European Journal of Operational Research 281 (2020) 36–49

Contents lists available at ScienceDirect

European Journal of Operational Research

journal homepage: www.elsevier.com/locate/ejor

Discrete Optimization

Parametric convex quadratic relaxation of the quadratic knapsack problem

M. Fampa[a,*], D. Lubke[a], F. Wang[b], H. Wolkowicz[c]

[a] PESC/COPPE, Universidade Federal do Rio de Janeiro, Caixa Postal 68511, Rio de Janeiro, RJ21941-972, Brazil
[b] Department of Mathematics, Royal Institute of Technology, Sweden
[c] Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Canada

ARTICLE INFO

Article history:
Received 20 January 2019
Accepted 16 August 2019
Available online 20 August 2019

Keywords:
Quadratic knapsack problem
Quadratic binary programming
Convex quadratic programming relaxations
Parametric optimization
Valid inequalities

ABSTRACT

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.

1. Introduction

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

$$(\textbf{QKP}) \qquad \begin{array}{rl} p^*_{\text{QKP}} := \max & x^T Q x \\ \text{s.t.} & w^T x \le c \\ & x \in \{0,1\}^n, \end{array} \tag{1}$$

where $Q \in \mathbb{S}^n$ is a symmetric $n \times n$ nonnegative integer profit matrix, $w \in \mathbb{Z}^n_{++}$ is a vector of positive integer weights for the items, and $c \in \mathbb{Z}_{++}$ is the knapsack capacity with $c \ge w_i$, for all $i \in N := \{1, \dots, n\}$. The binary (vector) variable $x$indicates 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 attentio0n 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, Faye, & 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

* Corresponding author.
E-mail addresses: fampa@cos.ufrj.br (M. Fampa), danielalubke@cos.ufrj.br (D. Lubke), fewa@kth.se (F. Wang), hwolkowicz@uwaterloo.ca (H. Wolkowicz).

https://doi.org/10.1016/j.ejor.2019.08.027
0377-2217/

the quadratic objective function in **QKP** with a linear function in X, namely, 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 $Q - Q_p \preceq 0$. 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 & Thoai, 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 $Q - Q_p \preceq 0$.

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.

Table 1
Equations number corresponding to acronyms.

QKP	(1)	**CI**	(27)
QKP$_{\text{lifted}}$	(2)	**ECI**	(28)
LPR	(3)	**LCI**	(29)
CQP$_{Q_p}$	(5)	**SCI**	(32)
LSDP	(21)	**CILS**	(34)
QSDP$_{Q_p}$	(15)	**SCILS**	(36)
		SKILS	(41)

Notation

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

$$\text{svec}(A) := (a_{11}, \dots, a_{n1}, a_{22}, \dots, a_{n2}, \dots, a_{nn})^T \in \mathbb{R}^{n(n+1)/2}.$$

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

We also denote by $\lambda_{\min}(A)$, the smallest eigenvalue of A and by $\lambda_i(A)$ the ith largest eigenvalue of A.

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

Table 2
List of abbreviations.

CQP	Convex Quadratic Programming
QKP	Quadratic Knapsack Problem
SDP	Semidefinite Programming
MIQP	Mixed Integer Quadratic Programming
MILP	Mixed Integer Linear Programming

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 $X := xx^T$.

$$(\mathbf{QKP}_{\text{lifted}}) \qquad \begin{array}{rl} p^*_{\text{QKP}_{\text{LIFTED}}} := \max & \text{trace}(QX) \\ \text{s.t.} & w^T x \le c \\ & X = xx^T \\ & x \in \{0,1\}^n. \end{array} \tag{2}$$

We consider an initial LP relaxation of **QKP**, given by

$$(\mathbf{LPR}) \qquad \begin{array}{rl} \max & \text{trace}(QX) \\ \text{s.t.} & (x, X) \in \mathcal{P}, \end{array} \tag{3}$$

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

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

$$Q - Q_p \preceq 0, \tag{4}$$

and we get

$$\begin{aligned} x^T Q x &= x^T (Q - Q_p) x + x^T Q_p x = x^T (Q - Q_p) x + \text{trace}(Q_p x x^T) \\ &= x^T (Q - Q_p) x + \text{trace}(Q_p X). \end{aligned}$$

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

$$(\mathbf{CQP}_{Q_p}) \qquad \begin{array}{rl} p^*_{\text{CQP}}(Q_p) := \max & x^T (Q - Q_p) x + \text{trace}(Q_p X) \\ \text{s.t.} & (x, X) \in \mathcal{P}. \end{array} \tag{5}$$

3. Optimizing the parametric problem over the parameter Q_p

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

$$param^*_{\text{QKP}} := \min_{Q - Q_p \preceq 0} p^*_{\text{CQP}}(Q_p). \tag{6}$$

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

$$\begin{array}{rll} \min & B_\mu(Q_p, Z) := p^*_{\text{CQP}}(Q_p) - \mu \log\det Z & \\ \text{s.t.} & Q - Q_p + Z = 0 & (: \Lambda) \\ & Z \succ 0, & \end{array} \tag{7}$$

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 $\mathbf{CQP}_{Q_p}$, 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 $\mathbf{CQP}_{Q_p}$ 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. Fiacco (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 $\mathbf{CQP}_{Q_p}$, and

$$x^T (Q - Q_p) x + \text{trace}(Q_p X) = x^T Q x + \text{trace}(Q_p (X - xx^T)),$$

we have

$$\nabla p^*_{\text{CQP}}(Q_p) = X - xx^T. \tag{8}$$

The optimality conditions for (7) are obtained by differentiating the Lagrangian L_μ with respect to Q_p, Λ, Z, respectively,

$$\begin{array}{rrcll} \dfrac{\partial L_\mu}{\partial Q_p} : & \nabla p^*_{\text{CQP}}(Q_p) - \Lambda & = & 0, & \\ \dfrac{\partial L_\mu}{\partial \Lambda} : & Q - Q_p + Z & = & 0, & \\ \dfrac{\partial L_\mu}{\partial Z} : & -\mu Z^{-1} + \Lambda & = & 0, & \text{(or) } Z\Lambda - \mu I = 0. \end{array} \tag{9}$$

This gives rise to the nonlinear system

$$G_\mu(Q_p, \Lambda, Z) = \begin{pmatrix} \nabla p^*_{\text{CQP}}(Q_p) - \Lambda \\ Q - Q_p + Z \\ Z\Lambda - \mu I \end{pmatrix} = 0, \qquad Z, \Lambda \succ 0. \tag{10}$$

We use a BFGS approximation for the Hessian of p^*_{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 $\nabla^2_{\text{BFGS}} p^*_{\text{CQP}}(Q_p)$ 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

$$Y_k := \nabla p^*_{\text{CQP}}(Q_p^{k+1}) - \nabla p^*_{\text{CQP}}(Q_p^k), \qquad S_k := Q_p^{k+1} - Q_p^k,$$

and,

$$\upsilon := \langle Y_k, S_k \rangle, \qquad \omega := \langle \text{svec}(S_k), B_k \text{svec}(S_k) \rangle.$$

Finally, we update the Hessian approximation with

$$B_{k+1} := B_k + \frac{1}{\upsilon}\left(\text{svec}(Y_k)\text{svec}(Y_k^T)\right) - \frac{1}{\omega}\left(B_k \text{svec}(S_k)\text{svec}(S_k)^T B_k\right).$$

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

The equation for the search direction is

$$G'_\mu(Q_p, \Lambda, Z) \begin{pmatrix} \Delta Q_p \\ \Delta\Lambda \\ \Delta Z \end{pmatrix} = -G_\mu(Q_p, \Lambda, Z), \tag{11}$$

where

$$G_\mu(Q_p, \Lambda, Z) = \begin{pmatrix} \nabla p^*_{\mathrm{CQP}}(Q_p) - \Lambda \\ Q - Q_p + Z \\ Z\Lambda - \mu I \end{pmatrix} =: \begin{pmatrix} R_d \\ R_p \\ R_c \end{pmatrix}. \tag{12}$$

If B is the current estimate of the Hessian, then (11) becomes

$$\begin{cases} \mathrm{sMat}(B\ \mathrm{svec}(\Delta Q_p)) - \Delta\Lambda = -R_d, \\ -\Delta Q_p + \Delta Z = -R_p, \\ Z\Delta\Lambda + \Delta Z\Lambda = -R_c. \end{cases}$$

We can substitute for the variables $\Delta\Lambda$ and ΔZ 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,

$$\Delta\Lambda = \mathrm{sMat}(B\ \mathrm{svec}(\Delta Q_p)) + R_d, \quad \Delta Z = -R_p + \Delta Q_p. \tag{13}$$

Accordingly, we have a single equation to solve, and the system finally becomes

$$Z\ \mathrm{sMat}(B\ \mathrm{svec}(\Delta Q_p)) + (\Delta Q_p)\Lambda = -R_c - ZR_d + R_p\Lambda.$$

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 $\mathbf{CQP}_{Q_p}$ for the current perturbation Q_p. Problem $\mathbf{CQP}_{Q_p}$ is thus solved at each iteration of the IPM method, each time for a new perturbation Q_p, such that $Q - Q_p \prec 0$.

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 **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, Gilbert, 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 μ tends to zero and strict complementarity holds.

Algorithm 1 Updating the perturbation Q_p.

Input: k, Q_p^k, Z^k, Λ^k, $x(Q_p^k)$, $X(Q_p^k)$, $\nabla p^*_{\mathrm{CQP}}(Q_p^k)$, B_k, μ^k, $\tau_\alpha := 0.95$, $\tau_\mu := 0.9$.

Compute the residuals:

$$\begin{pmatrix} R_d \\ R_p \\ R_c \end{pmatrix} := \begin{pmatrix} \nabla p^*_{\mathrm{CQP}}(Q_p^k) - \Lambda^k \\ Q - Q_p^k + Z^k \\ Z^k\Lambda^k - \mu^k I \end{pmatrix}.$$

Solve the linear system for ΔQ_p:

$$Z^k\ \mathrm{sMat}(B_k\ \mathrm{svec}(\Delta Q_p)) + (\Delta Q_p)\Lambda^k = -R_c - Z^k R_d + R_p\Lambda^k.$$

Set:

$$\Delta\Lambda := \mathrm{sMat}(B_k\ \mathrm{svec}(\Delta Q_p)) + R_d, \quad \Delta Z := -R_p + \Delta Q_p.$$

Update Q_p, Z and Λ:

$$Q_p^{k+1} := Q_p^k + \hat{\alpha}_p\Delta Q_p, \ Z^{k+1} := Z_p^k + \hat{\alpha}_p\Delta Z, \ \Lambda^{k+1} := \Lambda^k + \hat{\alpha}_d\Delta\Lambda,$$

where

$$\hat{\alpha}_p := \tau_\alpha \times \min\{1, \mathrm{argmax}_{\alpha_p}\{Z_p^k + \alpha_p\Delta Z \succeq 0\}\},$$
$$\hat{\alpha}_d := \tau_\alpha \times \min\{1, \mathrm{argmax}_{\alpha_d}\{\Lambda^k + \alpha_d\Delta\Lambda \succeq 0\}\}.$$

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

Update the gradient of p^*_{CQP}:

$$\nabla p^*_{\mathrm{CQP}}(Q_p^{k+1}) := X(Q_p^{k+1}) - x(Q_p^{k+1})x(Q_p^{k+1})^T.$$

Update the Hessian approximation of p^*_{CQP} (if $\upsilon > 0$):

$$Y_k := \nabla p^*_{\mathrm{CQP}}(Q_p^{k+1}) - \nabla p^*_{\mathrm{CQP}}(Q_p^k), \ S_k := Q_p^{k+1} - Q_p^k,$$
$$\upsilon := \langle Y_k, S_k\rangle, \ \omega := \langle \mathrm{svec}(S_k), B_k\mathrm{svec}(S_k)\rangle,$$
$$B_{k+1} := B_k + \frac{1}{\upsilon}\left(\mathrm{svec}(Y_k)\mathrm{svec}(Y_k^T)\right) - \frac{1}{\omega}\left(B_k\ \mathrm{svec}(S_k)\mathrm{svec}(S_k)^T B_k\right).$$

Update μ:

$$\mu^{k+1} := \tau_\mu \frac{\mathrm{trace}(Z^{k+1}\Lambda^{k+1})}{n}.$$

Output: Q_p^{k+1}, Z^{k+1}, Λ^{k+1}, $x(Q_p^{k+1})$, $X(Q_p^{k+1})$, $\nabla p^*_{\mathrm{CQP}}(Q_p^{k+1})$, B_{k+1}, μ^{k+1}.

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 $\mathbf{CQP}_{Q_p}$, 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_p 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 $\mathbf{CQP}_{Q_p}$. We could observe with our computational experiments that the best bounds were obtained by $\mathbf{CQP}_{Q_p}$, when we had $Q - Q_p \neq 0$, for all instances considered.

Consider the linear SDP problem given by

$$(\mathbf{LSDP}) \qquad \begin{array}{rll} p^*_{\mathrm{LSDP}} := & \sup & \mathrm{trace}(QX) \\ & \mathrm{s.t.} & (x, X) \in \mathcal{F} \\ & & X - xx^T \succeq 0, \end{array} \tag{14}$$

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

We now consider the parametric SDP problem given by

$$(\mathbf{QSDP}_{Q_p}) \qquad \begin{array}{rll} p^*_{\mathrm{QSDP}_{Q_p}} := & \sup & x^T(Q - Q_p)x + \mathrm{trace}(Q_pX) \\ & \mathrm{s.t.} & (x, X) \in \mathcal{F} \\ & & X - xx^T \succeq 0, \end{array} \tag{15}$$

where $Q - Q_p \preceq 0$.

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*

$$p^*_{\mathrm{QSDP}_{Q_p}} \geq p^*_{\mathrm{LSDP}}. \tag{16}$$

Moreover, $\inf\{p^*_{\mathrm{QSDP}_{Q_p}} : Q - Q_p \preceq 0\} = p^*_{\mathrm{LSDP}}$.

Proof. Let $(\tilde{x}, \tilde{X})$ be a feasible solution for **LSDP**. We have

$$p^*_{\mathrm{QSDP}_{Q_p}} \geq \tilde{x}^T(Q - Q_p)\tilde{x} + \mathrm{trace}(Q_p\tilde{X}) \tag{17}$$

$$= \mathrm{trace}((Q - Q_p)(\tilde{x}\tilde{x}^T - \tilde{X})) + \mathrm{trace}((Q - Q_p)\tilde{X}) + \mathrm{trace}(Q_p\tilde{X}) \tag{18}$$

$$= \mathrm{trace}((Q - Q_p)(\tilde{x}\tilde{x}^T - \tilde{X})) + \mathrm{trace}(Q\tilde{X}) \tag{19}$$

$$\geq \mathrm{trace}(Q\tilde{X}). \tag{20}$$

The inequality (17) holds because $(\tilde{x}, \tilde{X})$ is also a feasible solution for $\mathbf{QSDP}_{Q_p}$. The inequality in (20) holds because of the negative semidefiniteness of $Q - Q_p$ and $\tilde{x}\tilde{x}^T - \tilde{X}$. Because $p^*_{\mathrm{QSDP}_{Q_p}}$ is an upper bound on the objective value of **LSDP** at any feasible solution, we can conclude that $p^*_{\mathrm{QSDP}_{Q_p}} \geq p^*_{\mathrm{LSDP}}$. Clearly, $Q_p = Q$ satisfies $Q - Q_p = 0 \preceq 0$ and **LSDP** is the same as $\mathbf{QSDP}_{Q_p}$ for this choice of Q_p. Therefore, $\inf\{p^*_{\mathrm{QSDP}_{Q_p}} : Q - Q_p \preceq 0\} = p^*_{\mathrm{LSDP}}$. □

Notice that in Theorem 2 we do not require that $\mathcal{F}$ be convex nor bounded. Also, in principle, for some choices of Q_p, we could have $p^*_{\mathrm{QSDP}_{Q_p}} = +\infty$ with $p^*_{\mathrm{LSDP}} = +\infty$ or not.

Remark 3. As a corollary from Theorem 2, we have that the upper bound for **QKP**, given by the solution of the quadratic relaxation $\mathbf{CQP}_{Q_p}$, cannot be smaller than the upper bound given by the solution of the SDP relaxation obtained from it, by adding the SDP constraint $X - xx^T \succeq 0$ and setting Q_p equal to Q.

In Billionnet et al. (2016, Theorem 1), this result was already proven for the case where $\mathcal{F}$ is a particular convex set. The authors also claim that in this particular case, the best bound obtained by the CQP relaxation is exactly the same as the bound given by the linear SDP relaxation, and that the best perturbation can be derived from the optimal dual variables of the SDP problem. Nevertheless the proof presented in Billionnet et al. (2016) is based on an incorrect formulation of the dual SDP problem. In the following, we prove that the result holds, following the same idea used 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. The result then applies to the CQP relaxations that we use in this work.

Theorem 4. *Consider $\mathcal{F} \subset \mathbb{R}^n \times \mathbb{S}^n$ as a bounded polyhedron with nonempty interior, defined by:*

$$\mathcal{F} := \{(x, X) : \mathrm{trace}(\Gamma_k X) + \gamma_k^T x \leq b_k, \quad k = 1, \ldots, q\},$$

where $\Gamma_k \in \mathbb{S}^n$ and $\gamma_k \in \mathbb{R}^n$, for $k = 1, \ldots, q$.

Define

$$p^*_{\mathrm{POLCQP}}(Q_p) := \max\{x^T(Q - Q_p)x + \mathrm{trace}(Q_pX) \ : \ (x, X) \in \mathcal{F}\},$$

where $Q - Q_p \preceq 0$, and

$$p^*_{\mathrm{POLSDP}} := \max\{\mathrm{trace}(QX) \ : \ (x, X) \in \mathcal{F},\ X - xx^T \succeq 0\}. \tag{21}$$

Then

$$\min_{Q - Q_p \preceq 0} p^*_{\mathrm{POLCQP}}(Q_p) = p^*_{\mathrm{POLSDP}}.$$

Proof. First we consider the parametric problem

$$\begin{array}{lll} & \displaystyle\min_{Q-Q_p \preceq 0} & p^*_{\mathrm{POLCQP}}(Q_p) \\ = & \displaystyle\min_{Q-Q_p \preceq 0} & \displaystyle\max_{x,X} \quad x^T(Q - Q_p)x + \mathrm{trace}(Q_pX) \\ & & \mathrm{s.t.} \quad \mathrm{trace}(\Gamma_k X) + \gamma_k^T x \leq b_k,\ k = 1, \ldots, q. \\ & (: y_k \geq 0) & \end{array} \tag{22}$$

Considering $Q_n := Q_n(Q_p) := Q - Q_p$, the Lagrangian function of the inner maximization problem in (22) is defined as

$$L(x, X, y) := x^TQ_nx + \mathrm{trace}(Q_pX) + \sum_{k=1}^q y_k^T(b_k - \mathrm{trace}(\Gamma_kX) - \gamma_k^Tx).$$

The Lagrangian dual function is then defined as

$$\begin{aligned} g(y) &:= \max_{x,X} \quad L(x, X, y) \\ &= \max_{x,X} \quad x^TQ_nx + \mathrm{trace}(Q_pX) + \sum_{k=1}^q y_k(b_k - \mathrm{trace}(\Gamma_kX) - \gamma_k^Tx) \\ &= \max_{x,X} \quad \mathrm{trace}\left(\left(Q_p - \sum_{k=1}^q y_k\Gamma_k\right)X\right) + x^TQ_nx - \sum_{k=1}^q y_k\gamma_k^Tx + \sum_{k=1}^q y_kb_k \\ &= \max_x \begin{cases} x^TQ_nx - \sum_{k=1}^q y_k\gamma_k^Tx + \sum_{k=1}^q y_kb_k, & \text{if } Q_p - \sum_{k=1}^q y_k\Gamma_k = 0, \\ +\infty, & \text{otherwise.} \end{cases} \\ &= \begin{cases} -\frac{1}{4}\left(\sum_{k=1}^q y_k\gamma_k\right)^T Q_n^\dagger \left(\sum_{k=1}^q y_k\gamma_k\right) + y^Tb, & \\ \qquad \text{if } Q_p - \sum_{k=1}^q y_k\Gamma_k = 0 \text{ and } \sum_{k=1}^q y_k\gamma_k \in \mathrm{range}(Q_n), & \\ +\infty, \quad \text{otherwise,} & \end{cases} \end{aligned}$$

where $Q_n^\dagger$ is the pseudo-inverse of Q_n.

As $\mathcal{F}$ has nonempty interior, the Slater condition holds for the inner maximization problem in (22). Therefore, problem (22) has the same optimal value as

$$\begin{array}{ll} \displaystyle\min_{Q_p, Q_n, y} & -\frac{1}{4}\left(\sum_{k=1}^q y_k\gamma_k\right)^T Q_n^\dagger \left(\sum_{k=1}^q y_k\gamma_k\right) + y^Tb \\ \mathrm{s.t.} & Q_p - \sum_{k=1}^q y_k\Gamma_k = 0, \\ & \sum_{k=1}^q y_k\gamma_k \in \mathrm{range}(Q_n), \\ & Q_n = Q - Q_p \preceq 0,\ y \geq 0, \end{array}$$

which is equivalent to

$$\begin{array}{ll} -\displaystyle\max_{t, Q_p, y} & t \\ \mathrm{s.t.} & \frac{1}{4}\left(\sum_{k=1}^q y_k\gamma_k\right)^T (Q - Q_p)^\dagger \sum_{k=1}^q y_k\gamma_k - y^Tb - t \geq 0, \\ & Q - Q_p \preceq 0, \\ & \sum_{k=1}^q y_k\gamma_k \in \mathrm{range}(Q - Q_p), \\ & Q_p - \sum_{k=1}^q y_k\Gamma_k = 0, \\ & y \geq 0. \end{array}$$

By Schur complement (Horn & Zhang, 2005), this is equivalent to the following SDP problem

$$\begin{array}{ll} -\displaystyle\max_{t, Q_p, y} & t \\ \mathrm{s.t.} & \begin{bmatrix} -t - y^Tb & \left(\sum_{k=1}^q y_k\gamma_k\right)^T/2 \\ \left(\sum_{k=1}^q y_k\gamma_k\right)/2 & Q_p - Q \end{bmatrix} \succeq 0, \\ & Q_p - \sum_{k=1}^q y_k\Gamma_k = 0, \\ & y \geq 0. \end{array}$$

After substitution, this is equivalent to

$$\begin{array}{rll}\min\limits_{t,y} & -t & \\ \text{s.t.} & \begin{bmatrix} -t-y^Tb & \left(\sum_{k=1}^{q} y_k\gamma_k\right)^T/2 \\ \left(\sum_{k=1}^{q} y_k\gamma_k\right)/2 & \sum_{k=1}^{q} y_k\Gamma_k - Q \end{bmatrix} & \\ \succeq & 0. \left(: \begin{bmatrix} s & z^T \\ z & Z \end{bmatrix} \succeq 0\right) & \\ & y \geq 0. & \end{array} \tag{23}$$

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

$$\begin{aligned} & L(t,y,s,z,Z) \\ &= -t - \text{trace}\left(\begin{bmatrix} s & z^T \\ z & Z\end{bmatrix}\begin{bmatrix} -t-y^Tb & \left(\sum_{k=1}^{q} y_k\gamma_k\right)^T\Big/2 \\ \left(\sum_{k=1}^{q} y_k\gamma_k\right)\Big/2 & \sum_{k=1}^{q} y_k\Gamma_k - Q \end{bmatrix}\right) \\ &= -t - s(-t-y^Tb) - \left(\sum_{k=1}^{q} y_k\gamma_k\right)^T z - \text{trace}\left(Z\left(\sum_{k=1}^{q} y_k\Gamma_k - Q\right)\right) \\ &= t(s-1) + sy^Tb - \left(\sum_{k=1}^{q} y_k\gamma_k\right)^T z - \text{trace}\left(Z\left(\sum_{k=1}^{q} y_k\Gamma_k - Q\right)\right) \\ &= t(s-1) + \sum_{k=1}^{q} y_k(sb_k - \gamma_k^T z - \text{trace}(\Gamma_k Z)) + \text{trace}(QZ). \end{aligned}$$

The Lagrangian dual function is defined as

$$\begin{aligned} h(s,z,Z) &:= \min_{y\geq 0,t} \quad L(t,y,s,z,Z) \\ &= \min_{y\geq 0,t} \quad t(s-1) + \sum_{k=1}^{q} y_k(sb_k - \gamma_k^T z - \text{trace}(\Gamma_k Z)) + \text{trace}(QZ) \\ &= \begin{cases} \text{trace}(QZ), \\ \quad \text{if } s=1,\ sb_k - \gamma_k^T z - \text{trace}(\Gamma_k Z) \geq 0, k=1,\dots,q, \\ -\infty, \text{ otherwise.} \end{cases} \end{aligned}$$

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

$$\begin{array}{rll} \max\limits_{z,Z} & \text{trace}(QZ) & \\ \text{s.t.} & \text{trace}(\Gamma_k Z) + \gamma_k^T z \leq b_k, & k=1,\dots,q, \\ & \begin{bmatrix} 1 & z^T \\ z & Z \end{bmatrix} \succeq 0. & \end{array} \tag{24}$$

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 **QKP** in the lifted space determined by the lifting $X := xx^T$. Let us denote by **CRel**, any convex relaxation of **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 $\textbf{QKP}_{\text{lifted}}$

We note that if the inequality

$$\tau^T x \leq \beta \tag{25}$$

is valid for **QKP**, where $\tau \in \mathbb{Z}_+^n$ and $\beta \in \mathbb{Z}_+$, then, as $x$is nonnegative and $X := xx^T$,

$$(x\ X)\begin{pmatrix} -\beta \\ \tau \end{pmatrix} \leq 0 \tag{26}$$

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

$\textbf{KF} := \{x \in \{0,1\}^n : w^T x \leq c\}$.

Definition 5 (Zero-one knapsack polytope)**.**

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

Proposition 6. *The dimension*

$\dim(\textbf{KPol}) = n$,

*and **KPol** is an independence system, i.e.,*

$x \in \textbf{KPol}, y \in \{0,1\}^n, y \leq x \Rightarrow y \in \textbf{KPol}$.

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 **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

$$\sum_{j\in C} x_j \leq |C| - 1. \tag{27}$$

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

$E(C) := C \cup \{j \in N \backslash C : w_j \geq w^*\}$.

The **ECI** is

$$\sum_{j\in E(C)} x_j \leq |C| - 1. \tag{28}$$

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

$$\sum_{j\in C} x_j + \sum_{j\in N\backslash C} \alpha_j x_j \leq |C| - 1, \tag{29}$$

is a valid inequality for **KF**. Inequality (29) is a **LCI**.

Cover inequalities are extensively discussed in Hammer, Johnson, and Peled (1975), Balas and Zemel (1978), Balas (1975), Wolsey (1975), Nemhauser and Wolsey (1988), and Atamtürk (2005). Details about the computational complexity of **LCI** is presented in Zemel (1989) 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 **KPol** when C is a minimal cover and $\bar{t} = 1$.

Algorithm 2 Procedure to Lift Cover Inequalities.

Input: A cover C and a valid inequality

$$\sum_{j=1}^{\bar{t}-1} \alpha_{i_j} x_{i_j} + \sum_{i \in C} x_i \leq |C| - 1,$$

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

$$\begin{aligned} \zeta_t = \quad & \max \quad \sum_{j=1}^{t-1} \alpha_{i_j} x_{i_j} + \sum_{i \in C} x_i \\ & \text{s.t.} \quad \sum_{j=1}^{t-1} w_{i_j} x_{i_j} + \sum_{i \in C} w_i x_i \leq c - w_{i_t} \\ & \qquad x \in \{0, 1\}^{|C|+t-1}. \end{aligned} \tag{30}$$

Set $\alpha_{i_t} = |C| - 1 - \zeta_t$.

End

5.2. Adding cuts to the relaxation

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

$$\mathbf{cut}(\alpha) = \begin{pmatrix} -e^T \alpha + 1 \\ \alpha \end{pmatrix}.$$

To obtain such a **CI**, we solve the following linear knapsack problem,

$$v^* := \max_{\alpha} \{ e^T \bar{Y} \mathbf{cut}(\alpha) : w^T \alpha \geq c + 1,\ \alpha \in \{0, 1\}^n \}. \tag{31}$$

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

$$(x\, X) \begin{pmatrix} -e^T \alpha^* + 1 \\ \alpha^* \end{pmatrix} \leq 0. \tag{32}$$

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

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

Proof. Consider the **LCI** (29) derived from a **CI** (27) for **QKP**. The corresponding scaled cover inequalities (26) derived from the **CI** and the **LCI** are, respectively,

$$\sum_{j \in C} X_{ij} \leq (|C| - 1) x_i, \quad \forall i \in N,$$

and

$$\sum_{j \in C} X_{ij} + \sum_{j \in N \setminus C} \alpha_j X_{ij} \leq (|C| - 1) x_i, \quad \forall i \in N,$$

where $\alpha_j \geq 0$, $\forall j \in N \backslash C$. Clearly, as all X_{ij} 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 **QKP**, we may add the constraint (26) to **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 $x$is binary. In the following, we show how the idea can be applied to cover inequalities.

Let

$$\sum_{j \in C} x_j \leq \beta, \tag{33}$$

where $C \subset N$ and $\beta < |C|$, be a valid inequality for **KPol**.

Inequality (33) can be either a cover inequality, **CI**, an extended cover inequality, **ECI**, or a particular lifted cover inequality, **LCI**, where $\alpha_j \in \{0, 1\}$, $\forall j \in N \backslash C$ in (29). Furthermore, given a general **LCI**, where $\alpha_j \in \mathbb{Z}_+$, for all $j \in N \backslash C$, a valid inequality of type (33) can be constructed by replacing each α_j with $\min\{\alpha_j, 1\}$ in the **LCI**.

Definition 11 (Cover inequality in the lifted space, **CILS**)**.** Let $C \subset N$ and $\beta < |C|$ as in inequality (33), and also consider here that $\beta > 1$. We define

$$\sum_{i,j \in C, i<j} X_{ij} \leq \binom{\beta}{2}. \tag{34}$$

as the **CILS** derived from (33).

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

Proof. Considering (33), we conclude that at most $\binom{\beta}{2}$ 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 idea to what was used to construct the **CILS**, we conclude that it is possible to fix

$$X_{ij} = 0, \text{ for all } i, j \in C, i < j.$$

Given a solution $(\bar{x}, \bar{X})$ of **CRel**, the following MIQP problem is a separation problem, which searches for a **CILS** violated by $\bar{X}$.

$$\begin{array}{llll} z^* := & \max_{\alpha,\beta,K} \operatorname{trace}(\bar{X}K) - \beta(\beta - 1), & & (\mathbf{MIQP}_1) \\ \text{s.t.} & w^T \alpha \geq c + 1, & & \\ & \beta = e^T \alpha - 1, & & \\ & K(i,i) = 0, & i = 1, \ldots, n, & \\ & K(i,j) \leq \alpha_i, & i, j = 1, \ldots, n,\ i < j, & \\ & K(i,j) \leq \alpha_j, & i, j = 1, \ldots, n,\ i < j, & \\ & K(i,j) \geq 0, & i, j = 1, \ldots, n,\ i < j, & \\ & K(i,j) \geq \alpha_i + \alpha_j - 1, & i, j = 1, \ldots, n,\ i < j, & \\ & \alpha \in \{0, 1\}^n,\ \beta \in \mathbb{R},\ K \in \mathbb{S}^n. & & \end{array}$$

If α^*, β^*, K^* solves $\mathbf{MIQP}_1$, with $z^* > 0$, the **CILS** given by $\operatorname{trace}(K^* X) \leq \beta^*(\beta^* - 1)$ is violated by $\bar{X}$. The binary vector α^* defines the **CI** from which the cut is derived. The **CI** is specifically given by ${\alpha^*}^T x \leq e^T \alpha^* - 1$ and $\beta^*(\beta^* - 1)$ determines the right-hand side of the **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 **CILS** for* $\mathbf{QKP}_{\text{lifted}}$*, which is derived from a valid **LCI** in the form (33), dominates any **CILS** derived from a **CI** that can be lifted to the **LCI**.*

Proof. As X is nonnegative, it is straightforward to verify that if X satisfies a **CILS** derived from a **LCI**, X also satisfies any **CILS** derived from a **CI** that can be lifted to the **LCI**. □

Any feasible solution of $\textbf{MIQP}_1$ such that $\text{trace}(\bar{X}K) > \beta(\beta-1)$ generates a valid inequality for $\textbf{QKP}_{\text{lifted}}$ that is violated by $\bar{X}$. Therefore, we do not need to solve $\textbf{MIQP}_1$ to optimality to generate a cut. Moreover, to generate distinct cuts, we can solve $\textbf{MIQP}_1$ several times (not necessarily to optimality), each time adding to it, the following "no-good" cut to avoid the previously generated cuts:

$$\sum_{i\in N}\bar{\alpha}(i)(1-\alpha(i)) \geq 1, \tag{35}$$

where $\bar{\alpha}$ is the value of the variable α in the solution of $\textbf{MIQP}_1$ when generating the previous cut.

We note that, if α^*, β^*, K^* solves $\textbf{MIQP}_1$, then ${\alpha^*}^T x \leq e^T\alpha^* - 1$ 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 $\textbf{MIQP}_1$, the term $-\delta e^T\alpha$, 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 $\bar{X}$, then clearly, the **CILS** derived from the **LCI** will also be violated by $\bar{X}$.

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

$$\sum_{(i,j)\in C_s} X_{ij} \leq \left\lfloor \frac{\beta}{2} \right\rfloor, \tag{36}$$

for all partitions C_s defined as above.

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

Proof. The proof of the validity of **SCILS** is based on the lifting relation $X_{ij} = x_i x_j$. We note that if the binary variable x_i 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_s is a partition of C in exactly $|C|/2$ subsets with two elements each, and therefore, if at most β elements of C can be selected in the solution, clearly at most $\left\lfloor \frac{\beta}{2} \right\rfloor$ subsets of C_s can also be selected.
2. If $|C|$ and β are odd, C_s is a partition of $C\backslash\{i_0\}$ 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 β elements of C can be selected in the solution, clearly at most $\frac{\beta-1}{2}\left(= \left\lfloor \frac{\beta}{2} \right\rfloor\right)$ subsets of C_s can also be selected.
3. If $|C|$ is odd and β is even, C_s is the union of $\{(i_0, i_0)\}$ with a partition of $C\backslash\{i_0\}$ 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 β elements of C can be selected in the solution, clearly at most $\frac{\beta}{2}\left(= \left\lfloor \frac{\beta}{2} \right\rfloor\right)$ subsets of C_s can also be selected.

□

Given a solution $(\bar{x}, \bar{X})$ of **CRel**, we now present a mixed linear integer programming (MILP) separation problem, which searches for an inequality in **SCILS** that is most violated by $\bar{X}$. Let $A \in \{0,1\}^{n\times\frac{n(n+1)}{2}}$. 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 $n = 4$,

$$A := \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \end{pmatrix}.$$

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

$$\begin{aligned}
z^* := \max_{\alpha,v,K,y}\ & \text{trace}(\bar{X}K) - 2v, && (\textbf{MILP}_2)\\
\text{s.t. } & w^T\alpha \geq c+1, \\
& K(i,i) = 2y(i), && i = 1,\ldots,n,\\
& \sum_{i=1}^{n} y(i) \leq 1, \\
& K(i,j) = \sum_{t=n+1}^{n(n+1)/2} A(i,t)A(j,t)y(t), && i,j = 1,\ldots,n,\ i<j,\\
& v \geq (e^T\alpha - 1)/2 - 0.5, \\
& v \leq (e^T\alpha - 1)/2, \\
& y(t) \leq 1 - A(i,t) + \alpha(i), && i = 1,\ldots,n,\\
& && t = 1,\ldots,\tfrac{n(n+1)}{2},\\
& \alpha \leq Ay \leq \alpha + \left(\tfrac{n(n+1)}{2}\right)(1-\alpha), \\
& \alpha \in \{0,1\}^n,\ y \in \{0,1\}^{\frac{n(n+1)}{2}}, \\
& v \in \mathbb{Z},\ K \in \mathbb{S}^n.
\end{aligned}$$

If α^*, v^*, K^*, y^* solves $\textbf{MILP}_2$, with $z^* > 0$, then the particular inequality in **SCILS** given by

$$\text{trace}(K^*X) \leq 2v^* \tag{37}$$

is violated by $\bar{X}$. The binary vector α^* defines the **CI** from which the cut is derived. As the **CI** is given by $\alpha^* x \leq e^T\alpha^* - 1$, 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 $\textbf{MILP}_2$. The vector y^* defines a partition C_s as presented in case (3), if $\sum_{i=1}^n y(i) = 1$, and in case (1), 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 $\textbf{MIQP}_1$.

Any feasible solution of $\textbf{MILP}_2$ such that $\text{trace}(\bar{X}K) > 2v$ generates a valid inequality for **CRel**, which is violated by $\bar{X}$. Therefore, we do not need to solve $\textbf{MILP}_2$ to optimality to generate a cut. Moreover, to generate distinct cuts, we can solve $\textbf{MILP}_2$ several times (not necessarily to optimality), each time adding to it, the following suitable "no-good" cut to avoid the previously generated cuts:

$$\sum_{i=1}^{\frac{n(n+1)}{2}} \bar{y}(i)(1-y(i)) \geq 1, \tag{38}$$

where $\bar{y}$ is the value of the variable y in the solution of $\textbf{MILP}_2$, when generating the previous cut.

The **CI** ${\alpha^*}^T x \leq e^T\alpha^* - 1$ may not be a minimal cover. Aiming at generating stronger valid cuts, we might add again to the objective function of $\textbf{MILP}_2$, the term $-\delta e^T\alpha$, for some weight $\delta > 0$. The objective function would then favor minimal covers, which could be lifted to a facet-defining **LCI**. In this case, however, after computing the **LCI**, we have to solve $\mathbf{MILP}_2$ again, with α fixed at values that represent the **LCI**, and ν fixed so that the right-hand side of the inequality is equal to the right-hand side of the **LCI**. All components of y that were equal to 1 in the previous solution of $\mathbf{MILP}_2$ should also be fixed at 1. The new solution of $\mathbf{MILP}_2$ would indicate the other subsets of N to be added to C_s. 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 $\mathbf{MILP}_2$ should be modified accordingly. Specifically, the second and third constraints in $\mathbf{MILP}_2$, should be modified respectively to

$$K(i,i)=0, \qquad i=1,\ldots,n,$$
$$\sum_{i=1}^{n} y(i)=1.$$

Remark 17. Let $\gamma := |C|$. Then, the number of inequalities in the **SCILS** is

$$\frac{\gamma!}{2^{(\frac{\gamma}{2})}(\frac{\gamma}{2}!)},$$

if γ is even, or

$$\gamma \times \frac{(\gamma-1)!}{2^{(\frac{\gamma-1}{2})}(\frac{\gamma-1}{2}!)},$$

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 $\alpha_j \in \mathbb{Z}_+, \forall j \in N \backslash C$.

Let

$$\sum_{j\in N} \alpha_j x_j \le \beta. \tag{39}$$

be a valid knapsack inequality for **KPol**, with $\alpha_j, \beta \in \mathbb{Z}_+, \beta \ge \alpha_j, \forall j \in N$.

Definition 18 (Set of knapsack inequalities in the lifted space, SKILS)**.** Let α_j be the coefficient of x_j in (39). Let $\{C_1,\ldots,C_q\}$ be the partition of N, such that $\alpha_u=\alpha_v$, if $u,v\in C_k$ for some k, and $\alpha_u \neq \alpha_v$, otherwise. The knapsack inequality (39) can then be rewritten as

$$\sum_{k=1}^{q}\left(\tilde{\alpha}_k \sum_{j\in C_k} x_j\right) \le \beta. \tag{40}$$

Now, for $k=1,\ldots,q$, let $C_{l_k} := \{(i_{k_1}, j_{k_1}),\ldots,(i_{k_{p_k}}, j_{k_{p_k}})\}$, where $i<j$ for all $(i,j)\in C_{l_k}$, and

- C_{l_k} is a partition of C_k, if $|C_k|$ is even.
- C_{l_k} is a partition of $C_k \setminus \{i_{k_0}\}$, where $i_{k_0}\in C_k$, if $|C_k|$ is odd.

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

$$\sum_{k=1}^{q}\left(\tilde{\alpha}_k X_{i_{k_0} i_{k_0}} + 2\tilde{\alpha}_k \sum_{(i,j)\in C_{l_k}} X_{ij}\right) \le \beta, \tag{41}$$

for all partitions C_{l_k}, $k=1,\ldots,q$, defined as above, and for all $i_{k_0} \in C_k \setminus C_{l_k}$. (If $|C_k|$ is even, $C_k \setminus C_{l_k} = \emptyset$, and the term in the variable $X_{i_{k_0} i_{k_0}}$ does not exist.)

Remark 19. Consider $\{C_1,\ldots,C_q\}$ as in Definition 18. For $k=1,\ldots,q$, let $\gamma_k := |C_k|$ and define

$$NC_{l_k} := \frac{\gamma_k!}{2^{(\frac{\gamma_k}{2})}(\frac{\gamma_k}{2}!)},$$

if γ_k is even, or

$$NC_{l_k} := \gamma_k \times \frac{(\gamma_k-1)!}{2^{(\frac{\gamma_k-1}{2})}(\frac{\gamma_k-1}{2}!)},$$

if γ_k is odd.

Then, the number of inequalities in **SKILS** is

$$\prod_{k=1}^{q} NC_{l_k}.$$

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

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

Corollary 21. *If inequality (39) is valid for **QKP**, then the inequalities (41), in the **SKILS**, are valid for $\mathbf{QKP}_{\text{lifted}}$, 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 $X_{ij}=1$, 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 $\gamma := |C|$ to be even.*

1. *If $\beta=\gamma-1$, 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 $\beta<\gamma-1$, there is no dominance relation between **SCILS** and **CILS**.*

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

$$rhs(sum(\mathbf{SCILS})) = \frac{\gamma!}{2^{(\frac{\gamma}{2})}(\frac{\gamma}{2}!)} \times \left\lfloor\frac{\beta}{2}\right\rfloor.$$

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

$$coef_{ij} = \frac{(\gamma-2)!}{2^{(\frac{(\gamma-2)}{2})}(\frac{(\gamma-2)}{2}!)}$$

Dividing $rhs(sum(\mathbf{SCILS}))$ by $coef_{ij}$, we obtain

$$rhs(sum(\mathbf{SCILS}))/coef_{ij} = (\gamma-1)\times\left\lfloor\frac{\beta}{2}\right\rfloor. \tag{42}$$

On the other side, the rhs of **CILS** is:

$$rhs(\mathbf{CILS}) = \binom{\beta}{2} = \frac{\beta(\beta-1)}{2}. \tag{43}$$

1. Replacing β with $\gamma-1$, and $\left\lfloor\frac{\beta}{2}\right\rfloor$ with $\frac{\beta-1}{2}$ (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 **CILS** becomes:

$$X_{12}+ X_{13} + X_{14} + X_{15} + X_{16} + X_{23} + X_{24} + X_{25} + X_{26} + X_{34} + X_{35} + X_{36} + X_{45} + X_{46} + X_{56} \leq 3.$$

And a particular inequality in **SCILS** is

$$X_{12} + X_{34} + X_{56} \leq 1. \tag{44}$$

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:

$$X_{12}+ X_{13} + X_{14} + X_{15} + X_{16} + X_{23} + X_{24} + X_{25} + X_{26} + X_{34} + X_{35} + X_{36} + X_{45} + X_{46} + X_{56} \leq 6.$$

And a particular inequality in **SCILS** is

$$X_{12} + X_{34} + X_{56} \leq 2. \tag{45}$$

The solution $X_{1j} = 1$, for $j = 2, \ldots, 6$, $X_{2j} = 1$, for $j = 3, \ldots, 6$, and all other variables equal to zero, satisfies all inequalities in **SCILS**, 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 $\beta = 3$ (β odd). In this case, the **CILS** becomes:

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

And a particular inequality in **SCILS** is

$$X_{23} + X_{45} \leq 1. \tag{46}$$

The solution $X_{1j} = 1$, for $j = 1, \ldots, 5$, 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 $X_{23} = X_{45} = 1$, and all other variables equal to zero, satisfies **CILS**, but does not satisfy (46).

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

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

And a particular inequality in **SCILS** is

$$X_{11} + X_{23} + X_{45} \leq 2. \tag{47}$$

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 **SCILS**, 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

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

if β is odd, and

$$2X_{i_0 i_0} + 2 \sum_{(i,j)\in C_s} X_{ij} \leq \beta,$$

if β is even, and the inequalities in **SKILS** become

$$X_{i_0 i_0} + 2 \sum_{(i,j)\in C_s} X_{ij} \leq \beta,$$

for all β. In all cases, C_s is a partition of $C \backslash \{i_0\}$, where $i_0 \in C$.

Either with β even or odd, it becomes clear that **SCILS** is stronger than **SKILS**. □

6. Lower bounds from solutions of the relaxations for $QKP_{\textbf{lifted}}$

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 $\bar{\lambda}$ and $\bar{v}$, respectively. Then $\bar{\lambda}\bar{v}\bar{v}^T$ is a rank-one approximation of $\bar{X}$. We set $\bar{x} = \bar{\lambda}^{\frac{1}{2}}\bar{v}$ to be an approximation of the solution x of **QKP**. We note that $\bar{\lambda} > 0$ because $\bar{X}_{ii} > 0$ 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 $\bar{\lambda}$ and $\bar{v}$ be, respectively, the largest eigenvalue and the corresponding eigenvector of $\bar{X}$.
Set $\bar{x} = \bar{\lambda}^{\frac{1}{2}}\bar{v}$.
Round $\bar{x}$ to $\hat{x} \in \{0, 1\}^n$.
While $w^T\hat{x} > c$
  Set $i = \text{argmin}_{j\in N}\{\bar{x}_j | \bar{x}_j > 0\}$.
  Set $\bar{x}_i = 0$, $\hat{x}_i = 0$.
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_p 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 Mosek, version 8, to solve the relaxation $\mathbf{CQP}_{Q_p}$, and, to solve the separation problems $\mathbf{MIQP}_1$ and $\mathbf{MILP}_2$, we use Gurobi, 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 $\mathbf{CQP}_{Q_p}$, with $Q_p := Q_p^0$, we obtain $x(Q_p^0)$, $X(Q_p^0)$, as its optimal solution, and set $\nabla p^*_{\mathrm{CQP}}(Q_p^0) := X(Q_p^0) - x(Q_p^0)x(Q_p^0)^T$. Finally, the positive definiteness of Z^0 and Λ^0 are assured by setting: $Z^0 := Q_p^0 - Q$ and $\Lambda^0 := \nabla p^*_{\mathrm{CQP}}(Q_p^0) + (2|\lambda_{\min}(\nabla p^*_{\mathrm{CQP}}(Q_p^0)| + 0.1)I$.

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 $[50, \sum_{j=1}^n w_j]$. The procedure used by Cunha to generate the instances was based on previous works (Billionnet & Calmels, 1996; Caprara et al., 1999; Chaillou et al., 1989; Gallo et al., 1980; Michelon & Veillieux, 1996).

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

- OptGap (%):= ((upper bound − opt)/opt) × 100, where opt is the optimal solution value (the relative optimality gap),
- Time (seconds) (the computational time to compute the bound),
- DuGap (%) := (upper bound − lower bound)/(lower bound) × 100, where the lower bound is computed as described in Section 6 (the relative duality gap),
- Iter (the number of iterations),
- Cuts (the number of cuts added to the relaxation),
- $\mathrm{Time_{MIP}}$ (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

$$(\tilde{\mathbf{LPR}})\quad \begin{array}{lll} \max & \mathrm{trace}(QX) & \\ \text{s.t.} & \sum_{j=1}^{n} w_j x_j \le c, & \\ & 0 \le X_{ij} \le 1, & \forall i, j \in N \\ & 0 \le x_i \le 1, & \forall i \in N \\ & X \in \mathbb{S}^n. & \end{array} \tag{48}$$

In the first row of Table 3, the results correspond to the solution of the linear relaxation $\tilde{\mathbf{LPR}}$ with no cuts. In $\mathbf{SCI}_1$, we add only the most violated cut from the n cuts in **SCI** to $\tilde{\mathbf{LPR}}$ 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: $Q \in \mathbb{S}^n$, $max.n_{cuts}$.
$k := 0$, $B_0 := I$, $\mu^0 := 1$.
Let $\lambda_i(Q), v_i$ be the ith largest eigenvalue of Q and corresponding eigenvector.
$Q_n := \sum_{i=1}^n (-|\lambda_i(Q)| - 1) v_i v_i^T$ (or $Q_n := \sum_{i=1}^n (\min\{\lambda_i, -10^{-6}\}) v_i v_i^T$), $Q_p^0 := Q - Q_n$.
Solve $\mathbf{CQP}_{Q_p}$, with $Q_p := Q_p^0$, and obtain $x(Q_p^0)$, $X(Q_p^0)$.
$\nabla p^*_{\mathrm{CQP}}(Q_p^0) := X(Q_p^0) - x(Q_p^0)x(Q_p^0)^T$.
$Z^0 := Q_p^0 - Q$.
$\Lambda^0 := \nabla p^*_{\mathrm{CQP}}(Q_p^0) + (2|\lambda_{\min}(\nabla p^*_{\mathrm{CQP}}(Q_p^0)| + 0.1)I$.
While (stopping criterium is violated)
  Run Algorithm 1, where Q_p^{k+1} is obtained and relaxation $\mathbf{CQP}_{Q_p}$, with $Q_p := Q_p^{k+1}$ is solved. Let $(x(Q_p^{k+1}), X(Q_p^{k+1}))$ be its optimal solution.
  $upper.bound^{k+1} := p^*_{\mathrm{CQP}}(Q_p^{k+1})$.
  Run Algorithm 3, where $\hat{x}$ is obtained.
  $lower.bound^{k+1} := \hat{x}^T Q \hat{x}$.
  If k mod m == 0
    Solve problem (31) and obtain cuts **SCI** in (32).
    Add the $\max\{n, max.n_{cuts}\}$ cuts **SCI** with the largest violations at $(x(Q_p^{k+1}), X(Q_p^{k+1}))$, to $\mathbf{CQP}_{Q_p}$.
    $n_{cuts} := 0$.
    While ($n_{cuts} < max.n_{cuts}$ & $\mathbf{MIQP}_1$ feasible)
      Solve $\mathbf{MIQP}_1$ and add the **CI** and **CILS** obtained to $\mathbf{CQP}_{Q_p}$.
      Add the “no-good” cut (35) to $\mathbf{MIQP}_1$.
      $n_{cuts} := n_{cuts} + 1$.
    End
    $n_{cuts} := 0$.
    While ($n_{cuts} < max.n_{cuts}$ & $\mathbf{MILP}_2$ feasible)
      Solve $\mathbf{MILP}_2$ and add the **CI** and **SCILS** obtained to $\mathbf{CQP}_{Q_p}$.
      Add the “no-good” cut (38) to $\mathbf{MILP}_2$.
      $n_{cuts} := n_{cuts} + 1$.
    End
  End
  $k := k + 1$.
End
Output: Upper bound $upper.bound^k$, lower bound $lower.bound^k$, and feasible solution $\hat{x}$ to **QKP**.

Fig. 1 depicts the optimality gaps from Table 3. There is a trade-off between the quality of the cuts and the computational time needed to find them. Considering a unique cut of each type, we note that **SCILS** is the strongest cut (OptGap = 9.121%), but the computational time to obtain it, if compared to **CILS** and **SCI**, is bigger. Nevertheless, a decrease in the times could be achieved with a heuristic solution for the separation problems, and also by the application of better stopping criteria for the cutting plane algorithm. We point out that using all cuts together we find a better upper bound than using each type of cut separately (OptGap = 3.315%).

We now analyze the effectiveness of our IPM in decreasing the upper bound while optimizing the perturbation Q_p. To improve the bounds obtained, besides the constraints in (48), we also consider in the initial relaxation, the valid equations $X_{ii} = x_i$, the McCormick inequalities $X_{ij} \le X_{ii}$, and the valid inequalities obtained by

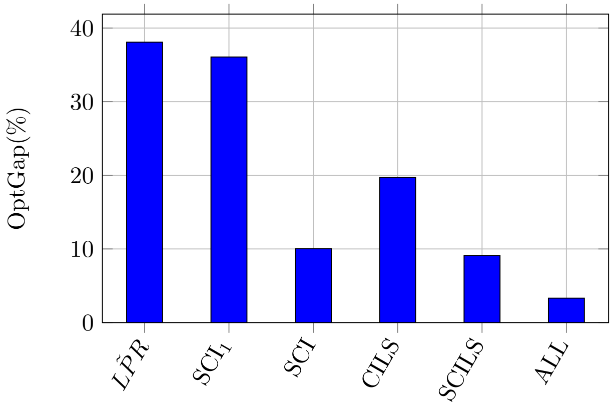

Fig. 1. Average optimality gaps from Table 3.

Table 3
Impact of the cuts added to $\tilde{\text{LPR}}$ on 10 small instances ($n = 10$).

Method	OptGap (%)	Time (seconds)	Iter	Cuts	Time_{MIP} (seconds)
$\tilde{\text{LPR}}$	38.082	0.35	1.0		
SCI_1	36.703	32.38	1.1	28.4	
SCI	10.036	39.98	3.0	364.1	
CILS	19.719	9.00	2.7	82.2	6.91
SCILS	9.121	266.81	50.0	794.3	198.12
ALL	3.315	315.82	28.3	646.6	264.91

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.

$$
(\textbf{QPR}) \quad
\begin{array}{lll}
\max & x^T(Q - Q_p^0)x + \text{trace}(Q_p^0 X) & \\
\text{s.t.} & \sum_{j=1}^{n} w_j x_j \le c, & \\
& \sum_{j=1}^{n} w_j X_{ij} \le c X_{ii}, & \forall i \in N \\
& \sum_{j=1}^{n} w_j (X_{jj} - X_{ij}) \le c(1 - X_{ii}), & \forall i \in N \\
& X_{ii} = X_{ii}, & \forall i \in N \\
& X_{ij} \le X_{ii}, & \forall i, j \in N \\
& 0 \le X_{ij} \le 1, & \forall i, j \in N \\
& 0 \le x_i \le 1, & \forall i \in N \\
& X \in \mathbb{S}^n. &
\end{array}
\qquad (49)
$$

In order to evaluate the influence of the initial decomposition of Q on the behavior of the IPM, we considered two initial decompositions. In both cases, we compute the eigendecomposition of Q, getting $Q = \sum_{i=1}^{n} \lambda_i v_i v_i^T$.

- For the first decomposition, we set $Q_n := \sum_{i=1}^{n}(-|\lambda_i| - 1)v_i v_i^T$, and $Q_p^0 := Q - Q_n/2$. We refer to this initial matrix Q_p^0 as Q_p^a.
- For the second, we set $Q_n := \sum_{i=1}^{n}(\min\{\lambda_i, -10^{-6}\})v_i v_i^T$, and $Q_p^0 := Q - Q_n/2$. We refer to this initial matrix Q_p^0 as Q_p^b.

In Table 4, we compare the bounds obtained by our IPM after 20 iterations ($boundIPM_{20}$), with the bounds given from the linear SDP relaxation obtained by taking $Q_p^0 = Q$ in (49), and adding to it the semidefinite constraint $X - xx^T \succeq 0$ ($boundSDP$). As mentioned in Section 4, these are the best possible bounds that can be obtained by the IPM algorithm. We also show in Table 4 how close to $boundSDP$, the bound computed with the initial decomposition Q_p^0 ($boundIPM_1$) in relaxation (49) is. The values presented in the table are

$$gap_1(\%) = (boundIPM_1 - boundSDP)/boundSDP * 100$$
$$gap_{20}(\%) = (boundIPM_{20} - boundSDP)/boundSDP * 100$$

For the experiment reported in Table 4, we consider 10 instances with $n = 50$ and 100. We see from the results in Table 4 that in 20 iterations, the IPM closed the gap to the SDP bounds for all instances. When starting from Q_p^a, we end up with an average bound less than 0.1% of the SDP bound, while when starting from Q_p^b, this percentage decreases to only 0.03%. We also start from better bounds when considering Q_p^b, and therefore, we use this matrix as the initial decomposition for the IPM in the next experiments. The results in Table 4 show that the IPM developed in this paper is effective to solve the parametric problem (6), converging to bounds very close to the solution of the SDP relaxation, which are their minimum possible values.

We finally present results obtained from the application of Algorithm 4, considering the parametric quadratic relaxation, the IPM, and the cuts. In Tables 5 and 6 we show the results for the same instances with $n = 50$ and $n = 100$ considered in the previous experiment. The cuts are added at every m iterations of the IPM and the numbers of cuts added at each iteration are n **SCI**,

Table 4
SDP bound vs IPM bound at iterations 1 and 20, for two initial matrices Q_p^0.

Q_p^0	Inst	n	$gap_1(\%)$	$gap_{20}(\%)$
Q_p^a	I1	50	0.30	0.01
	I2	50	0.73	0.03
	I3	50	0.14	0.00
	I4	50	1.02	0.21
	I5	50	0.59	0.09
	I1	100	1.47	0.14
	I2	100	0.59	0.04
	I3	100	0.51	0.05
	I4	100	1.38	0.26
	I5	100	0.73	0.06
Q_p^b	I1	50	0.01	0.00
	I2	50	0.30	0.09
	I3	50	0.08	0.03
	I4	50	0.10	0.02
	I5	50	0.03	0.03
	I1	100	0.04	0.00
	I2	100	0.02	0.01
	I3	100	0.03	0.01
	I4	100	0.12	0.04
	I5	100	0.02	0.01

Table 5
Results for Algorithm 4 ($n = 50$).

Inst	OptGap (%)	Time (seconds)	DuGap (%)	Iter	Time_{MIP} (seconds)
I1	0.23	1013.50	0.27	100	641.98
I2	**0.00**	632.50	**0.00**	64	411.67
I3	**0.00**	392.55	**0.00**	44	205.70
I4	**0.00**	289.97	**0.00**	31	160.37
I5	0.21	1093.60	0.37	10	698.04

Table 6
Results for Algorithm 4 ($n = 100$).

Inst	OptGap (%)	Time (seconds)	DuGap (%)	Iter	Time_{MIP} (seconds)
I1	**0.00**	2035.30	**0.00**	20	737.86
I2	0.25	2177.30	0.65	20	919.41
I3	**0.00**	2007.10	**0.00**	20	773.00
I4	0.12	1885.90	0.84	20	828.98
I5	0.04	2309.50	0.20	20	970.49

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 Q_p 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 Q_p 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 Q_p, such that $Q - Q_p \preceq 0$. Seeking for the best possible bound, the concave term $x^T(Q - Q_p)x,$ is then kept in the objective function of the relaxation and the remaining part, given by x^TQ_px is linearized through the standard approach that lifts the problem to space of symmetric matrices defined by $X := xx^T$.

We present a primal-dual interior point method (IPM), which update the perturbation Q_p 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 Q_p, 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 Q_p 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 $X - xx^T \succeq 0$ 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 Q_p 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.

Acknowledgments

We thank J. O. Cunha for providing us with the test instances used in our experiments. We greatly thank the anonymous referees and editor for their constructive comments that significantly improved the paper. M. Fampa was partially supported by CNPq (National Council for Scientific and Technological Development) Grant 303898/2016-0, D. C. Lubke did part of this research at the University of Waterloo, and was supported by Research Grants from CAPES (Brazilian Federal Agency for Support and Evaluation of Graduate Education) Grant 88881.131629/2016-01, CNPq Grant 142143/2015-4 and partially supported by PSR –Power Systems Research, Rio de Janeiro, Brazil.

References

Armand, P., Gilbert, J. C., & Jégou, S. J. (2000). A feasible BFGS interior point algorithm for solving convex minimization problems. *SIAM Journal on Optimization, 11*(1), 199–222.

Atamtürk, A. (2005). Cover and pack inequalities for (mixed) integer programming. *Annals of Operations Research, 139*(1), 21–38.

Balas, E. (1975). Facets of the knapsack polytope. *Mathematical Programming, 8*(1), 146–164.

Balas, E., & Zemel, E. (1978). Facets of the knapsack polytope from minimal covers. *SIAM Journal on Applied Mathematics, 34*(1), 119–148.

Billionnet, A., & Calmels, F. (1996). Linear programming for the 0–1 quadratic knapsack problem. *European Journal of Operational Research, 92*(2), 310–325.

Billionnet, A., Elloumi, S., & Lambert, A. (2012). Extending the QCR method to the case of general mixed integer programs. *Mathematical Programming, 131*(1), 381–401.

Billionnet, A., Elloumi, S., & Lambert, A. (2016). Exact quadratic convex reformulations of mixed-integer quadratically constrained problems. *Mathematical Programming, 158*(1–2), 235–266.

Billionnet, A., Elloumi, S., & Plateau, M. (2009). Improving the performance of standard solvers for quadratic 0–1 programs by a tight convex reformulation: The QCR method. *Discrete Applied Mathematics, 157*(6), 1185–1197.

Billionnet, A., Faye, A., & Soutif, E. (1999). A new upper bound for the 0–1 quadratic knapsack problem. *European Journal of Operational Research, 112*(3), 664–672.

Caprara, A., Pisinger, D., & Toth, P. (1999). Exact solution of the quadratic knapsack problem. *INFORMS Journal on Computing, 11*(2), 125–137.

Chaillou, P., Hansen, P., & Mahieu, Y. (1989). Best network flow bounds for the quadratic knapsack problem. In B. Simeone (Ed.), *Combinatorial optimization: Lectures given at the 3rd session of the centro internazionale matematico estivo (C.I.M.E.) Held at Como, Italy* (pp. 225–235). Berlin, Heidelberg: Springer. August 25–September 2, 1986

Cunha, J. O., Simonetti, L., & Lucena, A. (2016). Lagrangian heuristics for the quadratic knapsack problem. *Computational Optimization and Applications, 63*(1), 97–120.

Danskin, J. M. (1966). The theory of max-min, with applications. *SIAM Journal on Applied Mathematics, 14*(4), 641–664.

Fampa, M., Lee, J., & Melo, W. (2017). On global optimization with indefinite quadratics. *EURO Journal on Computational Optimization, 5*(3), 309–337. 09

Fiacco, A. V. (1983). Introduction to sensitivity and stability analysis in nonlinear programming. *Mathematics in science and engineering*. Academic Press 165.

Gallo, G., Hammer, P. L., & Simeone, B. (1980). Quadratic knapsack problems. In M. W. Padberg (Ed.), *Combinatorial optimization* (pp. 132–149). Berlin, Heidelberg: Springer.

Gu, Z., Nemhauser, G. L., & Savelsbergh, M. W. P. (1998). Lifted cover inequalities for 0–1 integer programs: Computation. *INFORMS Journal on Computing, 10*(4), 427–437.

Hammer, P. L., Johnson, E. L., & Peled, U. N. (1975). Facet of regular 0–1 polytopes. *Mathematical Programming, 8*(1), 179–206.

Helmberg, C., Rendl, F., & Weismantel, R. (1996). Quadratic knapsack relaxations using cutting planes and semidefinite programming. In *Integer programming and combinatorial optimization (Vancouver, BC, 1996)*. In *Lecture notes in comput. sci., pages 190–203: 1084*. Berlin: Springer.

Helmberg, C., Rendl, F., & Weismantel, R. (2000). A semidefinite programming approach to the quadratic knapsack problem. *Journal of Combinatorial Optimization, 4*(2), 197–215.

Hogan, W. W. (1973). The continuity of the perturbation function of a convex program. *Operations Research, 21*, 351–352.

Horn, R. A., & Zhang, F. (2005). Basic properties of the Schur complement. In F. Zhang (Ed.), *The Schur complement and its applications. Numerical methods and algorithms: 4*. Boston, MA, USA: Springer.

Horst, R., & Thoai, N. V. (1999). DC programming: Overview. *Journal of Optimization Theory and Applications, 103*, 1–43.

Jolliffe, I. (2010). *Principal component analysis* (2nd). Berlin: Springer.

Lemarchal, C., & Oustry, F. (1999). *Semidefinite relaxations and Lagrangian duality with application to combinatorial optimization*. INRIA Rhones-Alpes.

Lewis, A. S., & Overton, M. L. (2013). Nonsmooth optimization via quasi-newton methods. *Mathematical Programming, 141*(1), 135–163.

McCormick, G. P. (1976). Computability of global solutions to factorable nonconvex programs: part i convex underestimating problems. *Mathematical Programming, 10*, 147–175.

Michelon, P., & Veillieux, L. (1996). Lagrangean methods for the 0–1 quadratic knapsack problem. *European Journal of Operational Research, 92*(2), 326–341.

Nemhauser, G. L., & Wolsey, L. A. (1988). *Integer and combinatorial optimization*. New York, NY: John Wiley & Sons.

Pisinger, D. (2007). The quadratic knapsack problem: A survey. *Discrete Applied Mathematics, 155*(5), 623–648.

Turlach, B. A., & Wright, S. J. (2015). Quadratic programming. In *Wiley interdisciplinary reviews: Computational statistics: 7* (pp. 153–159). John Wiley & Sons, Inc.

Wolsey, L. A. (1975). Faces for a linear inequality in 0–1 variables. *Mathematical Programming, 8*(1), 165–178.

Wolsey, L. A. (1998). *Integer programming*. New York, NY, USA: Wiley-Interscience.

Zemel, E. (1989). Easily computable facets of the knapsack polytope. *Mathematics of Operations Research, 14*(4), 760–764.