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Quadratic Knapsack Relaxations Using Cutting Planes and Semidefinite Programming

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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.

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 [7, 1, 4] 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 $N = \{1, ..., n\}$ be a set of items, $a \in \mathbb{N}^n$ a vector of weights, $b \in \mathbb{N}$ a capacity, and $C \in \Re^{n \times n}$ a matrix of costs. The quadratic knapsack problem reads

(QK) Maximize
$$x^t C x$$

subject to $a^t x \le b$
 $x \in \{0, 1\}^n$.

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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, ..., 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 [3, 6].

Our approach builds up on [4], which concentrates on the quadratic 0/1 programming aspects. Here, we investigate quadratic representations of a linear constraint, as suggested in [7, 1, 4] and discuss various aspects of knapsack specific inequalities.

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. In Section 5 implementational issues are discussed. We also present our numerical results.

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 [4] which is based on [7] 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

$$\left(\begin{array}{cc} Y & y \\ y^t & 1 \end{array}\right) \succeq 0.$$

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

$$y_i y_j - \sqrt{y_i y_j (1 + y_i y_j - y_i - y_j)} \le y_{ij} \le y_i y_j + \sqrt{y_i y_j (1 + y_i y_j - y_i - y_j)}$$
(1)

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

Numerous facet defining inequalities are known for the boolean quadric polytope [8] and can be added to sharpen the relaxation. Some of the most popular inequalities are (for all possible i, j and k)

$$y_{ij} \geq 0 \tag{2}$$

$$y_{ij} \leq y_{ii} \tag{3}$$

$$y_{ii} + y_{jj} \leq 1 + y_{ij} \tag{4}$$

$$y_{ik} + y_{jk} \leq y_{kk} + y_{ij} \tag{5}$$

$$y_{ij} + y_{ik} + y_{jk} + 1 \ge y_{ii} + y_{jj} + y_{kk}$$
 (6)

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,

(SQK1) Maximize
$$\operatorname{tr}(CY)$$

subject to $\operatorname{tr}(\operatorname{Diag}(a)Y) \leq b$
 $Y - yy^t \succeq 0.$

Can we do better than (SQK1) by choosing some other representation of the knapsack inequality? Let us first consider a generic approach [7]. $b - a^t x \ge 0$ implies

$$(b - a^{t}x)(b - a^{t}x) = b^{2} - 2ba^{t}x + a^{t}xx^{t}a \ge 0.$$

So a possible representation for the knapsack inequality could read

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

However, this inequality is already implied by the semidefinite constraint $Y - y \# \succeq 0$. On the other hand exploiting the fact that $a^t x \ge -b$ on the feasible set we get a very useful representation in a very similar manner. We square both sides of $a^t x \le b$ and get

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

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

$$\begin{array}{lll} (\mathrm{SQK2}) & \mathrm{Maximize} & \mathrm{tr}(CY) \\ & \mathrm{subject \ to} & \mathrm{tr}(aa^tY) \leq b^{\sharp} \\ & Y - yy^t \succeq 0. \end{array}$$

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

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

$$a^t Za + (a^t y)^2 \le b^2 \tag{7}$$

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 $tr(aa^t Y) \leq b^2$ and $Y - yy^t \geq 0$, then a is in the null space of $Z = Y - yy^t$.

Another possibility to construct quadratic representations is to multiply the inequality by either x_i or $(1 - x_i)$ [7, 1]. If, for some fixed *i*, we sum up the two inequalities

$$\sum_{j=1}^{n} a_j y_{ij} \leq b y_i \tag{8}$$

$$\sum_{j=1}^{n} a_j (y_j - y_{ij}) \leq b(1 - y_i)$$
(9)

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

Lemma 2.3 The relaxation obtained by replacing $tr(Diag(a)Y) \leq b$ of (SQK1) with a pair of inequalities (8) and (9) for some i is tighter than (SQK1).

By including all n inequalities of type (8) and one additional inequality of type (9) we get

(SQK3) Maximize
$$\operatorname{tr}(CY)$$

subject to $\sum_{j=1}^{n} a_j y_{ij} \leq b y_i$ $i = 1 \dots n$
 $\sum_{j=1}^{n} a_j (y_{jj} - y_{1j}) \leq b(1 - y_1)$
 $Y - yy^t \succeq 0.$

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

Proof. By multiplying inequality i of type (8) with a_i

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

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

In practice it is more efficient to start with (SQK2) and to add Inequalities (8) and (9) in case of violation only.

Comparison With a Linear Relaxation

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

(LK) Maximize
$$c^t x$$

 $a^t x \le b$
 $0 \le x_i \le 1$ $i = 1, ..., n.$

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

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 5.

Our starting point is the polyhedron

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

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

$$\sum_{i \in S} x_i \le |S| - 1$$

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 be given and set r := b - a(T). The weight inequality with respect to T is defined as

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

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

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:

$$c_u := 1$$
 if $u \in T$; $c_u := \min\{|S|: S \subseteq T, a(S) \ge a_u\}$ 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 3.3 (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

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

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

Extended weight inequalities have been introduced and analyzed in [9]. For the purpose of this paper the following proposition is needed.

Proposition 3.4 [9] The extended weight inequality defined for $T \cup I \cup \{z\}$ is valid for \mathcal{P} .

It was also shown in [9] 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.

In the following we will study the polyhedron

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

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 3.5 Let N_1, \ldots, N_k be a partition of N. For every $v \in \{1, \ldots, k\}$ 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 $conv\{y \in \{0, 1\}^{n(n-1)/2}: \sum_{v=1}^k (\sum_{i \in N_v} a_i) [\sum_{ij \in T_v} y_{ij} + \sum_{i \in N_v} (1 - deg_i^v) y_{ii}] \leq b$ contains all the feasible points of Q.

Lemma 3.5 allows us to derive valid inequalities for Q via the following scheme: Generate a relaxation Q' of Q as stated in the Lemma. Find valid inequalities, like cover inequalities, weight inequalities or extended weight inequalities for Q. These inequalities are also valid for Q.

Example 3.6 Consider the knapsack polyhedron

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

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

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

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

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

A valid inequality for 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 Q. These are obtained by partitioning a subset $S = \{i_1, \ldots, i_s\}$ of N of even cardinality into elements of cardinality two, $S^1, \ldots, S^{\frac{s}{2}}, S^1 = \{i_1, i_2\}, S^2 = \{i_3, i_4\}, \ldots, S^{\frac{s}{2}} = \{i_{s-1}, i_s\}$, 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 3.5 the polyhedron

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

is a relaxation of 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

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

is a valid inequality for Q. We refer to this type of inequalities as cycle inequalities [3].

4 Various Aspects 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.

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 $x_i > 0$,

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

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 := \operatorname{conv}\{x \in \{0,1\}^4 : 4x_1 + 5x_2 + 6x_3 + 7x_4 \le 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

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

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

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

It is also interesting to investigate the dominance relation between different representations if we include triangle inequalities (2) to (6) in the basic relaxation. Consider the extended weight inequality for \mathcal{P}

$$\sum_{i \in T} (1 - x_i) + \sum_{i \in I} c_i (1 - x_i) - c_z x_z \ge 0.$$
(10)

Multiplication with x_z yields the quadratic representation

$$\sum_{i \in T} (y_{zz} - y_{iz}) + \sum_{i \in I} c_i (y_{zz} - y_{iz}) - c_z y_{zz} \ge 0.$$
(11)

We subtract this inequality from the diagonal representation of (10) (replace x_i with y_{ii}) and get

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

If we require the triangle inequalities (4) to hold, the latter expression is clearly nonnegative and (11) dominates the diagonal representation of (10).

We now turn towards valid inequalities for the polyhedron 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 Q and

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

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 (3) every cover inequality that is valid for C is dominated by a matching-cover-constraint.

The next lemma is another indication that matching-knapsack-constraints are a useful relaxation 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.

5 Implementation

For solving the semidefinite programs we use the primal-dual path-following interior point algorithm of [5]. 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 item 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.

We start the algorithm with (SQK2) as initial relaxation and compute its optimal solution. Then we improve the relaxation by adding n cutting planes and iterate. The current implementation supports the following cutting planes: representations of the knapsack constraint in the form of (8) and (9), all triangle inequalities (2) to (6), weight inequalities and extended weight inequalities with respect to the original knapsack constraint. An inequality of the latter two classes is checked for violation with respect to its quadratic representation and representations of the form (8) and (9). Especially the separation algorithm for extended weight inequalities is quite involved and includes an exact lifting procedure.

dim	rhs	sol	(SQK1)	(SQK2)	(SQK3)	cut
30	350	934	1412.2	1298.6	1257.4	972.8
30	450	1580	1783.5	1736.5	1733.1	1580.0
30	512	1802	2397.4	2050.3	2023.0	1824.3
45	350	2228	2561.1	2327.1	2296.9	2228.0
45	450	2840	3283.8	3086.0	3078.2	2873.8
45	512	3154	4082.5	3554.2	3554.2	3251.7
47	350	1192	1487.7	1406.6	1375.4	1192.0
47	450	1732	1848.7	1834.0	1832.9	1735.6
47	512	1932	2505.9	2162.0	2155.2	1951.6
61	350	22210	23738.7	23357.1	23352.8	22221.3
61	450	26996	27987.5	27654.3	27651.7	27000.2
61	512	29760	30353.7	30083.9	30083.0	29760.6

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As test problems we use some compiler design problems of [6]. For each example we compute solutions for right hand sides 350, 450, and 512. Results are given in Table 1. The first column is the dimension, the second the right hand side. The third column gives the best solution we know. Columns (SQK1), (SQK2), and (SQK3) give the optimal solution of the corresponding relaxations. Column *cut* displays the upper bound of the cutting plane approach after half an

hour of CPU-time.

Observe that there is a significant gap between (SQK1) and (SQK2) but only little improvement from (SQK2) to (SQK3). Typically the set of active constraints consists of numerous triangle inequalities and a few knapsack specific cuts. Regarding the possible representations of linear cuts there is a clear tendency in favor of multiplication with some x_i (8) which is not astonishing in view of the theoretical results.

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