

Consecutive Ones and A Betweenness Problem in Computational Biology

Thomas Christof and Marcus Oswald and Gerhard Reinelt

Institut für Angewandte Mathematik

Universität Heidelberg

Im Neuenheimer Feld 294

69120 Heidelberg, Germany

Thomas.Christof@IWR.Uni-Heidelberg.De

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Abstract. In this paper we consider a variant of the betweenness problem occurring in computational biology. We present a new polyhedral approach which incorporates the solution of consecutive ones problems and show that it supersedes an earlier one. A particular feature of this new branch-and-cut algorithm is that it is not based on an explicit integer programming formulation of the problem and makes use of automatically generated facet-defining inequalities.

1 Introduction

The general *Betweenness Problem* is the following combinatorial optimization problem. We are given a set of n objects $1, 2, \dots, n$, a set \mathcal{B} of betweenness conditions, and a set $\overline{\mathcal{B}}$ of non-betweenness conditions. Every element of \mathcal{B} (of $\overline{\mathcal{B}}$) is a triple (i, j, k) (a triple $\overline{(i, j, k)}$) requesting that object j should be placed (should not be placed) between objects i and k . The task is to find a linear order of all objects such that as many betweenness and non-betweenness conditions are satisfied, resp. to characterize all orders that achieve this minimum. If violations are penalized by weights, we call the problem of finding a linear order minimizing the sum of weights of violations *Weighted Betweenness Problem*. This problem is \mathcal{NP} -hard in general.

In this paper we consider a special variant of this problem occurring in computational molecular biology, namely in the physical mapping problem with end probes. For the purpose of this paper we do not elaborate on the biological background, but refer to [4]. We define the problem simply as follows. We are given a set of m so-called *clones* $1, 2, \dots, m$ to each of which two so-called *end probes* $t(i)$ and $h(i)$ are associated. These

$n = 2m$ probes are numbered such that $t(i) = 2i - 1$ and $h(i) = 2i$. Depending on the data, we have for every pair of a clone i and a probe $j \in \{1, 2, \dots, n\} \setminus \{t(i), h(i)\}$ either a betweenness condition $(t(i), j, h(i))$ or a non-betweenness condition $\overline{(t(i), j, h(i))}$. Violation of a betweenness condition is penalized with cost c_ρ , and violation of a non-betweenness constraint receives a penalty of c_μ . The problem is then to find a linear order of the probes minimizing the sum of penalties for violated constraints.

This weighted betweenness problem can also be stated in a different version. A 0/1 matrix $A \in \{0, 1\}^{m \times n}$ has the *consecutive ones property* (for rows) if the columns of A can be permuted so that the 1's in each row appear consecutively. For a 0/1 matrix $B \in \{0, 1\}^{m \times n}$ having the consecutive ones property let n_ρ^B (n_μ^B) denote the number of 1's (of 0's) that have to be switched to transform A into B . Let c_ρ and c_μ be some nonnegative numbers. The *Weighted Consecutive Ones Problem* is to find a matrix B with the consecutive ones property minimizing $c_\rho n_\rho^B + c_\mu n_\mu^B$. This problem is known to be \mathcal{NP} -hard [2]. All column permutations π of a feasible matrix B so that the 1's in each row of B^π appear consecutively can be found in time linear in the number of 1's in B by a so called *PQ-tree algorithm* [1].

For our discussion, we assume that the data is given as clone \times probe 0/1-matrix A where $a_{i,t(i)}$ and $a_{i,h(i)}$ are fixed to 1. The other entries are obtained from some experiment where an entry $a_{ij} = 1$ gives rise to a betweenness constraint $(t(i), j, h(i))$ and an entry $a_{ij} = 0$ corresponds to a non-betweenness constraint $\overline{(t(i), j, h(i))}$. A solution of the weighted betweenness problem corresponds then to a solution of the weighted consecutive ones problem with the additional constraint that in some column permuted matrix B^π (in which the 1's in each row appear consecutively) the first and the last one in each row i correspond to the end probes of clone i .

The weighted consecutive ones problem models the biological situation if the information that the probes are the ends of clones is missing [6]. Note that by introducing artificial variables the weighted consecutive ones problem can easily be transformed to a weighted betweenness problem.

The paper is organized as follows. Section 2 discusses our previous approach which could already be applied successfully. An improved approach is presented in section 3 leading to the definition of the betweenness polytope. This polytope is then studied in the following section. Separation in the context of a branch-and-cut algorithm to solve the betweenness problem to optimality is the topic of section 5. Computational results conclude this paper.

2 A first IP model

Our previous computational approach to the weighted betweenness problem was based on a different model. We state it here mainly for a comparison and for introducing some notations. In the following we will introduce 0/1 variables indicating whether a betweenness or non-betweenness constraint is violated. Since a betweenness condition (i, j, k) is violated if and only if the non-betweenness condition $\overline{(i, j, k)}$ is satisfied, we can just complement

variables and will speak only about betweenness conditions in the following. The objective function coefficients of the variables will then give the preference if the condition should be satisfied or violated.

Let m be the number of clones and n be the number of probes. In our special setup we have $n = 2m$ and we have $n - 2$ betweenness constraints $(t(i), j, h(i))$ for every clone i . We write, for short, (i, j) for the betweenness constraint $(t(i), j, h(i))$, and call (i, j) a *clone-probe pair*. The set \mathcal{B}_m of all possible clone-probe pairs is

$$\mathcal{B}_m := \{(i, j) \mid 1 \leq i \leq m, 1 \leq j \leq n, j \neq t(i), j \neq h(i)\}.$$

Obviously, $|\mathcal{B}_m| = 2m(m - 1)$.

We will develop an integer programming formulation with two types of variables. For every ordered pair (i, j) of probes, we introduce a 0/1 variable y_{ij} which has value 1 if and only if i precedes j in the order π . With every clone-probe pair $(i, j) \in \mathcal{B}_m$, we associate the 0/1 variable x_{ij} which has value 1 if and only if constraint $(t(i), j, h(i))$ is met in the order π . Equivalently, $x_{ij} = 0$ if and only if the non-betweenness constraint $(\overline{t(i), j, h(i)})$ is met.

To ensure that the variables y_{ij} encode a linear order π of the probes, the constraints of the IP formulation of the linear ordering problem have to be met, i.e., they have to satisfy

$$\begin{aligned} y_{ij} + y_{ji} &= 1, & \text{for all } 1 \leq i < j \leq n, \\ y_{ij} + y_{jk} + y_{ki} &\leq 2, & \text{for all triples } 1 \leq i, j, k \leq n. \end{aligned}$$

To ensure that the x_{ij} count violations of the betweenness and nonbetweenness constraints, we add the following inequalities. To force a $x_{ij} \in \mathcal{B}_m$ to be 0 if and only if $(t(i), j, h(i))$ is violated (or $(\overline{t(i), j, h(i)})$ is satisfied), we add

$$\begin{aligned} x_{ij} &\leq y_{jh(i)} + y_{jt(i)}, \\ x_{ij} &\leq y_{h(i)j} + y_{t(i)j}, \\ x_{ij} &\geq -y_{t(i)j} - y_{jh(i)} + 1 \\ x_{ij} &\geq y_{t(i)j} + y_{jh(i)} - 1. \end{aligned}$$

Thus, x_{ij} is 1 if and only if $y_{t(i)j} = y_{jh(i)}$.

We do not discuss the objective function here. Due to the positive parameters c_ρ and c_μ we can omit some of these inequalities depending on whether x_{ij} corresponds to an original betweenness or non-betweenness condition, and moreover, we only have to require

$$0 \leq x_{ij} \leq 1.$$

The objective function will force these variables to have integer values if the linear ordering variables are integer. Note that the objective function is zero on the linear ordering variables.

With every feasible solution of the problem, corresponding to a permutation π of the probes, we associate 0/1-vectors $\psi^\pi \in \{0, 1\}^{n(n-1)}$ and $\chi^\pi \in \{0, 1\}^{|\mathcal{B}_m|}$ with

$$\psi_{ij}^\pi = \begin{cases} 1 & \text{if } i \text{ precedes } j \text{ in the order } \pi, \\ 0 & \text{otherwise.} \end{cases}$$

and

$$\chi_{ij}^\pi = \begin{cases} 1 & \text{if constraint } (t(i), j, h(i)) \text{ is met in the order } \pi, \\ 0 & \text{otherwise.} \end{cases}$$

The polytope P_{LOBW}^m associated with the instance of the weighted betweenness problem is the convex hull of all possible vectors $\begin{pmatrix} \psi^\pi \\ \chi^\pi \end{pmatrix}$,

$$P_{LOBW}^m = \text{conv} \left(\left\{ \begin{pmatrix} \psi^\pi \\ \chi^\pi \end{pmatrix} \mid \pi \text{ is a permutation of the probes} \right\} \right).$$

Previous computations were based on partial descriptions of this polytope (see [4]).

3 Modelling without linear ordering variables

The formulation of the preceding section is somewhat redundant. Namely, let $\begin{pmatrix} \psi \\ \chi \end{pmatrix} \in P_{LOBW}^m \cap \{0, 1\}^{6m^2-4m}$ be an incidence vector of the weighted betweenness problem with $n = 2m$ probes and the set \mathcal{B}_m of betweenness constraints. Obviously χ can be retrieved from ψ , because

$$\chi_{ij} = 1 \Leftrightarrow \psi_{t(i)j} = \psi_{jh(i)}.$$

Conversely, for χ there exist one or more feasible settings of ψ . These settings cannot be obtained directly but in linear time by application of the *PQ*-tree algorithm [1]. For a given χ we define for every clone i three sets in the following way.

$$\begin{aligned} S_{i_1} &= \{j \mid \chi_{ij} = 1\} \cup \{t(i)\}, \\ S_{i_2} &= \{j \mid \chi_{ij} = 1\} \cup \{h(i)\}, \\ S_{i_3} &= \{j \mid \chi_{ij} = 1\} \cup \{t(i)\} \cup \{h(i)\}. \end{aligned}$$

The feasible settings of the linear ordering variables ψ correspond to all permutations of $\{1, \dots, n\}$ where the elements of every set introduced above occur in consecutive order.

We now define the projection of P_{LOBW}^m onto the χ variables

$$P_{BW}^m = \text{conv}(\{\chi \mid \text{there exists } \psi \text{ such that } \begin{pmatrix} \psi \\ \chi \end{pmatrix} \in P_{LOBW}^m\}).$$

It can easily be tested if a 0/1-vector χ is contained in P_{BW}^m . Namely if not, i.e. if $\chi \in \{0, 1\}^{2m(m-1)}$, $\chi \notin P_{BW}^m$, then with the sets defined above for the clones, the application of the *PQ*-tree algorithm would yield the result that no permutation exists in which the elements of the sets appear as consecutive subsequences. Otherwise, if $\chi \in P_{BW}^m$, then the *PQ*-tree provides all consistent permutations.

Because a feasible linear ordering can be derived from an $\chi \in P_{BW}^m$ and the objective function is zero for the linear ordering variables, they can be omitted. A solution of the weighted betweenness problem for physical mapping is obtained by solving

$$\begin{aligned} \max \quad & c^T x \\ x \quad & \in P_{BW}^m \\ x \quad & \in \{0, 1\}^{2m(m-1)} \end{aligned}$$

Now we want to derive an integer programming formulation of this problem from an integer programming formulation of the weighted consecutive ones problem.

For each χ the sets S_{i_k} can be written as rows of a matrix $M^\chi \in \{0, 1\}^{3m \times 2m}$. For $1 \leq i \leq m$ and $1 \leq j \leq n$ and $1 \leq k \leq 3$ an entry $m_{3(i-1)+k,j}^\chi$ of M^χ has the value 1 if and only if $j \in S_{i_k}$.

Proposition 3.1 $\chi \in P_{BW}^m \iff M^\chi$ has the consecutive ones property for rows.

Proof. Clear because of the construction of the sets S_{i_k} . \square

Corollary 3.2 *Each integer programming formulation of the weighted consecutive ones problem leads to an integer programming formulation of the weighted betweenness problem for physical mapping.*

Proof. It exists a linear transformation from χ to M^χ . \square

An IP formulation of the weighted consecutive ones problem can be derived from a theorem of Tucker [11]. In this paper it is shown that the 0/1 matrix M has the consecutive ones property for rows if and only if no submatrix of M is a member of $\{M_i\}$, where $\{M_i\}$ is a given set of 0/1 matrices. Now for each submatrix of M and each matrix M_i with the same size it is easy to derive an inequality, which is violated if and only if the submatrix is equal to M_i . The set of all these inequalities gives an IP formulation of the weighted consecutive ones problem.

Using the linear transformation from χ to M^χ we obtain an IP formulation of the weighted betweenness problem for physical mapping. For $m = 2$ the nontrivial inequalities of the formulation are

$$\begin{aligned} 2x_{1t(2)} + x_{2t(1)} + x_{2h(1)} &\leq 3 \\ 2x_{1t(2)} - 2x_{1h(2)} - x_{2t(1)} - x_{2h(1)} &\leq 1 \end{aligned}$$

and further inequalities which can be obtained by the symmetry operations described in section 4.2. Note that these two classes of inequalities do not define facets of P_{BW}^2 .

4 The polytope P_{BW}^m

In this section we will investigate some properties of the polytope P_{BW}^m (see also [9] for a more detailed discussion). In particular we are interested in exhibiting classes of facet-defining inequalities.

4.1 Dimension and lifting

We first determine the dimension of P_{BW}^m and address the question of trivial (node) lifting of facets.

Proposition 4.1 *Let $m > \overline{m} \geq 2$. An inequality $g^T x \leq g_0$ for P_{BW}^m , obtained by trivial lifting from an inequality $f^T x \leq f_0$ which is valid for $P_{BW}^{\overline{m}}$ is valid for P_{BW}^m .*

Proof. to be supplied in the final version □

To be more precise, we can also compute the dimension of a face of P_{BW}^m which is induced by an inequality resulting from trivial lifting of an inequality of $P_{BW}^{\overline{m}}$.

Theorem 4.2 *Let $f^T x \leq f_0$ be valid for $P_{BW}^{\overline{m}}$, and let $F = \{x \in P_{BW}^{\overline{m}} \mid f^T x = f_0\}$ be the induced face with $\dim F \geq 0$. Let $m > \overline{m}$ and let $g^T x \leq g_0$ be valid for P_{BW}^m , obtained from $f^T x \leq f_0$ by trivial lifting. Let $G = \{x \in P_{BW}^m \mid g^T x = g_0\}$. Then*

$$\dim G - \dim F = |\mathcal{B}_m| - |\mathcal{B}_{\overline{m}}| = 2m(m-1) - 2\overline{m}(\overline{m}-1).$$

Proof. to be supplied in the final version □

From these results we obtain that trivial lifting preserves the facet-defining property and that P_{BW}^m is full-dimensional.

Corollary 4.3 *Let $m > \overline{m} \geq 2$. An inequality $g^T x \leq g_0$ for P_{BW}^m , obtained by trivial lifting from a facet-defining inequality $f^T x \leq f_0$ of $P_{BW}^{\overline{m}}$ is facet-defining.*

Corollary 4.4 *For $m \geq 2$ the following holds*

$$\dim P_{BW}^m = 2m(m-1),$$

i.e., P_{BW}^m is full-dimensional.

Proof. P_{BW}^2 is full-dimensional. By application of Theorem 4.2. with $F = P_{BW}^2$ and $G = P_{BW}^m$ the corollary follows. □

4.2 Small instance relaxations

Because facet-defining inequalities of P_{BW}^m are trivially liftable, we can obtain from linear descriptions of polytopes associated with small instances of the problem, say for $2 \leq m \leq 4$ relaxations of P_{BW}^m for any m . We call such a relaxation *small instance relaxation*.

In order to characterize the symmetry properties of P_{BW}^m we use the following notation. Let $v \in \mathbb{R}^{|\mathcal{B}_m|}$. The entries of v can be placed in an m by m *clone-clone matrix* \tilde{v} of 2-dimensional vectors. The rows and columns of the matrix correspond to the clones, and an entry $\tilde{v}_{ij} \in \mathbb{R}^2$ of \tilde{v} is defined for $i \neq j$ as $\tilde{v}_{ij} = \begin{pmatrix} v_{it(j)} \\ v_{ih(j)} \end{pmatrix}$, i.e., an entry ij refers to the relations of the end-probes obtained from clone j with clone i .

Now, the set of incidence vectors in P_{BW}^m can be partitioned into equivalence classes with respect to the following two operations. First, for $\chi \in P_{BW}^m$ an arbitrary permutation of the clones is allowed. This corresponds to a simultaneous permutation of the rows and columns of the associated clone-clone matrix $\tilde{\chi}$. Second, for an arbitrary clone j its end-probes can be reversed. This corresponds to reversing in column j of the clone-clone matrix the entries of $\begin{pmatrix} \chi_{it(j)} \\ \chi_{ih(j)} \end{pmatrix}$ to $\begin{pmatrix} \chi_{ih(j)} \\ \chi_{it(j)} \end{pmatrix}$ for all $1 \leq i \leq m, i \neq j$.

We used the algorithms for facet enumeration discussed in [5] to get more insight into the facet structure of P_{BW}^m for $m \leq 4$. It is clear that also the facet-defining inequalities of P_{BW}^m can be assigned to equivalence classes.

P_{BW}^2 has 7 vertices and is completely described by the following 3 equivalence classes of facets $f^{iT} x \leq f_0^i$, \tilde{f}^i is the clone-clone matrix of f^i .

$$\begin{aligned} \tilde{f}^1 &= \begin{pmatrix} * & \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 1 \end{pmatrix} & * \end{pmatrix}, & \tilde{f}^2 &= \begin{pmatrix} * & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 \\ -1 \end{pmatrix} & * \end{pmatrix}, & \tilde{f}^3 &= \begin{pmatrix} * & \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ \begin{pmatrix} -1 \\ -1 \end{pmatrix} & * \end{pmatrix} \\ f_0^1 &= 2, & f_0^2 &= 0, & f_0^3 &= 0 \end{aligned}$$

P_{BW}^3 has 172 vertices and 241 facets in total which can be partitioned into 16 equivalence classes of facets.

The computation of the complete linear description of P_{BW}^4 which has 9,197 vertices was not possible. However, by an algorithm for parallel facet enumeration (see [5]) we found $1,16 \cdot 10^7$ (!) different equivalence classes of facet-defining inequalities, yielding a lower bound of $4.4 \cdot 10^9$ for the number of facets of P_{BW}^4 .

4.3 Cycle inequalities

We use the following notation. For $i \in \{1, \dots, n\}$, $c(i)$ describes the clone from which the probe i is extracted, i.e., $i = t(c(i))$ or $i = h(c(i))$. Moreover, $q(i)$ describes the second probe $q(i)$ which the clone $c(i)$ defines. Of course, we have $q(q(i)) = i$.

A class of valid inequalities can be motivated by the following observation. Given $n = 2m$ betweenness constraints $(t(i_1), 1, h(i_1)), \dots, (t(i_n), n, h(i_n)))$, such that every probe j , $j \in \{1, \dots, n\}$ is exactly once the probe between the ends of a clone $i_j \neq c(j)$. Then for any permutation π of the probes at least two betweenness constraints are violated, because the first probe $\pi(1)$ and the last probe $\pi(2m)$ are not between other probes. Hence, the inequality

$$\sum_{j=1}^n x_{i_j j} \leq n - 2, \quad i_j \neq c(j) \tag{1}$$

is valid for P_{BW}^m . The following cycle inequalities are a special case of these inequalities. In particular, they are facet-defining.

Theorem 4.5 *Let D_n be the complete directed graph on n nodes corresponding to all probes, and let R be a cycle in D_n with the property that if i in $V(R)$, then $q(i) \notin V(R)$.*

Then

$$\sum_{(i,j) \in R} x_{c(i)j} + x_{c(j)q(i)} \leq 2|R| - 2 \quad (2)$$

defines a facet of P_{BW}^m .

Proof. to be supplied in the final version □

5 Separation procedures

We do not use the IP formulation presented above in our computations, because on the one hand it is fairly complicated and on the other hand the inequalities do not define facets in general. Rather, we proceed as follows. As discussed before, we can check feasibility of an integer vector x^* by making use of the PQ -tree algorithm. If x^* is feasible, then the PQ -tree algorithm also generates all optimal solutions π^* . Otherwise, if x^* is not feasible (but binary), then one can construct a cutting plane, which is satisfied by all 0/1-vectors different from x^* . Let $P = \{x_i^* \mid x_i^* = 1\}$ and $Z = \{x_i^* \mid x_i^* = 0\}$, then

$$\sum_{i \in P} x_i - \sum_{i \in Z} x_i \leq |P| - 1$$

is a cutting plane with the desired properties.

5.1 Separation of cycle inequalities

The separation of the cycle inequalities can be done by a shortest path algorithm. Let x^* be an LP solution and $D_n = (V_n, A_n)$ be the complete directed graph on n nodes with edge weights

$$w_{ij} = 2 - x_{c(i)j}^* - x_{c(j)q(i)}^*.$$

Then it is easy to see by the following transformation that a cycle with weight less than 2 corresponds to a violated inequality. Let $y^* = 1 - x^*$. Then x^* violates a cycle inequality (2) if and only if y^* violates an inequality

$$\sum_{(i,j) \in R} x_{c(i)j} + x_{c(j)q(i)} \geq 2$$

which is true if and only if $w(R) < 2$ for the cycle R in $D_n = (V_n, A_n)$.

5.2 Separation of small instance relaxations

We also implemented separation heuristics for inequalities of small instance relaxations.

Let an LP solution $x^* \in \mathbb{R}^{|B_m|}$ and a facet-defining inequality $g^T x \leq g_0$ be given. For a permutation σ of $\{1, \dots, m\}$ we define

$$C(\sigma) = \sum_{i=1}^m \sum_{j=1, j \neq i}^m \begin{pmatrix} x_{it(j)}^* \\ x_{ih(j)}^* \end{pmatrix}^T \begin{pmatrix} g_{\sigma(i)t(\sigma(j))} \\ g_{\sigma(i)h(\sigma(j))} \end{pmatrix}.$$

It is clear that the set $\{\sigma \mid C(\sigma) > g_0\}$ gives all violated inequalities among all inequalities which are (by means of relabeling of the clones) equivalent to $g^T x \leq g_0$. Thus the separation problem for equivalent inequalities (relative to relabeling of the clones) is a quadratic assignment problem in which all entries are 2-dimensional vectors.

Because an inequality $g^T x \leq g_0$ of a small instance relaxation results from trivial node lifting of an inequality $f^T x \leq f_0$ which is facet-defining for $P_{BW}^{\overline{m}}$, $\overline{m} < m$ we have

$$C(\sigma) = \sum_{i=1}^{\overline{m}} \sum_{j=1, j \neq i}^{\overline{m}} \begin{pmatrix} x_{\sigma^{-1}(i)t(\sigma^{-1}(j))}^* \\ x_{\sigma^{-1}(i)h(\sigma^{-1}(j))}^* \end{pmatrix}^T \begin{pmatrix} f_{it(j)} \\ f_{ih(j)} \end{pmatrix}.$$

Since \overline{m} is rather small ($\overline{m} \leq 4$) the quadratic assignment problem is computationally tractable and can effectively be solved by heuristics; in our implementation we use a Grasp procedure similar to [8].

In order to separate all inequalities of one equivalence class this separation procedure has to be executed for at most $2^{\overline{m}}$ different inequalities $f_i^T x \leq f_0^i$ which are equivalent relative to the end-probe reversing symmetry property.

6 Computational results

In our branch-and-cut computations we used ABACUS [10] with LP solver CPLEX and an implementation of the PQ -tree algorithm [7]. Our computational experiments show that the new approach clearly supersedes our previous approach.

In [4] we used a set of 150 randomly generated problem instances with 42 to 70 probes which simulate the biological situation. Figure 1 compares our previous approach (using linear ordering variables) with the new model described here. The table displays the average CPU-times t_{tot} , the average number of nodes of the branch-and-cut tree n_{sub} , the average number of cutting planes which are added to the linear program n_{cut} and the average number of LP reoptimizations n_{lp} to solve the problem instances.

Model	t_{tot}	n_{sub}	n_{cut}	n_{lp}
Linear ordering based	0:44:32	3.2	22197.8	201.5
PQ -tree based	0:01:28	1.13	1022.0	6.3

Table 1: Average values for 150 problems.

In our new approach the following strategy for separating a fractional LP solution turned out to be favorable. If by exact enumeration of the nontrivial facet classes of P_{BW}^2 not enough cutting planes are found, we execute the heuristics of section 5.2 for a small subset (less than 15) of all equivalence classes of facet-defining inequalities of P_{BW}^4 . If this separation fails, then we separate the cycle inequalities.

A detailed investigation of different strategies for using small instance relaxations in sequential and parallel branch-and-cut algorithms can be found in [3]. In this work also the question is addressed which and how many equivalence classes of facet-defining should be used for separation.

Further details to be supplied in the final version.

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