Compact Linearization for Binary Quadratic Programs Comprising Linear Constraints

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Abstract

In this paper, the compact linearization approach originally proposed for binary quadratic programs with assignment constraints is generalized to such programs with arbitrary linear equations and inequalities that have positive coefficients and right hand sides. Quadratic constraints may exist in addition, and the technique may as well be applied if these impose the only nonlinearities, i.e., the objective function is linear. We present special cases of linear constraints (along with prominent combinatorial optimization problems where these occur) such that the associated compact linearization yields a linear programming relaxation that is provably as least as strong as the one obtained with a classical linearization method. Moreover, we show how to compute a compact linearization automatically which might be used, e.g., by general-purpose mixed-integer programming solvers.

1 Introduction

In this paper, we consider a class of binary quadratic programs (BQPs) that comprise a set of linear equations with positive coefficients and right hand sides. More formally, we study mixed-integer non-linear programs, that can (after applying some method of linearization to realize the identities (4)) be stated in the following general form that covers several NP-hard combinatorial optimization problems including, e.g., the quadratic assignment problem and the quadratic traveling salesman problem:

$$
\begin{aligned}
\min\ & c^T x + d^T y && && \\
\text{s.t.}\ & Cx + Dy && \geq e && && (1)\\
& \sum_{i \in A_k} \alpha_i^k x_i && = \beta^k && \text{for all } k \in K_E && (2)\\
& \sum_{i \in A_k} \alpha_i^k x_i && \leq \beta^k && \text{for all } k \in K_I && (3)\\
& y_{ij} && = x_i x_j && \text{for all } (i,j) \in P && (4)\\
& x_i && \in \{0,1\} && \text{for all } i \in N &&
\end{aligned}
$$

Here, the set of original binary variables x in the BQP is indexed by a set $N = \{1,\dots,n\}$ where $n \in \mathbb{N}^{>0}$. Without loss of generality, we assume all bilinear terms $x_i x_j$ to be collected in an ordered set $P \subset N \times N$ such that $i \leq j$ for each $(i, j) \in P$. These are permitted to occur in the objective function as well as in the set of constraints, i.e., there may be an arbitrary set of $m \geq 0$ equations or inequalities that can be brought into the form (1) after linearization and where $C \in \mathbb{R}^{m\times n}$ and $D \in \mathbb{R}^{m\times|P|}$. Apart from these, the BQP shall comprise a nonempty collection $K := K_E \cup K_I$ of linear equations (2) and linear inequalities (3), where, for each $k \in K$, A_k is an index set specifying the binary variables on the left hand side, $\alpha_i^k \in \mathbb{R}^{>0}$ for all $i \in A_k$, and $\beta^k \in \mathbb{R}^{>0}$. The central subject of this paper is a specialized and compact technique to implement the relations (4) for this particular type of a BQP. In this context, 'compact' means that the approach typically involves the addition of significantly less constraints to the problem formulation compared to the well-known and widely applied linearization method by Glover and Woolsey (1974) where relations (4) are implemented using a variable $y_{ij} \in [0,1]$ and three constraints:

$$y_{ij} \leq x_i \tag{5}$$

$$y_{ij} \leq x_j \tag{6}$$

$$y_{ij} \geq x_i + x_j - 1 \tag{7}$$

The only prerequisite to apply the technique being the subject of this paper is that, for each product $x_i x_j$, there need to exist indices $k, \ell \in K$ such that $i \in A_k$ and $j \in A_\ell$, i.e., for each variable being part of a bilinear term, there must be some linear equation (2) or inequality (3) involving it. It is however soft in the sense that single products not adhering to this requirement do not affect a consistent linearization of those that do, and these could still be linearized using, e.g., the method just described. Moreover, if the prerequisite is satisfied already by considering only the present equations K_E, inequalities K_I, or a subset of them, then it might be attractive to apply the technique only to these in order to obtain a strong continuous relaxation. Originally, the technique was proposed by Liberti (2007) and revised by Mallach (2017) for the case where the only equations (2) considered are assignment (or rather 'single selection') constraints, i.e., where for all $k \in K_E$ one has $\beta^k = 1$ and $a_i^k = 1$ for all $i \in A_k$.

In this paper, we show that the underlying methodology of the compact linearization technique can be generalized to BQPs of the form displayed above. We then investigate under which circumstances the linear programming relaxation of the obtained formulation is provably as least as strong as when using the linearization by Glover and Woolsey (1974). Moreover, we highlight some prominent combinatorial optimization problems where previously found mixed-integer programming formulations appear now as particular compact linearizations. Last but not least, we show how these can be computed automatically, e.g., as part of a general-purpose mixed-integer programming solver.

2 Related Linearization Methods for BQPs

Since linearizations of quadratic and, more generally, polynomial programming problems, enable the application of well-studied mixed-integer linear programming techniques, they have been an active field of research since the 1960s. The seminal idea to model binary conjunctions using additional (binary) variables and inequalities (7) combined with the inequalities $x_i + x_j - 2y_{ij} \geq 0$ is attributed to Fortet (1959, 1960), and discussed in several succeeding books and papers, e.g. by Balas (1964), Zangwill (1965), Watters (1967), Hammer and Rudeanu (1968), and by Glover and Woolsey (1973). Shortly thereafter, Glover and Woolsey (1974) found that an explicit integrality requirement on y_{ij} becomes obsolete when replacing the mentioned inequality with (5) and (6). This method, that is henceforth referred to as the 'Glover-Woolsey linearization', is until today regarded as 'the standard linearization technique'. Together with $y_{ij} \geq 0$, the Glover-Woolsey linearization appears as a special case of the convex envelopes for general nonlinear programming problems as proposed by McCormick (1976). Moreover, Padberg (1989) proved the corresponding four inequalities to be facet-defining for the polytope associated to unconstrained binary quadratic optimization problems:

$$QP^n = conv\{(x,y) \in \mathbb{R}^n \times \mathbb{R}^{n(n-1)/2} \mid x \in \{0,1\}^n,\ y_{ij} = x_i x_j \text{ for all } 1 \leq i < j \leq n\}$$

While the Glover-Woolsey linearization is always applicable, its inequalities do not couple related linearization variables (i.e., such sharing a common factor) if these are present. Depending on the concrete problem to be solved, this may result in rather weak linear programming relaxations. Refined techniques are however (almost) exclusively available for BQPs with no or only linear constraints. This is true, e.g., for the posiform-based techniques by Hansen and Meyer (2009), the 'Clique-Edge Linearization' by Gueye and Michelon (2009), the 'Extended Linear Formulation' by Furini and Traversi (2013), as well as earlier ones by Glover (1975), Oral and Kettani (1992a,b), Chaovalitwongse et al. (2004), and Sherali and Smith (2007). An exception is the well-known transformation between unconstrained binary quadratic optimization and the maximum cut problem (cf. Hammer (1965); De Simone (1990)) that, in principle, also allows for the translation of a (possibly quadratic) constraint set. The only other general methodology to convert quadratically constrained BQPs into mixed-integer linear programs is, to the best of our knowledge, the reformulation-linearization technique (RLT) by Adams and Sherali (1999).

The compact linearization technique can be interpreted as a particular and usually incomplete (or 'sparse') first level application of the RLT, and establishes a practical and general approach to linearize an important and rich subclass of BQPs.

3 Compact Linearization

The compact linearization approach for binary quadratic problems with linear constraints is as follows. With each linear equation of type (2), i.e., with its index set A_k, we associate a corresponding index set $B_k^E \subseteq N$, and with each linear inequality of type (3), we associate two such index sets $B_k^{I+} \subseteq N$ and $B_k^{I-} \subseteq N$. For ease of subsequent reference, let $B_k := B_k^E$ if $k \in K_E$, $B_k := B_k^{I+} \cup B_k^{I-}$ if $k \in K_I$, and $B := \bigcup_{k \in K} B_k$. For each $j \in B_k^E \cup B_k^{I+}$, we then multiply the respective equation or inequality by x_j, and for each $j \in B_k^{I-}$, we multiply the respective inequality by $1 - x_j$. We thus obtain the new constraints:

$$\sum_{i \in A_k} \alpha_i^k x_i x_j = \beta^k x_j \qquad \text{for all } j \in B_k^E, \text{ for all } k \in K_E \tag{8}$$

$$\sum_{i \in A_k} \alpha_i^k x_i x_j \leq \beta^k x_j \qquad \text{for all } j \in B_k^{I+}, \text{ for all } k \in K_I \tag{9}$$

$$\sum_{i \in A_k} \alpha_i^k x_i (1 - x_j) \leq \beta^k (1 - x_j) \qquad \text{for all } j \in B_k^{I-}, \text{ for all } k \in K_I \tag{10}$$

Each product $x_i x_j$ induced by any of these new equations or inequalities is then replaced by a continuous linearization variable y_{ij} (if $i \leq j$) or y_{ji} (otherwise). We denote the set of bilinear terms created this way with

$$Q = \{(i,j) \mid i \leq j \text{ and } \exists k \in K : i \in A_k \text{ and } j \in B_k, \text{ or } j \in A_k \text{ and } i \in B_k\}.$$

Rewriting (8)–(10) using Q, we obtain the linearization constraints:

$$\sum_{i \in A_k, (i,j) \in Q} \alpha_i^k y_{ij} + \sum_{i \in A_k, (j,i) \in Q} \alpha_i^k y_{ji} = \beta^k x_j \qquad \text{for all } j \in B_k^E, \text{ for all } k \in K_E \tag{11}$$

$$\sum_{i \in A_k, (i,j) \in Q} \alpha_i^k y_{ij} + \sum_{i \in A_k, (j,i) \in Q} \alpha_i^k y_{ji} \leq \beta^k x_j \qquad \text{for all } j \in B_k^{I+}, \text{ for all } k \in K_I \tag{12}$$

$$\sum_{i \in A_k, (i,j) \in Q} \alpha_i^k (x_i - y_{ij}) + \sum_{i \in A_k, (j,i) \in Q} \alpha_i^k (x_i - y_{ji}) \leq \beta^k (1 - x_j) \quad \text{for all } j \in B_k^{I-}, \text{ for all } k \in K_I \tag{13}$$

It is clear that the constraints (8)–(10) are valid for the original problem and so are thus as well the constraints (11)–(13) whenever the introduced linearization variables take on consistent values with respect to their two original counterparts, i.e., $y_{ij} = x_i x_j$ holds for all $(i,j) \in Q$. Since the original problem formulation comprises the bilinear terms defined by the set P, we need to choose the set B such that the induced set of variables Q will be equal to P or contain P as a subset. We will discuss how to determine such a set $Q \supseteq P$ in Sect. 5, but suppose for now that it is already at hand. We will show that a consistent linearization is obtained if and only if the following three conditions are satisfied:

Condition 1. *For each $(i,j) \in Q$, there is a $k \in K$ such that $i \in A_k$ and $j \in B_k^E \cup B_k^{I+}$.*

Condition 2. *For each $(i,j) \in Q$, there is an $\ell \in K$ such that $j \in A_\ell$ and $i \in B_\ell^E \cup B_\ell^{I+}$.*

Condition 3. *For each $(i,j) \in Q$, there is a $k \in K$ such that $i \in A_k$ and $j \in B_k^E \cup B_k^{I-}$* or *an $\ell \in K$ such that $j \in A_\ell$ and $i \in B_\ell^E \cup B_\ell^{I-}$.*

Importantly, $k = \ell$ is a valid choice for satisfying Conditions 1 and 2, and Condition 3 is implicitly satisfied whenever Condition 1 *or* Condition 2 is established using an equation. In particular, Condition 3 is obsolete if only linear equations (2) but no inequalities (3) are present in the program to be linearized.

Theorem 4. *For any integer solution $x \in \{0,1\}^n$, the linearization constraints (11)–(13) imply $y_{ij} = x_i x_j$ for all $(i,j) \in Q$ if and only if Conditions 1–3 are satisfied.*

Proof. Let $(i,j) \in Q$. By Condition 1, there is a $k \in K$ such that $i \in A_k$, $j \in B_k^E \cup B_k^{I+}$ and hence either the equation

$$\sum_{h \in A_k,(h,j)\in Q} \alpha_h^k y_{hj} + \sum_{h \in A_k,(j,h)\in Q} \alpha_h^k y_{jh} = \beta^k x_j \qquad (*_{Ej})$$

or the inequality

$$\sum_{h \in A_k,(h,j)\in Q} \alpha_h^k y_{hj} + \sum_{h \in A_k,(j,h)\in Q} \alpha_h^k y_{jh} \leq \beta^k x_j \qquad (*_{Ij+})$$

exists and has y_{ij} on its left hand side. Since $\alpha_h^k > 0$ for all $h \in A_k$ and $0 \leq y_{ij} \leq 1$, each of them establishes that $y_{ij} = 0$ whenever $x_j = 0$.

Similarly, by Condition 2, there is an $\ell \in K$ such that $j \in A_\ell$, $i \in B_\ell^E \cup B_\ell^{I+}$ and hence the equation

$$\sum_{h \in A_\ell,(h,i)\in Q} \alpha_h^\ell y_{hi} + \sum_{h \in A_\ell,(i,h)\in Q} \alpha_h^\ell y_{ih} = \beta^\ell x_i \qquad (*_{Ei})$$

or the inequality

$$\sum_{h \in A_\ell,(h,i)\in Q} \alpha_h^\ell y_{hi} + \sum_{h \in A_\ell,(i,h)\in Q} \alpha_h^\ell y_{ih} \leq \beta^\ell x_i \qquad (*_{Ii+})$$

exists and has y_{ij} on its left hand side. Since $\alpha_h^\ell > 0$ for all $h \in A_\ell$ and $0 \leq y_{ij} \leq 1$, each of them establishes that $y_{ij} = 0$ whenever $x_i = 0$.

Let now $x_i = x_j = 1$. By Condition 3, we either have at least one equation or at least one inequality relating y_{ij} to either x_i or x_j. Consider first the equation case, and suppose w.l.o.g. that equation $(*_{Ej})$ exists (the opposite case with $(*_{Ei})$ can be exploited analogously). If $y_{ij} = 1$, there is nothing to show, so suppose that $y_{ij} < 1$ which means that we are in the following situation:

$$\sum_{h \in A_k,(h,j)\in Q, h\neq i} \alpha_h^k y_{hj} + \sum_{h \in A_k,(j,h)\in Q, h\neq i} \alpha_h^k y_{jh} = \beta^k \underbrace{x_j}_{=1} - \alpha_i^k \underbrace{y_{ij}}_{<1} > \beta^k - \alpha_i^k \qquad (*'_{Ej})$$

At the same time, we also have $\sum_{h \in A_k, h \neq i} \alpha_h^k x_h = \beta^k - \alpha_i^k$ with $x_h \in \{0,1\}$. In order for the equation $(*_{Ej})$ to be satisfied, an additional amount of $(1 - y_{ij})\alpha_i^k > 0$ thus needs to be contributed by the other summands on the left hand side of $(*'_{Ej})$. This implies, however, that there must be some $h \in A_k$, $h \neq i$, such that $y_{hj} > 0$ (or $y_{jh} > 0$) while $x_h = 0$ – which is impossible since Conditions 1 and 2 are established for these variables as well.

Finally, we consider the inequality case and assume again w.l.o.g. that Condition 3 is satisfied by some $k \in K_I$ with $i \in A_k$ and $j \in B_k^{I-}$, i.e., such that the the inequality

$$\sum_{h \in A_k,(h,j)\in Q} \alpha_h^k (x_h - y_{hj}) + \sum_{h \in A_k,(j,h)\in Q} \alpha_h^k (x_h - y_{jh}) \leq \beta^k (1 - x_j) \qquad (*_{Ij-})$$

exists. Its right hand side now evaluates to zero since $x_j = 1$. Looking at the left hand side, for any $h \in A_k$ (including i) the terms $(x_h - y_{hj})$ respectively $(x_h - y_{jh})$ cannot be negative since y_{hj} (y_{jh}) must be zero if x_h is (by the arguments above) and cannot be larger than one if x_h is (by its upper bound). Moreover, since the right hand side is zero and $\alpha_h^k > 0$ for all $h \in A_k$, the terms cannot be positive as well. It follows that $x_h = y_{hj}$ for all $h \in A_k$ (including i) and thus $y_{ij} = 1$ as desired.

We have just shown the *sufficiency* of the equations induced by satisfying Conditions 1–3. Moreover, within a framework that constructs a linearization only by means of constraints of type (11)–(13), it is impossible to enforce $y_{ij} = 0$ if $x_i = 0$ other than by satisfying Condition 1, impossible to enforce $y_{ij} = 0$ if $x_j = 0$ other than by satisfying Condition 2, and no other way to ensure $y_{ij} = 1$ if both x_i and x_j are equal to one as well than by satisfying Condition 3, which implies their *necessity*. □

Theorem 4 establishes that Conditions 1–3 are the only relevant criteria for that inequalities (5)–(7) be implied for integer solutions $x \in \{0,1\}^n$ for a particular $(i,j) \in Q$ – allowing for the construction of 'compact' linearizations of a given demanded 'sparse' set of products $P \subseteq Q$ based on an arbitrary given linear constraint set. Known before from the RLT (cf. Adams and Sherali (1986)) has been the fact that inequalities (5)–(7) are implied for a *complete* P, i.e., $P = \{(i,j) \mid i,j \in N, i < j\}$ if a set of constraints comprising in total *all* x_i, $i \in N$, is multiplied by *all* these variables and, in case of inequalities, by their complements $(1 - x_i)$, which *obviously* satisfies Conditions 1–3.

4 LP Relaxation Strength of Compact Linearizations

While this is unfortunately not possible for the general case, we can prove that a compact linearization yields a linear programming relaxation that is as least as tight as the one obtained with the Glover-Woolsey linearization if the structure of the present linear constraints is more specific. In particular, the next two subsections together show that this is the case if Conditions 1–3 are satisfied based on a selection of 'assignment' and 'knapsack' constraints.

4.1 Compact Linearizations with Provably Strong LP Relaxations

4.1.1 Assignment or 'Single Selection' Equations

Let us first consider the case where the equations (2) are assignment (or rather 'single selection') constraints, i.e., $K = K_E$, $a_i^k = 1$ for all $i \in A_k$ and $\beta^k = 1$ for all $k \in K$. This was the application the compact linearization technique was originally proposed for by Liberti (2007). Later, Mallach (2017) clarified that a consistent linearization is obtained if and only if Conditions 1 and 2 are enforced. Accidentally, and in contrast to inequalities (5) and (6), the proof did not verify that inequalities (7) hold as well in case of fractional solutions $x \in [0,1]^n$. This is caught up on now by giving a complete proof of the following theorem.

Theorem 5. *Let $\beta^k = 1$ for all $k \in K$, and as well $a_i^k = 1$ for each $i \in A_k$, $k \in K$. Then for any solution $x \in [0,1]^n$, the inequalities $y_{ij} \leq x_i$, $y_{ij} \leq x_j$ and $y_{ij} \geq x_i + x_j - 1$ are implied by equations (11) for all $(i,j) \in Q$ if and only if Conditions 1 and 2 are satisfied.*

Proof. Let $(i,j) \in Q$. By Condition 1, there is a $k \in K_E$ such that $i \in A_k$, $j \in B_k^E$ and hence the equation

$$\sum_{h \in A_k, (h,j) \in Q} y_{hj} + \sum_{h \in A_k, (j,h) \in Q} y_{jh} = x_j \tag{14}$$

exists, has y_{ij} on its left hand side, and thus establishes $y_{ij} \leq x_j$.

Similarly, by Condition 2, there is an $\ell \in K_E$ such that $j \in A_\ell$, $i \in B^E_\ell$ and hence the equation

$$\sum_{h\in A_\ell,(h,i)\in Q} y_{hi} + \sum_{h\in A_\ell,(i,h)\in Q} y_{ih} = x_i \tag{15}$$

exists, has y_{ij} on its left hand side, and thus establishes $y_{ij} \le x_i$.

To show that $y_{ij} \ge x_i + x_j - 1$, consider equation (14) in combination with its original counterpart $\sum_{h\in A_k} x_h = 1$. For any y_{hj} (or y_{jh}) in (14), the Conditions 1 and 2 assure that there is an equation establishing $y_{hj} \le x_h$ ($y_{jh} \le x_h$). Thus we have

$$\sum_{h\in A_k,(h,j)\in Q,h\neq i} y_{hj} + \sum_{h\in A_k,(j,h)\in Q,h\neq i} y_{jh} \le \sum_{h\in A_k,h\neq i} x_h = 1 - x_i$$

Applying this upper bound within equation (14), we obtain:

$$y_{ij} + \underbrace{\sum_{h\in A_k,(h,j)\in Q,h\neq i} y_{hj} + \sum_{h\in A_k,(j,h)\in Q,h\neq i} y_{jh}}_{\le 1-x_i} = x_j \;\Leftrightarrow y_{ij} \ge x_i + x_j - 1$$

Finally, the necessity to satisfy Conditions 1 and 2 is given for the same reasons as mentioned after the proof of Theorem 4. □

Again, special cases of Theorem 5 where *all* present assignment constraints are multiplied by *all* variables x_i, $i \in N$ and where P contains *all* possible products of these, were shown before for the quadratic assignment (Adams and Johnson (1994)) and quadratic semi-assignment (Billionnet and Elloumi (2001)) problems.

4.1.2 'Knapsack' Inequalities

We now focus on the case where the only constraints taken into account are 'knapsack' constraints, i.e., $K = K_I$, $a^k_i = 1$ for all $i \in A_k$ and $\beta^k = 1$ for all $k \in K$.

Theorem 6. *Let $\beta^k = 1$ for all $k \in K$, and as well $a^k_i = 1$ for each $i \in A_k$, $k \in K$. Then for any solution $x \in [0,1]^n$, the inequalities $y_{ij} \le x_i$, $y_{ij} \le x_j$ and $y_{ij} \ge x_i + x_j - 1$ are implied by inequalities (12) and (13) for all $(i, j) \in Q$ if and only if the Conditions 1–3 are satisfied.*

Proof. Let $(i, j) \in Q$. By Condition 1, there is a $k \in K$ such that $i \in A_k$, $j \in B^{I+}_k$ and hence the inequality

$$\sum_{h\in A_k,(h,j)\in Q} y_{hj} + \sum_{h\in A_k,(j,h)\in Q} y_{jh} \le x_j \tag{16}$$

exists, has y_{ij} on its left hand side, and thus establishes $y_{ij} \le x_j$.

Similarly, by Condition 2, there is an $\ell \in K$ such that $j \in A_\ell$, $i \in B^{I+}_\ell$ and hence the equation

$$\sum_{h\in A_\ell,(h,i)\in Q} y_{hi} + \sum_{h\in A_\ell,(i,h)\in Q} y_{ih} \le x_i \tag{17}$$

exists, has y_{ij} on its left hand side, and thus establishes $y_{ij} \le x_i$.

Moreover, by Condition 3, there is, w.l.o.g., some $k \in K_I$ with $i \in A_k$ and $j \in B_k^{I-}$, i.e., such that the inequality

$$\sum_{h \in A_k, (h,j) \in Q} (x_h - y_{hj}) + \sum_{h \in A_k, (j,h) \in Q} (x_h - y_{jh}) \leq 1 - x_j \tag{18}$$

exists. Due to Conditions 1 and 2, we have that $x_h \geq y_{jh}$ for each $h \in A_k, (j,h) \in Q$ and $x_h \geq y_{hj}$ for each $h \in A_k, (h,j) \in Q$ in (18). By reordering the latter to

$$x_j + x_i - y_{ij} + \underbrace{\sum_{h \in A_k, (h,j) \in Q, h \neq i} (x_h - y_{hj}) + \sum_{h \in A_k, (j,h) \in Q, h \neq i} (x_h - y_{jh})}_{\geq 0} \leq 1,$$

we obtain the desired result. The necessity of Conditions 1–3 stems once more from the same reasons as mentioned in the proof of Theorem 4. □

4.1.3 'Double Selection' Equations with Induced Squares

Another important special case, where the equations induced by Conditions 1 and 2 imply the inequalities (5)–(7) also for fractional solutions, is obtained if the right hand sides of all the considered original equations K_E are equal to two and all (or a subset of) the products to be induced are exactly those given by $A_k \times A_k$ for all $k \in K_E$. In this case, Conditions 1 and 2 are implicitly satisfied for all these products by choosing $B_k = A_k$ for all $k \in K_E$. We will see in Sect. 6.2 an application where this case occurs in practice and that also gives an example where it is attractive to apply the compact linearization only to a subset of the present linear constraints.

Theorem 7. *If, for all $k \in K_E$, (i) $a_i^k = 1$ for all $i \in A_k$, (ii) $\beta^k = 2$, and (iii) $B_k^E = A_k$, then there is a compact linearization such that, for any solution $x \in [0,1]^n$, the inequalities $y_{ij} \leq x_i$, $y_{ij} \leq x_j$ and $y_{ij} \geq x_i + x_j - 1$ are implied by the equations (11) for all $(i,j) \in Q$, $i \neq j$.*

Proof. Due to (i)–(iii), the induced equations (11) look like:

$$y_{jj} + \sum_{h \in A_k, h<j} y_{hj} + \sum_{h \in A_k, j<h} y_{jh} = 2x_j \qquad \text{for all } j \in A_k, \text{ for all } k \in K_E$$

Since y_{jj} shall take on the same value as x_j, we may eliminate y_{jj} on the left and once subtract x_j on the right. We obtain:

$$\sum_{h \in A_k, h<j} y_{hj} + \sum_{h \in A_k, j<h} y_{jh} = x_j \qquad \text{for all } j \in A_k, \text{ for all } k \in K_E \tag{19}$$

These equations establish inequalities (5) and (6) for all y_{ij}, $(i,j) \in Q$, $i \neq j$. Combining them with the original equations $\sum_{a \in A_k} x_a = 2$ yields the following identities:

$$2 = \sum_{a \in A_k} x_a = \sum_{a \in A_k} \Big(\sum_{h \in A_k, h<a} y_{ha} + \sum_{h \in A_k, a<h} y_{ah} \Big) = 2 * \sum_{a \in A_k} \sum_{h \in A_k, a<h} y_{ah}$$

As an immediate consequence, it follows (even for fractional x) that:

$$\sum_{a \in A_k} \sum_{h \in A_k, a<h} y_{ah} = 1 \tag{20}$$

Since $\{i,j\} \subseteq A_k$, we obtain a subtotal of (20) if we sum the equations (19) expressed for i and for j (which both contain y_{ij} on their left hand sides). We can exploit this as follows (cf. Fischer (2013)) in order to show that $y_{ij} \geq x_i + x_j - 1$:

$$\begin{aligned} x_i + x_j &= \sum_{h\in A_k, i<h} y_{ih} + \sum_{h\in A_k, h<i} y_{hi} + \sum_{h\in A_k, j<h} y_{jh} + \sum_{h\in A_k, h<j} y_{hj} \\ &= y_{ij} + \sum_{h\in A_k, i<h\neq j} y_{ih} + \sum_{h\in A_k, j\neq h<i} y_{hi} + \sum_{h\in A_k, j<h} y_{jh} + \sum_{h\in A_k, h<j} y_{hj} \\ &\overset{(20)}{\leq} y_{ij} + \sum_{a\in A_k} \sum_{h\in A_k, a<h} y_{ah} \\ &= y_{ij} + 1 \end{aligned}$$

□

Remark 8. *If $\beta^k > 2$ in Theorem 7 or $\beta^k \geq 2$ in the general setting, then it is impossible to conclude $y_{ij} \leq x_i$ and $y_{ij} \leq x_j$ from the linearization equations for fractional x. Moreover, if $B_k \neq A_k$, then it is impossible to conclude $y_{ij} \geq x_i + x_j - 1$ from (20).*

4.2 A Scenario with a Strictly Stronger LP Relaxation

Sect. 4.1 displayed scenarios where the proposed technique provides a linear programming relaxation that is at least as strong as the one obtained using the Glover-Woolsey linearization. If the *equation* sets A_k, $k \in K_E$, and P allow to construct a compact linearization with $Q = P$ (after possible squares are eliminated), then it can be shown that the corresponding relaxation is even *strictly* stronger. For example, this is true for the applications presented in Sect. 6. Moreover, a set Q generated can sometimes also be *made* compliant to this case or at least strengthened and at the same time reduced in size by a postprocessing, if the particular problem at hand allows to fix the values of (some of) the variables in $Q \setminus P$ prior to solving it.

Observation 9. *Let $(i,j) \in P$ and suppose that $x_i > 0$, $x_j > 0$, and $x_i + x_j \leq 1$ hold in a given optimum solution to the linear programming relaxation obtained with the Glover-Woolsey linearization. Then inequalities (7) are dominated by the trivial ones, i.e., $y_{ij} \geq 0$. Thus, if $d_{ij} > 0$ and no other constraint enforces $y_{ij} > 0$, then $y_{ij} = 0$.*

Now, for a fixed $i \in N$, let $k \in K_E$ be an index such that $i \in B_k^E$. Under the assumptions made before, it is then readily seen that the corresponding induced equation

$$\sum_{h\in A_k, h<i} \alpha_h^k y_{hi} + \sum_{h\in A_k, i<h} \alpha_h^k y_{ih} = \beta^k x_i$$

of the associated compactly linearized program formulation cuts off any point where the situation described in Observation 9 applies to *all* products (i,h) or $(h,i) \in P$ with $h \in A_k$. Consequently, this is true for *all the points* whose components have non-zero entries for *at least one* x_i, $i \in N$, and all x_h, $h \in A_k$, associated to some $k \in K_E$ such that $i \in B_k^E$, and zero-entries for all corresponding products y_{ih} or y_{hi}. It also becomes visible, why a set $Q = P$ needs to be assumed for this construction, as otherwise the value $\beta^k x_i$ could be entirely assigned to some y_{hi} or y_{ih} for $h \in A_k$ where (h,i) respectively

(i,h) is in $Q \setminus P$. Such a point however cannot occur using a Glover-Woolsey linearization as it only linearizes the products in P. For a similar reason, it is also necessary to establish consistency, i.e. to satisfy Conditions 1–3, for all products in Q rather than just those in P.

5 Obtaining a Compact Linearization (Automatically)

We shall now elaborate on how to obtain a consistent linearization while inducing a minimum number of additional constraints and as well a set $Q \supseteq P$ as small as possible. Such a 'most compact' linearization can be computed by solving the following mixed-integer program:

$$\min \sum_{1\le i\le n} \left(\sum_{k\in K_E} w_E z_{ik}^E + \sum_{k\in K_I} \left(w_{I_+} z_{ik}^{I_+} + w_{I_-} z_{ik}^{I_-} \right) \right) + w_Q \left(\sum_{1\le i\le n} \sum_{i\le j\le n} f_{ij} \right)$$

$$
\begin{array}{llll}
\text{s.t.} & f_{ij} = 1 & \text{for all } (i,j)\in P & (21)\\
& f_{ij} \ge z_{jk}^E & \text{for all } k\in K_E, i\in A_k, j\in N, i\le j & (22)\\
& f_{ji} \ge z_{jk}^E & \text{for all } k\in K_E, i\in A_k, j\in N, j< i & (23)\\
& f_{ij} \ge z_{jk}^{I_+} & \text{for all } k\in K_I, i\in A_k, j\in N, i\le j & (24)\\
& f_{ji} \ge z_{jk}^{I_+} & \text{for all } k\in K_I, i\in A_k, j\in N, j< i & (25)\\
& f_{ij} \ge z_{jk}^{I_-} & \text{for all } k\in K_I, i\in A_k, j\in N, i\le j & (26)\\
& f_{ji} \ge z_{jk}^{I_-} & \text{for all } k\in K_I, i\in A_k, j\in N, j< i & (27)\\
& \sum_{k\in K_E: i\in A_k} z_{jk}^E + \sum_{k\in K_I: i\in A_k} z_{jk}^{I_+} \ge f_{ij} & \text{for all } 1\le i\le j\le n & (28)\\
& \sum_{k\in K_E: j\in A_k} z_{ik}^E + \sum_{k\in K_I: j\in A_k} z_{ik}^{I_+} \ge f_{ij} & \text{for all } 1\le i\le j\le n & (29)\\
& \sum_{k\in K_E: j\in A_k} z_{ik}^E + \sum_{k\in K_I: j\in A_k} z_{ik}^{I_-} + & & \\
& \sum_{k\in K_E: i\in A_k} z_{jk}^E + \sum_{k\in K_I: i\in A_k} z_{jk}^{I_-} \ge f_{ij} & \text{for all } 1\le i\le j\le n & (30)\\
& f_{ij} \in [0,1] & \text{for all } 1\le i\le j\le n & \\
& z_{ik}^E \in \{0,1\} & \text{for all } k\in K_E, 1\le i\le n & \\
& z_{ik}^{I_+} \in \{0,1\} & \text{for all } k\in K_I, 1\le i\le n & \\
& z_{ik}^{I_-} \in \{0,1\} & \text{for all } k\in K_I, 1\le i\le n &
\end{array}
$$

The formulation involves binary variables z_{ik}^E to be equal to 1 if $i \in B_k^E$ for $k \in K_E$ and equal to zero otherwise, and binary variables $z_{ik}^{I_+}$ and $z_{ik}^{I_-}$ to express whether $i \in B_k^{I_+}$ and $i \in B_k^{I_-}$ for $k \in K_I$. To account for whether $(i,j) \in Q$, there is a further continuous variable f_{ij} for all $1 \le i \le j \le n$ that will be equal to 1 in this case and equal to zero otherwise. Constraints (21) fix those f_{ij} to 1 where the corresponding pair (i,j) is contained in P. Whenever some $j \in N$ is assigned to some set B_k, then we induce the corresponding products $(i,j) \in Q$ or $(j,i) \in Q$ for all $i \in A_k$ which is established by inequalities (22)–(27). Finally, if $(i,j) \in Q$, then we require Conditions 1–3 to be satisfied by inequalities (28)–(30), respectively.

The Conditions 1–3 impose a certain minimum on the number of constraints $|B|$ which depends on P, the sizes of the sets A_k, $k \in K$, and the distribution of the variables x_i, $i \in N$, across them. In general, different solutions achieving this minimum may lead to different cardinalities of $|Q|$. A rational choice for the weights introduced in the objective function is thus $w_Q = 1$ and $w_E = w_{I_+} = w_{I_-} > \max_{k \in K} |A_k|$. This results in a solution with a minimum number of constraints that, among these, also induces a minimal number of variables. Also one might prefer equations by choosing w_E larger compared to the other weights.

The mixed-integer program is interesting especially for an automated linearization, e.g. as part of a mixed-integer programming solver. It can be significantly simplified if only equations are considered. Moreover, if in addition the equation comprising each x_i, $i \in N$ that is involved in a product is unique, i.e., $A_k \cap A_\ell = \emptyset$, for all $k, \ell \in K$, $\ell \neq k$, it reduces to a linear program with a totally unimodular (TU) constraint matrix and can alternatively be solved using a simple combinatorial algorithm as described in Mallach (2017). This algorithm might also be altered such that it is still applicable as a heuristic in the case of non-disjoint sets A_k, $k \in K$. When considering a particular problem formulation on a paper print, an associated (most) compact linearization is however typically 'recognized' easily by hand.

6 Applications

While the number of existing as well as prospective applications of the technique proposed is large, we highlight in this section two prominent combinatorial optimization problems where formulations found earlier appear now as compact linearizations.

6.1 Quadratic Assignment Problem

Consider a canonical integer programming formulation for the n-by-n quadratic assignment problem (QAP) in the form by Koopmans and Beckmann (1957), with variables $x_{ip} \in \{0,1\}$ for 'facilities' or 'items' $i \in \{1,\dots,n\}$ and 'locations' or 'positions' $p \in \{1,\dots,n\}$. Let y_{ipjq} represent the linearization variable of the product $x_{ip} \cdot x_{jq}$ of any two such variables. As already mentioned by Liberti (2007), the following formulation by Frieze and Yadegar (1983) can be obtained by applying the methodology of the compact linearization technique (and ignoring commutativity in the first place).

$$
\begin{aligned}
\min \; & \sum_{i=1}^{n}\sum_{p=1}^{n}\sum_{j=1}^{n}\sum_{q=1}^{n} d_{ijpq} y_{ipjq} + \sum_{i=1}^{n}\sum_{p=1}^{n} c_{ip} x_{ip} \\
\text{s.t.} \; & \sum_{i=1}^{n} x_{ip} = 1 && \text{for all } p \in \{1,\dots,n\} && (31)\\
& \sum_{p=1}^{n} x_{ip} = 1 && \text{for all } i \in \{1,\dots,n\} && (32)\\
& \sum_{i=1}^{n} y_{ipjq} = x_{jq} && \text{for all } p,j,q \in \{1,\dots,n\} && (33)\\
& \sum_{p=1}^{n} y_{ipjq} = x_{jq} && \text{for all } i,j,q \in \{1,\dots,n\} && (34)\\
& \sum_{j=1}^{n} y_{ipjq} = x_{ip} && \text{for all } i,p,q \in \{1,\dots,n\} && (35)\\
& \sum_{q=1}^{n} y_{ipjq} = x_{ip} && \text{for all } i,p,j \in \{1,\dots,n\} && (36)\\
& y_{ipip} = x_{ip} && \text{for all } i,p \in \{1,\dots,n\} && (37)\\
& y_{ipjq} \in [0,1] && \text{for all } i,p,j,q \in \{1,\dots,n\} \\
& x_{ip} \in \{0,1\} && \text{for all } i,p \in \{1,\dots,n\}
\end{aligned}
$$

For each y_{ipjq}, $i,p,j,q \in \{1,\dots,n\}$, the displayed formulation however satisfies each of the Conditions 1 and 2 *twice*, i.e., it is not a compact linearization of minimum size. There is an equivalent formulation by Adams and Johnson (1994) that comprises only (33) and (34), and thus satisfies Conditions 1 (twice) while Conditions 2 are only 'indirectly' satisfied by means of additional identity constraints $y_{ipjq} = y_{jqip}$ for all $i,p,j,q \in \{1,\dots,n\}$. Hence, this formulation cannot, at least not directly, be generated from the compact linearization approach.

To characterize a 'most compact' QAP linearization, let $K = K_P^E \cup K_I^E$, where K_P^E corresponds to the assignment constraints (31) and K_I^E corresponds to the assignment constraints (32). For each $p \in K_P^E$, we have $A_p = \{ip \mid i \in \{1,\dots,n\}\}$, and for each $i \in K_I^E$, we have $A_i = \{ip \mid p \in \{1,\dots,n\}\}$[1]. Hence, all the variables x_{ip}, $i,p \in \{1,\dots,n\}$, occur exactly once in $\bigcup_{p \in K_P^E} A_p$ as well as exactly once in $\bigcup_{i \in K_I^E} A_i$. Thus, in order to induce all products and to satisfy Conditions 1 and 2 for them, it suffices to set *either* $B_p = \bigcup_{q \in K_P^E} A_q$ for all $p \in K_P^E$ – which induces (33) and (35), *or* $B_i = \bigcup_{j \in K_I^E} A_j$ for all $i \in K_I^E$ – which induces (34) and (36). Moreover, since the identities (37) and all variables y_{ipiq} for all pairs $p,q \in \{1,\dots,n\}$ as well as all variables y_{ipjp} for all pairs $i,j \in \{1,\dots,n\}$ can be eliminated, it suffices to formulate (34) and (36) only for $i \neq j$, and (33) and (35) only for $p \neq q$. If one further identifies y_{jqip} with y_{ipjq} whenever $i < j$, it even suffices to have only exactly *one* of these four equation sets in order to satisfy Conditions 1 and 2. The total number of additional equations then reduces to $n^3 - n^2$ compared to $3 \cdot \left(\frac{1}{2}(n^2-n)(n^2-n)\right) = \frac{3}{2}(n^4 - 2n^3 + n^2)$

[1] To ease notation, we treat ip as an index that would of course truly be $i \cdot n + p$.

inequalities when using the Glover-Woolsey linearization and creating y_{ipjq} only for $i < j$ and $p \neq q$ as well. However, these most compact formulations have a considerably weaker linear programming relaxation than the ones by Frieze and Yadegar (1983) and Adams and Johnson (1994).

6.2 Symmetric Quadratic Traveling Salesman Problem

The symmetric quadratic traveling salesman problem asks for a tour $T \subseteq E$ in a complete undirected graph $G = (V,E)$ such that the objective $\sum_{\{i,j,k\} \subseteq V, j \neq i < k \neq j} c_{ijk} x_{ij} x_{jk}$ (where $x_{ij} = 1$ if and only if $\{i,j\} \in T$) is minimized.

Consider the following mixed-integer programming formulation for this problem as presented by Fischer and Helmberg (2013) and oriented at the integer programming formulation for the linear traveling salesman problem by Dantzig et al. (1954).

$$\begin{aligned}
\min \quad & \sum_{\{i,j,k\} \subseteq V, j \neq i < k \neq j} c_{ijk} y_{ijk} & & \\
\text{s.t.} \quad & \sum_{\{i,j\} \in E} x_{ij} = 2 & & \text{for all } i \in V & (38)\\
& x(E(W)) \leq |W| - 1 & & \text{for all } W \subsetneq V,\ 2 \leq |W| \leq |V| - 2 & \\
& y_{ijk} = x_{ij} x_{jk} & & \text{for all } \{i,j,k\} \subseteq V, j \neq i < k \neq j & (39)\\
& x_{ij} \in \{0,1\} & & \text{for all } \{i,j\} \in E &
\end{aligned}$$

In the context of the approach presented, we consider only the linear equations (38) so that we have $K = K_E = V$, $A_k = \{jk \mid j < k \text{ and } \{j,k\} \in E\}$, $\alpha_i^k = 1$ for all $i \in A_k$ and $\beta^k = 2$ for all $k \in K$. Since we are interested in the bilinear terms of the form as in (39), i.e. in each pair of edges with common index j, we need to set $B_k = A_k$ for all $k \in K$ in order to satisfy both Conditions 1 and 2 for each such pair. We thus comply to the requirements of the special case addressed in Theorem 7 (Sect. 4.1) and obtain the equations:

$$\sum_{\{i,j\} \in E} x_{ij} x_{jk} = 2x_{jk} \qquad \text{for all } \{j,k\} \in E, \text{ for all } j \in V$$

After introducing linearization variables with indices ordered as desired, these are resolved as:

$$\sum_{\{i,j,k\} \subseteq V, j \neq i \leq k \neq j} y_{ijk} = 2x_{jk} \qquad \text{for all } \{j,k\} \in E, \text{ for all } j \in V$$

Each of these equations induces one variable more than originally demanded, namely y_{kjk} as the linearized substitute for the square term $x_{jk} x_{jk}$. Thus we may safely subtract y_{kjk} from the left and x_{jk} from the right hand side and obtain

$$\sum_{\{i,j,k\} \subseteq V, j \neq i < k \neq j} y_{ijk} = x_{jk} \qquad \text{for all } \{j,k\} \in E, \text{ for all } j \in V$$

which are exactly the linearization constraints as presented by Fischer and Helmberg (2013).

7 Conclusion

As has been shown in this paper, the compact linearization technique can be applied not only to binary quadratic problems with assignment constraints, but to those with arbitrary linear constraints with positive coefficients and right hand sides. We discussed two particular cases where the continuous relaxation of the obtained compactly linearized problem formulation is provably as least as strong as the one obtained with the well-known linearization by Glover and Woolsey (1974). Moreover, we highlighted previously found formulations for the quadratic assignment problem and the symmetric quadratic traveling salesman problem that appear as special cases that result when applying the proposed method. Last but not least, we demonstrated how a compact linearization can be generated automatically.

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References

Adams WP, Johnson TA (1994) Improved linear programming-based lower bounds for the quadratic assignment problem. In: Pardalos PM, Wolkowicz H (eds) Quadratic Assignment and Related Problems, DIMACS Series on Discrete Mathematics and Computer Science, vol 16, AMS, Providence, RI, USA, pp 43–75

Adams WP, Sherali HD (1986) A tight linearization and an algorithm for zero-one quadratic programming problems. Management Science 32(10):1274–1290, DOI 10.1287/mnsc.32.10.1274

Adams WP, Sherali HD (1999) A Reformulation-Linearization Technique for Solving Discrete and Continuous Nonconvex Problems, Nonconvex Optimization and its Applications, vol 31. Springer, DOI 10.1007/978-1-4757-4388-3

Balas E (1964) Extension de l'algorithme additif à la programmation en nombres entiers et à la programmation non linéaire. Comptes rendus de l'Académie des Sciences Paris 258:5136–5139

Billionnet A, Elloumi S (2001) Best reduction of the quadratic semi-assignment problem. Discrete Applied Mathematics 109(3):197 – 213, DOI 10.1016/S0166-218X(00)00257-2

Chaovalitwongse W, Pardalos PM, Prokopyev OA (2004) A new linearization technique for multi-quadratic 0-1 programming problems. Oper Res Lett 32(6):517–522, DOI 10.1016/j.orl.2004.03.005

Dantzig G, Fulkerson R, Johnson S (1954) Solution of a large-scale traveling-salesman problem. Journal of the Operations Research Society of America 2(4):393–410, DOI 10.1287/opre.2.4.393

De Simone C (1990) The cut polytope and the boolean quadric polytope. Discrete Math 79(1):71–75, DOI 10.1016/0012-365X(90)90056-N

Fischer A (2013) A polyhedral study of quadratic traveling salesman problems. PhD thesis, Chemnitz University of Technology

Fischer A, Helmberg C (2013) The symmetric quadratic traveling salesman problem. Math Program 142(1-2):205–254, DOI 10.1007/s10107-012-0568-1

Fortet R (1959) L'algèbre de boole et ses applications en recherche opérationnelle. Cahiers du Centre d'Etudes de Recherche Opérationnelle 1:5–36

Fortet R (1960) Applications de l'algèbre de boole en recherche opérationnelle. Revue de la Société Française de Recherche Opérationnelle 4:17–26

Frieze AM, Yadegar J (1983) On the quadratic assignment problem. Discrete Appl Math 5(1):89–98, DOI 10.1016/0166-218X(83)90018-5

Furini F, Traversi E (2013) Extended linear formulation for binary quadratic problems. Optimization Online

Glover F (1975) Improved linear integer programming formulations of nonlinear integer problems. Manage Sci 22(4):455–460, DOI 10.1287/mnsc.22.4.455

Glover F, Woolsey E (1973) Further reduction of zero-one polynomial programming problems to zero-one linear programming problems. Oper Res 21(1):156–161

Glover F, Woolsey E (1974) Converting the 0-1 polynomial programming problem to a 0-1 linear program. Oper Res 22(1):180–182, DOI 10.1287/opre.22.1.180

Gueye S, Michelon P (2009) A linearization framework for unconstrained quadratic (0-1) problems. Discrete Appl Math 157(6):1255–1266, DOI 10.1016/j.dam.2008.01.028

Hammer PL (1965) Some network flow problems solved with pseudo-boolean programming. Operations Research 13(3):388–399

Hammer PL, Rudeanu S (1968) Boolean Methods in Operations Research and Related Areas, Ökonometrie und Unternehmensforschung / Econometrics and Operations Research, vol 7. Springer, Berlin, Heidelberg, DOI 10.1007/978-3-642-85823-9

Hansen P, Meyer C (2009) Improved compact linearizations for the unconstrained quadratic 0-1 minimization problem. Discrete Appl Math 157(6):1267–1290, DOI 10.1016/j.dam.2007.12.008

Koopmans TC, Beckmann M (1957) Assignment problems and the location of economic activities. Econometrica 25(1):53–76

Liberti L (2007) Compact linearization for binary quadratic problems. 4OR 5(3):231–245, DOI 10.1007/s10288-006-0015-3

Mallach S (2017) Compact linearization for binary quadratic problems subject to assignment constraints. 4OR pp 1–15, DOI 10.1007/s10288-017-0364-0

McCormick GP (1976) Computability of global solutions to factorable nonconvex programs: Part i — convex underestimating problems. Mathematical Programming 10(1):147–175, DOI 10.1007/BF01580665

Oral M, Kettani O (1992a) A linearization procedure for quadratic and cubic mixed-integer problems. Oper Res 40(1-supplement-1):S109–S116, DOI 10.1287/opre.40.1.S109

Oral M, Kettani O (1992b) Reformulating nonlinear combinatorial optimization problems for higher computational efficiency. European J Oper Res 58(2):236–249, DOI 10.1016/0377-2217(92)90210-Z

Padberg M (1989) The boolean quadric polytope: Some characteristics, facets and relatives. Mathematical Programming 45(1):139–172, DOI 10.1007/BF01589101

Sherali HD, Smith JC (2007) An improved linearization strategy for zero-one quadratic programming problems. Optim Lett 1(1):33–47, DOI 10.1007/s11590-006-0019-0

Watters LJ (1967) Reduction of integer polynomial programming problems to zero-one linear programming problems. Oper Res 15:1171–1174

Zangwill WI (1965) Media selection by decision programming. J Advert Res 5:23–37