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**A Semidefinite Programming Approach
to the Quadratic Knapsack Problem**

A Semidefinite Programming Approach to the Quadratic Knapsack Problem

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Abstract

We investigate dominance relations between basic semidefinite relaxations and classes of cuts. We show that simple semidefinite relaxations are tighter than corresponding linear relaxations even in case of linear cost functions. Numerical results are presented illustrating the quality of these relaxations.

Key words: Semidefinite programming, quadratic knapsack problem, cutting planes, 0/1 polytopes, relaxations.

1 Introduction

The quadratic knapsack problem is the easiest case of constrained 0/1 quadratic programming and is extremely difficult to solve by linear programming alone. Semidefinite programming is well known to provide powerful relaxations for quadratic 0/1 programming [11, 1, 6] and, as we intend to show, it is very useful for quadratic knapsack problems as well. We compare several possibilities for setting up initial relaxations and show that in the special case of linear cost functions some are even better than the canonical linear relaxation. We discuss possible strengthenings of these relaxations by polyhedral cutting plane approaches in theory and in practice. The main practical difficulty with semidefinite approaches is the high computational cost involved. These stem from the factorization of a completely dense symmetric positive definite matrix with dimension equal to the number of constraints. To keep the number of constraints small it is of major importance to understand the interaction and dominance relations between different classes of cuts. We give several theoretical results in this direction. Finally, we present computational results of this approach on practical data.

Let $N = \{1, \dots, n\}$ be a set of items, $a \in \mathbb{N}^n$ a vector of weights, $b \in \mathbb{N}$ a capacity, and $C \in \mathbb{R}^{n \times n}$ a matrix of costs. The quadratic knapsack problem reads

$$\begin{array}{ll} \text{(QK)} & \text{Maximize} \quad x^t C x \\ & \text{subject to} \quad a^t x \leq b \\ & \quad \quad \quad x \in \{0, 1\}^n. \end{array}$$

We can interpret this problem in graph theoretic terms: Given the complete graph on n vertices with node weights a_i and profit c_{ii} for all $i = 1, \dots, n$. Every edge ij in the complete graph is assigned an objective function coefficient c_{ij} . Find a set of nodes S with sum of the node weights not greater than the threshold b that maximizes the profit $\sum_{i \in S} c_{ii} + \sum_{i, j \in S, i < j} 2c_{ij}$. As in the case of the linear knapsack problem the quadratic knapsack problem often appears as a subproblem to more complex optimization problems. Typical applications arise in VLSI- and compiler design [5, 9].

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Our approach builds up on [6], which concentrates on the quadratic 0/1 programming aspects. Here, we investigate quadratic representations of a linear constraint, as suggested in [11, 1, 6] and discuss various aspects of knapsack specific inequalities. A preliminary version of this paper has been presented at the fifth IPCO conference [8].

The paper is structured as follows. Section 2 introduces several semidefinite relaxations obtained by different representations of the knapsack constraint and analyzes their strength. Section 3 surveys both well known and some new polyhedral concepts for generating knapsack specific cuts. In Section 4 we deal with the dominance relation between these cuts. Section 5 is dedicated to the special case when the knapsack constraint coincides with a generalized upper bound constraint. We discuss implementational issues and our numerical results in Section 6.

2 Semidefinite Relaxation

(QK) is a constrained quadratic 0/1 programming problem. The usual approach for designing relaxations is to linearize the quadratic cost function by switching to “quadratic space”. To this end we introduce variables y_{ij} for $i \leq j$ which are used to model the products $x_i x_j$. In the unconstrained case the convex hull of all feasible points in quadratic space is referred to as the boolean quadric polytope. The knapsack constraint cuts off part of this polytope. Although the convex hull of the restricted set of feasible integral points may differ substantially from the boolean quadric polytope it seems natural to start with a strong relaxation for the boolean quadric polytope and add knapsack specific inequalities on top.

Relaxation for the Boolean Quadric Polytope.

As a relaxation for the boolean quadric polytope we use the semidefinite framework of [6] which is based on [11] and [1]. We model the dyadic product xx^t by a (symmetric) matrix variable Y . We denote the diagonal of this matrix by y . Using this notation the feasible set of matrices can be restricted to those satisfying $Y - yy^t \succeq 0$, i.e. $Y - yy^t$ must be positive semidefinite. This condition is equivalent to

$$\begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \succeq 0. \quad (1)$$

The diagonal elements y_i are obviously bounded by 0 and 1 and correspond to x_i . Looking at the determinant of a 3×3 principal minor containing the last row we get

$$y_i y_j - \sqrt{y_i y_j (1 + y_i y_j - y_i - y_j)} \leq y_{ij} \leq y_i y_j + \sqrt{y_i y_j (1 + y_i y_j - y_i - y_j)} \quad (2)$$

which yields an absolute lower bound of $-\frac{1}{8}$ for y_{ij} .

Numerous facet defining inequalities are known for the boolean quadric polytope [13] and can be added to sharpen the relaxation. Some of the most popular inequalities are (for all possible i , j and k)

$$y_{ij} \geq 0 \quad (3)$$

$$y_{ij} \leq y_{ii} \quad (4)$$

$$y_{ii} + y_{jj} \leq 1 + y_{ij} \quad (5)$$

$$y_{ik} + y_{jk} \leq y_{kk} + y_{ij} \quad (6)$$

$$y_{ij} + y_{ik} + y_{jk} + 1 \geq y_{ii} + y_{jj} + y_{kk} \quad (7)$$

These correspond to the triangle inequalities of the max-cut polytope [2].

Modelling the Knapsack Constraint.

The easiest way to model the knapsack constraint $a^t x \leq b$ on Y is to restrict the diagonal elements of Y , yielding our first semidefinite relaxation,

$$\begin{aligned} \text{(SQK1)} \quad & \text{Maximize} \quad \text{tr}(CY) \\ & \text{subject to} \quad \text{tr}(\text{Diag}(a)Y) \leq b \\ & \quad \quad \quad Y - yy^t \succeq 0. \end{aligned}$$

Can we do better than (SQK1) by choosing some other representation of the knapsack inequality? Let us first consider a generic approach [11]. $b - a^t x \geq 0$ implies

$$(b - a^t x)(b - a^t x) = b^2 - 2ba^t x + a^t x x^t a \geq 0.$$

So a possible representation for the knapsack inequality could read

$$b^2 - 2ba^t y + a^t Y a \geq 0.$$

However, this inequality is already implied by the semidefinite constraint $Y - yy^t \succeq 0$. Because of the integrality of the coefficients a_i and b we can employ a combinatorial argument to sharpen this inequality. Observe that $|(2b-1) - 2a^t x|$ is at least one for all 0/1 vectors x and therefore the quadratic representation of $(2b-1 - 2a^t x)^2 \geq 1$ yields a valid inequality for the boolean quadric polytope which is best formulated with respect to (1),

$$\begin{pmatrix} -2a^t & 2b-1 \end{pmatrix} \begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \begin{pmatrix} -2a \\ 2b-1 \end{pmatrix} \geq 1. \quad (8)$$

This inequality is no more implied by $Y - yy^t \succeq 0$. Indeed, it can be worked out that it belongs to the class of hypermetric inequalities¹ and that for special choices of a and b it will yield a facet defining inequality for the boolean quadric polytope. Notice however that this inequality does not exclude 0/1 solutions that violate the knapsack constraint. However, it is tight for all x which satisfy $a^t x = b$ or $a^t x = b - 1$ and might therefore turn out to be a useful cutting plane.

To achieve our goal of cutting off a larger part of the boolean quadric polytope we exploit the fact that $a^t x \geq -b$ on the feasible set. Squaring both sides of $a^t x \leq b$ yields

$$a^t x x^t a \leq b^2.$$

Replacing $x x^t$ by Y we call this the square representation of the inequality and use it to form a second relaxation

$$\begin{aligned} \text{(SQK2)} \quad & \text{Maximize} \quad \text{tr}(CY) \\ & \text{subject to} \quad \text{tr}(aa^t Y) \leq b^2 \\ & \quad \quad \quad Y - yy^t \succeq 0. \end{aligned}$$

Lemma 2.1 *(SQK2) is tighter than (SQK1).*

Proof. With $Z = Y - yy^t$ we get

$$a^t Z a + (a^t y)^2 \leq b^2 \quad (9)$$

which implies $a^t y \leq b$ by the positive semidefiniteness of Z . ■

This proof suggests the following corollary.

Corollary 2.2 *If $a^t y = b$ for some Y satisfying $\text{tr}(aa^t Y) \leq b^2$ and $Y - yy^t \succeq 0$, then a is in the null space of $Z = Y - yy^t$.*

¹More precisely, the inequality corresponds to a hypermetric inequality of the max-cut polytope for any a and b such that there is a 0/1 vector x with $a^t x = b$ or $a^t x = b - 1$. For a survey on the facets of the max-cut polytope see [3, 4].

Another possibility to construct quadratic representations is to multiply the inequality by either x_i or $(1 - x_i)$ [11, 1]. If, for some fixed i , we sum up the two inequalities

$$\sum_{j=1}^n a_j y_{ij} \leq b y_i \quad (10)$$

$$\sum_{j=1}^n a_j (y_j - y_{ij}) \leq b(1 - y_i) \quad (11)$$

we get $a^t y \leq b$.

Lemma 2.3 *The relaxation obtained by replacing $\text{tr}(\text{Diag}(a)Y) \leq b$ of (SQK1) with a pair of inequalities (10) and (11) for some i is tighter than (SQK1).*

By including all n inequalities of type (10) and one additional inequality of type (11) we get

$$\begin{aligned} \text{(SQK3)} \quad & \text{Maximize} \quad \text{tr}(CY) \\ & \text{subject to} \quad \sum_{j=1}^n a_j y_{ij} \leq b y_i \quad i = 1 \dots n \\ & \quad \quad \quad \sum_{j=1}^n a_j (y_{jj} - y_{1j}) \leq b(1 - y_1) \\ & \quad \quad \quad Y - yy^t \succeq 0. \end{aligned}$$

Lemma 2.4 *(SQK3) is tighter than (SQK2).*

Proof. By multiplying inequality i of type (10) with a_i

$$\sum_{j=1}^n a_i a_j y_{ij} \leq b a_i y_i$$

and summing up over all n inequalities, we obtain $a^t Y a \leq b a^t y \leq b^2$. The right hand side inequality follows from Lemma 2.3. \blacksquare

In practice it is more efficient to start with (SQK2) and to add Inequalities (10) and (11) in case of violation only.

Example 2.5 *To illustrate that the gap between these relaxations may indeed be quite large consider the following problem for $k \leq n$,*

$$\begin{aligned} \text{Maximize} \quad & x^t (e e^t - I) x \\ \text{subject to} \quad & e^t x \leq k \\ & x \in \{0, 1\}^n. \end{aligned} \quad (12)$$

Here, e denotes the n -vector of all ones, and $x^T(e e^t - I)x = \sum_{i < j} 2x_i x_j$. The optimal value of (12) is $k(k - 1)$. Observe that, because of symmetry, in any quadratic relaxation there exists an optimal solution such that every on-diagonal element has the same value d and every off-diagonal element has the same value f , i.e., there is an optimal solution of the form $Y = d \cdot I + f \cdot (e e^t - I)$. Thus, it suffices to compute the maximal possible f for relaxations (SQK1) to (SQK3).

First consider (SQK1). The diagonal representation of $e^t x \leq k$ reads $e^t y \leq k$ which implies $d \leq \frac{k}{n}$. Because of the positive semidefiniteness of Y we certainly cannot choose f larger than d . For $f = d = \frac{k}{n}$ we have $Y - yy^t = (f - f^2)e e^t \succeq 0$ and so this choice of f is optimal. The optimal value of (SQK1) for (12) is $(n - 1)k$. Asymptotically, for $n \rightarrow \infty$, this bound gets arbitrarily bad.

For (SQK2) the quadratic representation reads $e^t Y e \leq k^2$. Again we get the largest possible f by choosing $f = d$ and $e^t Y e = n^2 f = k^2$. This leads to an optimal value of $\frac{n-1}{n} k^2$. For $k = 2$ we get an asymptotic error factor of 2.

In (SQK3) each line of type (10) leads to $(n - 1)f \leq (k - 1)d$. Because one pair of (10) and (11) implies the diagonal constraint we get that $d \leq \frac{k}{n}$. It is easy to check that we can indeed set both values to their respective upper bounds. In particular we get $f = \frac{k(k-1)}{n(n-1)}$ and the optimal value is $k(k - 1)$ which is exact.

As we will see in Section 6 for practical examples the gap between (SQK2) and (SQK3) is much smaller, and (SQK3) itself may still have a rather large relative gap.

Comparison With a Linear Relaxation.

We investigate the special case of a linear cost function $C = \text{Diag}(c)$, i.e. $C_{ij} = 0$ for $i \neq j$. The standard linear relaxation reads

$$\begin{aligned} \text{(LK)} \quad & \text{Maximize} && c^t x \\ & && a^t x \leq b \\ & && 0 \leq x_i \leq 1 \quad i = 1, \dots, n. \end{aligned}$$

(SQK1) is equivalent to (LK) because for any feasible x vector there is a feasible matrix Y having x as its diagonal. However, this is not true for (SQK2).

Lemma 2.6 *Let Y^* be an optimal solution of (SQK2) for $C = \text{Diag}(c)$. If (LK) has a unique optimal solution x^* which is not integral then $\text{tr}(Y^*C) < c^t x^*$.*

Proof. First notice that if x^* is not integral then $a^t x^* = b$. As x^* is unique it has exactly one element x_i with $0 < x_i < 1$. Consider a matrix Y satisfying $y = \text{diag}(Y) = x^*$ and $Y - yy^t \succeq 0$. Because of (2) $y_{ij} = y_i y_j$ for $i \neq j$. Therefore the only non zero element of $Z = Y - yy^t$ is $z_{ii} = x_i - x_i^2$. Obviously $a^t Z a = a_i^2 z_{ii}$ is greater than zero. Thus, by Corollary 2.2, Y is not feasible for (SQK2). Finally, the fact that $y^* = \text{diag}(Y^*)$ is feasible for (LK) completes the proof. \blacksquare

Because of this result we can expect that for numerous linear 0/1 programming problems we get better relaxations by simply translating the linear relaxation to the semidefinite representation.

3 Cutting Planes

In this section we introduce several classes of valid inequalities for the polyhedra associated with the linear and the quadratic representation. These classes serve as the basis for an algorithm to tighten bounds obtained from the semidefinite relaxation of a knapsack problem, see Section 6.

The Linear Knapsack Polyhedron.

Our starting point is the polyhedron

$$\mathcal{P} := \text{conv}\{x \in \{0, 1\}^n : \sum_{i \in N} a_i x_i \leq b\}.$$

A typical example of valid inequalities for \mathcal{P} are cover inequalities. Let S be a subset of N with $\sum_{i \in S} a_i > b$, then the cover inequality with respect to the cover S

$$\sum_{i \in S} x_i \leq |S| - 1 \tag{13}$$

is valid for \mathcal{P} . The original weights are completely ignored by cover inequalities.

Definition 3.1 (weight inequalities) *Let $T \subseteq N$ with $a(T) < b$ and set $r := b - a(T)$. The weight inequality with respect to T is defined as*

$$\sum_{i \in T} a_i x_i + \sum_{i \in N \setminus T} \max\{0, (a_i - r)\} x_i \leq a(T).$$

The name *weight inequality* expresses that the coefficients of the items in T equal their weights. The symbol $r := b - a(T)$ corresponds to the remaining capacity of the knapsack when $x_t = 1$ for all $t \in T$. The right hand side of the inequality is the weight of the set T . Hence, if for an item $i \in N \setminus T$ $a_i \leq r$ holds, then $x_t = 1$ for all $t \in T$ and $x_i = 1$ is a feasible solution. Therefore, the coefficient of i equals 0 in this case. For an item $i \in N \setminus T$ such that $a_i > r$, the value $a_i - r$ corresponds to the weight by which the knapsack capacity b is exceeded if we set $x_i = 1$ and $x_t = 1$ for all $t \in T$. These arguments can be made precise to yield Proposition 3.2.

Proposition 3.2 [14] For $T \subseteq N$, $a(T) < b$ and $r := b - a(T)$, the weight inequality with respect to T is valid for \mathcal{P} .

Example 3.3 For the knapsack polyhedron

$$SP_7 := \text{conv}\{x \in \{0, 1\}^7 : x_1 + x_2 + x_3 + 2x_4 + 2x_5 + 3x_6 + 4x_7 \leq 6,$$

the following weight inequalities are easily seen to be facet-defining:

$$\begin{aligned} x_1 + x_2 + x_3 + 2x_4 + x_5 + 2x_6 + 3x_7 &\leq 5 \\ x_i + x_j + 2x_k + x_6 + 2x_7 &\leq 4 \text{ for all } i, j \in \{1, 2, 3\}, i \neq j \text{ and for all } k \in \{4, 5\} \\ x_1 + x_2 + x_3 + x_7 &\leq 3. \end{aligned}$$

The idea of weight inequalities can be extended to more general cases. Instead of taking the values of the weights of the items into account, we introduce “relative” weights for all the items and derive an analogon of weight inequalities for these relative weights.

For disjoint subsets T and I such that $a(T \cup I) \leq b$, $a_t \leq a_i$ for all $t \in T$ and $i \in I$ and $a(T) \geq a_i$ for all $i \in I$, we define the relative weight c_u of an item $u \in T \cup I$ as follows:

$$c_u := 1 \text{ if } u \in T; \quad c_u := \min\{|S| : S \subseteq T, a(S) \geq a_u\} \text{ if } u \in I.$$

In words, we first normalize the weights of the items in T to the value 1; thereafter an item $i \in I$ obtains as a new weight the value that counts the number of items in T that one needs in order to cover the original weight a_i . Under these assumptions we define for $z \in N \setminus (T \cup I)$ the extended weight inequality with respect to $T \cup I \cup \{z\}$ as follows:

Definition 3.4 (extended weight inequalities) For $r := b - a(T) - a(I)$, the extended weight inequality with respect to $T \cup I \cup \{z\}$ is of the form

$$\sum_{i \in T} x_i + \sum_{i \in I} c_i x_i + c_z x_z \leq |T| + \sum_{i \in I} c_i,$$

where $c_z := \min\{|S| + \sum_{j \in J} c_j : S \subseteq T, J \subseteq I, a(S \cup J) \geq a_z - r\}$.

Extended weight inequalities have been introduced and analyzed in [14]. For the purpose of this paper the following proposition is needed.

Proposition 3.5 [14] The extended weight inequality defined for $T \cup I \cup \{z\}$ is valid for \mathcal{P} .

Example 3.6 We continue analyzing the knapsack polyhedron SP_7 . Setting $T := \{1, 2, 4\}$, $I = \emptyset$ and $z = 6$, the extended weight inequality for T , I and $\{z\}$ is the inequality

$$x_1 + x_2 + x_4 + x_6 \leq 3,$$

that happens to be a minimal cover inequality. This inequality lifts to the facet-defining inequality

$$x_1 + x_2 + x_4 + x_6 + x_7 \leq 3$$

of SP_7 . The extended weight inequality with respect to $T = \{1, 4\}$, $I = \{6\}$ and $z = 7$ is the inequality

$$x_1 + x_4 + 2x_6 + 3x_7 \leq 4.$$

After computing lifting coefficients according to the sequence $(7, 2, 5, 3)$, for instance, we obtain the inequality

$$x_1 + x_2 + x_4 + x_5 + 2x_6 + 3x_7 \leq 4.$$

This induces a facet of SP_7 .

It was also shown in [14] that for any extended weight inequality lifting coefficients can always be computed in polynomial time. In particular, the exact lifting coefficient of an item coincides either with a certain lower bound or its value equals this lower bound plus 1.

The Quadratic Knapsack Polyhedron.

In the following we will study the polyhedron

$$\mathcal{Q} := \text{conv}\{y \in \{0, 1\}^{n(n+1)/2} : \sum_{i \in N} a_i y_{ii} \leq b, y_{ij} = y_{ii} y_{jj} \ \forall i < j\}.$$

that we obtain by lifting the original polyhedron to the space of quadratic variables. In this higher dimensional space, there are novel ways to construct relaxations of \mathcal{Q} that, itself, allow for generating valid inequalities for \mathcal{Q} .

Lemma 3.7 *Let N_1, \dots, N_k be a partition of N . For every $v \in \{1, \dots, k\}$ we choose a spanning tree (N_v, T_v) in the complete graph $K(N_v)$ on the node set N_v . By deg_i^v we denote the degree of node i in the tree (N_v, T_v) . The polyhedron $\text{conv}\{y \in \{0, 1\}^{n(n+1)/2} : \sum_{v=1}^k (\sum_{i \in N_v} a_i) [\sum_{ij \in T_v} y_{ij} + \sum_{i \in N_v} (1 - \text{deg}_i^v) y_{ii}] \leq b\}$ contains all the feasible points of \mathcal{Q} .*

Proof. Let $y \in \mathcal{Q}$, integral, be given and choose a tree (N_v, T_v) , $v \in \{1, \dots, k\}$. We want to show that the corresponding summand $\sum_{ij \in T_v} y_{ij} + \sum_{i \in N_v} (1 - \text{deg}_i^v) y_{ii}$ is one if $y_{ii} = 1$ for all $i \in N_v$ and not greater than zero otherwise. First suppose $y_{ii} = 1$ for all $i \in N_v$. In this case

$$\sum_{ij \in T_v} 1 + \sum_{i \in N_v} 1 - \sum_{i \in N_v} \text{deg}_i^v = |N_v| - 1 + |N_v| - 2|N_v - 1| = 1.$$

Otherwise edges with $y_{ij} = 0$ decompose the tree into several subtrees which again satisfy $y_{ii} = 1$ for all nodes belonging to the same subtree and are maximal in this respect. However, the value deg_i^v of at least one node in such a subtree must exceed the degree within the subtree by at least one. This is due to the fact that each subtree is connected by at least one edge to a vertex $j \in N_v$ with $y_{jj} = 0$. Therefore the contribution of a subtree to the summand is not greater than zero. \blacksquare

Lemma 3.7 allows us to derive valid inequalities for \mathcal{Q} via the following scheme: Generate a relaxation \mathcal{Q}' of \mathcal{Q} as stated in the Lemma. Find valid inequalities, like cover inequalities, weight inequalities or extended weight inequalities for \mathcal{Q}' . These inequalities are also valid for \mathcal{Q} .

Example 3.8 *Consider the knapsack polyhedron*

$$\text{conv}\{x \in \{0, 1\}^6 : 5x_1 + 6x_2 + 7x_3 + 8x_4 + 9x_5 + 12x_6 \leq 21\}.$$

Partitioning into sets $\{1, 2\}, \{3, 4\}, \{5, 6\}$ and choosing the edge set of the complete graphs on two nodes for all elements in the partition yields the knapsack polyhedron

$$\mathcal{Q}' := \text{conv}\{y \in \{0, 1\}^{21} : 11y_{1,2} + 15y_{3,4} + 21y_{5,6} \leq 21\}.$$

A valid inequality for this polyhedron is given by the cover inequality $y_{1,2} + y_{3,4} + y_{5,6} \leq 1$. Partitioning N into the sets $\{1, 2, 3\}, \{4\}, \{5\}, \{6\}$ and choosing the edges $(1, 2), (1, 3)$ in the complete graph with vertices $1, 2, 3$ yields another knapsack polyhedron

$$\mathcal{Q}'' := \text{conv}\{y \in \{0, 1\}^{21} : 18[y_{1,2} + y_{1,3} - y_{1,1}] + 8y_{4,4} + 9y_{5,5} + 12y_{6,6} \leq 21\}.$$

A valid inequality for \mathcal{Q}'' is given, for instance, by the constraint $2[y_{1,2} + y_{1,3} - y_{1,1}] + y_{4,4} + y_{5,5} + y_{6,6} \leq 2$.

In the remainder of this paper we sometimes refer to special relaxations of \mathcal{Q} . These are obtained by partitioning a subset $S = \{i_1, \dots, i_s\}$ of N of even cardinality into elements of cardinality two, $S^1, \dots, S^{\frac{s}{2}}$, $S^1 = \{i_1, i_2\}$, $S^2 = \{i_3, i_4\}$, \dots , $S^{\frac{s}{2}} = \{i_{s-1}, i_s\}$, for instance. In other words, we choose a perfect matching M in the complete graph with node set S , or a matching M in the complete graph with node set N . By Lemma 3.7 the polyhedron

$$\text{conv}\left\{y \in \{0, 1\}^{n(n+1)/2} : \sum_{ij \in M} (a_j + a_i) y_{ij} + \sum_{i \in N \setminus S} a_{ii} y_{ii} \leq b\right\}$$

is a relaxation of \mathcal{Q} . The knapsack inequality

$$\sum_{ij \in M} (a_j + a_i)y_{ij} + \sum_{i \in N \setminus S} a_{ii}y_{ii} \leq b$$

is called the *matching-knapsack*-constraint associated with the matching M in the complete graph with node set N . We will refer to a cover inequality based on a matching-knapsack-constraint as *matching-cover*-constraint.

We conclude this section by introducing a quadratic representation for linear cover inequalities. Let $S \subset N$ define a valid cover inequality for \mathcal{P} and choose any hamiltonian cycle C_S in the complete graph over the vertex set S . Then

$$\sum_{ij \in C_S} y_{ij} \leq |C_S| - 2$$

is a valid inequality for \mathcal{Q} . We refer to this type of inequalities as cycle inequalities [5].

4 The Strength of Cutting Planes

In general (SQK2) and (SQK3) will not be tight enough to provide provably optimal solutions but it is possible to improve these semidefinite relaxations by adding further inequalities. We have already mentioned generic cuts from the boolean quadric polytope in Section 2. In this section we will consider knapsack specific inequalities.

Linear Cutting Planes.

We start with valid inequalities for \mathcal{P} as defined in Section 3. These are again linear constraints which have to be transformed into some quadratic representation. In principal we have the same possibilities as for modeling the knapsack inequality and the same results apply. Note, that in case of multiplication with x_i it may be worth to postpone the lifting procedure. Multiplication of $a^t x \leq b$ with x_i corresponds to a conditional inequality, which is effective only if $x_i > 0$,

$$x_i \sum_{j \neq i} a_j x_j \leq (b - a_i)x_i.$$

So for an extended weight inequality multiplied with x_i we can lift the remaining coefficients with respect to the reduced knapsack inequality $\sum_{j \neq i} a_j x_j \leq b - a_i$ instead of the original $a^t x \leq b$.

Example 4.1 *For the knapsack polyhedron*

$$\mathcal{SP}_4 := \text{conv}\{x \in \{0, 1\}^4 : 4x_1 + 5x_2 + 6x_3 + 7x_4 \leq 16\},$$

lifting the inequality $x_1 + x_2 + x_3 \leq 3$ with respect to the original inequality yields $x_1 + x_2 + x_3 + x_4 \leq 3$. By multiplying with x_3 we get

$$y_{13} + y_{23} - 2y_{33} + y_{34} \leq 0.$$

Lifting $x_1 + x_2 \leq 2$ with respect to $4x_1 + 5x_2 + 7x_3 \leq 10$ yields

$$y_{13} + y_{23} - 2y_{33} + 2y_{34} \leq 0.$$

It is also interesting to investigate the dominance relation between different representations if we include triangle inequalities (3) to (7) in the basic relaxation. Consider the extended weight inequality for \mathcal{P}

$$\sum_{i \in T} (1 - x_i) + \sum_{i \in I} c_i (1 - x_i) - c_z x_z \geq 0. \quad (14)$$

Multiplication with x_z yields the quadratic representation

$$\sum_{i \in T} (y_{zz} - y_{iz}) + \sum_{i \in I} c_i (y_{zz} - y_{iz}) - c_z y_{zz} \geq 0. \quad (15)$$

We subtract this inequality from the diagonal representation of (14) (replace x_i with y_{ii}) and get

$$\sum_{i \in T} (1 - y_{ii} - y_{zz} + y_{iz}) + \sum_{i \in I} c_i (1 - y_{ii} - y_{zz} + y_{iz}) \geq 0.$$

If we require the triangle inequalities (5) to hold, the latter expression is clearly nonnegative and (15) dominates the diagonal representation of (14). Intuitively, the triangle inequalities help to spread the influence of an inequality defined on a single row over the whole matrix.

Quadratic Cutting Planes.

We now turn towards valid inequalities for the polyhedron \mathcal{Q} . One question in terms of computations is to choose a relaxation of the original problem that allows to derive strong valid cuts for the quadratic knapsack problem. If we restrict the discussions to cuts that are cover inequalities, a precise statement can be made for a comparison of the polyhedra \mathcal{Q} and

$$\mathcal{C} := \text{conv}\{y \in \{0, 1\}^{n(n+1)/2} : \sum_{i \in N} a_i^2 y_{ii} + \sum_{i < j, i, j \in N} 2a_i a_j y_{ij} \leq b^2\}$$

that we associate with the form $a^t x a^t x \leq b^2$ of the given quadratic knapsack problem.

Lemma 4.2 *For (SQK1) combined with the triangle inequalities (4) every cover inequality that is valid for \mathcal{C} is dominated by a matching-cover-constraint.*

Proof. Consider a subset S of the set of variables $\bigcup_{i \in N} \{i\}$ and a subset T of the set of variables $\bigcup_{i < j, i, j \in N} \{ij\}$ such that $\sum_{i \in S} a_i^2 + \sum_{ij \in T} 2a_i a_j > b^2$. The cover inequality associated with S and T reads

$$\sum_{i \in S} y_{ii} + \sum_{ij \in T} y_{ij} \leq |S| + |T| - 1, \quad (16)$$

and is obviously valid for \mathcal{C} . Let I denote the set of indices appearing in S or, as an endpoint, in T . We first show that $\sum_{i \in I} a_i > b$. Assume otherwise, then

$$b^2 \geq \left(\sum_{i \in I} a_i\right)^2 \geq \sum_{i \in S} a_i^2 + \sum_{ij \in T} 2a_i a_j,$$

which is a contradiction to our assumptions on S and T . Now consider a maximum cardinality matching $M \subset T$ in the graph (I, T) . We denote by $J \subset I$ the indices not covered by an edge of M . Obviously,

$$\sum_{i \in J} y_{ii} + \sum_{ij \in M} y_{ij} \leq |J| + |M| - 1$$

is a valid matching-cover-constraint for \mathcal{Q} . Except for the variables y_{ii} with $i \in J \setminus S$ all variables of this inequality also appear in (16). For any $i \in J \setminus S$ there is at least one j such that $ij \in T$. Since we require (4) to hold and for all ij $y_{ij} \leq 1$ by the semidefiniteness constraint the matching-cover-constraint indeed dominates (16). \blacksquare

The next lemma is another indication that matching-knapsack-constraints yield useful relaxations for deriving valid inequalities.

Lemma 4.3 *Let $S \subset N$ be a cover. The square representation of the cover inequality with respect to S is dominated by the diagonal representation combined with*

- (a) *matching-cover-inequalities if $|S|$ is even,*

(b) *cycle inequalities if $|S|$ is odd.*

Proof. Let $S \subset N$ be a cover for \mathcal{P} . The square representation reads

$$\sum_{i \in S} y_{ii} + \sum_{i,j \in S, i < j} 2y_{ij} \leq (|S| - 1)^2. \quad (17)$$

We first assume that $|S|$ is even. For M a perfect matching in the complete graph with vertex set S we obtain the matching-cover constraint

$$\sum_{ij \in M} y_{ij} \leq \frac{|S|}{2} - 1.$$

Let $M_1, M_2, \dots, M_{\lfloor |S|/2 \rfloor}$ be a partition of the edge set of the complete graph with node set S into perfect matchings. Then

$$\sum_{k=1}^{\lfloor |S|/2 \rfloor} \sum_{ij \in M_k} y_{ij} \leq (|S| - 1) \left(\frac{|S|}{2} - 1 \right).$$

To cover the y_{ii} terms of (17) we add the diagonal representation of the underlying cover inequality and get

$$\begin{aligned} \sum_{i \in S} y_{ii} + \sum_{i,j \in S, i < j} 2y_{ij} &= 2 \sum_{k=1}^{\lfloor |S|/2 \rfloor} \sum_{ij \in M_k} y_{ij} + \sum_{i \in S} y_{ii} \\ &\leq 2(|S| - 1) \left(\frac{|S|}{2} - 1 \right) + |S| - 1 = (|S| - 1)^2. \end{aligned}$$

If $|S|$ is odd then we partition the edge set of the complete graph with node set S into $\frac{|S|-1}{2}$ hamiltonian cycles, $C_1, \dots, C_{\frac{|S|-1}{2}}$. With each cycle C_k we associate the cycle constraint

$$\sum_{ij \in C_k} y_{ij} \leq |S| - 2.$$

Summing up over all cycles we get

$$\sum_{k=1}^{\frac{|S|-1}{2}} \sum_{ij \in C_k} y_{ij} + y_{vv} = \sum_{i,j \in S, i < j} y_{ij} \leq \frac{|S|-1}{2} (|S| - 2).$$

Multiplying by two and adding the diagonal representation yields (17). ■

5 Upper Bound Constraints

A typical constraint that arises in many practical applications is that at most k items from a given ground set of n items may be selected,

$$e^t x \leq k.$$

This is known as an upper bound constraint. Even within our framework the importance of this class of inequalities is immediate since the most fundamental cutting planes, the cover inequalities (13), belong to it.

In the following we assume $k \geq 2$. We start with further investigating Example 2.5 which is a special case of an upper bound constrained problem. Consider the constraint associated with the cost matrix,

$$\text{tr}((ee^t - I)Y) \leq k(k - 1). \quad (18)$$

It forms a quadratic representation of $e^t x \leq k$ which together with the semidefiniteness constraint yields, as we will show, a tighter relaxation than (SQK2). Let us call this special relaxation the upper bound relaxation,

$$\begin{aligned} \text{(UBR)} \quad & \text{Maximize} \quad \text{tr}(CY) \\ & \text{subject to} \quad \text{tr}((ee^t - I)Y) \leq k(k-1) \\ & \quad \quad \quad Y - yy^t \succeq 0. \end{aligned}$$

In the next lemma we prove that on the feasible set of (UBR) the diagonal representation of $e^t x \leq k$ is satisfied.

Lemma 5.1 *(UBR) is tighter than the relaxation (SQK1) associated with $e^t x \leq k$.*

Proof. Consider any feasible Y of (UBR). Using (1) we have for any $\alpha \in \mathbb{R}$

$$\begin{pmatrix} e^t & \alpha \end{pmatrix} \begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \begin{pmatrix} e \\ \alpha \end{pmatrix} = e^t Y e + 2\alpha e^t y + \alpha^2 \geq 0.$$

Because of (18) we get $e^t Y e \leq k(k-1) + e^t y$ implying that

$$k(k-1) + (2\alpha + 1)e^t y + \alpha^2 \geq 0.$$

Setting $\alpha = -k$ (remember that $k \geq 2$) and rearranging terms shows $e^t y \leq k$. ■

Since for any feasible Y of (UBR)

$$e^t Y e = e^t (Y - \text{Diag}(y))e + e^t y \leq k(k-1) + k = k^2$$

we immediately get the following corollary.

Corollary 5.2 *(UBR) is tighter than the relaxation (SQK2) associated with $e^t x \leq k$.*

The relation between (UBR) and (SQK3) follows directly from Example 2.5 where we proved that we cannot violate (18) within the feasible set of (SQK3).

Corollary 5.3 *(SQK3) is tighter than (UBR).*

Although these results indicate that (18) is a reasonable way to model the upper bound constraint $e^t x \leq k$, it is not too hard to see that the face F induced by the set of all points satisfying (18) at equality does not define a facet of \mathcal{Q} . Indeed, every point in F is contained in the face induced by the set of all points $y \in \mathcal{Q}$ that satisfy

$$\sum_{i=1}^n y_{ii} - \frac{1}{k-1} \sum_{1 \leq i < j \leq n} y_{ij} \leq \frac{k}{2}$$

at equality. This inequality is valid for \mathcal{Q} and always facet-defining. It corresponds to the representation (8) of the upper bound constraint $e^t x \leq k$ and, therefore, defines a hypermetric inequality of the max-cut polytope.

Remark 5.4 *The face induced by the set of all points in \mathcal{Q} that satisfy the knapsack constraint $e^t x \leq k$ at equality is contained in the face induced by the set of all points in \mathcal{Q} that satisfy the hypermetric inequality*

$$\begin{pmatrix} -2e^t & 2k-1 \end{pmatrix} \begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \begin{pmatrix} -2e \\ 2k-1 \end{pmatrix} \geq 1. \tag{19}$$

at equality.

In the special case when $k = 2$, the hypermetric inequality associated with $e^t x \leq 2$ reads

$$\sum_{i \in N} y_{ii} - \sum_{i < j \in N} y_{ij} \leq 1$$

and the inequalities of the form (10) specialize to the family $\sum_{j \in N \setminus \{i\}} y_{ij} \leq y_{ii}$ for all $i \in N$. These inequalities plus the non-negativity constraints describe \mathcal{Q} .

theorem 5.5 *The polyhedron*

$$\mathcal{Q} := \text{conv}\{y \in \{0, 1\}^{n(n+1)/2} : \sum_{i \in N} c_i y_{ii} \leq 2, y_{ij} = y_{ii} y_{jj} \ \forall i < j\}$$

is described by the system of inequalities

$$y_{ij} \geq 0 \text{ for all } i, j \in N \tag{20}$$

$$\sum_{i \in N} y_{ii} - \sum_{i < j \in N} y_{ij} \leq 1 \tag{21}$$

$$\sum_{j \in N \setminus \{i\}} y_{ij} \leq y_{ii} \text{ for all } i \in N. \tag{22}$$

Proof. We have to show that for every objective function $c \neq 0$ the set of all optimal solutions is contained in the face induced by one of the inequalities (20), (21), (22), see [10]. Let $c \in \mathbb{R}^{n(n+1)/2}$, $c \neq 0$ be any objective function. By X^* we denote the set of optimal solutions in \mathcal{Q} with respect to c . The following cases are distinguished.

Case 1: $0 \notin X^*$, then every optimal solution $x \in X^*$ satisfies $e^t x = 1$ or $e^t x = 2$. Therefore X^* is contained in the face induced by the set of all points y in \mathcal{Q} for which $\sum_{i \in N} y_{ii} - \sum_{i < j \in N} y_{ij} = 1$.

Case 2: $0 \in X^*$ implying that $c_{ii} \leq 0$ for all $i \in N$ and $c_{ii} + c_{jj} + c_{ij} \leq 0$ for all $i < j \in N$. First note that we cannot have all these inequalities tight because this would imply $c = 0$. Therefore one of the following subcases must hold.

(i) $c_{i_0 i_0} < 0$ for some $i_0 \in N$. Then no $y \in X^*$ satisfies $y_{i_0 i_0} = 1$ and $y_{jj} = 0$ for all $j \in N \setminus \{i_0\}$. Hence, every $y \in X^*$ satisfies the inequality $\sum_{j \in N \setminus \{i_0\}} y_{i_0 j} \leq y_{i_0 i_0}$ at equality.

(ii) $c_{i_0 i_0} + c_{j_0 j_0} + c_{i_0 j_0} < 0$ for some $i_0 < j_0 \in N$. Then there is no optimal solution y in X^* such that $y_{i_0 j_0} = 1$. Therefore, $y_{i_0 j_0} = 0$ for all $y \in X^*$.

This completes the proof. ■

6 Implementation

For solving the semidefinite programs we use the primal-dual path-following interior point algorithm of [7]. To guarantee that there is no duality gap between primal and dual optimal solutions we have to ensure that at least one of both has a feasible point satisfying all inequalities strictly. To this end we add the constraint $y_{ij} = 0$ whenever $a_i + a_j > b$ for some $i \neq j$. The arithmetic mean of all zero, one, and two items solutions is now such a feasible point.

Each iteration of the interior point code requires the factorization of a dense positive definite matrix. The dimension of this matrix is the number of constraints of the semidefinite program. More than 60% of the overall computation time are spent in this routine. It is therefore extremely important to keep the set of constraints as small as possible. Even expensive separation routines will pay off if they help to achieve this goal.

To illustrate the quality of the relaxations we give numerical results in Table 1 for some compiler design problems taken from [9]. For all problems the cost matrix is nonnegative and sparse (e.g. the problem of dimension 61 has just 187 nonzeros), and both, costs and weights, vary over a wide range. We emphasize that we do not exploit the sparsity of the problem at all. For each example we compute solutions for right hand sides 450, 512, and 600.

The first column of Table 1 gives the dimension of the problem, the second the value of the right hand side of the knapsack constraint, the third gives the best feasible solution we found. All other columns display the relative gap

$$\% = \left(\frac{\text{upper bound}}{\text{feasible solution}} - 1 \right) \times 100$$

of the upper bound — obtained after at most 30 minutes of CPU time² using the specific relaxation — with respect to this feasible solution. Whenever the gap between feasible solution and upper bound is closed (relative gap $< 5 \cdot 10^{-6}$) we mark this by \triangleright and give the computation time, instead.

Table 1: Compiler design problems taken from [9]

dim	rhs	feas. sol.	SQK1 %	SQK2 %	SQK3 %	Δ -ineq. %/mm:ss	lin. cuts %/mm:ss	matching %/mm:ss
30	450	1580	41	17	13	0.23	\triangleright 00:19	\triangleright 00:24
	512	1802	39	20	17	5.60	0.35	\triangleright 26:10
	600	2326	24	12	11	2.64	\triangleright 1:55	\triangleright 1:31
45	450	2840	16	8.7	8.4	2.90	\triangleright 13:54	\triangleright 13:43
	512	3154	30	12.7	12.7	3.07	1.61	1.58
	600	3840	22	8.2	8.2	\triangleright 20:16	\triangleright 3:45	\triangleright 3:02
47	450	1732	7	5.9	5.8	2.51	\triangleright 15:02	\triangleright 31:10
	512	1932	30	12	11	1.30	\triangleright 16:59	\triangleright 8:20
	600	2186	31	18	17	8.89	6.02	4.09
61	450	26996	3.7	2.4	2.4	0.40	\triangleright 3:17	\triangleright 3:23
	512	29492	2.9	2.0	2.0	1.34	\triangleright 28:53	0.02
	600	32552	2.6	1.9	1.9	1.04	0.42	0.33

Columns (SQK1), (SQK2), and (SQK3) refer to the respective relaxations of Section 2. The performance of (SQK1) is rather poor, (SQK2) halves the gap of (SQK1) requiring the same amount of computation time, (SQK3) is just a little bit better than (SQK2) but takes about twice as long to compute.

For column Δ -ineq. we start the algorithm with (SQK2) as initial relaxation and compute its optimal solution. Then we improve the relaxation by adding n cutting planes of type (3)–(7), (10), or (11) and iterate. All these cutting planes are applicable for all quadratic 0/1 problems and do not exploit any special properties of the knapsack problem. Yet the bound is already acceptable.

In column *lin. cuts* we also include cutting planes which are quadratic representations of valid inequalities for the linear knapsack polytope. In particular we consider weight inequalities and extended weight inequalities. In our experiments (10) was clearly the most successful quadratic representation. Representation (11) will be of importance if the cost matrix contains negative entries as well. As we can see in Table 1 the addition of these cuts was sufficient to close the gap for most of our test problems within half an hour. In general the final relaxation included just a few knapsack specific cutting planes and lots of triangle inequalities (3)–(7).

Finally, column *matching* gives the results if we separate matching inequalities as well. We use a preliminary version of the maximum weighted matching code of LEDA [12] to find reasonable starting sets and derive extended weight inequalities for these sets. Although this separation procedure is computationally quite expensive total computation time is roughly the same. In view of the fact that we started only recently to experiment with matching inequalities these results are very promising.

7 Conclusions

We presented several basic semidefinite relaxations for the 0/1 quadratic programming problem and compared them with respect to their quality in theory and in practice. The straight forward

²Computation times refer to a Sun Sparcstation 10.

approach of modelling the constraint on the diagonal (SQK1) yields a rather poor bound. At the same computational cost we can get a much better bound by using the square representation (SQK2). For this relaxation we proved that in case of linear cost functions it is superior to the canonical linear relaxation. Slightly better than (SQK2) is the relaxation formed by using all representations obtained by “multiplying” the knapsack inequality with x_i for all i (SQK3). However, computationally it is more efficient to start with (SQK2) and to compute (SQK3) by successively adding violated inequalities.

Generic 0/1 cutting planes such as the triangle inequalities (3)–(7) significantly improve these relaxations and yield surprisingly good bounds without requiring any special knowledge about the nature of the problem itself. However, special polyhedral knowledge is indispensable to close the gap and speed up the computation.

A good way to model valid inequalities of the linear knapsack polyhedron in quadratic space is to multiply it with some x_i (10). In case of negative elements in the cost matrix it is worth considering representation (11) as well. Combining the semidefinite framework with quadratic representations of weight inequalities and extended weight inequalities yields a reasonable approach to solve rather dense, small to medium sized problems.

In Section 3 we introduced a large new class of valid inequalities for the quadratic knapsack polyhedron which allow for direct derivation of quadratic cutting planes. We presented some theoretical and computational evidence for their importance in cutting plane approaches. However, there is much room for improvement, and it can be expected that the quadratic knapsack polytope has still a lot to offer.

The good quality of the bounds, even without exploiting special properties of the problem at hand, gives rise to the hope that — in spite of the high computational cost involved — semidefinite programming will become a useful tool to model and solve difficult subproblems in integer programming.

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