A LAGRANGIAN RELAXATION APPROACH TO THE EDGE-WEIGHTED CLIQUE PROBLEM

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ABSTRACT. The b-clique polytope CP_b^n is the convex hull of the node and edge incidence vectors of all subcliques of size at most b of a complete graph on n nodes. Including the Boolean quadric polytope $QP^n = CP_n^n$ as a special case and being closely related to the quadratic knapsack polytope, it has received considerable attention in the literature. In particular, the max-cut problem is equivalent with optimizing a linear function over CP_n^n. The problem of optimizing linear functions over CP_b^n has so far been approached via heuristic combinatorial algorithms and cutting-plane methods.

We study the structure of CP_b^n in further detail and present a new computational approach to the linear optimization problem based on the idea of integrating cutting planes into a Lagrangian relaxation of an integer programming problem that Balas and Christofides had suggested for the traveling salesman problem. In particular, we show that the separation problem for tree inequalities becomes polynomial in our Lagrangian framework. Finally, computational results are presented.

1. INTRODUCTION

Consider the complete undirected graph $K_n = (V, E)$ on the set $V = \{1, \dots, n\}$ of nodes with edge set E. We assume that to every edge $e \in E$ a weight c_e and to every node $i \in V$ a weight d_i is assigned. The weighted maximal b-clique problem (WCP_b) is to find, among all complete subgraphs with at most b nodes, a subgraph (clique) for which the sum of the weights of all the nodes and edges in the subgraph is maximal.

The weighted maximal b-clique problem can be seen as a Boolean quadratic problem with a cardinality constraint (Mehrotra [1997]). On the other hand, (WCP_b) generalizes the well-studied maximum clique problem, which is known to be NP–hard.

Applications of (WCP_b) can be found, for example, in location theory (see Späth [1985], Kuby [1987], Erkut *et al.*[1990] and Ravi *et al.* [1994]).

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Other important applications of this optimization model arise in molecular biology (see Hunting [1998]).

Exact branch-and-cut algorithms for (WCP_b), based on linear programming have been proposed by Dijkhuizen and Faigle [1993], Park *et al.* [1996], Mehrotra [1997], and Macambira and De Souza [1996]. In these four papers several facet-defining inequalities are introduced which are used as cutting planes in order to improve the quality of the upper bounds. In Faigle *et al.* [1994] upper bounds derived from Lagrangian relaxation are proposed. The usual branch-and-cut approach can be quite successful for special types of problems (see, *e.g.*, Barahona *et al.* [1989] for the max-cut problem). The general case, however, appears to be much harder. The first three of the afore-mentioned studies deal with graphs with up to 30 nodes whereas – as formulated by Macambira and de Souza – "the real challenge is to solve problems with $n \geq 40$ nodes".

The weighted maximal b-clique polytope generalizes the Boolean quadric polytope, which has been studied extensively (see, *e.g.*, Padberg [1989], Deza and Laurent [1992a,b], Boros and Hammer [1993], Sherali *et al.* [1995] and Hardin *et al.* [1995]). The max-cut problem on graphs (*cf.* Barahona and Mahjoub [1986]) can be formulated as the problem of optimizing a linear function over the Boolean quadric polytope. On the other hand, the weighted maximal b-clique problem is a special case of the quadratic knapsack problem. Therefore, the corresponding polytopes are closely related. Various techniques have been proposed for solving quadratic knapsack problems (see Chaillou *et al.* [1986], Johnson *et al.* [1993], Bretthauer *et al.* [1995] and Helmberg *et al.* [1996]).

In the present paper, we propose a relaxation technique that has not been applied before to (WCP_b) or to the related problems mentioned above: we combine Lagrangian relaxation with the use of cutting planes. This idea has been suggested by Balas and Christofides [1981] for the traveling salesman problem and has been employed, *e.g.*, by Lucena [1992] for Steiner problems in graphs. We report computational results for the weighted clique problem with a branch-and-cut algorithm based on this relaxation. We expect that the technique can also be fruitfully applied to the related problems.

The paper is organized as follows. In Section 2, we give an integer programming formulation for (WCP_b) and review polyhedral results from the literature. In Section 3, we describe two new classes of facet-defining inequalities, which we will use in the (Lagrangian) branch-and-cut algorithm, namely the i-clique inequalities and the generalized clique inequalities. These inequalities turn out to define facets of the Boolean quadric polytope as well.

In Section 4, we formulate a Lagrangian problem for (WCP_b) which turns out to have solutions with nice properties. The upper bound obtained in this Lagrangian relaxation often is quite good. Adding cutting planes to the objective function, however, we can obtain even stronger bounds as our computational results show.

Using cutting planes in a Lagrangian relaxation offers a considerable advantage over the standard branch-and-cut approach: Because of the special structure of the Lagrangian solutions, we are able to use classes of inequalities for which the separation problem is NP-hard in general ($cf.$ the tree inequalities in Section 4) by adding violated inequalities to the objective function of the Lagrangian relaxation without changing the structure of the Lagrangian solutions.

2. The b-clique polytope

We formulate the weighted maximal b-clique problem (WCP_b) as an integer programming problem. We introduce for every node $i \in V$ a $(0,1)$-variable x_i and for every edge $e \in E$ a $(0,1)$-variable y_e. We think of an (undirected edge $e \in E$ as an (unordered) subset of V of cardinality 2. In particular, if $e = \{i, j\}$, we call i and j the *endpoints* of e.

Variable x_i equals 1 if node i is in the clique and 0 otherwise, and y_e equals 1 if edge e is in the clique and 0 if not. The weighted maximal b-clique problem can then be formulated as follows:

$$\max \sum_{i \in V} d_i x_i \; + \; \sum_{e \in E} c_e y_e \tag{1}$$

subject to the constraints

$$\sum_{i \in V} x_i \leq b \tag{2}$$

$$y_e - x_i \leq 0 \qquad \text{for all } e = \{i, j\} \in E \tag{3}$$

$$x_i + x_j - y_e \leq 1 \qquad \text{for all } e = \{i, j\} \in E \tag{4}$$

$$x_i \in \{0, 1\} \qquad \text{for all } i \in V \tag{5}$$

$$y_e \geq 0 \qquad \text{for all } e \in E \tag{6}$$

Note that the constraints (3)–(6), in fact, imply the seemingly stronger integrality property $y_e \in \{0, 1\}$ for all $e \in E$. Also observe that (2) becomes redundant if $b = n$.

We denote the convex hull of the feasible solutions by

$$CP_b^n = \text{conv}\{(x, y) \in \mathbb{R}^{n(n+1)/2} |\ (x, y) \text{ satisfies (2)– (6)}\} \tag{7}$$

and call it the *b-clique polytope*.

It is easy to see that the b-clique polytope is full-dimensional if $b \geq 2$, *i.e.*,

$$\dim\ CP_b^n = n(n+1)/2\ .$$

Consequently, each facet-defining inequality for $CP_b^n$is unique up to scalar multiplication. Because $CP_{b-1}^n \subseteq CP_b^n$, each inequality that is valid for CP_b^n is also valid for CP_{b-1}^n. Moreover, if a valid inequality for CP_b^n is facet-defining for CP_{b-1}^n, it is also facet-defining for CP_b^n.

Remark 2.1. *It is interesting to observe that the (valid) inequalities $x_i \geq 0$ and $x_i \leq 1$ are* not *facet-defining for CP_b^n whenever $n \geq 2$ as they are implied by the constraints (3), (4), and (6).*

Similarly, inequality (2) is not *facet-defining. The vertices (x, y) of CP_b^n corresponding to cliques of size b satisfy the two independent equations*

$$\sum_{i \in V} x_i = b \quad \text{and} \quad \sum_{e \in E} y_e = b(b-1)/2$$

and thus cannot generate a hyperplane. (See also Lemma 3.1 below).

The b-clique polytope is closely related to the Boolean quadric polytope and the quadratic knapsack polytope. Other polytopes related to the b-clique polytope are the clique partitioning polytope (Grötschel and Wakabayashi [1990]) and the cut polytope, which arises from the max-cut problem (see, *e.g.*, Barahona and Mahjoub or Deza and Laurent [1992a,b]).

¡For the rest of the paper, we introduce the following notation. Given a vector $(x, y) \in \mathbb{R}^{n(n+1)/2}$ and subset $S \subseteq V$, we denote by $E(S)$ the set of edges with both endpoints in S and let

$$x(S) = \sum_{i \in S} x_i \qquad \text{and} \qquad y(S) = \sum_{e \in E(S)} y_e. \tag{8}$$

Each $S \subseteq V$ with $|S| \leq b$ corresponds to a feasible solution (x^S, y^S) for (WCP_b) in the obvious way. We call (x^S, y^S) the *incidence vector* of S and x^S the *node incidence vector* of S.

2.1. **Relationship with the Boolean quadric polytope.** The *Boolean quadric polytope* QP^n was introduced by Padberg [1989] in his study of the unconstrained quadratic zero-one programming problem. In our notation, we have

$$QP^n \;=\; CP_n^n \,, \tag{9}$$

i.e., the Boolean quadric polytope is exactly the weighted b-clique polytope with parameter $b = n$.

Every valid inequality for QP^n is, of course, valid for CP_b^n for any $b \leq n$. However, not all facet-defining inequalities of QP^n also define facets of CP_b^n. Nevertheless, interesting special cases enjoying this property exist. Examples are the "trivial" inequalities mentioned in the following result due to Padberg [1989] and Park *et al.* [1996].

Proposition 2.1. *Let $n \geq 3$ and $b \geq 2$. Then for all $e = \{i, j\} \in E$:*

(i) *The inequality $y_e \geq 0$ defines a facet of CP_b^n.*
(ii) *The inequalities $y_e - x_i \leq 0$ and $x_i + x_j - y_e \leq 1$ define facets of CP_b^n if and only if $b \geq 3$.*

◇

The following proposition exhibits two more classes of inequalities that are facet-defining for both QP^n and CP_b^n.

Proposition 2.2.

(i) *For any $S \subseteq V$ with $|S| \geq 1$ and $T \subseteq V - S$ with $|T| \geq 2$, the* **cut inequality**

$$\sum_{i \in S, j \in T} y_{\{i,j\}} - y(S) - y(T) - x(S) \ \leq \ 0 \tag{10}$$

defines a facet of CP_b^n if and only if either $|S| = 1$ and $b \geq 3$ or $|S| \geq 2$ and $b \geq 4$.

(ii) *For any $S \subseteq V$ with $|S| \geq 3$ and integer α, $1 \leq \alpha \leq |S| - 2$, the* **clique inequality**

$$\alpha x(S) - y(S) \ \leq \ \frac{\alpha(\alpha+1)}{2} \tag{11}$$

defines a facet of CP_b^n if and only if either $\alpha \leq b - 2$ or $S = V$ and $\alpha \leq b - 1$.

◇

Remark 2.2. *The fact that the inequalities in Proposition 2.2 are facet-defining for CP_b^n was already observed by Park et al.[1996]. However, the statement and proof concerning the clique inequalities is not quite correct there. It is claimed that for every $1 \leq \alpha \leq |S| - 2$ inequality (11) with $S = V$ defines a facet, which is not true if $\alpha \geq b$ (cf. Hunting [1998]).*

Recently, Macambira and De Souza [1996] presented the following class of facet-defining inequalities for CP_b^n that generalizes the cut inequalities.

Proposition 2.3. *Let $S \subseteq V$ with $|S| \geq 1$ and $T \subseteq V - S$ with $|T| \geq 2$ be two disjoint subsets of nodes. For nonnegative integers α and β such that $\alpha - \beta = 1$, and $|T| \geq \alpha + 1$, the* **(α, β)-inequality**

$$\sum_{i \in S, j \in T} y_{\{i,j\}} - y(S) - y(T) - \alpha x(S) + \beta x(T) \ \leq \ \frac{1}{2}\alpha\beta \tag{12}$$

defines a facet of CP_b^n if $\alpha \leq b - 4$.

◇

Macambira and De Souza furthermore proved that the (α,β)-inequalities define facets of QP^n. Their result generalizes a result of Padberg [1989] for the so-called generalized cut-inequalities. We will derive a class of facet-defining inequalities that generalizes the clique inequalities in Section 3.

2.2. **Relationship with the quadratic knapsack polytope.** Given a vector $w = (w_1, \ldots, w_n) \in \mathbb{R}^n$, we define the *quadratic knapsack polytope* $QKP_b^n(w)$ as the convex hull of those vectors $(x,y) \in \mathbb{R}^{n(n+1)/2}$ satisfying the conditions (3)–(6) together with the following knapsack generalization of (2):

$$\sum_{i\in V} w_i x_i \ \le \ b\ . \tag{13}$$

The linear optimization problem over $QKP_b^n(w)$ generalizes the classical knapsack problem to quadratic objective functions. This general problem occurs, for example, as a subproblem in the work of Johnson *et al.* [1993].

Letting QKP_b^n denote the knapsack polytope $QKP_b^n(w)$ in the special case $w = (1, 1, \ldots, 1)$, *i.e.*, with (2) for (13), we obtain the weighted b-clique polytope as $CP_b^n = QKP_b^n$.

The two classes of inequalities mentioned in the following proposition are facet-defining for QKP_b^n (see Johnson *et al.* [1993] and Park *et al.* [1996]).

Proposition 2.4.

(i) *For any node $i \in V$ the* **star inequality**

$$\sum_{e\ni i} y_e - (b-1)x_i \le 0 \tag{14}$$

defines a facet of CP_b^n if and only if $b \le n-1$.

(ii) *Let T be a sub-tree of K_n with set of nodes $V(T)$, $|V(T)| = b+1$, and set of edges $E(T)$, $|E(T)| = b$. Let $3 \le b \le n-1$. Then the* **tree inequality**

$$\sum_{e\in E(T)} y_e - \sum_{i\in V(T)} (\delta_i - 1)x_i \le 0 \tag{15}$$

where δ_i is the degree of node i in T, defines a facet of CP_b^n if and only if T is not a star or $b = n-1$.

◇

Tree inequalities were also considered by Macambira and De Souza [1996]. They combined a tree inequality with an (α,β)-inequality for $\alpha = 2$ and $\beta = 1$, and showed that the resulting inequality is facet-defining if the underlying tree is a path. Since the resulting inequalities do not seem to be very useful in practice, we do not present them in detail here. We mention that the separation problem for the tree inequalities is NP–complete (Hunting [1998]).

3. New facets for the b-clique polytope

We say that the collection $\mathcal{C} = \{C_1, \ldots, C_m\}$ of nodes of K_n is a *generating system of cliques* if the associated clique incidence vectors (x^C, y^C), $C \in \mathcal{C}$, generate an (affine) hyperplane in $\mathbb{R}^{n(n+1)/2}$.

If $\mathcal{C}$ is a generating system of cliques, there exists a vector $a \neq 0$ and a number a_0 such that

$$a(x^C, y^C) = a_0 \text{ for all } C \in \mathcal{C} .$$

Moreover, up to scalar multiplication, (a, a_0) is uniquely determined by $\mathcal{C}$. We say in this case that $a(x, y) = a_0$ is a *feasible equality* for the generating system $\mathcal{C}$.

Let $a(x, y) = a_0$ be a linear equality. Restricting the vector a to the components corresponding to x and to y respectively, let us write the equality $a(x, y) = a_0$ as

$$a^{(1)}x + a^{(2)}y \ = \ a_0 .$$

Then we observe

Lemma 3.1. *Assume $n \geq 2$, and let $a^{(1)}x + a^{(2)}y = a_0$ be a feasible equality for the generating system $\mathcal{C}$ of cliques. Then $a^{(2)} \neq 0$.*

Proof. Suppose $a^{(2)} = 0$. We will derive a contradiction.

Notice that $a^{(1)} \neq 0$ must hold (otherwise $a = 0$ would contradict our assumption that $a(x, y) = a_0$ is a feasible equality). Suppose that $a^{(1)}$ has exactly *one* non-zero coefficient $a_1^{(1)}$, say. By scalar multiplication, we may assume $a^{(1)} = 1$.

Then the equality $a(x, y) = a_0$ can only be $x_1 = 1$ or $x_1 = 0$. In the case $x_1 = 1$, however, the cliques in $\mathcal{C}$ also satisfy the equality $x_2 - y_{\{12\}} = 0$. Hence, the incidence vectors (x^C, y^C), $C \in \mathcal{C}$, lie in the intersection of two distinct hyperplanes and, therefore, could not generate a hyperplane. Similarly, in the case $x_1 = 0$, the cliques $C \in \mathcal{C}$ would also satisfy the equality $y_{\{12\}} = 0$ and thus could not generate a hyperplane. So we conclude that $a^{(1)}$ has at least *two* non-zero coefficients $a_1^{(1)}$ and $a_2^{(1)}$, say.

Every incidence vector (x^C, y^C), $C \in \mathcal{C}$, satisfies $a(x^C, y^C) = a^{(1)}(x^C) = \sum_{i=1}^n a_i^{(1)} x_i^C = a_0$. Squaring this equality, we obtain

$$\sum_{i=1}^{n} [a_i^{(1)}]^2 [x_i^C]^2 \ + \ \sum_{i \neq j} a_i^{(1)} a_j^{(1)} x_i^C x_j^C \ = \ a_0^2 .$$

Because $[x_i^C]^2 = x_i^C$ and $x_i^C x_j^C = y_{\{i,j\}}^C$, we see that the vector (x^C, y^C) also satisfies the linear equation

$$\sum_{i \in V} [a_i^{(1)}]^2 x_i \; + \sum_{\{i,j\} \in E} 2a_i^{(1)} a_j^{(1)} y_{\{i,j\}} \; = \; a_0^2 \, .$$

Since $a_1^{(1)} a_2^{(1)} \neq 0$, the latter equation is independent from $a(x,y) = a_0$, which implies that the clique incidence vectors lie in the intersection of two distinct hyperplanes, a contradiction to our assumption that $\mathcal{C}$ is a generating system of cliques.

□

Lemma 3.2. *Assume $n \geq 2$, and let $\mathcal{C}$ be a generating system of cliques with associated incidence vectors (x^C, y^C), $C \in \mathcal{C}$. Then the projected node incidence vectors x^C, $C \in \mathcal{C}$, generate $\mathbb{R}^n$.*

Proof. If the Lemma were false, the vectors x^C would be contained in a hyperplane of $\mathbb{R}^n$, *i.e.*, we could find a vector $a^{(1)} \neq 0$ and a number a_0 such that $a^{(1)} x^C = a_0$ for all $C \in \mathcal{C}$. With $a = (a^{(1)}, 0)$, we see that the generating system $\mathcal{C}$ would thus satisfy the equality $a(x,y) = a_0$, which contradicts Lemma 3.1.

□

Let $\mathcal{C} = \{C_1, \ldots, C_{n+1}, C_{n+2}, \ldots, C_m\}$ be a generating system of cliques of K_n. In view of Lemma 3.2, we may assume that the node incidence vectors $x^{C_1}, \ldots, x^{C_{n+1}}$ are affinely independent. We say that $\mathcal{C}$ is *b-strong* if $|C_1| \leq \ldots \leq |C_{n+1}| \leq b-1$ holds.

Note that $|C_1| \leq b-2$ must hold if $\mathcal{C}$ is b-strong: otherwise, the $n+1$ vectors x^{C_k}, $1 \leq k \leq n+1$, would satisfy the linear equality $\sum_{i \in V} x_i = b-1$ and hence could not be affinely independent.

With the generating system $\mathcal{C}$ of cliques of K_n we associate its *canonical extension* $\overline{\mathcal{C}}$ relative to K_N, $N > n$, as follows. $\overline{\mathcal{C}}$ consists of the following collections of subsets of nodes of K_N:

$$\begin{array}{lcll} \mathcal{S}^0 & := & \{C \mid C \in \mathcal{C}\} & \\ \mathcal{S}^l & := & \{C_k \cup \{l\} \mid k = 1, \ldots, n+1\} & \quad (\text{for } l = n+1, \ldots, N) \\ \mathcal{T} & := & \{C_1 \cup \{l, s\} \mid n+1 \leq l < s \leq N\} & \end{array}$$

(Note that $\mathcal{T} = \emptyset$ if $N = n+1$ and that the cardinality of each clique in $\mathcal{S}^l$ and $\mathcal{T}$ is bounded by b if $\mathcal{C}$ is b-strong).

Theorem 3.1. ("Lifting Theorem"). *If $n \geq 2$ and $\mathcal{C}$ is a generating system relative to K_n, then the canonical extension $\overline{\mathcal{C}}$ is a generating system relative to K_N.*

Proof. Let $\mathcal{C} = \{C_1, \ldots, C_m\}$. The canonical extension $\overline{\mathcal{C}}$ of $\mathcal{C}$ cannot generate all of $\mathbb{R}^{N(N+1)/2}$ since the feasible equation $a(x,y) = a_0$ for $\mathcal{C}$ yields an equality satisfied by $\overline{\mathcal{C}}$ in an obvious way (*cf.* the "canonical extension" of an inequality below).

To see that $\overline{\mathcal{C}}$ does indeed generate a hyperplane, there is no loss of generality when we assume that the associated incidence vectors (x^C, y^C), $C \in \mathcal{C}$, are affinely independent. So $m = n(n+1)/2$ and hence $|\overline{\mathcal{C}}| = N(N+1)/2$. It then suffices to show that the clique incidence vectors associated with $\overline{\mathcal{C}}$ are affinely independent.

The incidence vectors corresponding to cliques in $\mathcal{T}$ are independent of all the others (due to their unique 1-entry in the y-coordinate (l,s)). Thus, suppose that there exists some non-trivial affine relation among the other incidence vectors:

$$\sum_{j=1}^{n(n+1)/2} \lambda_j (x^{C_j}, y^{C_j}) \ + \ \sum_{l=n+1}^{N} \sum_{k=1}^{n+1} \mu_{lk} (x^{C_k \cup \{l\}}, y^{C_k \cup \{l\}}) \ = \ 0$$

with $\sum \lambda_j + \sum \mu_{lk} \ = \ 0$.

By assumption, the incidence vectors corresponding to $\mathcal{S}^0$ are affinely independent. Hence we must have $\mu_{lk} \neq 0$ for some l and k. Considering the x-coordinate corresponding to node l, we conclude $\sum_k \mu_{lk} = 0$.

Moreover, considering the y-coordinates corresponding to edges joining l to a node in C_k, $k = 1, \ldots, n+1$, we note that these are in one-to-one correspondence with the node incidence vector of C_k. So the above relation actually implies an affine relation among the node incidence vectors of $C_1, \ldots, C_{n+1}$, which contradicts Lemma 3.2 and our labeling of $\mathcal{C}$.

□

We want to generalize Padberg's [1989] concept of a *canonical extension* of a valid inequality.

If $a(x,y) \leq a_0$ is a valid inequality for CP_b^n, we define its canonical extension $a^*(x,y) \leq a_0$ to K_N by

$$\begin{aligned} a_i^* &= a_i \quad \forall\, i \in V, & a_i^* &= 0 \quad \forall\, i \in V' \setminus V \\ a_e^* &= a_e \quad \forall\, e \in E(V), & a_e^* &= 0 \quad \forall\, e \in E(V') \setminus E(V)\ , \end{aligned}$$

where $V = \{1, \ldots, n\}$ and $V' = \{1, \ldots, N\}$. Trivially, the canonical extension of a valid inequality for CP_b^n is valid for CP_b^N.

If $a(x,y) \leq a_0$ is facet-defining for CP_b^n, then the system $\mathcal{C}$ of all cliques C such that $|C| \leq b$ and $a(x^C, y^C) = a_0$ is a generating system of cliques. We say that $a(x,y) \leq a_0$ is *b-strong* if the associated generating system $\mathcal{C}$ is b-strong.

Corollary 3.1. *Let $a(x,y) \leq a_0$ be a b-strong facet-defining inequality for CP_b^n, $n \geq 2$. Then its canonical extension is facet-defining for any CP_b^N with $N > n$.*

Proof. If $\mathcal{C}$ is the generating system of cliques associated with the facet-defining inequality $a(x,y) \leq a_0$, then the incidence vectors of the cliques $\overline{C}$ in the canonical extension $\overline{\mathcal{C}}$ of $\mathcal{C}$ obviously satisfy the equality $a^*(x^{\overline{C}}, y^{\overline{C}}) = a_0$. So $a^*(x,y) \leq a_0$ S must be facet-defining for CP_b^N.

□

Corollary 3.2. (Padberg [1989]). *If $a(x,y) \leq a_0$ is a facet-defining inequality for the Boolean quadric polytope QP^n, then its canonical extension $a^*(x,y) \leq a_0$ is facet-defining for QP^{n+1}.*

Proof. $a^*(x,y) \leq a_0$ is valid for $QP^{n+1} = CP_{n+1}^{n+1}$. By Theorem 3.1, it must be facet-defining.

□

3.1. **Reformulation-Linearization Technique.** A useful technique for finding new valid inequalities of a polytope corresponding to an integer zero-one programming problem is the so-called *Reformulation-Linearization Technique* (RLT) as introduced by Sherali and Adams [1990]. (This work is related to Lovász and Schrijver [1991].)

The RLT consists of two steps, namely a reformulation step and a linearization step. In the reformulation step problem constraints are multiplied with d-degree polynomial factors composed of the n binary variables (in our case $x_1, \ldots, x_n$) and their complements, for some fixed $d \in \{0, 1, \ldots, n\}$. The resulting nonlinear program is then linearized by introducing new variables. For our purposes, we use only degree-1 polynomial factors.

As an example, consider the inequality (2)

$$\sum_{j \in V} x_j \;\leq\; b \,,$$

which is not facet-defining (*cf.* Lemma 3.1). Multiplication by $(1 - x_i)$, for some fixed $i \in V$, yields

$$(b-1)x_i + \sum_{j \in V} x_j - \sum_{e \ni i} y_e \;\leq\; b \,,$$

which is easily seen to be facet-defining. (We again employ the relations $x_i^2 = x_i$ and $x_i x_j = y_{\{i,j\}}$ for the binary variables x_i and x_j).

As a second example, consider the clique inequality

$$\alpha x(V) - y(V) \;\leq\; \frac{\alpha(\alpha+1)}{2} \tag{16}$$

for some integer $1 \leq \alpha \leq b-1$. Multiplying (16) with x_i, we obtain

$$\alpha x_i + \alpha \sum_{e \ni i} y_e - x_i \sum_{f \in E} y_f \;\leq\; \frac{\alpha(\alpha+1)}{2} x_i \;.$$

Instead of introducing new variables $w_{if} = x_i y_f$, we just use the relation $x_i y_f \leq y_f$ in order to obtain the *i-clique inequality*

$$\alpha \sum_{e \ni i} y_e - y(V) - \frac{\alpha(\alpha-1)}{2} x_i \;\leq\; 0\;. \tag{17}$$

The way we derived (17) from (16) implies that (17) is a valid inequality for CP_b^n. (This can also be verified directly).

Theorem 3.2. *For every integer α, $2 \leq \alpha \leq b-1 \;\leq n-2$, the i-clique inequality (17) is facet-defining for CP_b^n.*

Proof. We will exhibit a set of $n(n+1)/2$ affinely independent elements of CP_b^n satisfying a given i-clique inequality with equality.

Consider the incidence vectors (x^C, y^C) for $C = \emptyset, C = \{j\}$, $j \neq i$, and all subsets $C \subseteq V$ with $i \in C$ and $|C| \in \{\alpha, \alpha+1\}$.

It is straightforward to check that all of these incidence vectors satisfy (17) with equality. We leave it to the reader to verify that these incidence vectors also span a subspace of co-dimension 1. (Because $\alpha \leq n-2$, there are "sufficiently many" candidate sets C).

□

The i-clique inequalities are obviously b-strong. So we can apply Corollary 3.1 in the case $n = b+1$ and obtain

Corollary 3.3. *Let $S \subseteq V$ and $2 \leq \alpha \leq \min\{b-1, |S|-2\}$. Then the* "lifted i-clique inequality"

$$\alpha \sum_{j \in S \setminus i} y_{\{i,j\}} - y(S) - \frac{\alpha(\alpha-1)}{2} x_i \;\leq\; 0$$

is facet-defining for CP_b^n.

◇

We refer the interested reader to Hunting [1998] for other classes of facet-inducing inequalities. Applying the technique of "sequential lifting" (*cf.* Wolsey [1975]), one can, for example derive the following class of *generalized* clique inequalities:

$$\alpha[x(S) - \sum_{i \in S, j \in T} y_{\{i,j\}}] - y(S) \;\leq\; \frac{\alpha(\alpha+1)}{2}[1 - x(T) + y(T)]$$

for $S \subseteq V$, $T \subseteq V \setminus S$ and $1 \leq \alpha \leq |S| - 2$.

4. Lagrangian relaxation

We now assume in our model for the weighted clique problem that we have a complete *directed* graph $\vec{K}_n = (V, A)$ that differs from K_n in that each edge $e = \{i, j\} \in E$ is split into two arcs: (i, j) and (j, i), both in A. We assume that each arc in $\vec{K}_n$ has a weight that equals half the weight of the corresponding edge in K_n.

For each arc (i, j) in $\vec{K}_n$, we define a $(0, 1)$-variable $\vec{y}_{ij}$ that takes the value 1 if the arc (i, j) is in the clique, and value 0 otherwise. With these new variables, (WCP_b) can be transformed into the problem

$$\max \quad \sum_{i=1}^{n} d_i x_i + \sum_{(i,j) \in A} \frac{c_{ij}}{2} \vec{y}_{ij} \tag{18}$$

subject to

$$x_i + x_j - \vec{y}_{ij} \leq 1, \qquad 1 \leq i < j \leq n \tag{19}$$

$$\vec{y}_{ij} = \vec{y}_{ji} \qquad 1 \leq i < j \leq n \tag{20}$$

$$\vec{y}_{ij} - x_i \leq 0, \qquad 1 \leq i \neq j \leq n, \tag{21}$$

the star inequalities

$$\sum_{\substack{j=1 \\ j \neq i}}^{n} \vec{y}_{ij} - (b-1) x_i \leq 0, \qquad 1 \leq i \leq n, \tag{22}$$

the clique inequalities for $S = V$, $1 \leq \alpha \leq b - 1$,

$$\alpha \sum_{i=1}^{n} x_i - \frac{1}{2} \sum_{(i,j) \in A} \vec{y}_{ij} \leq \frac{\alpha(\alpha+1)}{2}, \tag{23}$$

the i-clique inequalities for $1 \leq i \leq n$ and $2 \leq \alpha \leq b - 1$,

$$\alpha \sum_{\substack{j=1 \\ j \neq i}}^{n} \vec{y}_{ij} - \frac{1}{2} \sum_{(j,k) \in A} \vec{y}_{jk} - \frac{\alpha(\alpha-1)}{2} x_i \leq 0, \tag{24}$$

and the integrality constraints

$$x_i \in \{0, 1\}, \qquad 1 \leq i \leq n \tag{25}$$

$$\vec{y}_{ij} \in \{0, 1\}, \qquad 1 \leq i \neq j \leq n. \tag{26}$$

When we now dualize the (in)equalities (19) and (20) by using Lagrangian multipliers $u \geq 0$ and w, we obtain the Lagrangian problem $(L_{u,w})$:

$$\max \sum_{i=1}^{n} d_i x_i + \sum_{(i,j)\in A} \frac{c_{ij}}{2} \vec{y}_{ij} + \sum_{(i,j)\in A} u_{ij}(1 - x_i - x_j + \vec{y}_{ij}) + \sum_{(i,j)\in A} w_{ij}(\vec{y}_{ji} - \vec{y}_{ij}) \tag{27}$$

subject to (21) – (26).

An optimal solution of the Lagrangian relaxation $(L_{u,w})$ can be efficiently computed as a consequence of the following observation.

Lemma 4.1. *A* $(0,1)$*-vector* $(x, \vec{y})$ *satisfies the constraints (21) – (26) if and only if there exists an integer* $p \in \{0, 1, \dots, b\}$ *such that*

$$\sum_{i=1}^{n} x_i = p \tag{28}$$

$$\sum_{j\in V\setminus i} \vec{y}_{ij} = \begin{cases} p-1 & \textit{if } x_i = 1 \\ 0 & \textit{otherwise.} \end{cases} \tag{29}$$

Proof. Assume that the $(0,1)$-vector $(x, \vec{y})$ satisfies (28) and (29). Then the conditions (21), (22), (25) and (26) are clearly satisfied. Inequality (23) is equivalent with

$$(\alpha - p)(\alpha - p + 1) \geq 0 ,$$

which holds because α and p are integers. Inequality (24) follows in the same way.

Conversely, assume that the $(0,1)$-vector $(x, \vec{y})$ satisfies (21) – (26). Adding all the star inequalities (22) and twice the clique inequality (23) with $\alpha = b-1$, we deduce $\sum x_i \leq b$. Let $p := \sum x_i$.

If $p = 0$, then (29) is an immediate consequence of (21). If $p = b$, then (22) implies that "$\leq$" holds in (29). On the other hand, we see from (23) with $\alpha = b-1$ that $\sum_{i,j} \vec{y}_{ij} \geq b(b-1)$ must hold. So (29) is satisfied with equality.

Finally, consider the case $1 \leq p \leq b-1$. When we add all i-clique inequalities (24) with $x_i = 1$ for $\alpha = p$ (choose $\alpha = 2$ in the case $p = 1$), we obtain

$$\sum_{x_i=1} \sum_{j\in V\setminus i} \vec{y}ij = \sum_{i,j} \vec{y}_{ij} \leq p(p-1) .$$

On the other hand, (23) with $\alpha = p$ shows

$$\sum_{i,j} \vec{y}_{ij} \geq p(p-1) .$$

Hence equality holds. Substitution of this equality into (24) with $\alpha = p$ now yields the desired result.

□

In view of Lemma 4.1, we can solve problem $(L_{u,w})$ in a straightforward way in time $O(n^2 \log n)$:

Note that the objective function of $(L_{u,w})$ can be written as

$$\max \sum_{i \in V} \tilde{d}_i x_i \; + \sum_{(i,j) \in A} \tilde{c}_{ij} \vec{y}_{ij} \; .$$

Thus, for $p = 0, 1, \ldots, b$, we (greedily) choose the p "best" nodes $i \in V$, *i.e.*, those nodes i for which the weight $\tilde{d}_i$ plus the weights $\tilde{c}_{i,j}$ of the corresponding p heaviest arcs (i, j) is as large as possible). We finally compare these $b+1$ candidate solutions and we take the one with the best objective function value.

4.1. **Improving the Lagrangian Relaxation.** Let $L(u, w)$ denote the optimal value of the Lagrangian problem $(L_{u,w})$ with respect to the objective (27). Since $L(u, w)$ is an upper bound on the objective function value of our integer program (WCP_b) of Section 2, we are interested in solving the problem

$$\min\{L(u, w) \mid u \geq 0, w\}$$

in order to obtain good bounds for a branch-and-bound algorithm (see also Section 5).

Note that the solution $(x, \vec{y})$ of the Lagrangian subproblem is optimal if it satisfies all the inequalities we have dualized. In general, however, $(x, \vec{y})$ will violate some of the dualized inequalities and min $L(u, w)$ will be strictly larger than the integer optimum we are looking for.

One may try to improve this bound min $L(u, w)$ by including more inequalities that are known to be valid for the CP_b^n into the Lagrangian objective as this procedure cannot deteriorate the bound. Intuitively, it seems promising to add inequalities that are *violated* by the current Lagrangian solution although there is, of course, no guarantee that the solution of the subsequent Lagrangian subproblem will satisfy these. In order to do this, however, we need an efficient algorithm to detect violated inequalities. As an illustration, we give such a separation algorithm for the tree inequalities (*cf.* Proposition 2.4) below. We expect that, *e.g.*, the clique and cut inequalities can be treated similarly. (In our practical implemenation below, we restrict ourselves to triangle clique and triangle cut inequalities, where the separation problem can be solved by enumeration).

It is NP-hard to find a tree inequality that is violated by a given vector $(x, \vec{y}) \in \mathbb{R}^{n^2}$ (Hunting [1998]). We will show, however, that this separation problem can be solved in polynomial time when restricted to $(0,1)$-vectors $(x, \vec{y})$ satisfying inequalities (28) and (29). This means that we can solve the separation problem for tree inequalities with respect to the solutions of our Lagrangian relaxation of (WCP_b).

Let T be a tree in K_n with set $V(T)$ of nodes and set $E(T)$ of (undirected) edges. Denoting by $\delta_i(T)$ the degree of node $i \in V(T)$ with respect to T, we set

$$(30) \qquad \omega(T) := \sum_{\{i,j\} \in E(T)} \frac{1}{2}(\vec{y}_{ij} + \vec{y}_{ji}) \; - \sum_{i \in V(T)} (\delta_i(T) - 1) x_i \; .$$

Thus $(x, \vec{y})$ violates the tree inequality associated with the tree T if and only if $\omega(T) > 0$.

Proposition 4.1. *Assume that the $(0,1)$-vector $(x, \vec{y})$ satisfies the conditions of Lemma 4.1. Then $(x, \vec{y})$ satisfies all tree inequalities if and only if*

$$(31) \qquad \vec{y}_{ij} \;\le\; x_j \qquad 1 \le i \ne j \le n \; .$$

Proof. Assume that (31) holds for the vector $(x, \vec{y})$ and let T be a tree with $|V(T)| = b + 1$ nodes.

Since $\sum_i x_i \le b$, there exists a node $r \in V(T)$ with $x_r = 0$. Starting from this "root" r, we can compute $\omega(T)$ recursively by iteratively adding an edge (i, j) to the subtree T' of T already constructed. If T'' denotes this augmented tree with the new node j, we observe

$$\omega(T'') \;=\; \omega(T') + \frac{1}{2}(\vec{y}_{ij} + \vec{y}_{ji}) - x_j \; .$$

In view of (21) and (31) we conclude $(\vec{y}_{ij} + \vec{y}_{ji})/2 - x_j \;\le\; 0$ and therefore obtain inductively

$$\omega(T'') \le \omega(T') \;\le\; 0 \; .$$

Conversely, if (31) is violated at some node $r \in V$ (*i.e.*, $x_r = 0$ and $\vec{y}_{lr} = 1$ for some $l \in V$), we take T to a star with center r and l as one of its b leaves. Then $\omega(T) > 0$ holds.

□

5. Computational Results

We implemented a branch-and-bound algorithm for the edge-weighted clique problem (WCP_b) as follows. At each node of the search tree, we create subproblems by fixing some variable x_i to either 0 or 1. Following an idea of Lucena [1992], we compute upper bounds for the objective function of the subproblems by first (approximately) solving the corresponding Lagrangian dual problem

$$(D) \qquad \min\{L(u,w) \mid u \geq 0\}$$

and then adding new violated inequalities to the objective function of the Lagrangian problem. We then solve the Lagrangian dual problem relative to the new objective function and add new violated inequalities. We repeat this process a fixed number of times. In the following, we will refer to an execution of this process (*i.e.*, solving problem (D) and adding new violated inequalities) as a *cycle*.

In order to keep the number of dualized constraints manageable, we remove in each cycle those constraints from the objective function for which the associated Lagrangian multipliers are almost 0.

We solve the Lagrangian dual (D) via the subgradient method with step sizes either according Held *et al.* [1974] with

$$\lambda_k = \rho \frac{f(x^k) - \bar{f}}{\|\gamma^k\|}, \tag{32}$$

where $\bar{f}$ is an estimation of the optimal value f^*, and coefficient ρ satisfies $0 < \rho \leq 2$ and $\gamma^k \in \partial(f(x^k)$ is a subgradient, or according to the convergent series method (see Shor [1968] and Goffin [1977]) with

$$\lambda_k = \lambda_0 \alpha^k, \tag{33}$$

where $0 < \alpha < 1$, and λ_0 is the initial step size.

Several preliminary tests lead us to an implementation where we use the first rule for solving Lagrangian dual problems associated to node 0 of the search tree and use the convergent series method for search tree nodes at depth > 0.

As to the parameter setting, we observed that the correct choice of parameters depends on the type of inequalities we add. For example, the "original" Lagrangian dual (D) could be solved with the convergent series method and $\alpha = 0.95$, while we needed $\alpha = 0.99$ when we added all triangle clique and triangle cut inequalities. Such high values of α (we set $\lambda_0 = 100$) lead to a fairly large number of iterations (about 300) of the subgradient method. All of our computational results are obtained with a fixed setting of the parameters, chosen so as to optimize running times for the "hard instances". We noticed that the choice of a different setting could result in a faster solution for the "easy" problems. We used the number of iterations as our stopping criterion for subgradient optimization of the Lagrangian dual because of a lack of feasible alternatives: we did not have a reliable estimate for the distance to the optimum and we observed that the objective function typically fluctuated considerably.

Lower bounds are computed with a simple heuristic solution algorithm proposed by Späth [1985a]: we take the clique given the current solution and perform a sequence of simple exchange steps (exchange a node in the clique with a node outside) until a local maximum is reached. This heuristic performed extremely well: in all of our experiments, we found the global optimum before the first branching, *i.e.*, at depth 0.

Macambira and de Souza [1996] tested a branch-and-cut method on a set of instances with $40 \leq n \leq 48$ and $b = n/2$. Edge weights were generated by using a parameter $k \in \{1, 2, 3, 4, 5\}$. Our computational results for these instances are listed below in Table 1 (positive edge weights) and Table 2 (mixed, *i.e.*, positive and negative edge weights).

The column "gap %" displays the relative difference between the optimal solution and the upper bound computed at depth 0. The columns "max depth" and "# branch nodes" refer to the search tree.

The running time resulting from our approach seems to be at least comparable with the branch-and-cut method of Macambira and de Souza [1996]. On the hard instances, in particular, our approach led to an improvement by a factor of 2 or 3. Our computations were carried out on a HP 9000/735 (125 Mhz), whereas Macambira and de Souza implemented their algorithm on a SUN Sparc 1000 machine, using CPLEX 3.0. Because of the different implementation platforms, however, it is difficult to compare the relative speeds. In fact, we view our methodological approach to the weighted b-clique problem not so much as competitor but as a feasible (and promising) alternative and complement to existing techniques.

n	k	optimal value	1st node	gap %	max. depth	# branch nodes	time (sec.)
40	1	109346	109819.2	0.4	4	11	1677
	2	82451	82517.1	0.1	2	5	946
	3	68759	69339.4	0.8	5	23	2115
	4	60782	61601.3	1.3	5	37	2915
	5	60513	60561.7	0.1	1	3	917
42	1	120299	121308.0	0.8	5	43	3845
	2	87810	88950.6	1.3	6	47	4203
	3	76554	77081.3	0.7	11	39	3947
	4	69482	69644.5	0.2	2	7	1381
	5	67383	67453.5	0.1	1	3	1245
44	1	136525	136846.5	0.2	4	11	1912
	2	98186	99285.3	1.1	4	31	3672
	3	84675	84856.6	0.2	2	7	1332
	4	75274	75559.8	0.4	2	7	1403
	5	69540	69777.6	0.3	12	27	4113
46	1	142985	144377.5	1.0	7	57	5590
	2	108243	109777.5	1.4	6	81	7481
	3	94859	95213.7	0.4	4	15	2421
	4	78747	79674.4	1.2	5	41	4222
	5	72431	73297.8	1.2	8	43	4434
48	1	163397	164435.4	0.6	6	47	4959
	2	115471	118219.7	2.4	11	295	27479
	3	96666	98305.9	1.7	8	117	11166
	4	88728	89112.5	0.4	4	11	2122
	5	82117	82361.6	0.3	4	9	2093

TABLE 1. Results for Macambira/De Souza instances (positive weights)

n	k	optimal value	1st node	gap %	max. depth	# branch nodes	time (sec.)
40	1	70348	73580.6	4.6	8	175	14079
	2	45404	45743.8	0.7	5	11	1857
	3	34091	34502.9	1.2	4	9	1129
	4	27758	28180.3	1.5	3	15	2548
	5	27967	28076.3	0.4	5	13	2785
42	1	81633	84997.2	4.1	9	185	14841
	2	46828	48091.0	2.7	5	43	4159
	3	36689	37014.2	0.9	3	13	2130
	4	35987	36211.2	0.6	3	7	534
	5	35460	35710.3	0.7	3	7	1800
44	1	90620	94499.8	4.3	11	307	27445
	2	56960	57978.3	1.8	5	25	3329
	3	40697	41101.0	1.0	3	9	2142
	4	32601	33157.9	1.7	7	35	4208
	5	29407	29639.5	0.8	3	9	1502
46	1	99550	102398.6	2.9	12	101	10348
	2	58361	59539.5	2.0	8	37	4579
	3	43915	45109.0	2.7	6	49	5418
	4	32968	34354.0	4.2	14	97	10185
	5	31000	31252.6	0.8	3	9	2350
48	1	113478	118353.3	4.3	12	539	55917
	2	61768	65358.1	5.8	10	377	36963
	3	45941	46572.9	1.4	5	23	3277
	4	36903	37176.3	0.7	3	9	2257
	5	31351	32067.0	2.3	5	33	4505

TABLE 2. Results for Macambira/De Souza instances (mixed weights)

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