Abstract

In this paper it is shown that the compact linearization approach, that has been previously proposed only for binary quadratic problems with assignment constraints, can be generalized to arbitrary linear equations with positive coefficients which considerably enlarges its applicability. We discuss special cases of prominent quadratic combinatorial optimization problems where the obtained compact linearization yields a continuous relaxation that is provably as least as strong as the one obtained with an ordinary linearization.

1 Introduction

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 is attributed to Fortet (1959, 1960) and addressed by Hammer and Rudeanu (1968). This method, that is also proposed in succeeding works by Balas (1964), Zangwill (1965) and Watters (1967), and further discussed by Glover and Woolsey (1973), requires two inequalities per linearization variable. Only shortly thereafter, Glover and Woolsey (1974) found that the same effect can be achieved using continuous linearization variables when replacing one of these inequalities with two different ones. The outcome is a method that is until today regarded as ‘the standard linearization technique’ and where, in the binary quadratic case, each product $x_i x_j$ is modeled using a variable $y_{ij} \in [0,1]$ and three constraints:

$$
\begin{align*}
    y_{ij} &\leq x_i \\
    y_{ij} &\leq x_j \\
    y_{ij} &\geq x_i + x_j - 1
\end{align*}
$$

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While this approach is widely applicable, it is considered to be rather ‘weak’ in the sense that the inequalities couple the three involved variables only very loosely. Depending on the concrete problem formulation, this may result in linear programming relaxations that yield unsatisfactory bounds on the respective objective function.

Several attempts have been made to develop more sophisticated techniques that exploit the structure of a given problem formulation. For example, linearization methods for binary quadratic problems (BQPs) where all bilinear terms appear only in the objective function are proposed by Glover (1975), Oral and Kettani (1992a,b), as well as by Chaovalitwongse et al. (2004), Sherali and Smith (2007), Furini and Traversi (2013), and, for quadratic problems with general integer variables, by Billionnet et al. (2008). Adapted formulations for unconstrained BQPs were addressed by Gueye and Michelon (2009), and Hansen and Meyer (2009).

In this paper, we are concerned with a compact linearization technique for BQPs that comprise a collection \( K \) of linear equations

\[
\sum_{i \in A_k} a_{ik}^k x_i = b_k^k, \quad k \in K
\]

where \( A_k \) is an index set specifying the binary variables on the left hand side, \( a_{ik}^k \in \mathbb{R}^{>0} \) for all \( i \in A_k \), and \( b_k^k \in \mathbb{R}^{>0} \). For ease of notation, let the overall set of binary variables in the BQP be indexed by a set \( N = \{1, \ldots, n\} \) where \( n \in \mathbb{N}^{>0} \). Bilinear terms \( y_{ij} = x_i x_j \), are permitted to occur in the objective function as well as in the set of constraints. The technique proposed is compact in the sense that it typically adds less constraints than the ‘standard’ method. Its only prerequisite is that for each product \( x_i x_j \) there exist indices \( k, \ell \) such that \( i \in A_k \) and \( j \in A_\ell \), i.e., for each variable being part of a bilinear term there is some linear equation involving it. Without loss of generality, we also assume the bilinear terms to be collected in an ordered set \( P \subset N \times N \) such that \( i \leq j \) for each \( (i, j) \in P \). With an arbitrary set of \( m \geq 0 \) linear constraints \( Cx + Dy \geq e \) where \( C \in \mathbb{R}^{m \times n} \) and \( D \in \mathbb{R}^{m \times |E|} \), a general form of the mixed-integer programs considered can be stated as:

\[
\begin{align*}
\min & \quad c^T x + d^T y \\
\text{s.t.} & \quad \sum_{i \in A_k} a_{ik}^k x_i = b_k^k \quad \text{for all } k \in K \quad (4) \\
& \quad Cx + Dy \geq e \\
& \quad y_{ij} = x_i x_j \quad \text{for all } (i, j) \in P \quad (5) \\
& \quad x_i \in \{0, 1\} \quad \text{for all } i \in N 
\end{align*}
\]

This general mixed-integer program covers several NP-hard combinatorial optimization problems. For the case where the equations (4) are assignment constraints, i.e., for all \( k \in K \) we have \( b_k^k = 1 \) and \( a_{ik}^k = 1 \) for all \( i \in A_k \), Liberti (2007) and Mallach (2017) proposed a compact linearization approach that can be seen as a first level application of the so-called reformulation-linearization technique by Adams and Sherali (1999).

In this paper, we show how this approach can be generalized to the mentioned arbitrary linear equations with positive coefficients. This broadens the applicability of the approach in a strong sense. We then discuss under which circumstances the obtained compact linearization is provably at least as strong as the one obtained with the ‘standard linearization’. Finally, we highlight some prominent example applications where previously found linearizations appear as special cases of the proposed technique.
2 Compact Linearization

The compact linearization approach for binary quadratic problems with linear equations is as follows. With each linear equation of type (4), i.e., with each index set $A_k$, we associate a corresponding index set $B_k \subseteq N$ such that for each $j \in B_k$ the equation is multiplied with $x_j$. We thus obtain the new equations:

$$\sum_{i \in A_k} a_{ij}^k x_i x_j = b^k x_j \quad \text{for all } j \in B_k, \text{ for all } k \in K \quad (6)$$

Each product $x_i x_j$ induced by any of the equations (6) 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

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

Rewriting the equations (6) using $Q$, we obtain the linearization equations:

$$\sum_{i \in A_k, (j, i) \in Q} a_{ij}^k y_{ij} + \sum_{i \in A_k, (j, i) \in Q} a_{ji}^k y_{ij} = b^k x_j \quad \text{for all } j \in B_k, \text{ for all } k \in K \quad (7)$$

It is clear that the equations (7) are valid for the original problem and thus as well the equations (6) 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 $(i, j) \in Q$.

In order to obtain a linearization of the original problem formulation with the bilinear terms defined by the set $P$, we need to choose the sets $B_k$ such that the induced set of variables $Q$ will be equal to or contain $P$ as a subset. We will discuss how to obtain a set $Q \supseteq P$ later, but suppose for now that such a set $Q$ is already at hand. We will show that a consistent linearization is obtained if and only if the following two conditions (for which $k = \ell$ is a valid choice) are satisfied:

**Condition 1.** For each $(i, j) \in Q$, there is a $k \in K$ such that $i \in A_k$ and $j \in B_k$.

**Condition 2.** For each $(i, j) \in Q$, there is an $\ell \in K$ such that $j \in A_\ell$ and $i \in B_\ell$.

**Theorem 3.** If Conditions [1] and [2] are satisfied, then for any integer solution $x \in \{0, 1\}^N$, the inequalities $y_{ij} \leq x_i$, $y_{ij} \leq x_j$, and $y_{ij} \geq x_i + x_j - 1 \text{ hold for all } (i, j) \in Q$.

**Proof.** Let $(i, j) \in Q$. By Condition [1] there is a $k \in K$ such that $i \in A_k$, $j \in B_k$ and hence the equation

$$\sum_{h \in A_k, (h, j) \in Q} a_{hj}^k y_{hj} + \sum_{h \in A_k, (j, h) \in Q} a_{jh}^k y_{jh} = b^k x_j \quad (*)$$

exists and has $y_{ij}$ on its left hand side. Since $a_{hj}^k > 0$ for all $h \in A_k$ and $0 \leq y_{ij} \leq 1$, it establishes that $y_{ij} = 0$ whenever $x_j = 0$. Similarly, by Condition [2] there is an $\ell \in K$ such that $j \in A_\ell$, $i \in B_\ell$ and hence the equation

$$\sum_{h \in A_\ell, (h, i) \in Q} a_{hi}^\ell y_{hi} + \sum_{h \in A_\ell, (i, h) \in Q} a_{ih}^\ell y_{ih} = b^\ell x_i \quad (***)$$

for all $k \in K$. Therefore the solutions $x$ of the original problem and the solutions $x$ of the linearized problem are consistent.
exists and has \( y_{ij} \) on its left hand side. Since \( a_{ih}^k > 0 \) for all \( h \in A_k, 0 \leq y_{ij} \leq 1 \) it establishes that \( y_{ij} = 0 \) whenever \( x_i = 0 \).

Within a framework that constructs a linearization only by means of equations of type (7), there is no other way of establishing \( y_{ij} \leq x_j \) and \( y_{ij} \leq x_i \) than by satisfying conditions 1 and 2 – showing their necessity. We will now continue with showing also their sufficiency.

Since \( y_{ij} = 0 \) whenever \( x_i = 0 \) or \( x_j = 0 \), the inequality \( y_{ij} \geq x_i + x_j - 1 \) is satisfied as well in this case. So let now \( x_i = x_j = 1 \). Then the right hand sides of (2) and (2∗∗) are equal to \( b^k \) and \( b^f \) respectively. The variable \( y_{ij} \) (the only one that) occurs on the left hand sides of both of these equations. If \( y_{ij} = 1 \), this is consistent and correct. So suppose that \( y_{ij} < 1 \) which implies that, in the case of equation (2∗∗), we have:

\[
\sum_{h \in A_k, (h,j) \in Q, h \neq i} a_{ih}^k y_{hj} + \sum_{h \in A_k, (j,h) \in Q, h \neq i} a_{jh}^k y_{jh} = b^k x_j - a_i^k y_{ij} > b^k - a_i^k. \tag{∗′}
\]

At the same time, however, we have \( \sum_{h \in A_k, h \neq i} a_{ih}^k x_h = b^k - a_i^k \) with \( x_h \in \{0, 1\} \).

In order for the equation (2∗∗) to be satisfied, an additional amount of \( (1 - y_{ij})a_i^k > 0 \) must be contributed by the other summands on the left hand side of (2∗∗). 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 the conditions 1 and 2 are also established for these variables. An analogous result can be stated for equation (2∗∗∗).

Unfortunately, in the general case, Theorem 3 cannot be restated for fractional solutions \( x \in [0, 1]^N \) and thus we cannot conclude from the proof that the compact linearization yields a linear programming relaxation which is provably as least as tight as the one obtained with the ‘standard linearization’. This is in contrast to the special case where the equations (4) are assignment constraints, i.e., \( a_i^k = 1 \) for all \( i \in A_k \) and \( b^k = 1 \) for all \( k \in K \). As stated in the introduction, the compact linearization approach was originally proposed for this case, in [Liberati (2007)] and [Mallach (2017)]. Accidentally, the proof in [Mallach (2017)] lacks a verification that \( y_{ij} \geq x_i + x_j - 1 \) holds for all \( (i, j) \in Q \) also in the fractional case that we now catch up on.

**Theorem 4.** If, for all \( k \in K, a_i^k = 1 \) for all \( i \in A_k \) and \( b^k = 1 \), and the Conditions 1 and 2 are satisfied, then for any solution \( x \in [0, 1]^N \), the inequalities \( y_{ij} \leq x_i, y_{ij} \leq x_j \) and \( y_{ij} \geq x_i + x_j - 1 \) hold for all \( (i, j) \in Q \).

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

\[
\sum_{h \in A_k, (h,j) \in Q} y_{hj} + \sum_{h \in A_k, (j,h) \in Q} y_{jh} = x_j \tag{∗∗∗}
\]

exists, has \( y_{ij} \) on its left hand side, and thus establishes \( y_{ij} \leq x_j \). Similarly, by Condition 2 there is an \( \ell \in K \) such that \( j \in A_\ell, i \in B_\ell \) and thus the equation

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

exists, has \( y_{ij} \) on its left hand side, and thus establishes \( y_{ij} \leq x_i \).
To show that $y_{ij} \geq x_i + x_j - 1$, consider equation (9) in combination with its original counterpart $\sum_{h \in A_k} x_h = 1$. For any $y_{hj}$ (or $y_{jh}$) in (9), the conditions (1) and (2) assure that there is an equation establishing $y_{ij} \leq x_h \leq y_{hj}$. Thus we have

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

Applying this bound within equation (9), we obtain:

$$y_{ij} + \sum_{h \in A_k, (h,j) \in Q, h \neq i} y_{hj} + \sum_{h \in A_k, (j,h) \in Q, h \neq i} y_{jh} = x_j \iff y_{ij} \geq x_i + x_j - 1$$

If all the right hand sides of the original equations are equal to two and the products to be induced are exactly those given by $A_k \times A_k$ for all $k \in K$, we obtain another important special case where the equations induced by conditions (1) and (2) imply the inequalities (1), (2), and (3) also for fractional solutions. We will see an example application where this case occurs in practice in Sect. 3.2.

**Theorem 5.** If, for all $k \in K$, (i) $d^k_i = 1$ for all $i \in A_k$, (ii) $b^k = 2$, (iii) $B_k = A_k$, and the Conditions (1) and (2) are satisfied, 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 $y_{ij} \geq x_i + x_j - 1$ hold for all $(i, j) \in Q$, $i \neq j$.

**Proof.** Due to (iii), the induced equations (7) look like:

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

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:

$$\sum_{h \in A_k, h < j} y_{hj} + \sum_{h \in A_k, j < h} y_{jh} = x_j \quad \text{for all } j \in A_k, \text{ for all } k \in K \quad (8)$$

These equations establish inequalities (1) and (2) for all $y_{ij}$, $(i, j) \in Q$, $i \neq j$. Combining them with the original equations $\sum_{j \in A_k} x_j = 2$ yields:

$$2 = \sum_{j \in A_k} x_j = \sum_{j \in A_k} \left( \sum_{h \in A_k, h < j} y_{hj} + \sum_{h \in A_k, j < h} y_{jh} \right) = 2 \sum_{j \in A_k} \sum_{h \in A_k, h < j} y_{hj}$$

It follows that $\sum_{j \in A_k} \sum_{h \in A_k, h < j} y_{hj} = 1$ holds even when $x$ is fractional. Since we have for all $y_{ij}$, $(i, j) \in Q$, $i \neq j$ that $\{i, j\} \subseteq A_k$ and, except $y_{ij}$, no two variables in the equations (8) expressed for $i$ and for $j$ coincide, we conclude:

$$x_i + x_j = \sum_{h \in A_k, i < h} y_{ih} + \sum_{h \in A_k, j < h} y_{hj} + \sum_{h \in A_k, j < h} y_{ih} + \sum_{h \in A_k, i < h} y_{hj} \leq 1$$

$$y_{ij} + \sum_{h \in A_k, i < h} y_{hj} + \sum_{h \in A_k, j < h} y_{ih} \leq y_{ij} + 1$$

\[\square\]
For the general setting of linear equations, we shall now clarify on how to obtain a set \( Q \supseteq P \) as compact as possible and how to induce also a minimum number of additional linearization equations by minimizing \( \sum_{k \in K} |B_k| \). This works in the same fashion as presented in [Mallach 2017] for the case of assignment constraints. While the approach possibly involves creating more linearization variables as originally demanded by the set \( P \), the number of equations will typically be considerably smaller than it would be with the ‘standard’ approach as is discussed by Liberti (2007). Depending on \( P \) and the overlap among the sets \( A_k, k \in K \), the conditions [1] and [2] impose a certain minimum on the sum of cardinalities \( \sum_{k \in K} |B_k| \) and hence on the number of equations. Different solutions achieving this minimum may lead to different cardinalities of \( |Q| \).

In general, it is even possible that a minimum \( |Q| \) can only be achieved by adding more than a minimum number of equations. But, in practice, this is seldom the case as adding equations rather induces more variables.

A consistent linearization of minimum size can be computed by solving the following mixed-integer program that reduces to a linear program with totally unimodular constraint matrix whenever \( A_k \cap A_\ell = \emptyset \), for all \( k, \ell \in K, \ell \neq k \).

\[
\begin{align*}
\min w_{eqn} \left( \sum_{k \in K} \sum_{1 \leq i \leq n} z_{ik} \right) + w_{var} \left( \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq n} f_{ij} \right) \\
\text{s.t.} & \quad f_{ij} = 1 \quad \text{for all } (i, j) \in P \tag{9} \\
& \quad f_{ij} \geq z_{jk} \quad \text{for all } k \in K, i \in A_k, j \in N, i \leq j \tag{10} \\
& \quad f_{ij} \geq z_{jk} \quad \text{for all } k \in K, i \in A_k, j \in N, j < i \tag{11} \\
& \quad \sum_{k \in A_k} z_{jk} \geq f_{ij} \quad \text{for all } 1 \leq i \leq j \leq n \tag{12} \\
& \quad \sum_{j \in A_k} z_{jk} \geq f_{ij} \quad \text{for all } 1 \leq i \leq j \leq n \tag{13} \\
& \quad f_{ij} \in [0, 1] \quad \text{for all } 1 \leq i \leq j \leq n \\
& \quad z_{ik} \in \{0, 1\} \quad \text{for all } k \in K, 1 \leq i \leq n
\end{align*}
\]

The formulation involves binary variables \( z_{ik} \) to be equal to 1 if \( i \in B_k \) and equal to zero otherwise. Further, to account for whether \( (i, j) \in Q \), there is a (continuous) variable \( f_{ij} \) for all \( 1 \leq i \leq j \leq n \) that will be equal to 1 in this case and 0 otherwise. The constraints [9] 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 [10] and [11]. Finally, if \( (i, j) \in Q \), then we require Conditions [1] and [2] to be satisfied, namely that there is a \( k \in K \) such that \( i \in A_k \) and \( j \in B_k \) [12] and a (possibly different) \( k \in K \) such that \( j \in A_k \) and \( i \in B_k \) [13]. The weights \( w_{var} \) and \( w_{eqn} \) of the objective function allow to find the best compromise between a minimum number of variables and a minimum number of equations. A rational choice would be to set \( w_{var} = 1 \) and \( w_{eqn} > \max_{k \in K} |A_k| \). This results in a solution with a minimum number of additional equations that, among these, also induces a minimal number of additional variables.

In the mentioned case of disjoint supports, i.e., \( A_k \cap A_\ell = \emptyset \), for all \( k, \ell \in K, \ell \neq k \), the unique minimum-cardinality sets \( B_k \) satisfying conditions [1] and [2] for all \( (i, j) \in Q \) can as well be computed by a combinatorial algorithm as presented in [Mallach 2017].
So while it is possible to carry out the linearization problem in a very general form algorithmically (e.g. as part of a preprocessing step of a solver), the (most) compact linearization associated to a particular problem formulation is typically ‘recognized’ easily by hand as we will see exemplary in the following section.

3 Applications

In this section, we highlight some prominent quadratic combinatorial optimization problems where linearizations found earlier appear as special cases of the proposed compact linearization technique.

3.1 Quadratic Assignment Problem

As discussed by Liberti (2007), the linearization of the Koopmans-Beckmann formulation for the quadratic assignment problem as presented by Frieze and Yadegar (1983) is exactly the one that results when applying the compact linearization technique to it.

3.2 Symmetric Quadratic Traveling Salesman Problem

In the form as discussed by Fischer and Helmberg (2013), the symmetric quadratic traveling salesman problem asks for a tour \( T \) 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 \( \{i, j\} \in T \)) is minimized. Consider the following mixed-integer programming formulation for this problem that is oriented at the integer programming formulation for the linear traveling salesman problem by Dantzig et al. (1954).

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

In the context of the compact linearization approach proposed, we consider the linear equations \([14]\) where we have \( K = V, A_k = \{jk \mid j < k \} \in E, c_{ij} = 1 \) for all \( i \in A_k \) and \( b^k = 2 \) for all \( k \in K \). Since we are interested in the bilinear terms of the form as in \([15]\), i.e. 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 \([5]\) and obtain the equations:

\[
\sum_{\{i, j\} \in E} x_{ij}x_{jk} = 2x_{jk} \quad \text{for all } \{j, k\} \in E, \text{ for all } j \in V
\]
After introducing linearization variables with indices ordered as desired, these are resolved as:

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

Each of these equations induces one variable more than originally demanded which is $y_{jk}$ as the linearized substitute for the square term $x_{jk}^2$. Since this product is zero if $x_{jk} = 0$ and equal to one if $x_{jk} = 1$, we may safely subtract $y_{jk}$ from the left and $x_{jk}$ from the right hand side and obtain

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

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

4 Conclusion

We showed that the compact linearization approach can be applied not only to binary quadratic problems with assignment constraints, but to those with arbitrary linear equations with positive coefficients. We discussed two special cases under which the continuous relaxation of the obtained compactly linearized problem formulation is provably as least as strong as the one obtained with an ordinary linearization. This is true for the original case of assignment constraints, but also for another setting where the right hand sides of the equations are equal to two. Finally, we highlighted previously found linearizations that appear as special cases of the proposed compact linearization technique, namely the one by Frieze and Yadegar found for the quadratic assignment problem, and the one by Fischer and Helmberg for the symmetric quadratic traveling salesman problem.

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