A Semidefinite Programming Approach to the Quadratic Knapsack Problem*

C. Helmberg† F. Rendl‡ R. Weismantel*

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Abstract

In order to gain insight into the quality of semidefinite relaxations of constrained quadratic 0/1 programming problems we study the quadratic knapsack problem. We investigate several basic semidefinite relaxations of this problem and compare their strength in theory and in practice. Various possibilities to improve these basic relaxations by cutting planes are discussed. The cutting planes either arise from quadratic representations of linear inequalities or from linear inequalities in the quadratic model. In particular, a large family of combinatorial cuts is introduced for the linear formulation of the knapsack problem in quadratic space. Computational results on a small class of practical problems illustrate the quality of these relaxations and cutting planes.

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

Mathematics Subject Classification (MSC 1991). 90C25, 90C09, 90C10.

1 Introduction

The quadratic knapsack problem

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

with $a \in \mathbb{N}^n$, $b \in \mathbb{N}$ is one of the standard combinatorial optimization problems (in some works, the term quadratic knapsack problem has also been used for continuous versions of (QK) [29]). Typical applications of the discrete problem such as portfolio selection [22] or site selection [11] are of the following form. A few items have to be selected from a given ground set subject to budgetary constraints. The objective, profit/quality maximization or risk minimization, is strongly influenced by the pairwise interrelation between the items of the selected set. Besides these direct applications the quadratic knapsack problem also appears as a subproblem in several applications of constrained quadratic 0/1 programming, e.g. in VLSI- and compiler design [10, 21].

Current practical approaches for solving (QK) are branch and bound algorithms. The bounds are specially designed for the quadratic knapsack problem and often require special properties of the objective function such as nonnegativity of c_{ij} [14, 6]. These approaches are of little use if (QK) appears as a subproblem within general constrained quadratic 0/1 programming. This drawback can be overcome by resorting to a polyhedral approach. Typically, polyhedral methods work with linear relaxations of (QK). However, these often exhibit a large gap even for very small

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†Konrad Zuse Zentrum für Informationstechnik Berlin, Heilbronnerstraße 10, D-10711 Berlin, Germany (`http://www.zib-berlin.de/KombOpt/`)

‡Technische Universität Graz, Institut für Mathematik, Steyrergasse 30, A-8010 Graz, Austria

instances ($n = 20$). We design a polyhedral approach using semidefinite methods and show that this leads to reasonable bounds.

In recent years it became clear that for unconstrained quadratic 0/1 programming problems semidefinite programming yields strong bounds, in theory [12, 27] as well as in practice [16]. From a theoretical point of view there is a well established technique for including linear constraints in this semidefinite relaxation [1, 31, 24, 3]. The main ingredients of this technique are the pairwise multiplication of feasible inequalities and the substitution of products of variables by linear variables (the final projection step back into linear space is not needed in our context).

In this paper we go towards a practical realization of this theoretical approach. In Section 2 we set up various initial semidefinite relaxations of (QK) in the line of [1, 31, 24, 3] and compare them with respect to quality and efficiency. In particular we introduce the square representation of the knapsack inequality. For the practical examples tested, the semidefinte relaxation based on this single constraint achieves almost the bound of the standard semidefinite relaxation. The latter bound is much more expensive to compute, because it involves n additional inequalities. We show that in the special case of a linear cost function the semidefinite relaxation formed by the square representation of the knapsack inequality still suffices to beat the linear relaxation.

In order to improve an initial semidefinite relaxation it is necessary to add further inequalities that are valid for the linear formulation of the original program in quadratic space. Here there are two possibilities. One can derive valid inequalities that are valid for the polyhedron associated with the feasible region of the original problem and lift them into the quadratic model (by the technique of Lovász and Schrijver or alternatives) or develop a polyhedral understanding of the quadratic model itself. Some aspects of the quadratic knapsack polyhedron have been studied in [10]. In Section 3 we introduce a new large family of combinatorial cuts for the linear formulation of the knapsack problem in quadratic space and analyze their strength in comparison to quadratic representations of certain linear cutting planes.

A class of constraints that appears frequently within quadratic 0/1 programming problems is the family of generalized upper bound constraints of the form $\sum x_i \leq k$. For constraints of this form we construct a special quadratic representation, analyze its strength, and relate it to the hypermetric inequalities of the max-cut polytope. This is the topic of Section 4.

We discuss implementational issues and numerical results of the semidefinite programming code for the quadratic knapsack problem in Section 5. It will turn out that the semidefinite relaxations are of good quality. Computationally they are too expensive for solving larger instances of (QK) to optimality. However, the approach gives some insight on important classes of inequalities that may help to set up good initial relaxations of more complex problems. This is of particular importance in combination with new methods [5, 17] that can compute approximate solutions to semidefinite relaxations for large problem instances as well.

2 Modeling Linear Constraints for Semidefinite Relaxations

A common approach for designing relaxations for quadratic 0/1 programs is to linearize the quadratic cost function by switching to "quadratic space". Variables y_{ij} are introduced to model the products $x_i x_j$ for $i \leq j$. Stated differently, the dyadic product xx^t is replaced 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 [24, 4]. This condition is equivalent to

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

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

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

which bounds the offdiagonal variables by $-\frac{1}{8} \leq y_{ij} \leq 1$. Note, that the nonnegativity constraints $y_{ij} \geq 0$ are not implied by this semidefinite relaxation.

The easiest way to model a linear constraint $a^t x \leq b$, with $a \in \mathbb{N}^n$ and $b \in \mathbb{N}$ on Y is to restrict the diagonal elements of Y, yielding the **diagonal representation** of $a^t x \leq b$ and our first semidefinite relaxation,

$$\begin{array}{lll} \text{(SQK1)} & \text{Maximize} & \langle C, Y \rangle \\ & \text{subject to} & \langle \text{Diag}(a), Y \rangle \leq b \\ & & Y - yy^t \succeq 0. \end{array}$$

Can we do better than (SQK1) by choosing some other representation of the knapsack inequality? Let us first consider a particular case of the generic approach of [31, 24]. $b - a^t x \geq 0$ 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),

$$\begin{pmatrix} -2a^t & 2b-1 \end{pmatrix} \begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \begin{pmatrix} -2a \\ 2b-1 \end{pmatrix} \geq 1. \tag{3}$$

This inequality is no more implied by the condition $Y - yy^t \succeq 0$. Indeed, it can be worked out that (3) belongs to the class of hypermetric inequalities[1] and that for special choices of a and b it defines a facet of the boolean quadric polytope (for definition see Section 3). Notice, 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 xx^t by Y we call this the **square representation** of the inequality $a^t x \leq b$ and use it to form a second relaxation

$$\begin{array}{lll} \text{(SQK2)} & \text{Maximize} & \langle C, Y \rangle \\ & \text{subject to} & \langle aa^t, Y \rangle \leq b^2 \\ & & Y - yy^t \succeq 0. \end{array}$$

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

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

$$a^t Z a + (a^t y)^2 \leq b^2 \tag{4}$$

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

This proof suggests the following corollary.

[1] More 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 [8, 9].

Corollary 2.2 *If $a^t y = b$ for some Y satisfying $\langle aa^t, Y\rangle \leq b^2$ and $Y - yy^t \succeq 0$, 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 $(1 - x_i)$ [1, 31, 24, 3]. If, for some fixed i, we sum up the two inequalities

$$\sum_{j=1}^{n} a_j y_{ij} \quad \leq \quad by_i \tag{5}$$

$$\sum_{j=1}^{n} a_j (y_j - y_{ij}) \quad \leq \quad b(1 - y_i) \tag{6}$$

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

Lemma 2.3 *[1, 31, 24] The relaxation obtained by replacing $\langle Diag(a), Y\rangle \leq b$ of (SQK1) with a pair of inequalities (5) and (6) for some i is tighter than (SQK1).*

By including all n inequalities of type (5) and one additional inequality of type (6) we get

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

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

Proof. By multiplying inequality i of type (5) 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. ■

It is clear that (SQK3) can be improved at the expense of adding the remaining inequalities of the form (6) to the relaxation. The improvement of the latter relaxation towards (SQK3) is, in all our test examples, neglectable. This is the reason why we work with (SQK3). Our computational experiments have also revealed that among the relaxations (SQK2) and (SQK3), the first one has the best trade-off between running time and quality. In fact, it is usually more efficient to start with (SQK2) and to add Inequalities (5) and (6) in case of violation only, see Section 5.

One cannot expect that either of these initial relaxations yields an optimal solution of the original quadratic 0/1 program. A natural way to improve these relaxations is via cutting planes for the polyhedron associated with the 0/1 program. Such linear inequalities can be transformed into quadratic space using the three techniques outlined before: the diagonal representation, the square representation, and representations (5) and (6). On account of Lemma 2.1 the diagonal representation can be neglected. In practice it proved advantageous to work with violated inequalities of type (5) and (6), only.

In our code we included separation heuristics for several well known classes of valid inequalities of the linear knapsack polyhedron

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

We briefly introduce these classes in the following. For convenience we use the notation $N = \{1, \ldots, n\}$ and, for $T \subseteq N$, $a(T) = \sum_{i \in T} a_i$.

A typical example of valid inequalities for $\mathcal{P}$ are cover inequalities.

Definition 2.5 *[13, 33, 2][cover inequalities] Let $S \subseteq N$ with $\sum_{i\in S} a_i > b$. S is called a* cover *and the inequality*

$$\sum_{i\in S} x_i \leq |S| - 1 \tag{7}$$

is the cover inequality *with respect to S.*

Definition 2.6 *[32][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 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.

Definition 2.7 *[32][extended weight inequalities]*

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:

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

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

It was shown in [32] that for any extended weight inequality (this includes cover inequalities) lifting coefficients can always be computed in polynomial time.

Comparison with a Linear Relaxation.

Although (SQK2) does not yield the "best" initial semidefinite relaxation of a 0/1 knapsack problem, it is strong enough to improve the linear relaxation. Let $C = \mathrm{Diag}(c)$ be a linear cost function, i.e. $C_{ij} = 0$ for $i \neq j$. The standard linear relaxation reads

$$\begin{array}{lll} \text{(LK)} \qquad \text{Maximize} & c^t x & \\ & a^t x \leq b & \\ & 0 \leq x_i \leq 1 \qquad & i = 1, \ldots, n. \end{array}$$

(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 2.8 *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 $\langle Y^*, C\rangle < c^t x^*$.*

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 $y = \mathrm{diag}(Y) = x^*$ 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 $y^* = \mathrm{diag}(Y^*)$ is feasible for (LK) completes the proof. ■

This result indicates that for numerous linear 0/1 programming problems the linear relaxation can be improved by a semidefinite relaxation with the same number of constraints.

3 Quadratic Cutting Planes

In the case of an unconstrained quadratic 0/1 program the convex hull of all feasible points in quadratic space is referred to as the boolean quadric polytope,

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

Numerous facet defining inequalities are known for the boolean quadric polytope [28]. Some elementary inequalities are (for all possible i, j and k)

$$\begin{aligned} y_{ij} &\geq 0 && (8)\\ y_{ij} &\leq y_{ii} && (9)\\ y_{ii} + y_{jj} &\leq 1 + y_{ij} && (10)\\ y_{ik} + y_{jk} &\leq y_{kk} + y_{ij} && (11)\\ y_{ij} + y_{ik} + y_{jk} + 1 &\geq y_{ii} + y_{jj} + y_{kk} && (12) \end{aligned}$$

These correspond to the triangle inequalities of the max-cut polytope [7], and may also be derived by algebraic considerations [31, 24].

For a constrained quadratic 0/1 program valid inequalities for $\mathcal{B}$ remain valid and can be added to sharpen an initial semidefinite relaxation. For the quadratic 0/1 knapsack problem, the knapsack constraint cuts off part of the boolean quadric polytope. In the following we 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 $\mathcal{Q}$.

Theorem 3.1 *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* $\text{conv}\{y \in \{0,1\}^{n(n+1)/2} : \ \sum_{v=1}^{k} (\sum_{i \in N_v} a_i)[\sum_{ij \in T_v} y_{ij} + \sum_{i \in N_v}(1 - deg_i^v) y_{ii}] \leq b\}$ *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), $v \in \{1, \ldots, k\}$. We want to show that the corresponding summand $\sum_{ij \in T_v} y_{ij} + \sum_{i \in N_v}(1 - deg_i^v) y_{ii}$ 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

$$\sum_{ij \in T_v} 1 + \sum_{i \in N_v} 1 - \sum_{i \in N_v} deg_i^v = |N_v| - 1 + |N_v| - 2(|N_v| - 1) = 1.$$

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. ■

Theorem 3.1 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 3.2 *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 graph on two nodes for all elements in the partition yields the knapsack polyhedron*

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

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*

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

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 we sometimes refer to special relaxations of $\mathcal{Q}$. 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 Theorem 3.1 the polyhedron

$$\mathcal{M} = \text{conv}\left\{ y \in \{0,1\}^{n(n+1)/2} : \ \sum_{ij \in M} (a_j + a_i) y_{ij} + \sum_{i \in N \setminus S} a_i y_{ii} \leq b \right\} \tag{13}$$

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

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

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.

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 square representation $a^t x a^t x \leq b^2$ of the given quadratic knapsack problem.

Lemma 3.3 *For (SQK1) combined with the triangle inequalities (9) 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

$$\sum_{i \in S} y_{ii} + \sum_{ij \in T} y_{ij} \leq |S| + |T| - 1, \tag{14}$$

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

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

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 (14). For any $i \in J \setminus S$ there is at least one j such that $ij \in T$. Since we require (9) to hold and since for all $ij \in T$ we have that $y_{ij} \leq 1$ by the semidefiniteness constraint, the matching-cover-constraint indeed dominates (14). ■

The next lemma is a further indication that the polytope associated with a matching-knapsack-constraint gives rise to good valid inequalities for $\mathcal{Q}$. To state the lemma we need to introduce another quadratic representation of a linear cover inequality.

Definition 3.4 *[10][cycle inequalities] Let $S \subset N$ define a valid cover inequality for $\mathcal{P}$ and let C_S be an Hamiltonian cycle in the complete graph over the vertex set S. Then*

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

is called a cycle inequality.

Lemma 3.5 *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

$$\sum_{i \in S} y_{ii} + \sum_{i,j \in S, i<j} 2y_{ij} \leq (|S| - 1)^2. \tag{15}$$

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 $M_1, M_2, \ldots, M_{|S|-1}$ be a partition of the edge set of the complete graph with node set S into perfect matchings. Then

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

To cover the y_{ii} terms of (15) we add the diagonal representation of the underlying cover inequality and get

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

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, $C_1 \ldots, C_{\frac{|S|-1}{2}}$. 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

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

Multiplying by two and adding the diagonal representation yields (15). ■

4 Generalized Upper Bound Constraint

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

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

where e denotes the n-vector of all ones. This is known as a *generalized upper bound constraint.* Within our framework this class of inequalities plays an important role because the most fundamental cutting planes, the cover inequalities (7), belong to this class.

In the following we assume $k \geq 2$. We start investigating Example 4.1 that compares relaxations (SQK1) to (SQK3) in this special case.

Example 4.1 *For $k \leq n$ consider*

$$\begin{array}{ll} \textit{Maximize} & x^t(ee^t - I)x \\ \textit{subject to} & e^t x \leq k \\ & x \in \{0,1\}^n, \end{array} \tag{16}$$

with $x^T(ee^t - I)x = \sum_{i<j} 2x_i x_j$. The optimal value of (16) 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 $Y = d \cdot I + f \cdot (ee^t - I)$. 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 $Y - yy^t = (f - f^2)ee^t \succeq 0$ and so this choice of f is optimal. The optimal value of (SQK1) for (16) is $(n-1)k$. Asymptotically, for $n \to \infty$, 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 (5) leads to $(n-1)f \leq (k-1)d$. Because one pair of (5) and (6) implies the diagonal constraint we get that $d \leq \frac{k}{n}$. It 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.

Consider the constraint associated with the cost matrix,

$$\langle ee^t - I, Y \rangle \leq k(k-1). \tag{17}$$

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,

$$\begin{array}{lll} \text{(UBR)} & \text{Maximize} & \langle C, Y \rangle \\ & \text{subject to} & \langle ee^t - I, Y \rangle \leq k(k-1) \\ & & Y - yy^t \succeq 0. \end{array}$$

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 4.2 *(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 (17) 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)

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

we immediately get the following corollary.

Corollary 4.3 *(UBR) is tighter than the relaxation (SQK2) associated with $e^t x \leq k$.*

The relation between (UBR) and (SQK3) follows directly from Example 4.1 where we proved that we cannot violate (17) within the feasible set of (SQK3).

Corollary 4.4 *(SQK3) is tighter than (UBR).*

Although these results indicate that (17) 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 (17) 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 (3) of the upper bound constraint $e^t x \leq k$ and, therefore, defines a hypermetric inequality of the max-cut polytope.

Remark 4.5 *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*

$$\begin{pmatrix} -2e^t & 2k-1 \end{pmatrix} \begin{pmatrix} Y & y \\ y^t & 1 \end{pmatrix} \begin{pmatrix} -2e \\ 2k-1 \end{pmatrix} \geq 1. \tag{18}$$

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 (5) 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 4.6 *The polyhedron*

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

is described by the system of inequalities

$$y_{ij} \geq 0 \text{ for all } i, j \in N \tag{19}$$

$$\sum_{i \in N} y_{ii} - \sum_{i<j \in N} y_{ij} \leq 1 \tag{20}$$

$$\sum_{j \in N \setminus \{i\}} y_{ij} \leq y_{ii} \text{ for all } i \in N. \tag{21}$$

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 (19), (20), (21), see [23]. 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. ■

5 Implementation

For solving the semidefinite programs we use the primal-dual path-following interior point algorithm of [18] (for a survey on the use of interior point methods in combinatorial optimization see [25]). 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 the solutions associated with all zero, one, and two elementary subsets of items is 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 tables 1 and 2 for some compiler design problems taken from [21]. 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. In each table the first column gives the dimension of the problem, the second the value of the right hand side of the knapsack constraint. *feas.* refers to the best feasible solution we found. Computation times are given with respect to a Sun SPARCstation 10 Model 41. % refers to the relative gap

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

of the upper bound.

In Table 1 we compare the three basic semidefinite relaxations (SQK1), (SQK2), and (SQK3). The computation times of (SQK1) and (SQK2) are roughly the same, it takes about twice as long to compute (SQK3). On the other hand the bound of (SQK3) is only marginally better than (SQK2), whereas (SQK1) is drastically worse.

			relative gap (%)			time(sec)		
dim	rhs	feas.	SQK1	SQK2	SQK3	SQK1	SQK2	SQK3
30	450	1580	41	17	13	1	1	2
	512	1802	39	20	17	1	1	2
	600	2326	24	12	11	1	1	2
45	450	2840	16	8.7	8.4	3	3	6
	512	3154	30	12.7	12.7	3	3	6
	600	3840	22	8.2	8.2	3	3	6
47	450	1732	7	5.9	5.8	3	3	7
	512	1932	30	12	11	3	3	7
	600	2186	31	18	17	3	3	7
61	450	26996	3.7	2.4	2.4	8	9	17
	512	29492	2.9	2.0	2.0	9	9	18
	600	32552	2.6	1.9	1.9	8	9	17

Table 1: Comparison of relaxations (SQK1), (SQK2), and (SQK3). The instances are based on compiler design problems taken from [21]. *dim* is the number of 0-1 variables, each problem was examined for the three capacities of column *rhs*. *feas.* gives the best solution we know. The relative gap is computed via $100 \cdot (\frac{\text{upper bound}}{\text{feas.}} - 1)$. All times refer to a Sun SPARCstation 10 Model 41.

Table 2 presents our results with the cutting plane algorithm. The problems are the same as in Table 1, for better comparison we have copied the results of (SQK2) into this Table as well. In all cases (SQK2) is the starting relaxation and the algorithm terminates when the gap between feasible solution and upper bound is closed (relative gap $< 5 \cdot 10^{-6}$) or a time limit of 30 minutes is reached.

For column $\triangle$-*ineq.* we improve (SQK2) by adding in each phase of the cutting plane algorithm at most n constraints that are either triangle inequalities (8)–(12) or inequalities of the form (5) or (6). Although these cutting planes do not rely on the analysis of the polyhedron associated with the original 0/1 problem, the bound that this relaxation gives is reasonable.

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 (for a detailed description of the separation heuristics we refer to [20]). In our experiments, (5) was clearly the most successful quadratic representation. Representation (6) might play a role if the cost matrix contains negative entries as well. As we can see in Table 2 the addition of these cuts was sufficient to close the gap for most of our test problems within half an hour. This demonstrates that special polyhedral knowledge is indispensable to close the gap and speed up the computation.

Finally, column *matching* shows the results when we also incorporate quadratic cutting planes as discussed in Section 3. We use a preliminary version of the maximum weighted matching code of LEDA [26] to find a relaxation in form of the convex hull of all 0/1 points that satisfy a matching-knapsack-constraint, see (13). Once a polyhedron of this form is constructed, we apply our separation routines for the linear knapsack polytope $\mathcal{M}$. Although the construction of a relaxation of the form (13) is computationally very expensive the computation time shows that one can slightly gain in terms of quality and running time.

Summarizing, the semidefinite approach is probably too expensive to solve pure quadratic knapsack problems to optimality. However, the study of the quadratic knapsack polytope is not only theoretically interesting, but also practically it offers insights which inequalities may be worth to include or to separate in the relaxation of more general constrained quadratic 0/1 programming problems.

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dim	rhs	feas.	SQK2	$\triangle$-ineq.		lin. cuts		matching	
		feas.	%	%	mm:ss	%	mm:ss	%	mm:ss
30	450	1580	17	0.23	30:00	0	00:19	0	00:24
	512	1802	20	5.60	30:00	0.35	30:00	0	26:10
	600	2326	12	2.64	30:00	0	1:55	0	1:31
45	450	2840	8.7	2.90	30:00	0	13:54	0	13:43
	512	3154	12.7	3.07	30:00	1.61	30:00	1.58	30:00
	600	3840	8.2	0	20:16	0	3:45	0	3:02
47	450	1732	5.9	2.51	30:00	0	15:02	0	31:10
	512	1932	12	1.30	30:00	0	16:59	0	8:20
	600	2186	18	8.89	30:00	6.02	30:00	4.09	30:00
61	450	26996	2.4	0.40	30:00	0	3:17	0	3:23
	512	29492	2.0	1.34	30:00	0	28:53	0.02	30:00
	600	32552	1.9	1.04	30:00	0.42	30:00	0.33	30:00

Table 2: Improvement of the bound by adding cutting planes for the examples of Table 1. The initial relaxation is (SQK2). For each solution we eliminate inequalities with small dual variables, add n violated inequalities, and iterate. Nonzero relative gaps refer to the bound after 30 minutes of computation time, otherwise the relative gap was closed to $5 \cdot 10^{-6}$ within this time limit. In $\triangle$-*ineq.* the inequalities of (SQK3) and the triangle inequalities are used as cutting planes. In *lin. cuts* the knapsack specific linear cutting planes are separated, as well. In *matching* we consider all inequalities together, including the matching constraints.