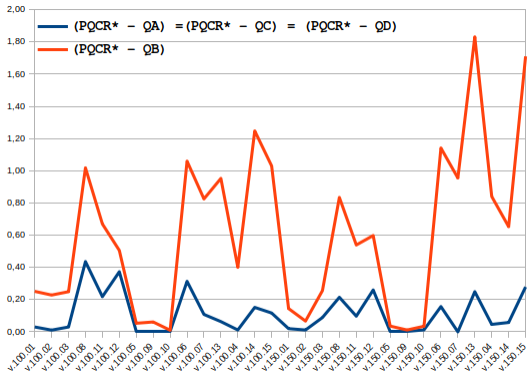
Table 3: Characteristics of the image restoration instances

We present the same graphs as in Section 6.1 (Figures 8 to 9), comparing the CPU times and initial gaps of the different combinations of the quadratization schemes, quadratic reformulations and convexifications. We only report the detailed results of the best performing methods (PQCR*$^{\mathcal{S}}$), (FOR-L$^{\mathcal{S}}$) and (ROS-C$^{\mathcal{S}}$). In particular methods (FOR-Q*$^{\mathcal{S}}$), (ROS-Q*$^{\mathcal{S}}$), and (ABCG-Q*$^{\mathcal{S}}$) were not able to solve any of the 30 instances within the time limit of 3 hours. We observe that the quadratization scheme has only a limited impact on the CPU times of (FOR-L$^{\mathcal{S}}$) (Figure 8c) and (ROS-C$^{\mathcal{S}}$) (Figure 8e), while its choice strongly affects the CPU times of (PQCR*$^{\mathcal{S}}$) (Figure 8a). Indeed, the total CPU time of (PQCR*$^{\mathcal{S}}$) goes on average from about 1600 seconds for QD to 32 seconds for QB, and the CPU time of (FOR-L$^{\mathcal{S}}$) ((ROS-C$^{\mathcal{S}}$) resp.) goes from 5 seconds for QA (5 seconds for QB and QC resp.) to 21 seconds for QD (26 seconds for QA resp.). On these sparse instances, the quadratization scheme QB, which has the smallest number of auxiliary variables, is the best scheme for (PQCR*$^{\mathcal{S}}$). Note that most of the CPU time of (PQCR*$^{\mathcal{S}}$) is used to solve (SDP') since the average CPU time for the branch-and-bound is 5 seconds for QB within an average total CPU time of 32 seconds. Concerning the initials gaps, we observe that (PQCR*$^{\mathcal{S}}$) (Figure 8b) always has an initial gap lower than 2%, for all quadratization schemes, whereas (FOR-L$^{\mathcal{S}}$) (Figure 8d) and (ROS-C$^{\mathcal{S}}$) (Figure 8f) always have gaps higher than 175%. Moreover, for (PQCR*$^{\mathcal{S}}$) the initial gaps are identical for the quadratization schemes QA, QC and QD; this is also the case for (FOR-L$^{\mathcal{S}}$) with the quadratization schemes QA and QB.

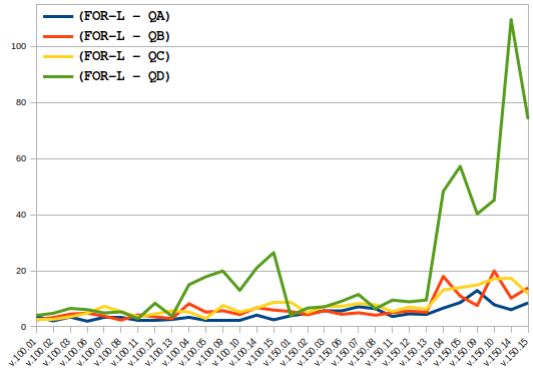
The quadratization scheme that is most efficient globally on all the methods is QB, we therefore compare in Figure 9 the performance of different methods when QB is selected. As in Section 6.1, we compare the CPU time (Figure 9a) and the initial gaps (Figure 9b) for the three best performing methods: (PQCR*$^{\text{QB}}$), (ROS-C$^{\text{QB}}$) and (FOR-L$^{\text{QB}}$) with the performance of the standard linearization (SL). We observe that (ROS-C$^{\text{QB}}$) and (FOR-L$^{\text{QB}}$) outperform (PQCR*$^{\text{QB}}$) and (SL) in terms of CPU times, in spite of the fact that (PQCR*$^{\text{QB}}$) has a significant smaller initial gap than the other methods. Finally, for the standard linearization (SL), we observe that despite an initial gap comparable to that of (FOR-L$^{\text{QB}}$), it is the slower method. Then, we present in Figure 9d a comparison of the initial gaps of all the considered methods and we observe that the quadratic reformulation and convexification steps have a clear impact on these gaps. Finally, we present in Figure 9c an illustration of the improvement in computing time obtained with the compact linearization (ROS-C$^{\text{QB}}$) when compared with the reformulation (ROS$^{\text{QB}}$) (which is identical to (ABCG$^{\text{QB}}$) for the scheme QB). We observe that the new linearization is slightly faster on average.



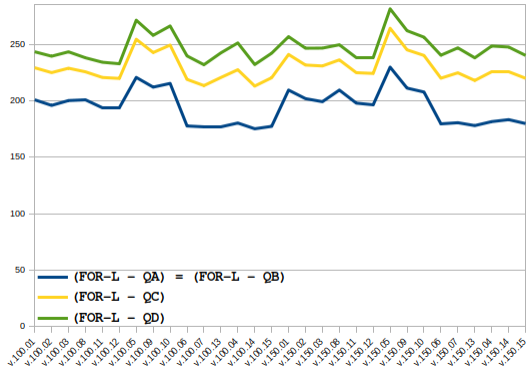
(a) CPU times: (PQCR*$^{\mathcal{S}}$) with QA, QB, QC and QD



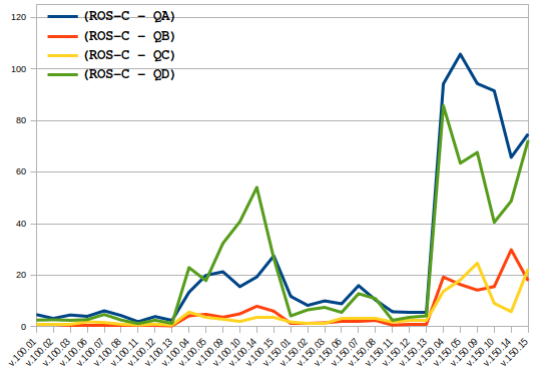
(b) Initial gaps: (PQCR*$^{\mathcal{S}}$) with QA, QB, QC and QD



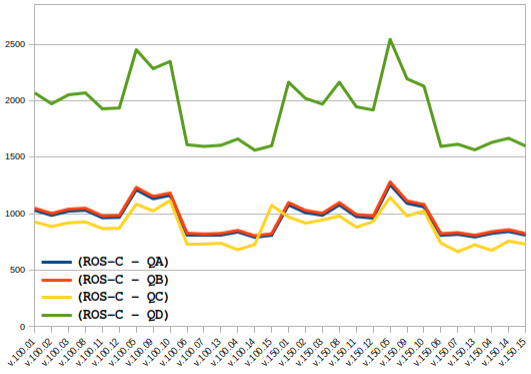
(c) CPU times: (FOR-L$^{\mathcal{S}}$) with QA, QB, QC and QD



(d) Initial gaps: (FOR-L$^{\mathcal{S}}$) with QA, QB, QC and QD



(e) CPU times: (ROS-C$^{\mathcal{S}}$) with QA, QB, QC and QD



(f) Initial gaps: (ROS-C$^{\mathcal{S}}$) with QA, QB, QC and QD

Figure 8: Image restoration instances: CPU time and initial gaps comparison of the quadratizations QA, QB, QC and QD. Time limit: 10800 seconds.

(a) CPU times: best performing methods with `QB`

(b) Initial gaps for all methods with `QB`

(c) CPU times for linearizations with `QB`

(d) All methods : Initial gap for `QB`

Figure 9: Image restoration: CPU times and initial gaps with quadratization scheme `QB`

7 Conclusion

In this paper, we have examined a generic framework for the exact solution of the polynomial unconstrained binary programming problem. The framework consists of three phases: the first one determines a *quadratization scheme* of the polynomial which is used, in a second phase, to produce a *quadratic reformulation* of the initial problem. The resulting quadratic problem is in general non-convex. The third phase of the solution process is the *convexification* of the quadratic reformulation. For each phase, we present several possible approaches that we compare from the theoretical point of view and that we relate to the literature. In particular, we present in a unified way various concepts that were previously introduced independently of each other, and we explicitly show which quadratic reformulations can be meaningfully combined with existing convexification methods.

We illustrate our findings through a set of computational experiments. Our numerical results clearly demonstrate that the choice of the quadratization scheme, of the quadratic reformulation step and of the convexification method should not be made arbitrarily and independently of each other. In particular, in our experiments, the smaller quadratization schemes `QA` and `QB` rather

consistently outperformed the denser schemes QC and QD in terms of CPU time. Regarding the quadratic reformulation methods, the constraint-based approaches proved more robust than the penalty approaches. Finally, for the convexification methods, QCR struggled and was never competitive, neither in terms of gap nor in terms of CPU time, whereas PQCR was best able to reduce the duality gap and to provide a tight reformulation. However, this small gap came at the cost of long computing times, mostly spent in setting up the large-size reformulation. For the (relatively easy) image restoration instances, this time was prohibitively large, so that the reduction of the gap and the associated tighter relaxation were not sufficient to make PQCR really competitive: it was generally outperformed by simpler, more primitive methods like (FOR-L$^{\mathcal{S}}$) or (ROS-C$^{\mathcal{S}}$) or, in spite of their much larger initial gap.

In summary, we conclude that within the three-phase framework for polynomial unconstrained binary optimization, the performance of a global solution method depends very much on the combination of its constituting elements, as well as on the features of the instances to be solved. The combined method should always be designed accordingly. In particular, for sparse instances, applying linearization methods that do not require expensive pre-processing and whose size remains moderate is probably a wise choice. On the other hand, for very dense instances, the size of linearizations increases drastically, and thus convexifications that are very stable in both size and gap are likely to perform more efficiently.

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