Discrete Optimization

Parametric convex quadratic relaxation of the quadratic knapsack problem

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\textbf{A B S T R A C T}

We consider a parametric convex quadratic programming (CQP) relaxation for the quadratic knapsack problem (QKP). This relaxation maintains partial quadratic information from the original QKP by perturbing the objective function to obtain a concave quadratic term. The nonconcave part generated by the perturbation is then linearized by a standard approach that lifts the problem to matrix space. We present a primal-dual interior point method to optimize the perturbation of the quadratic function, in a search for the tightest upper bound for the QKP. We prove that the same perturbation approach, when applied in the context of semidefinite programming (SDP) relaxations of the QKP, cannot improve the upper bound given by the corresponding linear SDP relaxation. The result also applies to more general integer quadratic problems. Finally, we propose new valid inequalities on the lifted matrix variable, derived from cover and knapsack inequalities for the QKP, and present separation problems to generate cuts for the current solution of the CQP relaxation. Our best bounds are obtained alternating between optimizing the parametric quadratic relaxation over the perturbation and applying cutting planes generated by the valid inequalities proposed.

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1. Introduction

We study a convex quadratic programming (CQP) relaxation of the quadratic knapsack problem (QKP),

\begin{equation}
\begin{aligned}
P_{\text{QKP}}^C := \max_{x \in \mathbb{R}^n} & \quad x^T Q x \\
\text{s.t.} & \quad W x \leq c,
\end{aligned}
\end{equation}

where \(Q \in \mathbb{S}^n\) is a symmetric \(n \times n\) nonnegative integer profit matrix, \(W \in \mathbb{Z}^{n \times n}\) is a vector of positive integer weights for the items, and \(c \in \mathbb{Z}^n\) is the knapsack capacity with \(c_i \geq w_i\) for all \(i \in \mathbb{N} := \{1, \ldots, n\}\). The binary (vector) variable xindicates which items are chosen for the knapsack, and the inequality in the model, known as a knapsack inequality, ensures that the selection of items does not exceed the knapsack capacity. We note that any linear costs in the objective can be included on the diagonal of \(Q\) by exploiting the \(\{0,1\}\) constraints and, therefore, are not considered.

The QKP was introduced in Gallo, Hammer, and Simeone (1980) and was proved to be NP-Hard in the strong sense by reduction from the clique problem. The quadratic knapsack problem is a generalization of the knapsack problem, which has the same feasible set of the QKP, and a linear objective function in \(x\). The linear knapsack problem can be solved in pseudo-polynomial time using dynamic programming approaches with complexity of \(O(nc)\).

The QKP appears in a wide variety of fields, such as biology, logistics, capital budgeting, telecommunications and graph theory, and has received a lot of attention in the last decades. Several papers have proposed branch-and-bound algorithms for the QKP, and the main difference between them is the method used to obtain upper bounds for the subproblems (Billionnet & Calmels, 1996; Billionnet, Fay& Soutif, 1999; Caprara, Pisinger, & Toth, 1999; Chaillou, Hansen, & Mahieu, 1989; Helmberg, Rendl, & Weismantel, 1996; 2000). The well known trade-off between the strength of the bounds and the computational effort required to obtain them is intensively discussed in Pisinger (2007), where semidefinite programming (SDP) relaxations proposed in Helmberg et al. (1996) and Helmberg, Rendl, and Weismantel (2000) are presented as the strongest relaxations for the QKP. The linear programming (LP) relaxation proposed in Billionnet and Calmels (1996), on the other side, is presented as the most computationally inexpensive.

Both the SDP and the LP relaxations have a common feature, they are defined in the symmetric matrix lifted space determined by the equation \(X = xx^T\), and by the replacement of
the quadratic function in \textbf{QKP} with a linear function in \( X \), namely, \( \text{trace}(QX) \). As the constraint \( X = xx^T \) is nonconvex, it is relaxed by convex constraints in the relaxations. The well known McCormick inequalities [McCormick, 1976], and also the semidefinite constraint, \( X - xx^T \succeq 0 \), have been extensively used to relax the nonconvex constraint \( X = xx^T \), in relaxations of the QKP.

In this paper, we investigate a CQP relaxation for the QKP, where instead of linearizing the objective function, we perturb the objective function Hessian \( Q \), and maintain the (concave) perturbed version of the quadratic function in the objective, linearizing only the remaining part derived from the perturbation. Our relaxation is a parametric convex quadratic problem, defined as a function of a matrix parameter \( Q_p \), such that \( Q - Q_p \succeq 0 \). This matrix parameter is iteratively optimized by a primal-dual interior point method (IPM) to generate the best possible bound for the QKP. During this iterative procedure, valid cuts are added to the formulation to strengthen the relaxation, and the search for the best perturbation is adapted accordingly. Our procedure alternates between optimizing the matrix parameter and applying cutting planes generated by valid inequalities. At each iteration of the procedure, a new bound for the QKP is computed, considering the updated matrix parameter and the cuts already added to the relaxation.

In Billionnet, Elloumi, and Lambert (2016) (see also Billionnet, Elloumi, & Lambert, 2012; Billionnet, Elloumi, & Plateau, 2009 for previous results), a similar parametric convex quadratic problem was investigated for the more general problem of minimizing a quadratic function of bounded integer variables subject to a set of quadratic constraints. However, the authors consider a unique perturbation of the Hessian of each quadratic function in the model, to reformulate it as a mixed integer quadratic programming (MIQP) problem with a CQP continuous relaxation. They propose to solve the reformulated problem by an MIQP solver. To reformulate the problem, the authors also seek the best possible perturbations of the Hessians, which are considered as the ones, such that the solution of the continuous relaxation of the MIQP is maximal. In other words, they seek perturbations that lead to the best bound at the root node of a branch-and-bound algorithm. The authors claim that these perturbations can be computed from an optimal dual solution of a standard SDP relaxation of the problem. However, the dual SDP problem is not correctly formulated in the paper, and the proof presented is not correct. In this paper, we prove the result following the idea presented in Billionnet et al. (2009), which is based on Lemarchal and Oustry (1999, Theorem 4.4). Furthermore, we show that the result is valid to the more general problem where the feasible set is any bounded polyhedron with nonempty interior. We also note that, if no cuts are added to the relaxation during the iterations of our interior point method, it becomes an alternative way of obtaining the optimal perturbation considered in Billionnet et al. (2016).

Another similar approach to handle nonconvex quadratic functions consists in decomposing it as a difference of convex (DC) quadratic function (Horst & Thaoi, 1999). DC decompositions have been extensively used in the literature to generate convex quadratic relaxations of nonconvex quadratic problems. See, for example, Fampa, Lee, and Melo (2017) and references therein. Unlike the approach used in DC decompositions, we do not necessarily decompose \( x^TQx \) as a difference of convex functions, or equivalently, as a sum of a convex and a concave function. Instead, following the approach introduced in Billionnet et al. (2016), we decompose it as a sum of a concave function and a quadratic term derived from the perturbation applied to \( Q \). This perturbation can be any symmetric matrix \( Q_p \), such that \( Q - Q_p \succeq 0 \).

In an attempt to obtain stronger bounds, we also investigated the parametric convex quadratic SDP problem, where we add to our CQP relaxation, the positive semidefinite constraint \( X - xx^T \succeq 0 \). An IPM could also be applied to this parametric problem in order to generate the best possible bound. Nevertheless, we prove an interesting result concerning the relaxations, in case the constraint \( X - xx^T \succeq 0 \) is imposed: the tightest bound generated by the parametric quadratic SDP relaxation is obtained when the perturbation \( Q_p \) is equal to \( Q \), or equivalently, when we linearize the entire objective function, obtaining the standard linear SDP relaxation. We conclude, therefore, that keeping the (concave) perturbed version of the quadratic function in the objective of the SDP relaxation does not lead to a tighter bound. A result that could be derived from our analysis is that the CQP relaxation cannot generate a tighter bound than the standard linear SDP relaxation. This result was already proved in Billionnet et al. (2016), and we show that it still holds for unbounded and nonconvex feasible set.

Another contribution of this work is the development of valid inequalities for the CQP relaxation on the lifted matrix variable. The inequalities are first derived from cover inequalities for the knapsack problem. The idea is then extended to knapsack inequalities. Taking advantage of the lifting \( X := xx^T \), we propose new valid inequalities that can also be applied to more general relaxations of binary quadratic programming problems that use the same lifting. We discuss how cuts for the quadratic relaxation can be obtained by the solution of separation problems, and investigate possible dominance relation between the inequalities proposed.

Finally, we present an algorithmic framework, where we iteratively improve the upper bound for the QKP by optimizing the choice of the perturbation of the objective function and adding cutting planes to the relaxation. At each iteration, lower bounds for the problem are also generated from feasible solutions constructed from a rank-one approximation of the solution of the CQP relaxation.

In Section 2, we introduce our parametric convex quadratic relaxation for the QKP. In Section 3, we explain how we optimize the parametric problem over the perturbation of the objective; i.e., we present the IPM applied to obtain the perturbation that leads to the best possible bound. In Section 4, we present our conclusion about the parametric quadratic SDP relaxation, and relate our results to the results presented in Billionnet et al. (2016). In Section 5, we introduce new valid inequalities on the lifted matrix variable of the convex quadratic model, and we describe how cutting planes are obtained by the solution of separation problems. In Section 6, we present the heuristic used to generate lower bounds to the QKP. In Section 7, we discuss our numerical experiments and in Section 8, we present our final remarks.

**Notation**

If \( A \in \mathbb{S}^n \), then \( \text{svec}(A) \) is a vector whose entries come from \( A \) by stacking up its ‘lower half’, i.e.,

\[
\text{svec}(A) := (a_{11}, \ldots, a_{11}, a_{22}, \ldots, a_{n2}, \ldots, a_{nn})^T \in \mathbb{R}^{n(n+1)/2}.
\]

The operator \( \text{sMat} \) is the inverse of \( \text{svec} \), i.e., \( \text{sMat}(\text{svec}(A)) = A \).

We also denote by \( \lambda_{\min}(A) \), the smallest eigenvalue of \( A \) and by \( \lambda_{i}(A) \) the \( i \)-th largest eigenvalue of \( A \).

To facilitate the reading of the paper, Table 1 relates the acronyms used with the associated equations numbers.

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Equation Number</th>
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<tbody>
<tr>
<td>QKP</td>
<td>(1)</td>
</tr>
<tr>
<td>QP,full</td>
<td>(2)</td>
</tr>
<tr>
<td>LPR</td>
<td>(3)</td>
</tr>
<tr>
<td>CQP</td>
<td>(5)</td>
</tr>
<tr>
<td>LSDP</td>
<td>(21)</td>
</tr>
<tr>
<td>QSDP</td>
<td>(15)</td>
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<tr>
<td>CI</td>
<td>(27)</td>
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<tr>
<td>ECI</td>
<td>(28)</td>
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<tr>
<td>LCI</td>
<td>(29)</td>
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<tr>
<td>SCI</td>
<td>(32)</td>
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<tr>
<td>CHS</td>
<td>(34)</td>
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<td>SCILS</td>
<td>(36)</td>
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<tr>
<td>SKILS</td>
<td>(41)</td>
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We also show the standard abbreviations used in the paper in Table 2.

2. A parametric convex quadratic relaxation

In order to construct a convex relaxation for QKP, we start by considering the following standard reformulation of the problem in the lifted space of symmetric matrices, defined by the lifting $X := xx^T$.

\[
p_{\text{QKP, lift}} := \max_{X \in \mathbb{S}^n} \text{trace}(QX) \quad \text{s.t.} \quad w^TX \leq c, \quad X = xx^T, \quad x \in \{0, 1\}^n. \tag{2}
\]

We consider an initial LP relaxation of QKP, given by

\[
\max_{(x,X) \in \mathcal{P}} \text{trace}(QX) \quad \text{s.t.} \quad (x,X) \in \mathcal{P},
\]

where $\mathcal{P} \subseteq \{0, 1\}^n \times \mathbb{S}^n$ is a bounded polyhedron, such that $\{(x,X) : w^TX \leq c, X = xx^T, x \in \{0, 1\}^n \} \subseteq \mathcal{P}$.

2.1. The perturbation of the quadratic objective

Next, we propose a convex quadratic relaxation with the same feasible set as LPR, but maintaining a concave perturbed version of the quadratic objective function of QKP, and linearizing only the remaining nonconcave part derived from the perturbation. More specifically, we choose $Q_p \in \mathbb{S}^n$ such that $Q - Q_p \succeq 0$, and we get

\[
x^T(Q - Q_p)x + \text{trace}(Q_pxx^T) = x^T(Q - Q_p)x + \text{trace}(Q_pX).
\]

Finally, we define the parametric convex quadratic relaxation of QKP:

\[
p_{\text{CQP}}(Q_p) := \max_{(x,X) \in \mathcal{P}} x^T(Q - Q_p)x + \text{trace}(Q_pXX^T)
\]

3. Optimizing the parametric problem over the parameter $Q_p$

The upper bound $p_{\text{CQP}}(Q_p)$ in the convex quadratic problem CQP depends on the feasible perturbation $Q_p$ of the Hessian $Q$. To find the best upper bound, we consider the parametric problem

\[
\text{param}^{\text{CQP}} := \min_{Q - Q_p \succeq 0} p_{\text{CQP}}(Q_p).
\]

We solve (6) with a primal-dual interior-point method (IPM), and we describe in this section how the search direction of the algorithm is obtained at each iteration.

We start with minimizing a log-barrier function. We use the barrier function $B_{\mu}(Q_p, Z)$ with barrier parameter $\mu > 0$, to obtain the barrier problem

\[
\min_{Q - Q_p \succeq 0} B_{\mu}(Q_p, Z) := p_{\text{CQP}}(Q_p) - \mu \log \det Z \quad \text{s.t.} \quad Z > 0, \quad Z \succeq 0.
\]

where $Z \in \mathbb{S}^n$ and $\Lambda \in \mathbb{S}^n$ denote, respectively, the slack and the dual symmetric matrix variables. We consider the Lagrangian function

\[
L_{\mu}(Q_p, Z, \Lambda) := p_{\text{CQP}}(Q_p) - \mu \log \det Z + \text{trace}((Q - Q_p + Z)\Lambda).
\]

Some important points should be emphasized here. We first note that the objective function for $p_{\text{CQP}}(Q_p)$ is linear in $Q_p$, i.e., this function is the maximum of linear functions over feasible points $x, X$. Therefore, this is a convex function.

Moreover, as will be detailed next, the search direction of the IPM, computed at each iteration of the algorithm, depends on the optimum solution $x = x(Q_p), X = X(Q_p)$ of CQP, for a fixed matrix $Q_p$. At each iteration of the IPM, we have $Z \succ 0$, and therefore $Q - Q_p \prec 0$. Thus, problem CQP maximizes a strictly concave quadratic function, subject to linear constraints over a compact set $\mathcal{P}$, and consequently, has a unique optimal solution (see e.g. Turlach & Wright, 2015). From standard sensitivity analysis results, e.g. Facco (1983, Corollary 3.4.2), Hogan (1973), and Danskin (1966, Theorem 1), as the optimal solution $x = x(Q_p), X = X(Q_p)$ is unique, the function $p_{\text{CQP}}(Q_p)$ is differentiable, and therefore, the Lagrangian function is also differentiable.

Since $Q_p$ appears only in the objective function in CQP, and

\[
x^T(Q - Q_p)x + \text{trace}(Q_pXX^T) = x^TQx + \text{trace}(Q_pX(x - xx^T)),
\]

we have

\[
\nabla p_{\text{CQP}}(Q_p) = x - xx^T.
\]

The optimality conditions for (7) are obtained by differentiating the Lagrangian $L_{\mu}$ with respect to $Q_p, \Lambda, Z$, respectively,

\[
\begin{align*}
\frac{\partial L_{\mu}}{\partial Q_p} &= \nabla p_{\text{CQP}}(Q_p) - \Lambda = 0, \\
\frac{\partial L_{\mu}}{\partial \Lambda} &= Q - Q_p + Z = 0, \\
\frac{\partial L_{\mu}}{\partial Z} &= -\mu Z^{-1} = 0 \quad \text{or} \quad Z \Lambda - \mu I = 0.
\end{align*}
\]

This gives rise to the nonlinear system

\[
G_{\mu}(Q_p, \Lambda, Z) = \left(\begin{array}{c}
Q - Q_p + Z \\
Z \Lambda - \mu I
\end{array}\right) = 0, \quad Z, \Lambda > 0.
\]

We use a BFGS approximation for the Hessian of $p_{\text{CQP}}$, since it is not guaranteed to be twice differentiable everywhere, and update it at each iteration (see Lewis & Overton, 2013). We denote the approximation of $\nabla^2_{BFGS} p_{\text{CQP}}(Q_p)$ by $B$, and begin with the approximation $B_0 = I$. Recall that if $Q_p^k, Q_p^{k+1}$ are two successive iterates with gradients $\nabla p_{\text{CQP}}(Q_p^k), \nabla p_{\text{CQP}}(Q_p^{k+1})$, respectively, with current Hessian approximation $B_k \in \mathbb{S}^{n(n+1)/2}$, then we set

\[
Y_k := \nabla p_{\text{CQP}}(Q_p^{k+1}) - \nabla p_{\text{CQP}}(Q_p^k),
\]

\[
S_k := Q_p^{k+1} - Q_p^k
\]

and,

\[
\omega := (Y_k, S_k), \quad \omega := \{\text{svec}(S_k), B_k \text{svec}(S_k)\}.
\]

Finally, we update the Hessian approximation with

\[
B_{k+1} := B_k + \frac{1}{\omega} (\text{svec}(Y_k) \text{svec}(Y_k) - \frac{1}{\omega} B_k \text{svec}(S_k) \text{svec}(S_k)^T B_k).
\]

We note that the curvature condition $\omega > 0$ should be verified to guarantee the positive definiteness of the updated Hessian. In our implementation, we address this by skipping the BFGS update when $\omega$ is negative or too close to zero.

The equation for the search direction is

\[
G_{\mu}(Q_p, \Lambda, Z) \begin{pmatrix} \Delta Q_p \\ \Delta \Lambda \\ \Delta Z \end{pmatrix} = -G_{\mu}(Q_p, \Lambda, Z).
\]

Table 2

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>CQP</td>
<td>Convex Quadratic Programming</td>
</tr>
<tr>
<td>QKP</td>
<td>Quadratic Knapsack Problem</td>
</tr>
<tr>
<td>SDP</td>
<td>Semidefinite Programming</td>
</tr>
<tr>
<td>MIQP</td>
<td>Mixed Integer Quadratic Programming</td>
</tr>
<tr>
<td>MILP</td>
<td>Mixed Integer Linear Programming</td>
</tr>
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</table>
where
\[ G_{\mu}(Q_p, Z) = \begin{pmatrix} \nabla p^*_\text{CP}(Q_p) - \Lambda \\ Q - Q_p + Z \\ Z \Lambda - \mu I \end{pmatrix} \] = \begin{pmatrix} R_d \\ R_p \\ R_c \end{pmatrix}. \tag{12} \]

If \( B \) is the current estimate of the Hessian, then (11) becomes
\[ \begin{align*}
&\begin{bmatrix}
\text{sMat}(B \text{ svec}(\Delta Q_p)) - \Delta \Lambda = -R_d, \\
-\Delta Q_p + \Delta Z = -R_p, \\
Z \Delta \Lambda + Z \Delta Z = -R_c
\end{bmatrix}
\end{align*} \]

We can substitute for the variables \( \Delta \Lambda \) and \( \Delta Z \) in the third equation of the system. The elimination gives us a simplified system, and therefore, we apply it, using the following two equations for elimination and backsolving,
\[ \Delta \Lambda = \text{sMat}(B \text{ svec}(\Delta Q_p)) + R_d, \quad \Delta Z = -R_p + \Delta Q_p. \tag{13} \]

Accordingly, we have a single equation to solve, and the system finally becomes
\[ Z \text{sMat}(B \text{ svec}(\Delta Q_p)) + (\Delta Q_p) \Lambda = -R_c - ZR_d + R_p \Lambda. \]

We emphasize that to compute the search direction at each iteration of our IPM, we need to update the residuals defined in (12), and therefore we need the optimal solution \( x = x(Q_p), X = X(Q_p) \) of the convex quadratic relaxation \( \text{CQP}_{Q_p} \) for the current perturbation \( Q_p \). Problem \( \text{CQP}_{Q_p} \) is thus solved at each iteration of the IPM method, each time for a new perturbation \( Q_p \), such that \( Q - Q_p < \epsilon \).

In Algorithm 1, we present in details an iteration of the IPM. The algorithm is part of the complete framework used to generate bounds for \( \text{QKP} \), as described in Section 7.

**Remark 1.** Algorithm is an interior-point method with a quasi-Newton step (BFGS). The object function we are minimizing is differentiable with exception possibly at the optimum. A complete convergence analysis of the algorithm is not in the scope of this paper, however, convergence analysis for some similar problems can be found in the literature. In Armand, Gilber, and Jégou (2000), it is shown that if the objective function is always differentiable and strongly convex, then it is globally convergent to the analytic center of the primal-dual optimal set when \( \mu \) tends to zero and strict complementarity holds.

### 4. The parametric quadratic SDP relaxation

In an attempt to obtain tighter bounds, a promising approach might seem to be to include the positive semidefinite constraint \( X - xx^T \succeq 0 \) in our parametric quadratic relaxation \( \text{CQP}_{Q_p} \), and solve a parametric convex quadratic SDP relaxation, also using an IPM. Nevertheless, we show in this section that the convex quadratic SDP relaxation cannot generate a better bound than the linear SDP relaxation, obtained when we set \( Q_0 \) equal to \( Q \). In fact, as shown below, the result applies not only to the QKP, but to more general problems as well. We emphasize here that the same result does not apply for \( \text{CQP}_{Q_p} \). We could observe with our computational experiments that the best bounds were obtained by \( \text{CQP}_{Q_p} \), when we had \( Q - Q_p \neq 0 \), for all instances considered.

Consider the linear SDP problem given by
\[ \begin{align*}
\min \quad & p_{\text{LSDP}} := \sup \quad \text{trace}(QX) \\
\text{s.t.} \quad & (x, X) \in \mathcal{F} \\
& X - xx^T \succeq 0,
\end{align*} \tag{14} \]

where \( x \in \mathbb{R}^n \), \( X \in \mathbb{S}^n \), and \( \mathcal{F} \) is any subset of \( \mathbb{R}^n \times \mathbb{S}^n \).

#### Algorithm 1: Updating the perturbation \( Q_p \)

**Input:** \( k, Q_p^k, Z^k, \Lambda^k, x(Q_p^k), X(Q_p^k), \nabla p^*_\text{CP}(Q_p^k), B_k, \mu^k, \tau_\mu := 0.95, \tau_\mu := 0.9. \)

**Compute the residuals:**
\[ \begin{bmatrix}
R_d \\
R_p \\
R_c
\end{bmatrix} := \begin{bmatrix}
\nabla p^*_\text{CP}(Q_p^k) - \Lambda^k \\
Q - Q_p^k + Z^k \\
Z^k \Lambda^k - \mu^k I
\end{bmatrix}. \]

**Solve the linear system for \( \Delta Q_p^k \):**
\[ Z^k \text{sMat}(B_k \text{ svec}(\Delta Q_p^k)) + (\Delta Q_p^k) \Lambda^k = -R_c - Z^k R_d + R_p \Lambda^k. \]

Set:
\[ \Delta \Lambda := \text{sMat}(B_k \text{ svec}(\Delta Q_p^k)) + R_d, \quad \Delta Z := -R_p + \Delta Q_p^k. \]

Update \( Q_p, Z \) and \( \Lambda \):
\[ Q_p^{k+1} := Q_p^k + \alpha_p \Delta Q_p^k, \quad Z^{k+1} := Z_p^k + \alpha_p \Delta Z, \quad \Lambda^{k+1} := \Lambda^k + \alpha_d \Delta \Lambda, \]
where
\[ \alpha_p := \tau_\mu \times \min\{1, \arg \max_{\alpha \in [0, 1]} \{Z^k + \alpha \Delta Z \geq 0\} \}, \]
\[ \alpha_d := \tau_\mu \times \min\{1, \arg \max_{\alpha \in [0, 1]} \{ \Lambda^k + \alpha \Delta \Lambda \geq 0 \} \}. \]

Obtain the optimal solution \( x(Q_p^{k+1}), X(Q_p^{k+1}) \) of relaxation \( \text{CQP}_{Q_p^k} \), where \( Q_p := Q_p^{k+1} \).

**Update the gradient of \( p^*_\text{CP} \):**
\[ \nabla p^*_\text{CP}(Q_p^{k+1}) := x(Q_p^{k+1}) - x(Q_p^k)X(Q_p^k)X(Q_p^{k+1})^T. \]

**Update the Hessian approximation of \( p^*_\text{CP} \) (if \( v > 0 \)):**
\[ Y_k := \nabla^2 p^*_\text{CP}(Q_p^{k+1}) - \nabla^2 p^*_\text{CP}(Q_p^k), \quad S_k := Q_p^{k+1} - Q_p^k, \quad v := \| Y_k \|_2, \quad \omega := \text{svec}(S_k), \quad B_k := \text{svec}(S_k)^T S_k. \]

Update \( \mu^k \):
\[ \mu^{k+1} := \tau \mu \frac{\text{trace}(Z^{k+1} \Lambda^{k+1})}{\| S_k \|_2}. \]

**Output:** \( Q_p^{k+1}, Z^{k+1}, \Lambda^{k+1}, x(Q_p^{k+1}), X(Q_p^{k+1}), \nabla p^*_\text{CP}(Q_p^{k+1}), B_k, \mu^{k+1} \).

We now consider the parametric SDP problem given by
\[ p^*_{\text{SDP}_{Q_p}} := \sup_{X \in \mathbb{S}^n} \text{trace}(Q X) \quad \text{s.t.} \quad (x, X) \in \mathcal{F}, \quad X - xx^T \succeq 0, \tag{15} \]

where \( Q - Q_p \succeq 0 \).

**Theorem 2.** Let \( \mathcal{F} \) be any subset of \( \mathbb{R}^n \times \mathbb{S}^n \). For any choice of matrix \( Q_p \) satisfying \( Q - Q_p \preceq 0 \), we have
\[ p^*_{\text{SDP}_{Q_p}} \geq p^*_{\text{LSDP}}. \tag{16} \]

Moreover, \( \inf [p^*_{\text{SDP}_{Q_p}} : Q - Q_p \preceq 0] = p^*_{\text{LSDP}}. \)

**Proof.** Let \( (\bar{x}, \bar{X}) \) be a feasible solution for \( \text{LSDP} \). We have
\[ p^*_{\text{SDP}_{Q_p}} \geq \bar{x}^T (Q - Q_p) \bar{x} + \text{trace}(Q_p \bar{X}). \tag{17} \]
\[ L(x, X, y) := x^T Q x + \text{trace}(Q_pX) \]
\[ + \sum_{k=1}^{q} y_k^T (b_k - \text{trace}(\Gamma_k X) - \gamma_k^T x). \]

The Lagrangian dual function is then defined as
\[ g(y) := \max_{x \in F} L(x, X, y) \]
\[ = \max_{x \in F} x^T Q x + \text{trace}(Q_pX) + \sum_{k=1}^{q} y_k (b_k - \text{trace}(\Gamma_k X) - \gamma_k^T x) \]
\[ = \max_{x \in F} \text{trace} \left( Q - \sum_{k=1}^{q} y_k \Gamma_k X \right) x^T + x^T Q_pX - \sum_{k=1}^{q} y_k b_k \]
\[ = \max_{x \in F} \left[ x^T Q x - \sum_{k=1}^{q} y_k \Gamma_k^T x + \sum_{k=1}^{q} y_k b_k \right] \]
\[ + \infty, \quad \text{if } Q_p - \sum_{k=1}^{q} y_k \Gamma_k = 0, \]
\[ = \left[ \sum_{k=1}^{q} y_k \right] Q_p \]
\[ + \infty, \quad \text{if } Q_p - \sum_{k=1}^{q} y_k \Gamma_k = 0 \text{ and } \sum_{k=1}^{q} y_k \gamma_k \in \text{range}(Q_p). \]

where \( Q_p \) is the pseudo-inverse of \( Q_p \).

As \( F \) has nonempty interior, the Slater condition holds for the inner maximization problem in (22). Therefore, problem (22) has the same optimal value as
\[ \min_{Q_p, y, \gamma} -\frac{1}{2} \left( \sum_{k=1}^{q} y_k \gamma_k \right)^T Q_p \left( \sum_{k=1}^{q} y_k \gamma_k \right) + y^T b \]
\[ \text{s.t. } Q_p - \sum_{k=1}^{q} y_k \Gamma_k = 0, \]
\[ \sum_{k=1}^{q} y_k \gamma_k \in \text{range}(Q_p), \]
\[ Q_p - Q_p \geq 0, \quad y \geq 0. \]

which is equivalent to
\[ \max_{t, Q_p, y} t \]
\[ \text{s.t. } \frac{1}{2} \left( \sum_{k=1}^{q} y_k \gamma_k \right)^T (Q - Q_p) \left( \sum_{k=1}^{q} y_k \gamma_k - y^T b - t \geq 0, \right. \]
\[ Q - Q_p \leq 0, \]
\[ \sum_{k=1}^{q} y_k \gamma_k \in \text{range}(Q - Q_p), \]
\[ Q_p - \sum_{k=1}^{q} y_k \Gamma_k = 0, \]
\[ y \geq 0. \]

By Schur complement (Horn & Zhang, 2005), this is equivalent to the following SDP problem
\[ \max_{t, Q_p, y} t \]
\[ \text{s.t. } \begin{bmatrix} -t - y^T b & \left( \sum_{k=1}^{q} y_k \gamma_k \right)^T / 2 \\ \sum_{k=1}^{q} y_k \gamma_k / 2 & Q_p - Q \end{bmatrix} \geq 0, \]
\[ Q_p - \sum_{k=1}^{q} y_k \Gamma_k = 0, \]
\[ y \geq 0. \]
After substitution, this is equivalent to

\[
\begin{aligned}
\min_{t, y} & \quad -t \\
\text{s.t.} & \quad \begin{bmatrix}
-t - y^T b & \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T / 2 \\
\left(\sum_{k=1}^{q} y_k \gamma_k\right)/ 2 & \sum_{k=1}^{q} y_k \Gamma_k - Q
\end{bmatrix} \begin{bmatrix}
y \\
z
\end{bmatrix} \geq 0 \\
y & \geq 0
\end{aligned}
\]

(23)

We can now derive the dual problem of (23), considering the Lagrangian function, defined as

\[
L(t, y, s, z, Z) = -t - \text{trace}\left(\begin{bmatrix}
s & z^T \\
z & Z
\end{bmatrix}\begin{bmatrix}
-t - y^T b & \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T / 2 \\
\left(\sum_{k=1}^{q} y_k \gamma_k\right)/ 2 & \sum_{k=1}^{q} y_k \Gamma_k - Q
\end{bmatrix}\begin{bmatrix}
y \\
z
\end{bmatrix}\right)
\]

\[
=-t - s(-t - y^T b) - \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T z - \text{trace}\left(\begin{bmatrix}
s & z^T \\
z & Z
\end{bmatrix}\begin{bmatrix}
-t - y^T b & \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T / 2 \\
\left(\sum_{k=1}^{q} y_k \gamma_k\right)/ 2 & \sum_{k=1}^{q} y_k \Gamma_k - Q
\end{bmatrix}\begin{bmatrix}
y \\
z
\end{bmatrix}\right)
\]

\[
=t(s - 1) + s y^T b - \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T z - \text{trace}\left(\begin{bmatrix}
s & z^T \\
z & Z
\end{bmatrix}\begin{bmatrix}
-t - y^T b & \left(\sum_{k=1}^{q} y_k \gamma_k\right)^T / 2 \\
\left(\sum_{k=1}^{q} y_k \gamma_k\right)/ 2 & \sum_{k=1}^{q} y_k \Gamma_k - Q
\end{bmatrix}\begin{bmatrix}
y \\
z
\end{bmatrix}\right)
\]

\[
=t(s - 1) + \sum_{k=1}^{q} y_k (sb_k - y_k^T z - \text{trace}(\Gamma_k Z)) + \text{trace}(QZ).
\]

The Lagrangian dual function is defined as

\[
h(s, z, Z) := \min_{y \geq b} L(t, y, s, z, Z)
\]

\[
= \min_{y \geq b} t(s - 1) + \sum_{k=1}^{q} y_k (sb_k - y_k^T z - \text{trace}(\Gamma_k Z)) + \text{trace}(QZ)
\]

\[
= \begin{cases}
\text{trace}(QZ) & \text{if } s = 1, \ \text{otherwise.}
\end{cases}
\]

Therefore, the dual problem of (23) is given by the maximization of the Lagrangian dual function over the SDP cone, as in

\[
\max_{y, z} \text{trace}(QZ)
\]

\[
\text{s.t.} \quad \text{trace}(\Gamma_k Z) + y_k^T z \leq b_k, \quad k = 1, \ldots, q,
\]

\[
\begin{bmatrix}
1 & z^T \\
z & Z
\end{bmatrix} \geq 0.
\]

(24)

We finally note that problems (24) and (21) are the same. Since \( \mathcal{F} \) has nonempty interior, then (21) is strictly feasible. Therefore, strong duality holds for problem (21), and the result of the theorem follows.

5. Valid inequalities

We are now interested in finding valid inequalities to strengthen relaxations of \( \text{QKP} \) in the lifted space determined by the lifting \( X := xx^T \). Let us denote by \( \text{CRel} \), any convex relaxation of \( \text{QKP} \) in the lifted space, where the equation \( X = xx^T \) was relaxed in some manner, by convex constraints, i.e., any convex relaxation of \( \text{QKP}_{\text{lifted}} \).

We note that if the inequality

\[
\tau^T x + b \leq \beta
\]

is valid for \( \text{QKP} \), where \( \tau \in \mathbb{Z}^n_+ \) and \( \beta \in \mathbb{R}_+ \), then, as xis nonnegative and \( X := xx^T \),

\[
(x X)(\frac{-\beta}{\tau}) \leq 0
\]

(26)

is a valid inequality for \( \text{QKP}_{\text{lifted}} \). In this case, we say that (26) is a valid inequality for \( \text{QKP}_{\text{lifted}} \) derived from the valid inequality (25) for \( \text{QKP} \).

5.1. Preliminaries: knapsack polytope and cover inequalities

We begin by recall the concepts of knapsack polytopes and cover inequalities.

The knapsack polytope is the convex hull of the feasible points of the knapsack problem,

\[
\text{KF} := \{ x \in \{0, 1\}^n : w^T x \leq c \}.
\]

Definition 5 (Zero-one knapsack polytope).

\[
\text{KPol} := \text{conv}(\text{KF}) = \text{conv}(\{ x \in \{0, 1\}^n : w^T x \leq c \})
\]

Proposition 6. The dimension

\[
\dim(\text{KPol}) = n.
\]

and \( \text{KPol} \) is an independence system, i.e.,

\[
x \in \text{KPol}, \ y \in \{0, 1\}^n, \ y \leq x \Rightarrow y \in \text{KPol}.
\]

Proof. Recall that \( w_i \leq c \forall i \). Therefore, all the unit vectors \( e_i \in \mathbb{R}^n \), as well as the zero vector, are feasible, and the first statement follows. The second statement is clear.

Cover inequalities were originally presented in Balas (1975), Wolsey (1975), see also Nemhauser and Wolsey (1988, Section II.2). These inequalities can be used in general optimization problems with knapsack inequalities and binary variables and, particularly, in \( \text{QKP} \).

Definition 7 (Cover inequality, CI). The subset \( C \subseteq N \) is a cover if it satisfies

\[
\sum_{j \in C} w_j > c.
\]

The (valid) CI is

\[
\sum_{j \in C} x_j \leq |C| - 1.
\]

(27)

A cover \( C \) is minimal if no proper subset of \( C \) is a cover.

Definition 8 (Extended CI, ECI). Let \( w^* := \max_{j \in C} w_j \) and define the extension of \( C \) as

\[
E(\text{C}) := C \cup \{ j \in N \setminus C : w_j \geq w^* \}.
\]

The ECI is

\[
\sum_{j \in E(\text{C})} x_j \leq |C| - 1.
\]

(28)

Definition 9 (Lifted CI, LCI). Given a cover \( C \), let \( \alpha_j \geq 0, \forall j \in N \setminus C \), and \( \alpha_j > 0 \), for some \( j \in N \setminus C \), such that

\[
\sum_{j \in C} x_j + \sum_{j \in N \setminus C} \alpha_j x_j \leq |C| - 1.
\]

(29)

is a valid inequality for \( \text{KF} \). Inequality (29) is a LCI.

Cover inequalities are extensively discussed in Hammer, Johnson, and Peled (1975), Balas and Nemhauser (1978), Balas (1975), Wolsey (1975), Nemhauser and Wolsey (1988), and Atamtürk (2005). Details about the computational complexity of \( \text{LCI} \) is presented in Nemhauser and Wolsey (1988), and Gu, Nemhauser, and Savelsbergh (1998). Algorithm 2 (Wolsey, 1998, p.17), shows how to lift a LCI. It provides a facet-defining inequality for \( \text{KPol} \) when \( C \) is a minimal cover and \( \bar{f} = 1 \).
Algorithm 2  Procedure to Lift Cover Inequalities.

Input: A cover $C$ and a valid inequality
\[ \sum_{j=1}^{t-1} \alpha_i x_i + \sum_{i \in C} x_i \leq |C| - 1. \]

for $\mathbf{KF}$, for some $t \in [1, r]$, where $r := |N \setminus C|$.
Sort the elements $i \in N \setminus C$ in ascending $w_i$ order, defining \{i_1, i_2, \ldots, i_t\}.
For: $t = 1$ to $r$

\[ \zeta_t = \max_{i \in C} \left\{ \sum_{j=1}^{t-1} \alpha_i x_i + \sum_{i \in C} x_i \right\} \]
\[ \text{s.t.} \sum_{j=1}^{t-1} w_i x_j + \sum_{i \in C} w_i x_i \leq \zeta - w_i, \quad x \in \{0, 1\}^{C \setminus i_{t-1}}. \]

Set $\alpha_i = |C| - 1 - \zeta_t$.
End

5.2. Adding cuts to the relaxation

Given a solution $(\tilde{x}, \tilde{X})$ of $\text{CRel}$, our initial goal is to obtain a valid inequality for $\text{QKP}_{\text{lifted}}$ derived from a $\text{CI}$ that is violated by $(\tilde{x}, \tilde{X})$. A $\text{CI}$ is formulated as $\alpha^T x \leq \alpha^T \beta - 1$, where $\alpha \in \{0, 1\}^n$ and enumerates the vector of ones. We then search for the $\text{CI}$ that maximizes the sum of the violations among the inequalities in $\text{Ycut}(\alpha) \leq 0$, where $\text{Y} := (\tilde{x}, \tilde{X})$.

\[ \text{cut}(\alpha) = \left( -e^T \alpha + 1 \right) \alpha \]

To obtain such a $\text{CI}$, we solve the following linear knapsack problem,
\[ \nu^* := \max_{\alpha} e^T \text{Ycut}(\alpha) : w^T \alpha \geq 1, \alpha \in \{0, 1\}^n. \]

Let $\alpha^*$ solve (31). If $\nu^* > 0$, then at least one valid inequality in the following set of $ns$ scaled cover inequalities, denoted in the following by $\text{SCI}$, is violated by $(\tilde{x}, \tilde{X})$.

\[ (x \ X) \left( \begin{array}{c} -e^T \alpha^* + 1 \\ \alpha^* \end{array} \right) \leq 0. \]

Based on the following theorem, we note that to strengthen cut (32), we may apply Algorithm 2 to the $\text{CI}$ obtained, lifting it to an LCI, and finally add the valid inequality (26) derived from the LCI to $\text{CRel}$.

Theorem 10. The valid inequality (26) for $\text{QKP}_{\text{lifted}}$, which is derived from a valid $\text{LCl}$, dominates all inequalities derived from a $\text{CI}$ that can be lifted to the $\text{LCI}$.

Proof. Consider the $\text{LCI}$ (29) derived from a $\text{CI}$ (27) for $\text{QKP}$. The corresponding scaled cover inequalities (26) derived from the $\text{CI}$ and the $\text{LCI}$ are, respectively,
\[ \sum_{j \in C} x_j \leq (|C| - 1) x_i, \quad \forall i \in N, \]
and
\[ \sum_{j \in C} x_j + \sum_{j \in N \setminus C} \alpha_j x_j \leq (|C| - 1) x_i, \quad \forall i \in N, \]
where $\alpha_j \geq 0$, $\forall j \in N \setminus C$. Clearly, as all $X_j$ are nonnegative, the second inequality dominates the first, for all $i \in N$.

5.3. New valid inequalities in the lifted space

As discussed, after finding any valid inequality in the form of (25) for $\text{QKP}$, we may add the constraint (26) to $\text{CRel}$ when aiming at better bounds. We observe now, that besides (26) we can also generate other valid inequalities in the lifted space by taking advantage of the lifting $X := xx^T$, and also of the fact that xis binary. In the following, we show how the idea can be applied to cover inequalities.

Let
\[ \sum_{j \in C} x_j \leq \beta, \]
where $C \subseteq N$ and $\beta < |C|$, be a valid inequality for $\text{KPol}$. Inequality (33) can be either a cover inequality, $\text{CI}$, an extended cover inequality, $\text{LCI}$, or a particular lifted cover inequality, $\text{LCI}$, where $\alpha_j \in \{0, 1\}, \forall j \in N \setminus C$ in (29). Furthermore, given a general $\text{LCI}$, where $\alpha_j \in \mathbb{Z}_+$, for all $j \in N \setminus C$, a valid inequality of type (33) can be constructed by replacing each $\alpha_j$ with min $\{\alpha_j \}$ in the $\text{LCI}$.

Definition 11 (Cover inequality in the lifted space, $\text{CILS}$). Let $C \subseteq N$ and $\beta < |C|$ as in inequality (33), and also consider here that $\beta > 1$. We define
\[ \sum_{i,j \in C, i < j} X_{ij} \leq \left( \frac{\beta}{2} \right). \]

as the $\text{CILS}$ derived from (33).

Theorem 12. If inequality (33) is valid for $\text{QKP}$, then the $\text{CILS}$ (34) is a valid inequality for $\text{QKP}_{\text{lift}}$.

Proof. Considering (33), we conclude that at most $\binom{n}{2}$ products of variables $x_i x_j$, where $i, j \in C$, can be equal to 1. Therefore, as $X_{ij} := x_i x_j$, the result follows.

Remark 13. When $\beta = 1$, inequality (33) is well known as a clique cut, widely used to model decision problems, and frequently used as a cut in branch-and-cut algorithms. In this case, using similar ideas to what was used to construct the $\text{CILS}$, we conclude that it is possible to fix $X_{ij} = 0$ for all $i \in C, i < j$.

Given a solution $(\tilde{x}, \tilde{X})$ of $\text{CRel}$, the following MiQP problem is a separation problem, which searches for a $\text{CILS}$ violated by $\tilde{X}$.
\[ z^* := \max \alpha, \beta, \kappa \delta(\tilde{X} \bar{K}) - \beta (\bar{\beta} - 1), \quad \text{MIQP}_1 \]
\[ \text{s.t.} \quad w^T \alpha \geq c + 1, \quad \beta = e^T \alpha - 1, \]
\[ K(i, j) = 0, \quad i = 1, \ldots, n. \]
\[ K(i, j) \leq \alpha_i, \quad i = 1, \ldots, n, \quad i < j. \]
\[ K(i, j) \leq \alpha_j, \quad i = 1, \ldots, n, \quad i < j. \]
\[ K(i, j) \geq 0, \quad i = 1, \ldots, n, \quad i < j. \]
\[ K(i, j) \geq \alpha_i + \alpha_j - 1, \quad i = 1, \ldots, n, \quad i < j. \]
\[ \alpha \in \{0, 1\}^n, \quad \beta \in \mathbb{R}^n. \]

If $\alpha^*, \beta^*, \kappa^*$ solves $\text{MIQP}_1$, with $z^* > 0$, the $\text{CILS}$ given by $\delta(K\bar{X}) \leq \beta^* (\beta^* - 1)$ is violated by $\tilde{X}$. The binary vector $\alpha^*$ defines the $\text{Cl}$ from which the cut is derived. The $\text{Cl}$ is specifically given by $\alpha^* x \leq e^T \alpha^* - 1$ and $\beta^* (\beta^* - 1)$ determines the right-hand side of the $\text{CILS}$. The inequality is multiplied by 2 because we consider the variable $K$ as a symmetric matrix, in order to simplify the presentation of the model.

Theorem 14. The valid inequality $\text{CILS}$ for $\text{QKP}_{\text{lifted}}$, which is derived from a valid $\text{LCI}$ in the form (33), dominates any $\text{CILS}$ derived from a $\text{CI}$ that can be lifted to the $\text{LCI}$.

Proof. As $X$ is nonnegative, it is straightforward to verify that if $X$ satisfies a $\text{CILS}$ derived from a $\text{LCI}$, it also satisfies any $\text{CILS}$ derived from a $\text{CI}$ that can be lifted to the $\text{LCI}$.
Any feasible solution of MIQP\textsubscript{1} such that \( \text{trace}(\tilde{X}X) > \beta(\beta - 1) \) generates a valid inequality for QKP\textsubscript{lifted} that is violated by \( \tilde{X} \). Therefore, we do not need to solve MIQP\textsubscript{1} to optimality to generate a cut. Moreover, to generate distinct cuts, we can solve MIQP\textsubscript{1} several times (not necessarily to optimality), each time adding to it, the following "no-good" cut to avoid the previously generated cuts:
\[
\sum_{i \in N} \tilde{a}(i)(1 - \alpha(i)) \geq 1, \quad (35)
\]
where \( \tilde{a} \) is the value of the variable \( \alpha \) in the solution of MIQP\textsubscript{1} when generating the previous cut.

We note that, if \( \alpha^*, \beta^*, K^* \) solves MIQP\textsubscript{1}, then \( \alpha^*\top x \leq \varepsilon^T \alpha^* - 1 \) is a valid CI for QKP, however it may not be a minimal cover. Aiming at generating stronger valid cuts, based in Theorem 14, we might add to the objective function of MIQP\textsubscript{1}, the term \(-\delta \varepsilon^T \alpha\), for some weight \( \delta > 0 \). The objective function would then favor minimal covers, which could be lifted to a facet-defining LCI, that would finally generate the CILS. We should also emphasize that if the CILS derived from a CI is violated by a given \( \tilde{X} \), then clearly, the CILS derived from the LCI will also be violated by \( \tilde{X} \).

Now, we also note that, besides defining one cover inequality in the lifted space considering all possible pairs of indexes in \( C \), we can also define a set of cover inequalities in the lifted space, considering for each partition, a partition of the indexes in \( C \) into subsets of cardinality 1 or 2. In this case, the right-hand side of the inequalities is never greater than \( \beta/2 \). The idea is made precise below.

**Definition 15** (Set of cover inequalities in the lifted space, SCILS). Let \( C \subset N \) and \( \beta < |C| \) as in inequality (33). Let

1. \( C_i := \{(i_1, j_1), \ldots, (i_p, j_p)\} \) be a partition of \( C \), if \( |C| \) is even.
2. \( C_i := \{(i_1, j_1), \ldots, (i_p, j_p)\} \) be a partition of \( C \{i_0\} \) for each \( i_0 \in C \), if \( |C| \) is odd and \( \beta \) is odd.
3. \( C_i := \{(i_0, i_0), (i_1, j_1), \ldots, (i_p, j_p)\} \), where \( (i_1, j_1), \ldots, (i_p, j_p) \) is a partition of \( C \{i_0\} \) for each \( i_0 \in C \), if \( |C| \) is odd and \( \beta \) is even.

In all cases, \( i_k < j_k \) for all \( k = 1, \ldots, p \).

The inequalities in the SCILS derived from (33) are given by
\[
\sum_{(i,j) \in C_i} x_{ij} \leq \left\lfloor \frac{\beta}{2} \right\rfloor, \quad (36)
\]
for all partitions \( C_i \) defined above.

**Theorem 16.** If inequality (33) is valid for QKP, then the inequalities in the SCILS (36) are valid for QKP\textsubscript{lifted}.

**Proof.** The proof of the validity of the SCILS is based on the lifting relation \( x_{ij} = x_{ij} \). We note that if the binary variable \( x_{ij} \) indicates whether or not the item \( i \) is selected in the solution, the variable \( x_{ij} \) indicates whether or not the pair of items \( i \) and \( j \) are both selected in the solution.

1. If \( |C| \) is even, \( C_1 \) is a partition of \( C \) in exactly \( |C|/2 \) subsets with two elements each, and therefore, if at most \( \beta \) elements of \( C \) can be selected in the solution, clearly at most \( \left\lfloor \frac{\beta}{2} \right\rfloor \) subsets of \( C_1 \) can also be selected.
2. If \( |C| \) and \( \beta \) are odd, \( C_1 \) is a partition of \( C \{i_0\} \) in exactly \( |C| - 1)/2 \) subsets with two elements each, where \( i_0 \) can be any element of \( C \). In this case, if at most \( \beta \) elements of \( C \) can be selected in the solution, clearly at most \( \left\lfloor \frac{\beta - 1}{2} \right\rfloor \) \( \left\lfloor \frac{\beta}{2} \right\rfloor \) subsets of \( C_1 \) can also be selected.
3. If \( |C| \) is odd and \( \beta \) is even, \( C_1 \) is the union of \( \{i_0, i_0\} \) with a partition of \( C \{i_0\} \) in exactly \( |C| - 1)/2 \) subsets with two elements each, where \( i_0 \) can be any element of \( C \). In this case, if at most \( \beta \) elements of \( C \) can be selected in the solution, clearly at most \( \left\lfloor \frac{\beta - 1}{2} \right\rfloor \) \( \left\lfloor \frac{\beta}{2} \right\rfloor \) subsets of \( C_1 \) can also be selected.

Given a solution \((x, \tilde{X})\) of CRel, we now present a mixed linear fractional graph coloring (SCILS) algorithm, that searches for an inequality in SCILS that is most violated by \( \tilde{X} \). Let \( A \in \{0, 1\}^{3n \times (n+1)/2} \). In the first \( n \) columns of \( A \) we have the \( n \times n \) identity matrix. In the remaining \( n(n-1)/2 \) columns of the matrix, there are exactly two elements equal to 1 in each column. All columns are distinct. For example, for \( n = 4 \),
\[
A := \begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
\end{pmatrix}
\]

The columns of \( A \) represent all the subsets of items in \( N \) with one or two elements.

Let
\[
z^* := \max_{x \in X_N} \text{trace}(\tilde{X}X) - 2\nu, \quad \text{(MILP\textsubscript{2})}
\]
\[\text{s.t. } w^T \alpha \geq c + 1, \quad (i = 1, \ldots, n),
\]
\[
\sum_{i = 1}^{n} y(i) \leq 1, \quad (i = 1, \ldots, n, i < j),
\]
\[
v(1) \leq (e^\top \alpha - 1)/2 - 0.5, \quad v \leq (e^\top \alpha - 1)/2,
\]
\[
y(t) \leq 1 - A(i, t) + \alpha(t), \quad (t = 1, \ldots, n(n+1)/2, i = 1, \ldots, \nu, v \in \mathbb{Z}, K \in \mathbb{N}^n).
\]

If \( \alpha^*, \nu^*, K^*, y^* \) solves MILP\textsubscript{2}, with \( z^* > 0 \), then the particular inequality in SCILS given by
\[
\text{trace}(K^*X) \leq 2\nu
\]
(37)
is violated by \( \tilde{X} \). The binary vector \( \alpha^* \) defines the CI from which the cut is derived. As the CI is given by \( \alpha^*x \leq e^\top \alpha^* - 1 \), we can conclude that the cut generated either belongs to case (1) or (3) in Definition 15. This fact is considered in the formulation of MILP\textsubscript{2}. The vector \( y^* \) defines a partition \( C_i \) as presented in case (3), if \( \sum_{i = 1}^{n} y(i) = 1 \). In this case, otherwise. We finally note that the number 2 in the right-hand side of (37) is due to the symmetry of the matrix \( K^* \).

We now may repeat the observations made for MIQP\textsubscript{1}.

Any feasible solution of MILP\textsubscript{2} such that \( \text{trace}(\tilde{X}X) > 2\nu \) generates a valid inequality for CRel, which is violated by \( \tilde{X} \). Therefore, we do not need to solve MILP\textsubscript{2} to optimality to generate a cut. Moreover, to generate distinct cuts, we can solve MILP\textsubscript{2} several times (not necessarily to optimality), each time adding to it, the following suitable "no-good" cut to avoid the previously generated cuts:
\[
\sum_{i = 1}^{n(n+1)/2} y(i)(1 - y(i)) \geq 1, \quad (38)
\]
where \( y \) is the value of the variable \( y \) in the solution of MILP\textsubscript{2}, when generating the previous cut.
lifted to a facet-defining LCI. In this case, however, after computing the LCI, we have to solve MILP₂ again, with α fixed at values that represent the LCI, and γ fixed so that the right-hand side of the inequality is equal to the right-hand side of the LCI. All components of γ that were equal to 1 in the previous solution of MILP₂ should also be fixed at 1. The new solution of MILP₂ would indicate the other subsets of N to be added to C. One last detail should be taken into account. If the cover C corresponding to the LCI, is such that |C| is odd and the right-hand side of the LCI is also odd, then the cut generated should belong to case (2) in Definition 15, and MILP₂ should be modified accordingly. Specifically, the second and third constraints in MILP₂, should be modified respectively to

\[ K(i, i) = 0, \quad i = 1, \ldots, n, \]

\[ \sum_{i=1}^{n} y(i) = 1. \]

Remark 17. Let γ := |C|. Then, the number of inequalities in the SCILS is

\[ \frac{1}{2} \frac{(\gamma - 1)!}{2^{(\gamma - 1)/2} (\frac{\gamma}{2} - 1)!} \]

if γ is even, or

\[ \frac{1}{2} \frac{(\gamma - 1)!}{2^{(\gamma - 1)/2} (\frac{\gamma}{2} - 1)!} \]

if γ is odd.

Finally, we extend the ideas presented above to the more general case of knapsack inequalities. We note that the following discussion applies to a general LCI, where α_j ∈ Z⁺, ∀ j ∈ N\C.

Let

\[ \sum_{j \in C} \alpha_j x_j \leq \beta. \tag{39} \]

be a valid knapsack inequality for KPol, with α_j, β ∈ Z⁺, β ≥ α_j, ∀ j ∈ N.

Definition 18 (Set of knapsack inequalities in the lifted space, SKILS). Let α_j be the coefficient of x_j in (39). Let \{C₁, \ldots, C_q\} be the partition of N, such that α_u = α_v, if u, v ∈ C_k for some k, and α_u ≠ α_v, otherwise. The knapsack inequality (39) can then be rewritten as

\[ \sum_{k=1}^{q} \left( \bar{\alpha}_k \sum_{j \in C_k} x_j \right) \leq \beta. \tag{40} \]

Now, for k = 1, \ldots, q, let C_k := \{(i_1, j_1), \ldots, (i_{k_h}, j_{k_h})\}, where i_j for all (i, j) ∈ C_k, and

• C_k is a partition of C_k, if |C_k| is even.
• C_k is a partition of C_k \{i_{k_h}\}, if i_{k_h} ∈ C_k, if |C_k| is odd.

The inequalities in the SKILS corresponding to (39) are given by

\[ \sum_{k=1}^{q} \left( \bar{\alpha}_k \sum_{(i, j) \in C_k} X_{i_j} + 2 \bar{\alpha}_k \sum_{(i, j) \in C_k} X_{i_j} \right) \leq \beta. \tag{41} \]

for all partitions C_k, k = 1, \ldots, q, defined as above, and for all i_{k_h} ∈ C_k \ C_k. (If |C_k| is even, C_k \ C_k = ∅, and the term in the variable X_{i_{k_h}} does not exist.)

Remark 19. Consider \{C₁, \ldots, C_q\} as in Definition 18. For k = 1, \ldots, q, let γ_k := |C_k| and define

\[ NC_k := \frac{\gamma_k!}{2^{(\gamma_k - 1)/2}}. \]

if γ_k is even, or

\[ NC_k := \frac{\gamma_k!}{2^{(\gamma_k - 1)/2}}. \]

if γ_k is odd.

Then, the number of inequalities in SKILS is

\[ \prod_{k=1}^{q} NC_k. \]

Remark 20. If \bar{\alpha}_k is even for every k, such that γ_k := |C_k| is odd, then the right-hand side β of inequality (41) may be replaced with 2 × \left[ \frac{\beta}{2} \right], which will strengthen the inequality in case β is odd.

Note the case where γ_k is even for every k, is a particular case contemplated by this remark, where the tightness of the inequality can also be applied.

Corollary 21. If inequality (39) is valid for KPol, then the inequalities (41), in the SKILS, are valid for KPol, whether or not the modification suggested in Remark 20 is applied.

Proof. The result is again verified, by using the same argument used in the proof of Theorem 16, i.e., considering that X_{i_j} = 1, iff x_i = x_j = 1.

5.4. Dominance relation among the new valid inequalities

We start this subsection investigating whether SCILS dominates CILS or vice versa.

Theorem 22. Let C be the cover in (33) and consider γ := |C| to be even.

1. If β = γ − 1, then the sum of all inequalities in SCILS is equivalent to CILS. Therefore, in this case, the set of inequalities in SCILS dominates CILS.

2. If β < γ − 1, there is no dominance relation between SCILS and CILS.

Proof. Let sum(SCILS) denote the inequality obtained by adding all inequalities in SCILS, and let rhs(sum(SCILS)) denote its right-hand side (rhs). We have that rhs(sum(SCILS)) is equal to the number of inequalities in SCILS multiplied by the rhs of each inequality, i.e.,

\[ \text{rhs}(\text{sum}(\text{SCILS})) = \frac{(\gamma - 1)!}{2^{(\gamma - 1)/2} (\frac{\gamma}{2} - 1)!} \times \left\lfloor \frac{\beta}{2} \right\rfloor. \]

The coefficient of each variable X_{i_j} in \text{sum}(\text{SCILS}) (coef_{i_j}) is given by the number of inequalities in the set SCILS in which X_{i_j} appears, i.e.,

\[ \text{coef}_{i_j} = \frac{(\gamma - 2)!}{2^{(\gamma - 2)/2} (\frac{\gamma - 2}{2} - 1)!} \times \left\lfloor \frac{\beta}{2} \right\rfloor. \]

Dividing rhs(sum(SCILS)) by coef_{i_j}, we obtain

\[ \text{rhs}(\text{sum}(\text{SCILS})) / \text{coef}_{i_j} = (\gamma - 1) \times \left\lfloor \frac{\beta}{2} \right\rfloor. \tag{42} \]

On the other side, the rhs of CILS is:

\[ \text{rhs}(\text{CILS}) = \left( \frac{\beta}{2} \right) = \frac{\beta(\beta - 1)}{2}. \tag{43} \]

1. Replacing β with γ − 1, and \left[ \frac{\beta}{2} \right] with \left[ \frac{\beta - 1}{2} \right] (since β is odd), we obtain the result.
2. Consider, for example, $C = \{1, 2, 3, 4, 5, 6\}$ and $\beta = 3$ ($\beta < \gamma - 1$ and odd). In this case, the SCILS becomes:

$$\begin{align*}
X_{12} + X_{13} + X_{14} + X_{15} + X_{16} + X_{23} + X_{24} \\
+ X_{25} + X_{36} + X_{34} + X_{35} + X_{36} + X_{45} + X_{46} + X_{56} \leq 3.
\end{align*}$$

And a particular inequality in SCILS is

$$X_{12} + X_{34} + X_{56} \leq 1. \quad (44)$$

The solution $X_{1j} = 1$, for $j = 2, \ldots, 6$, and all other variables equal to zero, satisfies all inequalities in SCILS, because only one of the positive variables appears in each inequality in the set. However, the solution does not satisfy CILS. On the other side, the solution $X_{12} = X_{34} = X_{56} = 1$, and all other variables equal to zero, satisfies CILS, but does not satisfy (44).

Now, consider $C = \{1, 2, 3, 4, 5, 6\}$ and $\beta = 4$ ($\beta < \gamma - 1$ and even). In this case, the CILS becomes:

$$\begin{align*}
X_{12} + X_{13} + X_{14} + X_{15} + X_{16} + X_{23} + X_{24} \\
+ X_{25} + X_{36} + X_{34} + X_{35} + X_{36} + X_{45} + X_{46} + X_{56} \leq 6.
\end{align*}$$

And a particular inequality in CILS is

$$X_{12} + X_{34} + X_{56} \leq 2. \quad (45)$$

The solution $X_{1j} = 1$, for $j = 2, \ldots, 6$, and all other variables equal to zero, satisfies all inequalities in CILS, because at most two of the positive variables appear in each inequality in the set. However, the solution does not satisfy CILS. On the other side, the solution $X_{12} = X_{34} = X_{56} = 1$, and all other variables equal to zero, satisfies CILS, but does not satisfy (45).

Theorem 23. Let $C$ be the cover in (33) and consider $\gamma := |C|$ to be odd. Then there is no dominance relation between SCILS and CILS.

Proof. Consider, for example, $C = \{1, 2, 3, 4, 5\}$ and $\beta = 3$ ($\beta$ odd). In this case, the CILS becomes:

$$\begin{align*}
X_{12} + X_{13} + X_{14} + X_{15} + X_{23} + X_{24} + X_{25} + X_{34} + X_{35} + X_{45} \leq 3.
\end{align*}$$

And a particular inequality in CILS is

$$X_{23} + X_{45} \leq 1. \quad (46)$$

The solution $X_{1j} = 1$, for $j = 1, \ldots, 5$, and all other variables equal to zero, satisfies all inequalities in CILS, because only one of the positive variables appears in each inequality in the set. However, the solution does not satisfy CILS. On the other side, the solution $X_{23} = X_{45} = 1$, and all other variables equal to zero, satisfies CILS, but does not satisfy (46).

Now, consider $C = \{1, 2, 3, 4, 5\}$ and $\beta = 4$ ($\beta$ even). In this case, the CILS becomes:

$$\begin{align*}
X_{12} + X_{13} + X_{14} + X_{15} + X_{23} + X_{24} + X_{25} + X_{34} + X_{35} + X_{45} \leq 6.
\end{align*}$$

And a particular inequality in CILS is

$$X_{11} + X_{23} + X_{45} \leq 2. \quad (47)$$

The solution $X_{1j} = 1$, for $j = 1, \ldots, 5$, $X_{2j} = 1$, for $j = 2, \ldots, 5$, and all other variables equal to zero, satisfies all inequalities in CILS, because at most two of the positive variables appear in each inequality in the set. However, the solution does not satisfy CILS. On the other side, the solution $X_{11} = X_{23} = X_{45} = 1$, and all other variables equal to zero, satisfies CILS, but does not satisfy (47).

Now, we investigate if SCILS is just a particular case of SKILS, when $\alpha_j \in \{0, 1\}$, for all $j \in N$ in (39).

Theorem 24. In case the modification suggested in Remark 20 is applied, then if $|C|$ is even in (33), SCILS becomes just a particular case of SKILS. In case $|C|$ is odd, however, the inequalities in SCILS are stronger.

Proof. If $|C|$ is even, the result is easily verified. If $|C|$ is odd, the inequalities in SCILS become

$$2 \sum_{i,j \in C} X_{ij} \leq \beta - 1,$$

if $\beta$ is odd, and

$$2X_{i0} + 2 \sum_{i,j \in C} X_{ij} \leq \beta,$$

if $\beta$ is even, and the inequalities in SKILS become

$$X_{i0} + 2 \sum_{i,j \in C} X_{ij} \leq \beta,$$

for all $\beta$. In all cases, $C_i$ is a partition of $C \setminus \{i_0\}$, where $i_0 \in C$.

Either with $\beta$ even or odd, it becomes clear that SCILS is stronger than SKILS.

6. Lower bounds from solutions of the relaxations for QKP$_{lifted}$

In order to evaluate the quality of the upper bounds obtained with CRel, we compare them with lower bounds for QKP, given by feasible solutions constructed by a heuristic. We assume in this section that all variables in CRel are constrained to the interval $[0,1]$. Let $(\bar{x}, \bar{X})$ be a solution of CRel. We initially apply principal component analysis (PCA) (Jolliffe, 2010) to construct an approximation to the solution of QKP and then apply a special rounding procedure to obtain a feasible solution from it. PCA selects the largest eigenvalue and the corresponding eigenvector of $\bar{X}$, denoted by $\lambda$ and $\bar{v}$, respectively. Then $\lambda \bar{v} \bar{v}$ is a rank-one approximation of $\bar{X}$. We set $\bar{x} = \frac{1}{\lambda} \bar{v} \bar{v}$ to be an approximation of the solution $x$ of QKP. We note that $\lambda > 0$ because $\bar{X}_{i0} > 0$ for at least one index $i$ in the optimal solutions of the relaxations, and therefore, $\bar{x}$ is not negative semidefinite. Finally, we round $\bar{x}$ to a binary solution that satisfies the knapsack capacity constraint, using the simple approach described in Algorithm 3.

Algorithm 3 A heuristic for the QKP.

Input: the solution $\bar{x}$ from CRel, the weight vector $w$, the capacity $c$.

Let $\lambda$ and $\bar{v}$ be, respectively, the largest eigenvalue and the corresponding eigenvector of $\bar{X}$.

Set $\bar{x} = \frac{1}{\lambda} \bar{v} \bar{v}$.

Round $\bar{x}$ to $\hat{x} \in \{0, 1\}^n$.

While $w^T \hat{x} > c$

Set $i = \arg\min_{j \in N} [\bar{x}_j \hat{x}_j > 0]$.

Set $\hat{x}_i = 0, \hat{x}_i = 1$.

End

Output: a feasible solution $\hat{x}$ of QKP.

7. Numerical experiments

We summarize our algorithmic framework in Algorithm 4, where at each iteration we update the perturbation $Q_0$ of the parametric relaxation and, at every $m$ iterations, we add to the relaxation, the valid inequalities considered in this paper, namely, SCI, defined in (32), CILS, defined in (34), and SCILS, defined in (36).

The numerical experiments performed had the following main purposes,
• verify the impact of the valid inequalities, SCI, CILS, and SCILS, when iteratively added to cut the current solution of a relaxation of QKP.
• verify the effectiveness of the IPM described in Section 3 in decreasing the upper bound while optimizing the perturbation $Q_p$.
• compute the upper and lower bounds obtained with the proposed algorithmic approach described in Algorithm 4, and compare them, with the optimal solutions of the instances.

We coded Algorithm 4 in MATLAB, version R2016b, and ran the code on a notebook with an Intel Core i5-4200U CPU 2.30 gigahertz, 6 gigabytes RAM, running under Windows 10. We used the primal-dual IPM implemented in Mosesk, version 8, to solve the relaxation $\text{CQP}_{Q_p}$, and, to solve the separation problems $\text{MIQP}_1$ and MILP$_2$, we use Garubi, version 8.

The input data used in the first iteration of the IPM described in Algorithm 1 (k = 0) are: $B_0 = I$, $\mu^0 = 1$. We start with a matrix $Q_p^0$ such that $Q - Q_p^0$ is negative definite. By solving $\text{CQP}_{Q_p}$, with $Q_p := Q_p^0$, we obtain $x(Q_p^0)$, $X(Q_p^0)$, as its optimal solution, and set $\nabla \text{P}_{\text{CQP}}(Q_p^0) := X(Q_p^0) - x(Q_p^0)x(Q_p^0)^T$. Finally, the positive definiteness of $Z_0$ and $A^0$ are assured by setting: $Z_0 := Q - Q_p^0$ and $A^0 := \nabla \text{P}_{\text{CQP}}(Q_p^0) + (2\lambda_{\min}(\nabla \text{P}_{\text{CQP}}(Q_p^0)) + 0.1).$

Our randomly generated test instances were also used by Cunha, Simonetti, and Lucena (2016), who provided us with the instances data and with their optimal solutions. Each weight $w_j$, for $j \in N$, was randomly selected in the interval [1, 50], and the capacity c, of the knapsack, was randomly selected in [50, $\sum_{j\in N} w_j$]. The procedure used by Cunha to generate the instances was based on previous works (Billonnet & Calmels, 1996; Caprara et al., 1999; Chaillou et al., 1989; Gallo et al., 1989; Michelon & Veilleux, 1996).

The following labels identify the results presented in Tables 3, 5 and 6.

- OptGap: $\alpha_{\text{upper}} - \alpha_{\text{opt}}$ (the relative optimality gap).
- Time: (seconds) (the computational time to compute the bound).
- DuGap: $\frac{\text{upper} - \text{bound}}{\text{lower} \text{bound}}$ (the relative duality gap).
- Iter (the number of iterations).
- Cuts (the number of cuts added to the relaxation).
- Time$_{\text{MIQP}}$: (seconds) (the computational time to obtain cuts CILS and SCILS).

To get some insight into the effectiveness of the cuts proposed, we initially applied them to 10 small instances with $n = 10$. In Table 3 we present average results for this preliminary experiment, where we iteratively add the cuts to the following linear relaxation

$$\text{max } \text{trace}(QX)$$

s.t. \begin{align*}
&\sum_{j=1}^{n} w_j x_j \leq c, \\
&0 \leq x_j \leq 1, \quad \forall j \in N \\
&0 \leq x_i \leq 1, \quad \forall i \in N \\
&X \in S^n.
\end{align*}

(LPR)

In the first row of Table 3, the results correspond to the solution of the linear relaxation LPR with no cuts. In SCI, we add only the most violated cut from the $n$ cuts in SCI to LPR at each iteration, and in the SCI we add all $n$ cuts. In CILS and SCILS, we solve MIQP and MILP problems to find the most violated cut of each type. The last row of the table (All) corresponds to results obtained when we add all $n$ cuts in SCI, and one cut of each type, CILS and SCILS. In these initial tests, we run up to 50 iterations, and in most cases, stop the algorithm when no more cuts are found to be added to the relaxation.

Algorithm 4 A cutting plane algorithm for the QKP.

Input: $Q \in S^n$, $\max_{n \text{cuts}}$.

$k := 0$, $B_0 := I$, $\mu^0 := 1$.

Let $\lambda_0(Q)$, $v_i$ be the $i$th largest eigenvalue of $Q$ and corresponding eigenvector.

$Q_p := \sum_{i=1}^{n} (-\lambda_i(Q) - 1) v_i v_i^T$ (or $Q_p := \sum_{i=1}^{n} (\text{min}[-\lambda_i(Q), -10^{-6}]) v_i v_i^T$)

$Q_p^0 := Q - Q_p$.

Solve $\text{CQP}_{Q_p}$, with $Q_p := Q_p^0$, and obtain $x(Q_p^0)$, $X(Q_p^0)$.

$\nabla \text{P}_{\text{CQP}}(Q_p^0) := X(Q_p^0) - x(Q_p^0)x(Q_p^0)^T$.

$Z_0 := Q - Q_p$.

$A_0 := \nabla \text{P}_{\text{CQP}}(Q_p^0) + (2\lambda_{\min}(\nabla \text{P}_{\text{CQP}}(Q_p^0)) + 0.1).$

While (stopping criterion is violated)

Run Algorithm 1, where $Q_p^{k+1}$ is obtained and relaxation $\text{CQP}_{Q_p}$, with $Q_p := Q_p^{k+1}$ is solved. Let $(x(Q_p^{k+1}), X(Q_p^{k+1}))$ be its optimal solution.

$\text{upperbound}^{k+1} := \text{P}_{\text{CQP}}(Q_p^{k+1})$.

Run Algorithm 3, where $x$ is obtained.

$\text{lowerbound}^{k+1} := x^T Q x$.

If $k \mod m = 0$

Solve problem (31) and obtain cuts SCI in (32).

Add the $\min(n, \max_{n \text{cuts}})$ cuts SCI with the largest violations at $(x(Q_p^{k+1}), X(Q_p^{k+1}))$ to $\text{CQP}_{Q_p}$.

$n_{\text{cuts}} := 0$.

While ($n_{\text{cuts}} < \max_{n \text{cuts}}$ and MIQP 1 feasible)

Solve $\text{MIQP}_1$ and add the CI and CILS obtained to $\text{CQP}_{Q_p}$.

Add the “no-good” cut (35) to $\text{MIQP}_1$.

$n_{\text{cuts}} := n_{\text{cuts}} + 1$.

End

$n_{\text{cuts}} := 0$.

While ($n_{\text{cuts}} < \max_{n \text{cuts}}$ and MILP 2 feasible)

Solve $\text{MILP}_2$ and add the CI and CILS obtained to $\text{CQP}_{Q_p}$.

Add the “no-good” cut (38) to $\text{MILP}_2$.

$n_{\text{cuts}} := n_{\text{cuts}} + 1$.

End

End

$k := k + 1$.

End

Output: Upper bound $\text{upperbound}^d$, lower bound $\text{lowerbound}^d$, and feasible solution $\hat{x}$ to QKP.

Fig. 1 depicts the impact of the validity inequalities, SCI, CILS, and SCILS, when iteratively added to cut the current solution of a relaxation of QKP.
multiplying the capacity constraint by each nonnegative variable $x_i$, and also by $(1 - x_i)$, and then replacing each bilinear term $x_i x_j$ by $X_{ij}$. We then start the algorithm solving the following relaxation.

$$\max \quad x^T (Q - Q_0^p) x + \operatorname{trace}(Q_0^p X)$$

$$\text{s.t.} \quad \sum_{j=1}^n W_j x_j \leq C,$$

$$\sum_{j=1}^n W_j x_{ij} \leq C x_i, \quad \forall i \in N$$

$$\sum_{j=1}^n \sum_{j=1}^n W_{ij} (x_{ij} - X_{ij}) \leq c (1 - X_{ij}), \quad \forall i \in N \quad (49)$$

$$X_0 = X_{ii}, \quad \forall i \in N$$

$$X_{ij} \leq X_{ii}, \quad \forall i, j \in N$$

$$0 \leq X_{ij} \leq 1, \quad \forall i, j \in N$$

$$X \in \mathbb{R}^n.$$
5 CILS and 5 SCILS. Note that when solving each MIQP or MILP problem, besides the cut CILS or SCILS, we also obtain a cover inequality CI. We check if this CI was already added to the relaxation, and if not, we add it as well. We stop Algorithm 4 when a maximum number of iterations is reached or when DuGap is sufficiently small.

For the results presented in Table 5 (n = 50), we set the maximum number of iterations of the IPM equal to 100, and m = 10. The execution of each separation problem was limited to 3 seconds, and the best solutions obtained in this time limit was used to generate the cuts.

For the results presented in Table 6 (n = 100), we set the maximum number of iterations of the IPM equal to 20, and m = 4. In this case, the execution of each separation problem was limited to 10 seconds.

We note from the results in Tables 5 and 6, that the alternation between the iterations of the IPM to improve the perturbation Qp of the relaxation and the addition of cuts to the relaxation, changing the search direction of the IPM, is an effective approach to compute bounds for QKP. Considering the stopping criterion imposed to Algorithm 4, it was able to converge to the optimum solution of three out of five instances with n = 50 and of two out of five instances with n = 100. The average optimality gap for all ten instances is less than 0.1%. The heuristic applied also computed good solutions for the problem. The average duality gap for the 10 instances is less than 0.25%.

We note that our algorithm spends a high percentage of its running time solving the separation problems, and also solving the linear systems to define the direction of improvement in the IPM algorithm. The running time of both procedures can be improved by a more judicious implementation. There are two parameters in Algorithm 4 that can also be better analyzed and tuned to improve the results, namely, m and the time limit for the execution of the separation problems. As mentioned before, these problems could still be solved by heuristics. Finally, we note that the alternation between the IPM iterations and addition of cuts to the relaxation could be combined with a branch-and-bound algorithm in an attempt to converge faster to the optimal solution. In this case, the cuts added to the relaxations would include the cuts that define the branching and the update on Qp would depend on the branch of the enumeration tree. These are directions for the continuity of the research on this work.

8. Conclusion

In this paper we present a cutting plane algorithm (CPA) to iteratively improve the upper bound for the quadratic knapsack problem (QKP). The initial relaxation for the problem is given by a parametric convex quadratic problem, where the Hessian Q of the objective function of the QKP is perturbed by a matrix parameter Qp such that Q − Qp \geq 0. Seeking for the best possible bound, the concave term xT(Q − Qp)x, is then kept in the objective function of the relaxation and the remaining part, given by xTQpx, is linearized through the standard approach that lifts the problem to space of symmetric matrices defined by X := xxT.

We present a primal-dual interior point method (IPM), which update the perturbation Qp at each iteration of the CPA aiming at reducing the upper bound given by the relaxation. We also present new classes of cuts that are added during the execution of the CPA, which are defined on the lifted variable X, and derived from cover inequalities and the binary constraints.

We show that both the IPM and the cuts generated are effective in improving the upper bound for the QKP and note that these procedures could be applied to more general binary indefinite quadratic problems as well. The separation problems described to generate the cuts could also be solved heuristically, in order to accelerate the process.

We note that the search for the best perturbation Qp, by our IPM, is updated with the inclusion of cuts to the relaxation. In the set of cuts added, we could also consider cuts defined by the branching procedure in a branch-and-bound algorithm. In this case, we could have the perturbation Qp optimized during all the descend on the branch-and-bound tree, considering the cuts the have been added to the relaxations.

Finally, we show that if the positive semidefinite constraint X − xTQx = 0 was introduced in the relaxation of the QKP, or any other indefinite quadratic problem (maximizing the objective function), then the decomposition of objective function, that leads to a convex quadratic SDP relaxation, where a perturbed concave part of the objective is kept, and the remaining part is linearized, is not effective. In this case the best bound is always attained when the whole objective function is linearized, i.e., when the perturbation Qp is equal to Q. This observation also relates to the well known DC (difference of convex) decomposition of indefinite quadratics that have been used in the literature to generate bounds for indefinite quadratic problems. Once more, in case the positive semidefinite constraint is added to the relaxation, the DC decomposition is not effective anymore, and the alternative linear SDP relaxation leads to the best possible bound. As corollary from this result, we see that the bound given by the convex quadratic relaxation cannot be better than the bound given by the corresponding linear SDP relaxation. This last result was already proved in the literature, as mentioned in Section 4.

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