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Polyhedral Aspects of Self-Avoiding Walks

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POLYHEDRAL ASPECTS OF SELF-AVOIDING WALKS

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ABSTRACT. In this paper, we study self-avoiding walks of a given length on a graph. We consider a formulation of this problem as a binary linear program. We analyze the polyhedral structure of the underlying polytope and describe valid inequalities. Proofs for their facial properties for certain special cases are given. In a variation of this problem one is interested in optimal configurations, where an energy function measures the benefit if certain path elements are placed on adjacent vertices of the graph. The most prominent application of this problem is the protein folding problem in biochemistry. On a set of selected instances, we demonstrate the computational merits of our approach.

1. INTRODUCTION

A path in a graph is a sequence of adjacent vertices. A path is called simple if multiple occurrence of vertices is prohibited. Paths in graphs give rise to various optimization questions. One of the most prominent is the shortest-path problem, where one is interested in an optimal connection between two given distinct vertices of the graph with respect to certain edge weights. If the edge weights are all positive or, more general, if there is no cycle with negative total weight, then an optimal path is automatically a simple path. Moreover, in this case, the solution of the shortest-path problem can be obtained in polynomial time complexity.

Our work is motivated by a field of applications in physical chemistry, where linear polymer molecules are modeled as simple paths in graphs featuring a certain regularity. These graphs are then referred to as *lattices*, and a simple path in this context is called a *self-avoiding walk* on the lattice. A prominent example is the protein folding problem which refers to the assembly (“*folding*”) of a three-dimensional structure of a polypeptide molecule, which is a linear polymer consisting of amino acids, in an aqueous solvent. Formulations of this problem as binary linear programs were given in [10, 17]. Our work contributes to a deeper understanding of the respective underlying polytopes. In particular, we are interested in the convex hull of the incidence vectors of self-avoiding walks. To the best of our knowledge, a polyhedral analysis of families of valid inequalities was not done so far. Under certain conditions we are able to prove facet-defining criteria for some substructures of interest.

The outline of the remainder of this article is the following. In Section 2 we introduce the necessary mathematical description of the problem. In Section 3, we state a complete outer description for $P^{(2)}$ by facet-defining inequalities. In the general case, one technical difficulty arising with the description of the facial structure of $P^{(n)}$ is the lack of dimensionality of these polytopes. We therefore consider their *down-monotonization* as a full-dimensional relaxation. The down-monotonization of $P^{(n)}$ yields the submonotone SAW- n polytope $P^{(n;\leq)}$ which we study in Section 4. We describe the structure of valid inequalities, and we provide a facet characterization for two special cases. In Section 5, we demonstrate the application of cutting planes derived from the polyhedral structures of $P^{(2)}$ and $P^{(n;\leq)}$, respectively. Section 6 contains a conclusion and an outlook to further research opportunities.

2. PROBLEM DESCRIPTION

Let $G = (V, E)$ be a graph. A path in G is a sequence

$$\omega = (\omega_0, \dots, \omega_m)$$

with $\omega_i \in V$ for all $i \in \{0, \dots, m\}$ and $\{\omega_{i-1}, \omega_i\} \in E$ for all $i \in \{1, \dots, m\}$. We alternatively call ω an m -step path (which refers to the number of its edges) or a path of length $m + 1$ (which refers to the number of its vertices). A self-avoiding walk (SAW) on G is a path in G without repetition of vertices, i.e., $\omega_i \neq \omega_j$ for $i \neq j$. At this point, we remark that the term “self-avoiding walk” is typically associated with a *lattice*, which can be seen as an infinite graph featuring a certain regular structure (usually originating from a regular tiling of the plane or space). Although the results of this paper are valid for general graphs, we put the focus on finite subgraphs of regular lattices, which we denote as $x \times y$ ($\times z$) lattices. Examples of regular grid graphs include $x \times y$ square ($Q_{x \times y}$) and triangular ($T_{x \times y}$) lattices in two dimensions, as well as $x \times y \times z$ cubic ($Q_{x \times y \times z}$) and tetrahedral ($T_{x \times y \times z}$) lattices in three dimensions. As an example, the 3×3 square lattice $Q_{3 \times 3}$ is shown in Figure 1. As a convention, we number the vertices consecutively, starting with zero, as indicated in Figure 1.

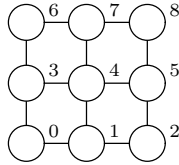


FIGURE 1. 3×3 square lattice

In order to emphasize the connection to lattice graphs, we use the term “self-avoiding walk” instead of “path”. In the following, we consider SAWs in the context of their vertices and therefore denote the set of all SAWs of length n on G (or $(n - 1)$ -step SAWs, respectively) by $\Omega_G^{(n)}$. We set $S^{(n)} = \{0, \dots, n - 1\}$ and define the incidence vector for an SAW $\omega \in \Omega_G^{(n)}$ as

$$x(\omega) = (x(\omega)_v^s)_{v \in V, s \in S^{(n)}} \quad \text{with} \quad x(\omega)_v^s = \begin{cases} 1, & \text{if } \omega_s = v, \\ 0, & \text{otherwise.} \end{cases}$$

The aim of this paper is the investigation of the convex hull $P^{(n)}$ of the incidence vectors for all SAWs of length n on a given graph G , i.e., we are going to study the structure of the polytope

$$P^{(n)} = \text{conv} \{x(\omega) \mid \omega \in \Omega_G^{(n)}\}$$

which we call the *SAW- n polytope*.

We start with the introduction of a terminology which enables a set-based representation for SAWs of length n on a graph $G = (V, E)$. For the remainder of this paper, we assume that G is connected and consists of at least two vertices, and we assume $n \geq 2$ to be fixed. Next, we introduce the *SAW- n graph* associated to a graph G as the expansion

$$G^{(n)} = (V^{(n)}, E^{(n)})$$

where $V^{(n)} = V \times S^{(n)}$ and $E^{(n)} = \bigcup_{j \in S^{(n)} \setminus \{0\}} \{\{(v, j - 1), (v, j)\} \mid \{v, w\} \in E\}$.

In the following, we mention two properties of the SAW- n graph. The proofs for the respective statements can be found in [16].

Property 2.1. *The SAW- n graph $G^{(n)}$ is bipartite with the partition*

$$V^{(n)} = V \times S_0^{(n)} \dot{\cup} V \times S_1^{(n)},$$

where $S_0^{(n)}$ contains all even and $S_1^{(n)}$ all odd elements of $S^{(n)}$, i.e.,

$$S_k^{(n)} = \left\{ j \in S^{(n)} \mid j \equiv k \pmod{2} \right\} \quad \text{for } k = 0, 1.$$

Property 2.2.

- a) The number $\kappa(G^{(n)})$ of connected components of $G^{(n)}$ is at most two.
- b) $G^{(n)}$ is connected if and only if G is non-bipartite.

Example 2.3. Consider the 3×3 square lattice $G = Q_{3 \times 3}$. Since G is bipartite, the corresponding SAW- n graph $G^{(n)}$ consists of two connected components for each $n \geq 2$. Figure 2 shows the corresponding SAW-4 graph and the decomposition into its two connected components.

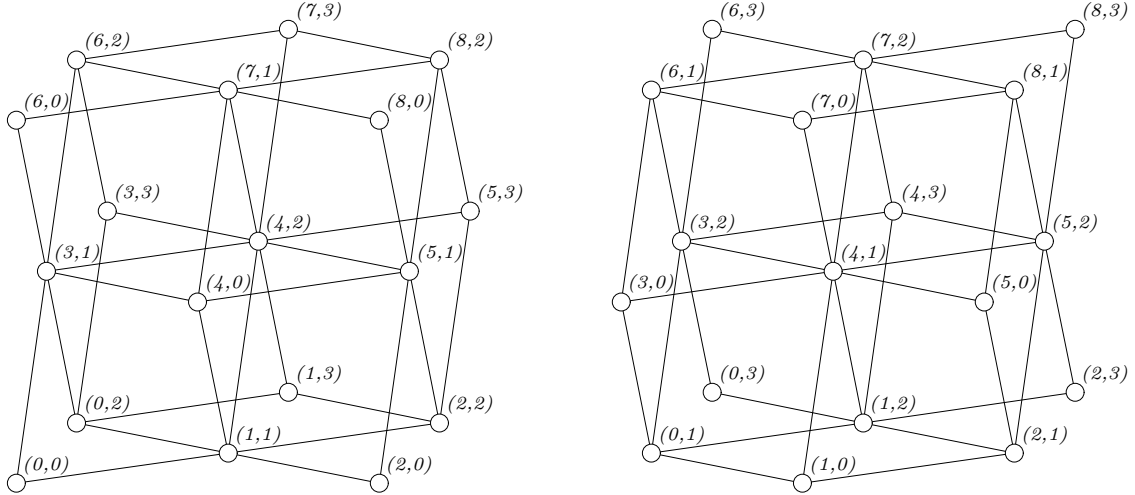


FIGURE 2. Connected components of the SAW-4 graph corresponding to the 3×3 square lattice

The SAW- n graph enables the representation of an SAW of length n on G as a subset of its vertices. For this, we introduce the following terminology.

Definition 2.4. Let $G = (V, E)$ be a graph and $G^{(n)}$ the corresponding SAW- n graph.

- a) An SAW- n conformation in $G^{(n)}$ is a set

$$\psi = \left\{ (v, s) \in V^{(n)} \mid \omega_s = v \text{ for some } \omega \in \Omega_G^{(n)} \right\}.$$

- b) We denote the set of all SAW- n conformations in $G^{(n)}$ with $\Psi_G^{(n)}$.
- c) For an SAW- n conformation $\psi \in \Psi_G^{(n)}$ in $G^{(n)}$, the corresponding SAW- n vector is given by the incidence vector $\chi^\psi \in \{0, 1\}^{|V^{(n)}|}$.
- d) We denote the set of SAW- n vectors in $G^{(n)}$ with $X_G^{(n)} = \{\chi^\psi \mid \psi \in \Psi_G^{(n)}\}$.

Thus the SAW- n polytope $P^{(n)}$ is given by $P^{(n)} = \text{conv}(X_G^{(n)})$. In the sequel, we present a straightforward description of $P^{(n)}$ by linear constraints and integrality conditions which has already been stated in [10, 17]. Throughout this article we will refer to this as the classical 0/1 model.

For each vertex $v \in V$ and for each element $s \in S^{(n)}$, we introduce a binary variable x_v^s with

$$(1) \quad x_v^s = \begin{cases} 1, & \text{if } \omega_s = v, \\ 0, & \text{otherwise.} \end{cases}$$

In order to guarantee the correct representation of a SAW of length n by the x -variables, the set of possible assignments of these variables has to be restricted by the following constraints:

- **Total Deployment**

Each element $s \in S^{(n)}$ must occupy exactly one vertex $v \in V$:

$$(2) \quad \sum_{v \in V} x_v^s = 1, \quad \forall s \in S^{(n)}.$$

• **Self-Avoidance**

Each vertex $v \in V$ can be occupied by at most one element $s \in S^{(n)}$:

$$(3) \quad \sum_{s \in S^{(n)}} x_v^s \leq 1, \quad \forall v \in V.$$

• **Contiguity**

Successive elements $s, s+1 \in S^{(n)}$ have to occupy adjacent vertices of G :

$$(4) \quad x_v^s \leq \sum_{w \in \delta_G(v)} x_w^{s+1}, \quad \forall v \in V, s \in S^{(n)} \setminus \{n-1\},$$

where $\delta_G(v)$ denotes the set of all vertices adjacent to v in G .

In the sections below, we are going to study certain polytopes related to $P^{(n)}$. Of particular interest in this context are the inequalities defining their facets. Having regard to this issue, we introduce the following notation which will be used throughout this article.

Definition 2.5. Let P be a polyhedron and $a^T x \leq \alpha$ an inequality.

- a) An element $\bar{x} \in P$ is called a **root** of $a^T x \leq \alpha$ if $a^T \bar{x} = \alpha$. The set of all such roots is denoted as $\text{eq}(P; a^T x \leq \alpha)$.
- b) We call (a subset of) an SAW- n conformation ψ an **SAW- n root (sub-) conformation** of $a^T x \leq \alpha$ for the associated polytope P if its incidence vector χ^ψ constitutes a root of $a^T x \leq \alpha$.

3. THE SAW-2 POLYTOPE

The aim of this section is the investigation of a class of polytopes for the representation of one-step paths (which are naturally self-avoiding). For these polytopes, we provide a complete outer description by facet-defining inequalities. We observe that the set of 1-step SAWs on a graph G can be bijectively mapped to the set of edges of the SAW-2 graph $G^{(2)}$ in the sense that an edge $e = \{(v, s), (w, 1-s)\} \in E^{(2)}$ is assigned the 1-step SAW $\omega \in \Omega_G^{(2)}$ given by $\omega_s = v, \omega_{1-s} = w$. Thus an SAW-2 conformation in $G^{(2)}$ is equivalent to an edge of $G^{(2)}$.

3.1. Dimension. We provide an upper bound for the dimension of $P^{(n)}$ which is given by a linear independent set of valid equations.

Theorem 3.1. For a given graph G , an upper bound for the dimension of the corresponding SAW- n polytope $P^{(n)}$ is given by

$$\dim P^{(n)} \leq \begin{cases} n \cdot |V| - n - (n-1), & \text{if } G \text{ is bipartite,} \\ n \cdot |V| - n, & \text{if } G \text{ is not bipartite.} \end{cases}$$

Proof. Since $P^{(n)} \subseteq [0, 1]^{|V^{(n)}|}$, its dimension is at most $|V^{(n)}| = n \cdot |V|$. Each vertex of $P^{(n)}$ satisfies the total deployment conditions (2). For $S^{(n)} = \{0, \dots, n-1\}$, we denote the deployment condition for the element $s \in S^{(n)}$ with $\text{TD}(s)$. The set $\{\text{TD}(s) \mid s \in S^{(n)}\}$ of all deployment equations is linearly independent. Consequently, each of these n equations reduces the upper bound of the dimension of $P^{(n)}$ by one. If moreover $G = (V, E)$ is bipartite with vertex partition $V = V_I \dot{\cup} V_{II}$, there are $n-1$ additional parity equations

$$(5) \quad \sum_{v \in V_I} (x_v^{s-1} + x_v^s) = 1 \quad \forall s \in S^{(n)} \setminus \{0\}.$$

Then this set $\{\text{PAR}_I(s) \mid s \in S^{(n)} \setminus \{0\}\}$ of equations, joined with the set $\{\text{TD}(s) \mid s \in S^{(n)}\}$ of deployment equations, is linearly independent, yielding the theorem. \square

The equations causing the reduction in the dimension can be represented as the two total deployment conditions from the classical 0/1 model

$$(6) \quad \sum_{v \in V} x_v^0 = 1,$$

$$(7) \quad \sum_{v \in V} x_v^1 = 1,$$

and, in the case of a bipartite graph G , the parity equation

$$(8) \quad \sum_{v \in V_I} x_v^0 - \sum_{v \in V_{II}} x_v^1 = 0.$$

Remark 3.2. For bipartite lattices $G = (V, E)$ with vertex partition $V = V_I \dot{\cup} V_{II}$, the parity equation (8) can be replaced by an equivalent parity equation by exchanging the assignments of $s \in \{0, 1\}$ to the partitions V_I and V_{II} . In terms of the equations introduced above, we replace (8) by (8) - (6) + (7). The resulting equation reads

$$(9) \quad \sum_{v \in V_{II}} x_v^0 - \sum_{v \in V_I} x_v^1 = 0.$$

In the following, we derive the lower bound for $P^{(2)}$ by stating affine independence of SAW-2 vectors. This lower bound turns out to be equal to the upper bound for $P^{(2)}$.

Definition 3.3. Let $X \subseteq X_G^{(2)}$ be a set of SAW-2 vectors, i.e., a subset of incidence vectors of the edges set of the SAW-2 graph $G^{(2)}$. Then we define

$$G_X = \left(V^{(2)}, E_X \right) \quad \text{with} \quad E_X = \left\{ e \in E^{(2)} \mid \exists x \in X : x = \chi^e \right\}.$$

Lemma 3.4. Let $X \subseteq X_G^{(2)}$ be a set of SAW-2 vectors. X is linearly independent if and only if G_X does not contain a cycle.

Proof. It suffices to show that X is linearly dependent if and only if G_X contains a cycle of even length, since G_X is included in $G^{(2)}$ which is bipartite, and each cycle in a bipartite graph has even length.

" \Leftarrow ": We show that X is linearly dependent if G_X contains a cycle of even length.

Let $X = (x_1, \dots, x_n)$ and $E_X = \{e_1, \dots, e_n\}$ be the set of edges of G_X . Let w.l.o.g. $C = (e_1, \dots, e_l)$, $l \leq n$, l even, be a cycle of even length in G_X with corresponding SAW-2 vectors $x_j = \chi^{e_j}$ for $j \in \{1, \dots, l\}$. W.l.o.g. we assume that the sequence (e_1, \dots, e_l) is chosen in such a manner that the successor edge of e_j in the cycle is given by e_{j+1} , and that of e_l by e_1 .

For each pair (x_j, x_{j+1}) , $j \in \{1, \dots, l-1\}$ of successive columns, including (x_l, x_1) in the matrix X_C having x_1, \dots, x_l as its columns, there is a row index i such that $x_j^i = x_{j+1}^i = 1$. Set $\lambda_j = (-1)^j$, $j \in \{1, \dots, l\}$ and consider the sum $\lambda_1 x_1 + \dots + \lambda_l x_l$. Due to the sequence of (x_1, \dots, x_l) , the ones in each pair of successive columns are eliminated in this sum. Since l is even, also the remaining ones in the columns x_l and x_1 are eliminated. Consequently, $\lambda_1 x_1 + \dots + \lambda_l x_l = 0$, which means that the vectors (x_1, \dots, x_l) are linearly dependent.

" \Rightarrow ": We show that G_X contains a cycle of even length if X is linearly dependent.

Let $X = \{x_1, \dots, x_n\}$ be linearly dependent and $\lambda_1 x_1 + \dots + \lambda_n x_n = 0$ and $(\lambda_1, \dots, \lambda_n) \neq 0$. We assume that G_X does not contain a cycle of even length, that means, as G_X is bipartite, it does not contain any cycle at all. Consequently, G_X consists of a set of trees. Let $e_j = \{i_1, i_2\}$ be an edge incident to a leaf of G_X which we w.l.o.g. assume to be i_1 . Consider the corresponding vector $x_j = \chi^{e_j}$ with $x_j^{i_1} = x_j^{i_2} = 1$. Therefore, in the matrix (x_1, \dots, x_l) in the row i_1 there is only one 1. To obtain $\lambda_1 x_1 + \dots + \lambda_n x_n = 0$, λ_{i_1} has to be zero. Now we remove the edge e_j from G_X . The remaining graph is also a set of trees, so we can gradually apply the procedure to all $\lambda \in \{\lambda_1, \dots, \lambda_n\}$, yielding $\lambda_i = 0$ for all i , a contradiction to our assumption. Consequently, G_X must contain a cycle of even length. \square

Corollary 3.5. *Let $X \subseteq X_G^{(2)}$ be a set of vertices of $P^{(2)}$. Then the affine rank of X equals the number of edges in a spanning tree of G_X .*

Now we can supply a lower bound for the dimension of $P^{(2)}$:

Theorem 3.6. *A lower bound for dimension of the SAW-2 polytope of a given graph G is given by*

$$\dim P^{(2)} \geq |V^{(2)}| - \kappa(G^{(2)}) - 1.$$

Proof. Consider the set $X = X_G^{(2)}$. Then we have $G_X = G_{X_G^{(2)}} = G^{(2)}$. The number of edges in each spanning tree of $G^{(2)}$ is $|V^{(2)}| - \kappa(G^{(2)})$, which, according to Corollary 3.5, equals the affine rank of $X_G^{(2)}$. Since $X_G^{(2)} \subseteq P^{(2)}$, the dimension of $P^{(2)}$ is at least $|V^{(2)}| - \kappa(G^{(2)}) - 1$. \square

Thus we obtain the dimension of $P^{(2)}$:

Theorem 3.7.

$$\dim P^{(2)} = |V^{(2)}| - \kappa(G^{(2)}) - 1.$$

Proof. As a consequence of Property 2.2 and Theorem 3.1, we obtain $\dim P^{(2)} \leq |V^{(2)}| - \kappa(G^{(2)}) - 1$. Concurrently, Theorem 3.6 states $\dim P^{(2)} \geq |V^{(2)}| - \kappa(G^{(2)}) - 1$, which yields the dimension of $P^{(2)}$. \square

3.2. Valid and Facet-Defining Inequalities. Now we are ready to introduce a class of valid inequalities for $P^{(2)}$ arising by a generalization of the contiguity constraints (4) of the classical 0/1 model. We investigate their structure and characterize the facets-defining inequalities among these.

Definition 3.8. *Let G be a graph, $G^{(2)}$ the corresponding SAW-2 graph, and $s \in \{0, 1\}$. An inequality of the form*

$$(10) \quad \sum_{(v,s) \in L} x_v^s \leq \sum_{(w,1-s) \in \delta_{G^{(2)}}(L)} x_w^{1-s}$$

is called an SAW-2 inequality with left-hand side $L \subseteq V^{(2)}$, if $L \subseteq V \times \{s\}$. For such an inequality, we set

$$V_L = \{v \in V \mid (v, s) \in L\}.$$

In other words, an SAW-2 inequality with left-hand side L enforces that once an element s occupies some vertex $v \in V_L$ in G , its neighbor $(1-s)$ occupies a vertex in the neighborhood of V_L . This fact gives rise for the validity of an SAW-2 inequality for $P^{(2)}$. Note that the SAW-2 inequalities with $|L| = 1$ exactly correspond to the contiguity constraints (4) of the classical 0/1 model. Hence, the entirety of SAW-2 inequalities can be seen as a generalization of the contiguity constraints. Obviously, an SAW-2 inequality is defined by its left-hand side L . Next we turn to the problem of identifying facet-defining inequalities for $P^{(2)}$ among the SAW-2 inequalities. To this end, we relate the roots of an SAW-2 inequality to a subgraph of the SAW-2 graph.

Definition 3.9. *Let*

$$(11) \quad \sum_{(v,s) \in V^{(2)}} a_v^s x_v^s \leq \alpha$$

be a generic inequality with coefficients corresponding to the vertices of the SAW-2 graph $G^{(2)}$. Then we define the SAW-2 root graph G^\equiv of (11) as $G_{\text{eq}(P^{(2)}; (11))}$.

If (11) is an SAW-2 inequality defined by $L \subseteq V^{(2)}$, we relate the terms “root” and “SAW-2 root graph” directly to L . In this case, we denote the set of roots by X_L and the SAW-2 root graph by G_L^\equiv .

We will use the SAW-2 root graph for some statements on the dimension of an SAW-2 inequality with left-hand side L . Here we state the dimension of an SAW-2 inequality as the affine rank of the set of its roots. For ease of exposition, we denote this affine rank with $\dim L$.

Theorem 3.10. *Let $G^{(2)}$ be an SAW-2 graph, and let $L \subseteq V^{(2)}$ be the left-hand side of an SAW-2 inequality. Then*

$$\dim L = |V^{(2)}| - \kappa(G_L^-).$$

Proof. According to Corollary 3.5, the dimension of L equals the number of edges in a spanning tree of G_L^- . Using the general formula $|\mathcal{T}| = |V| - \kappa(G)$ for a spanning tree \mathcal{T} of a graph $G = (V, E)$ we obtain the theorem. \square

Corollary 3.11. *An SAW-2 inequality whose root graph consists of exactly $\kappa(G^{(2)}) + 1$ connected components defines a facet of $P^{(2)}$.*

Proof. Let L be the left-hand side of an SAW-2 inequality whose root graph consists of $\kappa(G^=)$ components. According to Theorem 3.10, we have $\dim L = |V^{(2)}| - \kappa(G^=)$. Since $\kappa(G^=) = \kappa(G^{(2)}) + 1$, the SAW-2 inequality defined by L is facet-defining for $P^{(2)}$. \square

Example 3.12. *Consider the 3×3 square lattice $G = Q_{3 \times 3}$ as shown in Figure 1. The SAW-2 inequality $x_1^0 \leq x_2^1 + x_3^1$ defines a facet of $P^{(2)}$, since its root graph consists of $3 = \kappa(G^{(2)}) + 1$ connected components (see Figure 3). However, the SAW-2 inequality $x_5^0 \leq x_2^1 + x_4^1 + x_6^1 + x_8^1$ does not define a facet of $P^{(2)}$, since its root graph consists of $6 > \kappa(G^{(2)}) + 1$ components (see Figure 4).*

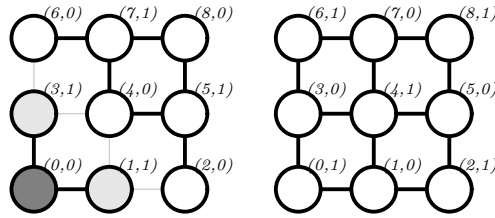


FIGURE 3. Root graph for a facet-defining SAW-2 inequality. The vertices $(v, s) \in L$ (left-hand side of the inequality) are colored in dark gray, the vertices $(w, 1-s) \in \delta_{G^{(2)}}(L)$ (right-hand side) in light gray.

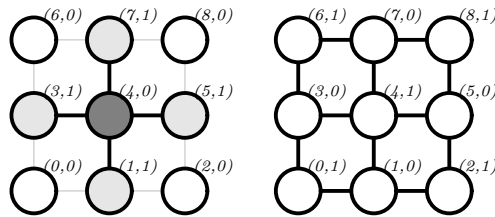


FIGURE 4. Root graph for a non-facet-defining SAW-2 inequality

3.3. Complete Description. At this stage, the classification of facet-defining SAW-2 inequalities is complete. In the following, we show that the facet-defining SAW-2 inequalities, together with the nonnegativity constraints, the deployment equations (6) and (7), and, if applicable, the parity equation (8), provide a complete outer description of $P^{(2)}$.

Theorem 3.13. *Let G be a graph. Then the SAW-2 polytope $P^{(2)}$ for G , i.e., the convex hull of all SAW-2 conformations in $G^{(2)}$, is completely described by the two equations (6) and (7) and, if G is bipartite, equation (8), the nonnegativity constraints, and the set of SAW-2 inequalities whose root graph consists of $\kappa(G^{(2)}) + 1$ connected components.*

The proof of this theorem requires the results of several lemmata. These are stated below and finally lead to the actual proof on page 10. We start with a statement on the representation of facet-defining inequalities for $P^{(2)}$.

Lemma 3.14. *Any facet-defining inequality for $P^{(2)}$ can be written in the form*

$$(12) \quad \sum_{(v,s) \in V_L} b_v^s x_v^s \leq \sum_{(w,t) \in V_R} b_w^t x_w^t$$

with $V_L, V_R \subseteq V^{(2)}$, $V_L \cap V_R = \emptyset$, as well as $b_v^s > 0$ for $(v, s) \in V_L$ and $b_w^t > 0$ for $(w, t) \in V_R$.

Proof. Let

$$(13) \quad \sum_{(v,s) \in V^{(2)}} a_v^s x_v^s \leq \alpha$$

with $a_v^s \in \mathbb{Z}$ for all $(v, s) \in V^{(2)}$ and $\alpha \in \mathbb{Z}$ be an inequality inducing a facet of $P^{(2)}$.

In order to obtain an inequality with right-hand side $\alpha = 0$, we choose $\alpha_0, \alpha_1 \in \mathbb{Z}$ with $\alpha_0 + \alpha_1 = \alpha$, and subtract $[\alpha_0 \cdot (6) + \alpha_1 \cdot (7)]$ from (13). The result is an inequality

$$(14) \quad \sum_{(v,s) \in V^{(2)}} \beta_v^s x_v^s \leq 0$$

with $\beta_v^s = a_v^s - \alpha_s$. This transformed inequality is equivalent to the original one with respect to the vertices of $P^{(2)}$ whose incidence vectors are roots of it. From the form (14), it is straightforward to achieve (12). \square

Next, we deal with the number of connected components of the SAW-2 root graph of a facet-defining inequality for $P^{(2)}$.

Lemma 3.15. *Consider an inequality (12) defining a facet of $P^{(2)}$, and let $X = \text{eq}(P^{(2)}; (12))$ denote the set of its roots. Then the number of connected components of the SAW-2 root graph G_X is given by*

$$\kappa(G_X) = \kappa(G^{(2)}) + 1.$$

Proof. G_X is a subgraph of the SAW-2 graph $G^{(2)}$. According to Corollary 3.5 the affine rank of X is $|V^{(2)}| - \kappa(G_X)$. On the other hand, X is a set of roots of a facet-defining inequality, and hence its affine rank is

$$\dim P^{(2)} - 1 = |V^{(2)}| - \kappa(G^{(2)}) - 2$$

according to Theorem 3.7. Consequently, $\kappa(G_X) = \kappa(G^{(2)}) + 1$. \square

In a further step, we investigate the coefficients b within the connected components of G_X .

Lemma 3.16. *Let G_X be the SAW-2 root graph of a facet-defining inequality (12). Let further $(v, s), (w, t) \in V^{(2)}$ belong to the same connected component $(K, E(K))$ of G_X . Then*

$$|b_v^s| = |b_w^t| =: b_K.$$

Proof. We distinguish two cases.

(i) $\{(v, s), (w, t)\} \in E_X^{(2)}$:

Then $t = 1 - s$, and there exists an SAW-2 vector $\bar{x} \in X$ with $\bar{x}_v^s = \bar{x}_w^{1-s} = 1$. For \bar{x} plugged in (12), we obtain the following requirements for the coefficients b : If $(v, s) \in V_N$, \bar{x} can be a root of (12) if $(w, 1 - s) \in V_N$, i.e., both sides of the equation are zero, and

$b_v^s = b_w^{1-s} = 0$. If $b_v^s \neq 0$, i.e., $(v, s) \in V_L$ or $(v, s) \in V_R$, we get $b_w^{1-s} = -b_v^s$. Consequently, we have $|b_v^s| = |b_w^{1-s}|$.

(ii) $\{(v, s), (w, t)\} \notin E_X^{(2)}$:

Since (v, s) and (w, t) belong to the same connected component $(K, E(K))$, there exists a path $((v, s) =: (v_0, s_0), (v_1, s_1), \dots, (v_{n-1}, s_{n-1}), (v_n, s_n) := (w, t))$ with $(v_j, s_j) \in K$ for $j = 0, \dots, n$, and $\{(v_{j-1}, s_{j-1}), (v_j, s_j)\} \in E(K)$ for $j = 1, \dots, n$. For $j \in \{1, \dots, n\}$ we consider $\{(v_{j-1}, s_{j-1}), (v_j, s_j)\}$ and apply (i). This yields $b_{v_j}^{s_j} = -b_{v_{j-1}}^{s_{j-1}}$, or $|b_{v_j}^{s_j}| = |b_{v_{j-1}}^{s_{j-1}}|$. Successively applying this argument for all $j \in \{1, \dots, n\}$, we obtain $|b_v^s| = |b_w^{1-s}|$. \square

In the following, we show that (12) can be transformed so that it has nonzero coefficients on only one connected component of G_X . For this, we remark that according to Lemma 3.15 and Corollary 2.2, the number of connected components of G_X is two if G is non-bipartite, and it is three if G is bipartite.

Lemma 3.17. *Let G_X be the SAW-2 root graph of a facet-defining inequality (12). Let $K_{X;0}$, $K_{X;1}$, and, if applicable, $K_{X;2}$ denote the vertex sets of its connected components. Then (12) has a representation such that its support is contained in only one component (w.l.o.g. $K_{X;1}$), i.e.,*

$$(15) \quad \hat{b}_{K_{X;1}} \sum_{(v,s) \in V_L \cap K_{X;1}} x_v^s \leq -\hat{b}_{K_{X;1}} \sum_{(w,t) \in V_R \cap K_{X;1}} x_w^t,$$

Proof. We first remark that we can w.l.o.g. claim that

$$(16a) \quad V_L \subseteq V \times \{0\} \quad \text{and}$$

$$(16b) \quad V_R \subseteq V \times \{1\}.$$

This can be justified by the following argument: Assume $V_L = V_{L;0} \dot{\cup} V_{L;1}$ and $V_R = V_{R;0} \dot{\cup} V_{R;1}$ where $V_{L;i}, V_{R;i} \subseteq V \times \{i\}$ for $i = 0, 1$. Then (12) can be written as

$$(17) \quad \sum_{(v,s) \in V_{L;0}} b_v^s x_v^s + \sum_{(v,s) \in V_{L;1}} b_v^s x_v^s \leq \sum_{(w,t) \in V_{R;0}} b_w^t x_w^t + \sum_{(w,t) \in V_{R;1}} b_w^t x_w^t.$$

Since per definition $V_L \cap V_R = \emptyset$, (17) is the sum of two valid inequalities with disjoint coefficient sets

$$(18a) \quad \sum_{(v,s) \in V_{L;0}} b_v^s x_v^s \leq \sum_{(w,t) \in V_{R;1}} b_w^t x_w^t \quad \text{and}$$

$$(18b) \quad \sum_{(v,s) \in V_{L;1}} b_v^s x_v^s \leq \sum_{(w,t) \in V_{R;0}} b_w^t x_w^t.$$

Now we have to distinguish between bipartite and non-bipartite graphs G .

(i) We consider the case that G is bipartite, i.e., $\kappa(G^{(2)}) = 2$ (see Theorem 2.2). We denote these components with K_0 and K_1 . Then G_X consists of three connected components $K_{X;0}, K_{X;1}, K_{X;2}$. W.l.o.g., $K_0 \subseteq K_{X;0}$ (otherwise, G_X would consist of more than three components). Since $K_{X;0}$ as a subgraph of $G^{(2)}$ is bipartite, we can add linear combinations of the equations (8) and (9) to (12) without reducing the dimension of (12). Furthermore, using the notation of (8) and (9), we have (w.l.o.g.) $V_L \subseteq V_I \times \{0, 1\}$ and $V_R \subseteq V_{II} \times \{0, 1\}$. Adding $(b_{K_{X;0}} \cdot ((8) - (9)))$ to (12) yields an inequality

$$(19) \quad \sum_{(v,s) \in V_L} \tilde{b}_v^s x_v^s \leq \sum_{(w,t) \in V_R} \tilde{b}_w^t x_w^t,$$

where $\tilde{b}_{K_{X;0}} = 0$.

Now we consider the remaining two components $K_{X;1}$ and $K_{X;2}$ of G_X .

Then (19) reads

$$(20) \quad \sum_{i \in \{1,2\}} \sum_{(v,s) \in V_L \cap K_{X;i}} \tilde{b}_v^s x_v^s \leq \sum_{i \in \{1,2\}} \sum_{(w,t) \in V_R \cap K_{X;i}} -\tilde{b}_w^t x_w^t$$

or equivalently,

$$(21) \quad \sum_{i \in \{1,2\}} \tilde{b}_{K_{X;i}} \sum_{(v,s) \in V_L \cap K_{X;i}} x_v^s \leq \sum_{i \in \{1,2\}} -\tilde{b}_{K_{X;i}} \sum_{(w,t) \in V_R \cap K_{X;i}} x_w^t$$

Now we consider the equations (8) and (9). We remark that the coefficients of each of these equations are completely zero on one connected component of $G^{(2)}$. With the notation used in (8) and (9), this can w.l.o.g. be expressed as

$$(22a) \quad V_{II} \times \{0\} \cup V_I \times \{1\} \subseteq K_0,$$

$$(22b) \quad V_I \times \{0\} \cup V_{II} \times \{1\} \subseteq K_1.$$

Since $(V_{II} \times \{0\} \cup V_I \times \{1\}) \cup (V_I \times \{0\} \cup V_{II} \times \{1\}) = V^{(2)}$, the " \subseteq " in (22a) and (22b) can be replaced by " $=$ ".

With $K_{X;1} \cup K_{X;2} \subseteq K_1 = V_I \times \{0\} \cup V_{II} \times \{1\}$, subtraction of $\tilde{b}_{K_{X;2}} \cdot (8)$ from (21) yields an inequality of the form (15) which reads

$$(23) \quad \hat{b}_{K_{X;1}} \sum_{(v,s) \in V_L \cap K_{X;1}} x_v^s \leq -\hat{b}_{K_{X;1}} \sum_{(w,t) \in V_R \cap K_{X;1}} x_w^t$$

with coefficients $\hat{b}_{K_{X;1}} = \tilde{b}_{K_{X;1}} - \tilde{b}_{K_{X;2}}$. The coefficients on $K_{X;2}$ are zero, and the coefficients on $K_{X;0}$ remain zero, since $K_{X;0}$ is not affected by (8). In other words, (15) has nonzero coefficients only in $K_{X;1}$.

- (ii) In the case that G is non-bipartite, the root graph G_X consists of two connected components $K_{X;0}$ and $K_{X;1}$. For the transformation of (12) we have the two equations (6) and (7) at our disposal. Using the assumption $V_L \subseteq V \times \{0\}$ and $V_R \subseteq V \times \{1\}$ we subtract $(b_{K_{X;0}} \cdot ((6) - (7)))$ from (12). This yields an inequality of the form (15) whose coefficients are zero on $K_{X;0}$ and $\pm \hat{b}_{K_{X;1}}$ on $K_{X;1}$, where $\hat{b}_{K_{X;1}} = b_{K_{X;1}} - b_{K_{X;0}}$.

□

Now we have all prerequisites to prove Theorem 3.13.

Proof of Theorem 3.13. Given a facet-defining inequality for $P^{(2)}$, Lemmata 3.14, 3.15, 3.16, and 3.17 provide a transformation into an equivalent inequality (15) with nonzero coefficients on exactly one connected component of its root graph (w.l.o.g. $K_{X;1}$).

We scale (15) by $\hat{b}_{K_{X;1}}$ and obtain an inequality

$$(24) \quad \sum_{(v,s) \in V_L \cap K_{X;1}} x_v^s \leq \sum_{(w,t) \in V_R \cap K_{X;1}} x_w^t.$$

It remains to show that (24) has the form of an SAW-2 inequality. In particular, we have to show that

$$\forall (v,s) \in V_L \cap K_{X;1} : \delta_{G^{(2)}}((v,s)) \subseteq V_R \cap K_{X;1}.$$

Consider $(v,s) \in V_L \cap K_{X;1}$. Assume there exists $(w,t) \in \delta_{G^{(2)}}((v,s))$ with $(w,t) \notin V_R \cap K_{X;1}$. Then the SAW-2 conformation defined by the edge $e = \{(v,s), (w,t)\} \in E^{(2)}$ violates (24). However, this is a contradiction to the assumption that (24) defines a facet of $P^{(2)}$ which in particular has to be valid for all vertices of $P^{(2)}$.

□

4. SUBMONOTONE SAW- n POLYTOPES

In this section, we explore the down-monotonization of the SAW- n polytopes $P^{(n)}$ yielding the *submonotone SAW- n polytopes* $P^{(n;\leq)}$. For these, we derive a class of valid inequalities, and for a subclass we prove facet property.

Definition 4.1. Let $G = (V, E)$ be a graph and $P^{(n)}$ the corresponding SAW- n polytope. The down-monotonization of $P^{(n)}$ is given by

$$P^{(n;\leq)} = \left\{ y \in \mathbb{R}^{|V^{(n)}|} \mid \exists x \in P^{(n)} : 0 \leq y \leq x \right\}.$$

We remark that $P^{(n;\leq)}$ is a polytope again. In the following, we refer to it as the *submonotone SAW- n polytope*.

4.1. Vertices. We provide a description of $P^{(n;\leq)}$ as the convex hull of its vertices. To this end, we consider the set of all SAW- n sub-conformations which contains all SAW- n conformations and all subsets of $V^{(n)}$ that can be extended to SAW- n conformations.

Definition 4.2. Let $G = (V, E)$ be a graph and $G^{(n)}$ the corresponding SAW- n graph.

a) An SAW- n sub-conformation in $G^{(n)}$ is a set

$$\zeta \subseteq V^{(n)} \quad \text{with} \quad \exists \psi \in \Psi_G^{(n)} : \zeta \subseteq \psi.$$

b) We denote the set of all SAW- n sub-conformations in $G^{(n)}$ with $\Psi_G^{(n;\leq)}$.

c) For an SAW- n sub-conformation $\zeta \in \Psi_G^{(n;\leq)}$ in $G^{(n)}$, the corresponding SAW- n subvector is given by the incidence vector $\chi^\zeta \in \{0, 1\}^{|V^{(n)}|}$.

d) We denote the set of SAW- n subvectors in $G^{(n)}$ with $X_G^{(n;\leq)} = \{\chi^\zeta \mid \zeta \in \Psi_G^{(n;\leq)}\}$.

It can be shown that the submonotone SAW- n polytope is the convex hull of all SAW- n subvectors in $G^{(n)}$, i.e.,

$$P^{(n;\leq)} = \text{conv}(X_G^{(n;\leq)}).$$

The proof for this statement can be found in [16]. According to the results of Balas and Fischetti [5], the submonotone SAW- n polytope is full-dimensional, i.e., its dimension is

$$\dim(P^{(n;\leq)}) = |V^{(n)}|.$$

4.2. Valid and Facet-Defining Inequalities. We first remark that according to the results in [5], the nonnegativity constraints

$$(25) \quad x_v^s \geq 0 \quad \forall (v, s) \in V^{(n)}$$

are valid and facet-defining for $P^{(n;\leq)}$. A further consequence from [5] is the nonnegativity of the coefficients of any facet-defining inequality for $P^{(n;\leq)}$.

In order to describe valid inequalities for $P^{(n;\leq)}$, we introduce the following notation.

Definition 4.3. Let G be a graph, $G^{(n)}$ the corresponding SAW- n graph, $\alpha \in \{1, \dots, n-1\}$, and (V_0, \dots, V_α) a partition of $V^{(n)}$. An inequality of the form

$$(26) \quad \sum_{a=1}^{\alpha} a \cdot \sum_{(v,s) \in V_a} x_v^s \leq \alpha$$

which is valid for $P^{(n;\leq)}$ is called a *submonotone SAW- n inequality with right-hand side α* . In this case, we call (V_0, \dots, V_α) a *valid partition of $V^{(n)}$* .

In the following, we investigate criteria required for a submonotone SAW- n inequality (26) to define a facet of $P^{(n;\leq)}$. First, we recall that, according to Theorem 2.2, the SAW- n graph $G^{(n)}$ is connected for non-bipartite graphs G , and it consists of two connected components if G is bipartite. For the upcoming considerations, we introduce a terminology which enables a uniform approach to the problem of stating criteria concerning the facet property of an inequality (26) both for bipartite

and non-bipartite graphs G . For the former case, we have the following statement for which a proof can be found in [16].

Remark 4.4. *Let $G = (V, E)$ be a bipartite graph and $G^{(k)}$ the corresponding SAW- n graph. Denote the vertex sets inducing the two connected components of $G^{(n)}$ by $V_I^{(n)}$ and $V_{II}^{(n)}$. Then each SAW- n conformation in $G^{(n)}$ is entirely included in one of the connected components $G_I^{(n)}$ or $G_{II}^{(n)}$, i.e.,*

$$\forall \psi \in \Psi_G^{(n)} : \psi \cap V_I^{(n)} \neq \emptyset \Leftrightarrow \psi \cap V_{II}^{(n)} = \emptyset.$$

Obviously, the above statement holds analogously when for substituting the term ‘‘SAW- n conformation’’ by ‘‘SAW- n sub-conformation’’. This fact leads to the following definition of *restrictions* of the set of SAW- n conformations and the set of SAW- n sub-conformations, respectively, to the connected components of $G^{(n)}$.

Definition 4.5. *Let G be a bipartite graph and $R \in \{I, II\}$. Then we call the set*

$$\Psi_{G_R}^{(n)} = \left\{ \psi \in \Psi_G^{(n)} \mid \psi \cap V_R^{(n)} \neq \emptyset \right\}$$

the restriction of $\Psi_G^{(n)}$ to $G_R^{(n)}$. Analogously, we define the restriction of $\Psi_G^{(n, \leq)}$ to $G_R^{(n)}$ as

$$\Psi_{G_R}^{(n, \leq)} = \left\{ \zeta \in \Psi_G^{(n, \leq)} \mid \zeta \cap V_R^{(n)} \neq \emptyset \right\}.$$

The restrictions of the set of SAW- n (sub-) conformations define two polytopes.

Definition 4.6. *Let G be a bipartite graph, $G^{(n)}$ the corresponding SAW- n graph consisting of the connected components $G_I^{(n)}$ and $G_{II}^{(n)}$, and $R \in \{I, II\}$. We define*

a) *the reduced SAW- n polytope with respect to $G_R^{(n)}$ as*

$$P_R^{(n)} = \text{conv} \left\{ \chi^\psi \mid \psi \in \Psi_{G_R}^{(n)} \right\},$$

and

b) *the reduced submonotone SAW- n polytope with respect to $G_R^{(n)}$ as*

$$P_R^{(n, \leq)} = \text{conv} \left\{ \chi^\zeta \mid \zeta \in \Psi_{G_R}^{(n, \leq)} \right\}.$$

Next, we introduce a decomposition of a submonotone SAW- n inequality with respect to the connected components of $G^{(n)}$. First, we consider bipartite graphs G (for which $G^{(n)}$ consists of two connected components).

Definition 4.7. *Let G be a bipartite graph and $G^{(n)}$ the corresponding SAW- n graph. Let further (26) be a submonotone SAW- n inequality with $\alpha \in \{1, \dots, n-1\}$ and a corresponding valid partition (V_0, \dots, V_α) of $V^{(n)}$. For $R \in \{I, II\}$ we call the inequality*

$$(27) \quad \sum_{a=1}^{\alpha} a \cdot \sum_{(v,s) \in V_a \cap V_R^{(n)}} x_v^s \leq \alpha$$

the restriction of the submonotone SAW- n inequality (26) to $G_R^{(n)}$.

For a non-bipartite graph G with corresponding SAW- n graph $G^{(n)}$, we set $G_R^{(n)} = G^{(n)}$ and accordingly $V_R^{(n)} = V^{(n)}$.

In the following, we show that the decision whether a submonotone SAW- n inequality (26) is facet-defining for $P^{(n, \leq)}$ can be reduced to the separate examination of its restrictions. First of all, we observe that each restriction of a submonotone SAW- n inequality is valid for $P^{(n, \leq)}$.

The following theorem relates the property of being facet-defining from a submonotone SAW- n inequality to its restrictions.

Theorem 4.8. *Let G be a graph and $G^{(n)}$ the corresponding SAW- n graph. A submonotone SAW- n inequality (26) with $\alpha \in \{1, \dots, n-1\}$ and a valid partition (V_0, \dots, V_α) of $V^{(n)}$ is facet-defining for $P^{(n;\leq)}$ if and only if each of its restrictions (27) is facet-defining for the associated reduced submonotone SAW- n polytope $P_R^{(n;\leq)}$.*

Proof. For $R \in \{I, II\}$ and $x \in \{0, 1\}^{|V^{(n)}|}$, we set

$$f_R(x) = \sum_{a=1}^{\alpha} a \cdot \sum_{(v,s) \in V_a \cap V_R^{(n)}} x_v^s.$$

Then (26) can be written as

$$(28) \quad f_I(x) + f_{II}(x) \leq \alpha,$$

and its restrictions (27) as

$$(29) \quad f_R(x) \leq \alpha, \quad R \in \{I, II\}.$$

Furthermore, we denote by Φ the set of SAW- n root sub-conformations of (28) and by $F_\Phi = \text{eq}(P^{(n;\leq)}; (28)) \cap X_G^{(n;\leq)}$ the set of corresponding SAW- n subvectors. Analogously, we denote by Φ_R the set of SAW- n root sub-conformations of (29) and by $F_{\Phi_R} = \text{eq}(P_R^{(n;\leq)}; (29)) \cap X_{G_R}^{(n;\leq)}$ the set of corresponding SAW- n subvectors.

" \Leftarrow ": Assume that w.l.o.g. restriction (29) for $R = I$ is not facet-defining for $P_I^{(n;\leq)}$. Then F_{Φ_I} is contained in a facet of $P_I^{(n;\leq)}$ which is defined by the equation $g_I(x) = \alpha$ where g_I is linearly independent from f_I . (Note that we can assume that the right-hand side of the equation is α after appropriate scaling of its coefficients.) For $\zeta \in \Phi_I$, according to Remark 4.4, $\zeta \cap V_{II}^{(n)} = \emptyset$ which implies that $f_{II}(\chi^\zeta) = 0$ and hence the incidence vector \bar{x} of ζ in $\{0, 1\}^{|V^{(n)}|}$ is a root of (28), i.e.,

$$f_I(\bar{x}) + f_{II}(\bar{x}) = \alpha.$$

Thus f_I can be substituted by g_I in (28), and the equality

$$g_I(\bar{x}) + f_{II}(\bar{x}) = \alpha$$

holds. This, however, means that the set F_Φ is contained in a face of $P^{(n;\leq)}$ induced by the inequality

$$g_I(x) + f_{II}(x) \leq \alpha,$$

and consequently, (28) cannot be facet-defining for $P^{(n;\leq)}$.

" \Rightarrow ": Let (29) be facet-defining inequalities for $P_I^{(n;\leq)}$ and $P_{II}^{(n;\leq)}$, respectively. Let Φ and F_Φ as introduced above describe the set of roots of (28). Now consider a generic hyperplane

$$(30) \quad F = \left\{ x \in \mathbb{R}^{|V^{(n)}|} \mid \sum_{(v,s) \in V^{(n)}} b_v^s x_v^s = \beta \right\}$$

containing F_Φ . Since for each $\zeta \in \Phi$ there exists $R \in \{I, II\}$ with $\zeta \in \Phi_R$, we have $\dim(\Phi) = \dim(\Phi_I) + \dim(\Phi_{II}) = n$ which means that (28) is facet-defining for $P^{(n;\leq)}$.

Since F_{Φ_R} is contained in the facet of $P_R^{(n;\leq)}$ induced by the inequality $f_R(x) \leq \alpha$, for $(v, s) \in V_R^{(n)}$ the coefficients b_v^s in (30) are determined by the coefficients of this facet-defining inequality. \square

In the following, we prove certain facet criteria for restrictions (27) of submonotone SAW- n inequalities for the special cases $\alpha = 1$ and $\alpha = 2$. We start with $\alpha = 1$.

For the characterization of the facet property of those inequalities of the form (27) with $\alpha = 1$, we introduce a generalization of stable sets. Whereas a stable set in G is a set of vertices with the property that each edge of G is incident to at most one of its elements, we generalize this term for SAW- n conformations in $G^{(n)}$ in the following way:

Definition 4.9. Let G be a graph and $V_R^{(n)}$ the vertex set inducing the connected component $G_R^{(n)}$ of its SAW- n graph. A set $Z \subseteq V_R^{(n)}$ is called an **SAW- n stable set** in $G_R^{(n)}$ if each SAW- n conformation in $G_R^{(n)}$ contains at most one of its elements, i.e.,

$$\forall \psi \in \Psi_{G_R^{(n)}}^{(n)} : |Z \cap \psi| \leq 1.$$

We denote the set of all SAW- n stable sets in $G_R^{(n)}$ by $\mathcal{S}_{G_R^{(n)}}$.

The term of SAW- n stable sets can be used for a characterization of the facet property of an inequality (27) in the case $\alpha = 1$.

Theorem 4.10. Let G be a graph and $V_R^{(n)}$ the vertex set inducing the connected component $G_R^{(n)}$ of its SAW- n graph. Let further $Z \in \mathcal{S}_{G_R^{(n)}}$ be an SAW- n stable set in $G_R^{(n)}$. Then the inequality

$$(31) \quad \sum_{(v,s) \in Z} x_v^s \leq 1$$

is facet-defining for $P_R^{(n;\leq)}$ if and only if the set Z is maximal with respect to vertex inclusion.

Applied to (27) with $\alpha = 1$, the theorem states that (27) is facet-defining for $P_R^{(n;\leq)}$ if and only if $V_1 \cap V_R^{(n)}$ (which is the only set occurring in the sum) is an SAW- n stable set in $G_R^{(n)}$.

Proof. Let $(v, s) \in Z$, and set

$$\Psi[(v, s)] = \{\zeta \in \Psi_{G_R^{(n)}}^{(n;\leq)} \mid (v, s) \in \zeta\}.$$

To ensure the validity of (31), any $\zeta \in \Psi[(v, s)]$ must not contain any further element $(w, t) \in Z$. This is true since

$$\begin{aligned} & \forall \zeta \in \Psi[(v, s)] \forall (w, t) \in \zeta \setminus \{(v, s)\} : (w, t) \notin Z \\ \Leftrightarrow & \zeta \cap Z = \{(v, s)\} \\ \Leftrightarrow & |\zeta \cap Z| = 1 \leq 1. \end{aligned}$$

Next, we show the facet property of (31) for $P_R^{(n;\leq)}$. Let thus $Z \in \mathcal{S}_{G_R^{(n)}}$ be a maximal SAW- n stable set in $G_R^{(n)}$ defining the submonotone SAW- n inequality (31) and $F_Z = \text{eq}(P_R^{(n;\leq)}; (31))$. We consider a generic hyperplane

$$(32) \quad F_{b,\beta} = \left\{ x \in \mathbb{R}^{|V_R^{(n)}|} \mid \sum_{(v,s) \in V_R^{(n)}} b_v^s x_v^s = \beta \right\}$$

with $F_Z \subseteq F_{b,\beta}$. The coefficients b_v^s are nonnegative for $(v, s) \in V_R^{(n)}$. For $(v, s) \in Z$, consider the SAW- n sub-conformation $\{(v, s)\} \subseteq Z$. The corresponding SAW- n subvector $\chi^{\{(v,s)\}}$ is an element of F_Z , and consequently $\chi^{\{(v,s)\}} \in F_{b,\beta}$. It follows that $b_v^s = \beta$. For each $(w, t) \notin Z$ there is an SAW- n conformation $\psi \in \Psi_{G_R^{(n)}}^{(n)}$ such that $\psi \cap Z \neq \emptyset$ and $(w, t) \in \psi$ (otherwise, (w, t) could be added to Z which is a contradiction to the maximality of Z). Now consider an SAW- n sub-conformation ζ in $G_R^{(n)}$ containing both $(v, s) \in Z$ and $(w, t) \in V_R^{(n)} \setminus Z$ and the corresponding SAW- n subvector $\chi^{\{(v,s),(w,t)\}}$ which is an element of F_Z . Application of (32) on the difference $\chi^{\{(v,s),(w,t)\}} - \chi^{\{(v,s)\}}$ yields

$$\begin{aligned} 0 &= \langle b, \chi^{\{(v,s),(w,t)\}} \rangle - \langle b, \chi^{\{(v,s)\}} \rangle \\ &= \langle b, \chi^{\{(v,s),(w,t)\}} - \chi^{\{(v,s)\}} \rangle \\ &= \langle b, \chi^{\{(w,t)\}} \rangle = b_w^t. \end{aligned}$$

Consequently, $b_w^t = 0$ which means that the (generic) facet-defining inequality

$$(33) \quad \sum_{(v,s) \in Z} b_v^s x_v^s \leq \beta$$

is a positive multiple of (31), which is therefore facet-defining for $P_R^{(n;\leq)}$.

It remains to show that (31) is not facet-defining for non-maximal $Z \in \mathcal{S}_{G_R^{(n)}}$. Let thus $\tilde{Z} \in \mathcal{S}_{G_R^{(n)}}$ be a non-maximal SAW- n stable set in $G_R^{(n)}$ and

$$(34) \quad \sum_{(v,s) \in \tilde{Z}} x_v^s \leq 1$$

the corresponding submonotone SAW- n inequality. Now consider a maximal SAW- n stable set $Z \in \mathcal{S}_{G_R^{(n)}}$ with $\tilde{Z} \subset Z$ and the corresponding submonotone SAW- n inequality

$$(35) \quad \sum_{(v,s) \in Z} x_v^s \leq 1.$$

As shown above, (35) is facet-defining for $P_R^{(n;\leq)}$. However, addition of the nonnegativity constraints

$$-x_v^s \leq 0 \quad \text{for } (v,s) \in Z \setminus \tilde{Z}$$

to (35) yields (34), which consequently cannot be facet-defining for $P_R^{(n;\leq)}$. \square

Example 4.11. Consider the submonotone SAW-3 inequality

$$x_0^1 + x_1^1 + x_3^1 + x_5^0 + x_5^2 + x_6^1 + x_8^0 + x_8^2 \leq 1$$

on the 3×3 square lattice $G = Q_{3 \times 3}$. Its restrictions to the connected components $G_I^{(3)}$ and $G_{II}^{(3)}$, respectively, read

$$\begin{aligned} x_1^1 + x_3^1 + x_8^0 + x_8^2 &\leq 1, \\ x_0^1 + x_5^0 + x_5^2 + x_6^1 &\leq 1. \end{aligned}$$

Figure 5 shows the SAW-3 graph with the vertices constituting the support of the inequality colored in light gray. For both restrictions, the supporting vertices in $V_R^{(3)}$ constitute a maximum SAW-3 stable set in the respective graph $G_R^{(3)}$. Consequently, both restrictions are facet-defining for the respective polytopes $P_R^{(3;\leq)}$, and according to Theorem 4.8, the entire inequality is facet-defining for $P^{(3;\leq)}$.

Let us now discuss the case $\alpha = 2$. We consider submonotone SAW- n inequalities of the form

$$(36) \quad \sum_{(v,s) \in V_1} x_v^s + 2 \cdot \sum_{(v,s) \in V_2} x_v^s \leq 2$$

with appropriate subsets $V_1, V_2 \subseteq V^{(n)}$. For the investigation of the facet property of a submonotone SAW- n inequality (36), we consider a restriction of (36) and set

$$W_1 = V_1 \cap V_R^{(n)}, \quad W_2 = V_2 \cap V_R^{(n)}.$$

Hence we consider the inequality

$$(37) \quad \sum_{(v,s) \in W_1} x_v^s + 2 \cdot \sum_{(v,s) \in W_2} x_v^s \leq 2.$$

In the following, we state some facet criteria for (37). First, we observe that the distribution of coefficients occurring in (37) can appear in two cases. In the case $W_1 = \emptyset$, i.e., all coefficients have value 2, we consider inequalities of the form

$$(38) \quad 2 \cdot \sum_{(v,s) \in W_2} x_v^s \leq 2.$$

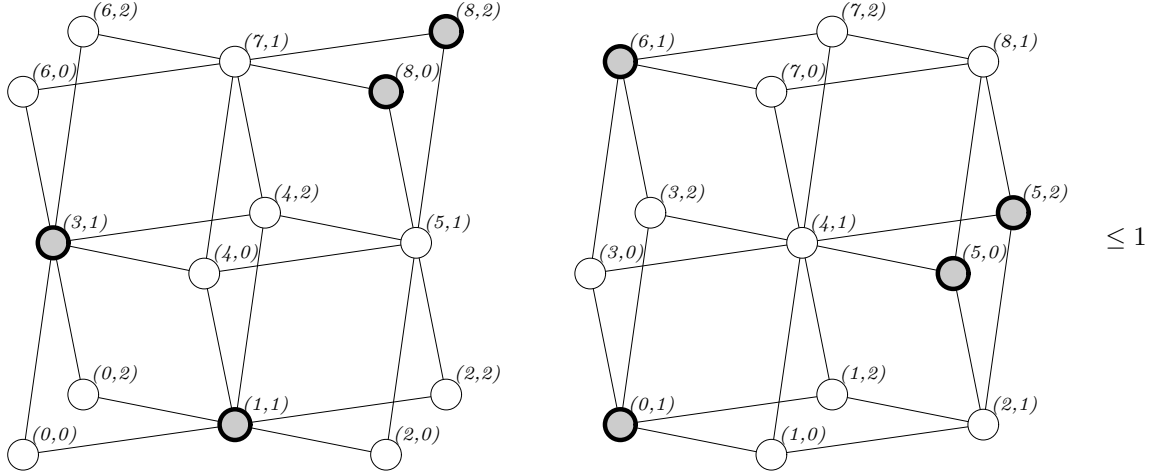


FIGURE 5. Example of a facet-defining submonotone SAW-3 inequality for $P^{(3;\leq)}$

which, after re-scaling, are equivalent to inequalities with right-hand side $\alpha = 1$. As a consequence of Theorem 4.10 we derive that (38) is facet-defining for $P_R^{(n;\leq)}$ if and only if W_2 is a maximal SAW- n stable set in $G_R^{(n)}$.

Next, we turn to the more complicated case $W_1 \neq \emptyset$ where we consider inequalities of the form

$$(39) \quad \sum_{(v,s) \in W_1} x_v^s + 2 \cdot \sum_{(v,s) \in W_2} x_v^s \leq 2.$$

We define the graph

$$H_{W_1}^{(n)} := (W_1, E_1)$$

$$\text{with } E_1 = \left\{ \{(v,s), (w,t)\} \subseteq W_1 \mid \exists \psi \in \Psi_{G_R^{(n)}}^{(n)} : \{(v,s), (w,t)\} \subseteq \psi \right\}.$$

A first necessary condition for W_1 and W_2 to define a facet-defining inequality for $P_R^{(n;\leq)}$ is a maximality condition which we specify below.

Definition 4.12. Let $W_1, W_2 \subseteq V_R^{(n)}$ such that (39) is valid for $P_R^{(n;\leq)}$. We denote (W_1, W_2) as maximal in $G_R^{(n)}$ if any of the following operations on (W_1, W_2) makes (39) invalid for $P_R^{(n;\leq)}$.

- (i) Addition of an element $(v,s) \in V_R^{(n)} \setminus (W_1 \cup W_2)$ to W_1 , or
- (ii) addition of an element $(v,s) \in V_R^{(n)} \setminus (W_1 \cup W_2)$ to W_2 , or
- (iii) transfer of an element $(v,s) \in W_1$ to W_2 .

Now we can formulate a necessary requirement to the coefficients of an inequality (39) in order to be facet-defining for $P_R^{(n;\leq)}$.

Lemma 4.13. Let (39) be a valid inequality for $P_R^{(n;\leq)}$. If (39) defines a facet of $P_R^{(n;\leq)}$, (W_1, W_2) is maximal in $G_R^{(n)}$.

The proof is basically straightforward and is omitted here. For details, we refer to [16].

The following theorem provides a characterization of facet-defining inequalities for $P_R^{(n;\leq)}$.

Theorem 4.14. Let $G = (V, E)$ be a graph and $G^{(n)}$ the corresponding SAW- n graph. Let further $R \in \{I, II\}$ and $W_1 \subseteq V_R^{(n)}$. An inequality (39) is facet-defining for $P_R^{(n;\leq)}$ if and only if (W_1, W_2) is maximal in $G_R^{(n)}$ and $H_{W_1}^{(n)}$ is both connected and non-bipartite.

Proof. Consider the set

$$F = \left\{ x \in P_R^{(n;\leq)} \mid \sum_{(v,s) \in W_1} x_v^s + 2 \cdot \sum_{(v,s) \in W_2} x_v^s = 2 \right\}$$

of roots of (39) as well as a generic hyperplane

$$(40) \quad F_{b,\beta} = \left\{ x \in \mathbb{R}^{|V_R^{(n)}|} \mid \sum_{(v,s) \in V_R^{(n)}} b_v^s x_v^s = \beta \right\}$$

with $F \subseteq F_{b,\beta}$. Let now (W_1, W_2) be maximal in $G_R^{(n)}$, and $H_{W_1}^{(n)}$ connected and non-bipartite.

First, we consider the coefficients b_v^s for $(v, s) \in W_1$. Due to its non-bipartition, $H_{W_1}^{(n)}$ contains an odd cycle $C = (v_{j_1}, v_{j_2}, \dots, v_{j_{2l+1}}, v_{j_1})$ with $v_{j_k} \in W_1$ for $k \in \{1, \dots, 2l+1\}$. Each of the incidence vectors

$$\chi^{\{v_{j_1}, v_{j_2}\}}, \dots, \chi^{\{v_{j_{2l+1}}, v_{j_1}\}}$$

is a root of (39) and consequently an element of $F_{b,\beta}$. From $\chi^{\{v_{j_i}, v_{j_k}\}} \in F_{b,\beta}$ we derive $b_{v_{j_i}} + b_{v_{j_k}} = \beta$. Then the system of linear equations

$$\begin{array}{rcccc} b_{v_{j_1}} & +b_{v_{j_2}} & & & = \beta \\ & b_{v_{j_2}} & +b_{v_{j_3}} & & = \beta \\ & & \dots & & = \beta \\ & & & b_{v_{j_{2l}}} & +b_{v_{j_{2l+1}}} & = \beta \\ & & & & b_{v_{j_{2l+1}}} & +b_{v_{j_1}} & = \beta \end{array}$$

yields the unique solution $b_{v_{j_i}} = \frac{\beta}{2}$ for $v_{j_i} \in C$.

Now we consider those vertices in W_1 that are not included in an odd cycle in $H_{W_1}^{(n)}$. For this, consider $w \in W_1$ and an odd cycle $C = (v_{j_1}, v_{j_2}, \dots, v_{j_{2l+1}}, v_{j_1})$ in $H_{W_1}^{(n)}$ where $w \notin C$. Since per assumption $H_{W_1}^{(n)}$ is connected, there exists a path p in $H_{W_1}^{(n)}$ connecting w to a vertex $v_{j_i} \in C$. Denote the series of vertices defining p by $w = w_{i_0}, w_{i_1}, \dots, w_{i_k} = v_{j_i}$. Each of the incidence vectors

$$\chi^{\{w_{i_0}, w_{i_1}\}}, \dots, \chi^{\{w_{i_{k-1}}, w_{i_k} = v_{j_i}\}}$$

is a root of (39) and consequently an element of $F_{b,\beta}$. From $\chi^{\{w_{i_{k-1}}, v_{j_i}\}} \in F_{b,\beta}$, we get $b_{w_{i_{k-1}}} = \frac{\beta}{2}$, and recursively $b_{w_{i_{k-1}}} = b_{w_{i_{k-2}}} = \dots = b_w = \frac{\beta}{2}$. With this, we have

$$b_v^s = \frac{\beta}{2} \quad \text{for all } (v, s) \in W_1.$$

Next, let $(v, s) \in W_2$. Then the incidence vector χ^ζ of the SAW- n sub-conformation $\zeta = \{(v, s)\}$ is a root of (39) and hence contained in $F_{b,\beta}$. Consequently,

$$b_v^s = \beta \quad \text{for all } (v, s) \in W_2.$$

Finally, consider $(v, s) \in V_R^{(n)} \setminus (W_1 \cup W_2)$. Since (W_1, W_2) is maximal in $G_R^{(n)}$, there exists at least one SAW- n sub-conformation $\zeta \in \Psi_{G_R^{(n)}}^{(n;\leq)}$ containing (v, s) which fulfills one of the following conditions:

- (i) ζ contains two elements $(w_1, t_1), (w_2, t_2) \in W_1$, i.e., $\langle \chi^\zeta, \chi^{W_1} \rangle = 2$. Now consider the SAW- n sub-conformations $\zeta_1 = \{(w_1, t_1), (w_2, t_2)\}$ and $\zeta_2 = \{(v, s), (w_1, t_1), (w_2, t_2)\}$ which are both contained in ζ and whose incidence vectors both are roots of (39) and are hence contained in $F_{b,\beta}$. Thus we obtain

$$\langle b, \chi^{\zeta_1} \rangle = \beta = \langle b, \chi^{\zeta_2} \rangle,$$

which implies

$$\begin{aligned}
b_v^s &= \langle b, \chi^{\{(v,s)\}} \rangle \\
&= \langle b, \chi^{\zeta_2 \setminus \zeta_1} \rangle \\
&= \langle b, \chi^{\zeta_2} \rangle - \langle b, \chi^{\zeta_1} \rangle \\
&= 0.
\end{aligned}$$

- (ii) ζ contains one element $(w, t) \in W_2$, i.e., $\langle \chi^\zeta, \chi^{W_2} \rangle = 1$. Now consider the SAW- n sub-conformations $\zeta_1 = \{(w, t)\}$ and $\zeta_2 = \{(v, s), (w, t)\}$ which are both contained in ζ and whose incidence vectors both are roots of (39) and are hence contained in $F_{b,\beta}$. Thus we obtain

$$\langle b, \chi^{\zeta_1} \rangle = \beta = \langle b, \chi^{\zeta_2} \rangle,$$

which implies

$$\begin{aligned}
b_v^s &= \langle b, \chi^{\{(v,s)\}} \rangle \\
&= \langle b, \chi^{\zeta_2 \setminus \zeta_1} \rangle \\
&= \langle b, \chi^{\zeta_2} \rangle - \langle b, \chi^{\zeta_1} \rangle \\
&= 0.
\end{aligned}$$

Consequently, we have

$$b_v^s = 0 \quad \text{for all } (v, s) \in V_R^{(n)} \setminus (W_1 \cup W_2).$$

Altogether, we have shown that (39) is a positive multiple of the equation defining the generic hyperplane (40) and is therefore facet-defining for $P_R^{(n;\leq)}$.

It remains to show that (39) cannot be a facet-defining inequality for $P_R^{(n;\leq)}$ if $H_{W_1}^{(n)}$ is not connected or bipartite. First, assume $H_{W_1}^{(n)}$ is bipartite with vertex partition $W_1 = W_1^I \dot{\cup} W_1^{II}$, and consider the inequalities

$$(41a) \quad \sum_{(v,s) \in W_1^I} x_v^s \leq 1 \quad \text{and}$$

$$(41b) \quad \sum_{(v,s) \in W_1^{II}} x_v^s \leq 1.$$

Due to the bipartition of $H_{W_1}^{(n)}$, both W_1^I and W_1^{II} are stable sets in $H_{W_1}^{(n)}$ which implies that they are SAW- n stable sets in $G_R^{(n)}$. (Note that they need not be maximal, even though W_1 is maximal; Example 4.16 shows such an instance.) Consequently, both (41a) and (41b) are valid for $P_R^{(n;\leq)}$, and since (39) is their sum, it cannot be a facet-defining inequality for $P_R^{(n;\leq)}$.

Next, assume $H_{W_1}^{(n)}$ is not connected. Then there exists a vertex $z \in V_R^{(n)} \setminus W_1$ whose addition to W_1 would entail the appearance of an edge in $H_{W_1}^{(n)}$ joining two or more connected components of $H_{W_1}^{(n)}$. We denote the set of all such vertices in $H_{W_1}^{(n)}$ by Z_{W_1} . (Note that the inequality $\sum_{(v,s) \in W_1 \cup Z_{W_1}} x_v^s \leq 2$ is invalid for $P_R^{(n;\leq)}$.) Then each root of (39) also fulfills the equation

$$\sum_{(v,s) \in Z_{W_1}} x_v^s = 0,$$

which means that (39) cannot be facet-defining for $P_R^{(n;\leq)}$. \square

Below, the statements of Theorems 4.8 and 4.14 are illustrated by a couple of examples. We start with an example of a facet-defining inequality for the submonotone SAW-3 polytope on the 3×3 square lattice $G = Q_{3 \times 3}$.

Example 4.15. Consider the submonotone SAW-3 inequality

$$(42) \quad 2x_0^1 + x_2^0 + 2x_2^1 + x_2^2 + x_3^1 + x_4^0 + 2x_4^1 + x_4^2 + 2x_6^1 + x_8^0 + 2x_8^1 + x_8^2 \leq 2$$

on the 3×3 square lattice $G = Q_{3 \times 3}$. Its restrictions to the connected components of $G^{(3)}$ read

$$(43a) \quad f_I(x) = x_2^0 + x_2^2 + x_3^1 + x_4^0 + x_4^2 + x_8^0 + x_8^2 \leq 2 \quad \text{and}$$

$$(43b) \quad f_{II}(x) = 2x_0^1 + 2x_2^1 + 2x_4^1 + 2x_6^1 + 2x_8^1 \leq 2.$$

The coefficients of the restriction (43a) of (42) to $G_I^{(3)}$ are uniformly one ($W_2 = \emptyset$), and those of the restriction (43b) to $G_{II}^{(3)}$ are uniformly two ($W_1 = \emptyset$). Figure 6 shows the SAW-3 graph $G^{(3)}$ where the vertices of W_1 are colored in light gray, and the vertices of W_2 in dark gray. For the restriction to $G_I^{(3)}$, furthermore the corresponding graph $H^{(3)}$ is shown.

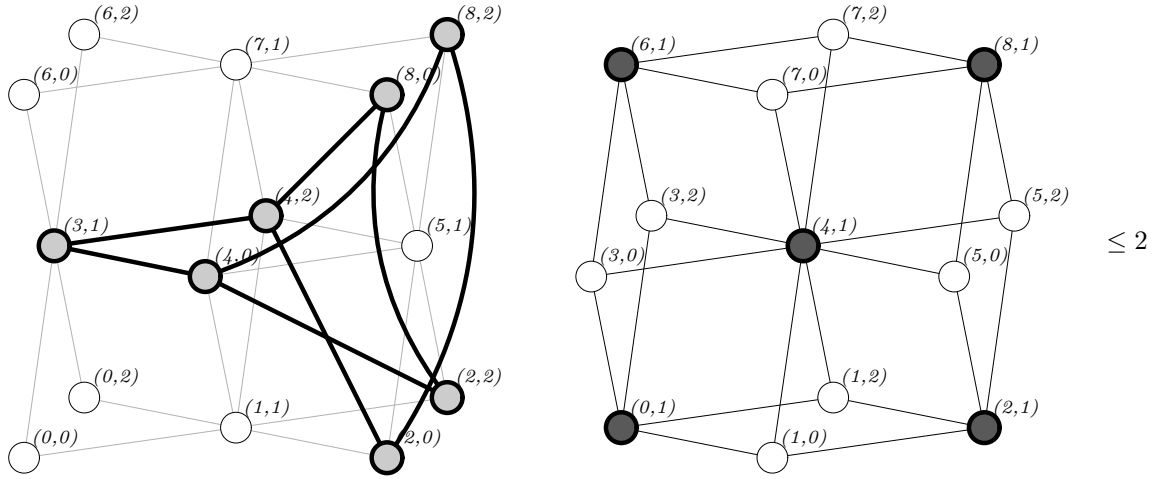


FIGURE 6. Example of a facet-defining submonotone SAW-3 inequality for $P^{(3;\leq)}$ with $H^{(3)}$ for both connected components of $G^{(3)}$

The restriction (43a) to $G_I^{(3)}$ is facet-defining for $P_I^{(3;\leq)}$, since (W_1, W_2) is maximal in $G_I^{(3)}$, and $H^{(3)}$ is both connected and non-bipartite.

Now consider restriction (43b) to $G_{II}^{(3)}$ which can be scaled by two and then reads

$$(44) \quad x_0^1 + x_2^1 + x_4^1 + x_6^1 + x_8^1 \leq 1.$$

This is a submonotone SAW-3 inequality with right-hand side $\alpha = 1$. The vertices defining its support constitute a maximum SAW-3 stable set in $G_{II}^{(3)}$. Hence, according to Theorem 4.10, the inequality (43b) is facet-defining for $P_{II}^{(3;\leq)}$. Thus both restrictions of (42) are facet-defining for the respective reduced polytopes, and hence, according to Theorem 4.8, (42) defines a facet of $P^{(3;\leq)}$.

The next example documents an instance of a submonotone SAW-3 inequality on the 3×3 square lattice $G = Q_{3 \times 3}$ which is not facet-defining for $P^{(3;\leq)}$ since $H_{W_1}^{(3)}$ is bipartite.

Example 4.16. Consider the inequality

$$(45) \quad f_I(x) + f_{II}(x) \leq 2$$

on the 3×3 square lattice $G = Q_{3 \times 3}$ whose restrictions are given by

$$(46a) \quad f_I(x) = 2x_0^0 + x_2^0 + x_4^0 + x_6^0 + x_8^0 + x_1^1 + x_7^1 \leq 2,$$

$$(46b) \quad f_{II}(x) = x_0^1 + x_1^1 + x_2^1 + x_3^0 + x_4^1 + x_5^0 + x_6^1 + x_7^0 + x_8^1 \leq 2.$$

Figure 7 shows the inequality (45) together with the corresponding graphs $H_{W_1}^{(3)}$ for both of its restrictions. First, consider the restriction (46a) to $G_I^{(3)}$. There we have

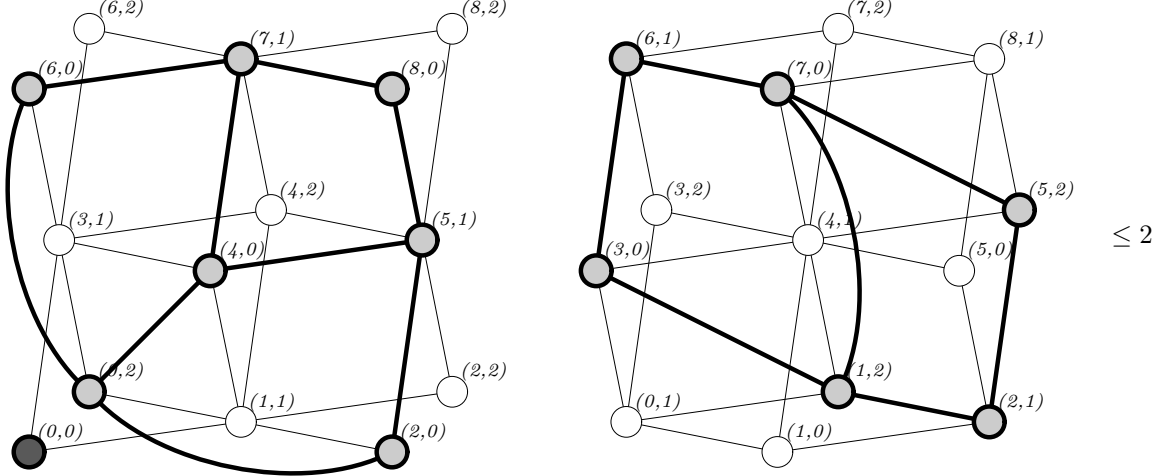


FIGURE 7. Example of a non-facet-defining inequality for $P_I^{(3;\leq)}$

$$W_1 = \{(0, 2), (2, 0), (4, 0), (5, 1), (6, 0), (7, 1), (8, 0)\} \quad \text{and}$$

$$W_2 = \{(0, 0)\}.$$

In the present case, (W_1, W_2) is maximal in $G_I^{(3)}$. Furthermore, the corresponding graph $H_{W_1}^{(3)}$ is connected. However, $H_{W_1}^{(3)}$ is bipartite with vertex partition $W_1 = W_1^I \dot{\cup} W_1^{II}$ where $W_1^I = \{(0, 2), (5, 1), (7, 1)\}$ and $W_1^{II} = \{(2, 0), (4, 0), (6, 0), (8, 0)\}$. Hence (46a) has a representation as the sum of the two inequalities

$$\begin{aligned} x_0^0 + x_2^0 + x_5^1 + x_7^1 &\leq 1 \quad \text{and} \\ x_0^0 + x_2^0 + x_4^0 + x_6^0 + x_8^0 &\leq 1 \end{aligned}$$

which are both valid for $P_I^{(3;\leq)}$. Hence (46a) cannot be facet-defining for $P_I^{(3;\leq)}$. Consequently, the entire inequality (45) cannot be facet-defining for $P^{(3;\leq)}$ any more, regardless whether (46b) is facet-defining for $P_{II}^{(3;\leq)}$ or not.

Nevertheless let us have a look at the restriction (46b) to $G_{II}^{(3)}$. There we have

$$W_1 = \{(1, 2), (2, 1), (3, 0), (5, 2), (6, 1), (7, 0)\} \quad \text{and}$$

$$W_2 = \emptyset.$$

The corresponding graph $H_{W_1}^{(3)}$ is bipartite with vertex partition $W_1 = W_1^I \dot{\cup} W_1^{II}$ where $W_1^I = \{(1, 2), (5, 2), (6, 1)\}$ and $W_1^{II} = \{(2, 1), (3, 0), (7, 0)\}$. Hence (46b) has a representation as the sum of the two inequalities

$$\begin{aligned} x_1^2 + x_5^2 + x_6^1 &\leq 1 \quad \text{and} \\ x_2^1 + x_3^0 + x_7^0 &\leq 1 \end{aligned}$$

which are both valid for $P_{II}^{(3;\leq)}$. Hence (46b) cannot be facet-defining for $P_{II}^{(3;\leq)}$.

5. COMPUTATIONAL RESULTS

In the previous sections, we studied self-avoiding walks from a polyhedral point of view. In this section, we show how our results can be embedded into a branch-and-cut framework, and we demonstrate the computational benefits of our approach.

The optimization problem at hand is the protein folding problem originating from molecular biology. It is believed that in principle the three-dimensional structure of a protein can be predicted (computed) solely from the sequence of amino acids, taking into account the physical forces between the atoms within the polypeptide and in the solvent. In a quite simple and abstract version, the protein folding problem can be formulated as an optimization problem, where an optimal self-avoiding walk with respect to a certain measure is sought. This approach is due to Dill [14], who named this the HP protein folding model. The about 20 different types of amino acids are grouped into two classes, the hydrophobic (**h**) and the polar (**p**) ones. Furthermore, the model assumes that the folding takes place on a regular lattice graph, such as a two- or three-dimensional square or triangular lattice. Only one type of physical force is considered, namely the attraction between hydrophobic amino acids resulting in a minimization of the contact surface between hydrophobic amino acids and the solvent. In the HP model, two non-adjacent hydrophobic elements are said to form a hydrophobic contact if they occupy adjacent vertices (connected by an edge) in the lattice graph. Folding a protein in this model thus means the computation of a self-avoiding walk that maximizes the number of hydrophobic contacts. This problem is known to be NP-hard [6, 13], hence one cannot expect a polynomial-time algorithm for its solution to proven optimality.

The protein folding problem in the HP model can be translated into a binary linear program. Respective formulations can be found in literature. Chandru, Rao, and Swaminathan [10] describe the set of self-avoiding walks by linear equality and inequality constraints as well as additional integrality conditions on the variables. Further variables and constraints are introduced to count the number of hydrophobic contacts. The objective function to be maximized counts their number. Using this formulation and standard integer programming solvers, global optimal solutions can be found for sequences consisting of up to 11 elements on two-dimensional square lattices. The same formulation is mentioned by Greenberg, Hart, and Lancia [17]. Carr, Hart, and Newman [9] describe improvements to this model by removing symmetries, lifting further variables into the constraints, and by extending the model with a network flow formulation.

We remark that several other approaches to tackle the HP model can be found in literature. Examples include approximation algorithms with a guaranteed solution quality [2, 18, 24, 25], exhaustive enumeration [11, 19, 20, 21, 22], constraint programming [3, 4], and various heuristic approaches [7, 8, 12, 15, 23, 26].

We give a formulation of the HP protein folding model that has also been stated in [17]. Let $\sigma \in \{\mathbf{h}, \mathbf{p}\}^n$ be an HP string of length n and $G = (V, E)$ a lattice graph. We consider this HP string as a self-avoiding walk ω on G . In order to count the number of hydrophobic contacts in ω , we need to introduce an additional binary variable $y_{v,w}$ for each edge $\{v, w\} \in E$. This variable indicates whether hydrophobic (**h**) elements are assigned to both v and w . To this end we introduce the following additional constraints. Denote by $(x_v^s)_{v \in V, s \in S^{(n)}}$ and by $H = \{i \in S^{(n)} : \sigma_i = \mathbf{h}\}$ the subset of hydrophobic elements of σ . The coupling of the y -variables with the x -variables is given by the following constraints which enforce that an edge $\{v, w\} \in E$ holds a hydrophobic contact if and only if on both vertices v and w an element of H is placed:

$$(47a) \quad y_{v,w} \leq \sum_{s \in H} x_v^s,$$

$$(47b) \quad y_{v,w} \leq \sum_{s \in H} x_w^s,$$

$$(47c) \quad \sum_{s \in H} (x_v^s + x_w^s) \leq 1 + y_{v,w}, \quad \forall \{v, w\} \in E.$$

An optimal self-avoiding walk is characterized by a maximal number of hydrophobic contacts. It can be obtained from a solution of the optimization problem

$$(48) \quad \begin{aligned} \max \quad & \sum_{\{v,w\} \in E} y_{v,w} \\ \text{s.t.} \quad & (47a), (47b), (47c), \\ & x \in P^{(n)}, \\ & y \in \{0, 1\}^{|E|}. \end{aligned}$$

In principle, common MIP solvers (such as ILOG CPLEX [1]) can be used to find global optimal solutions. However, even for small instances with HP strings of length about 20, the computing times are tremendous. This behavior is, amongst others, supported by the highly symmetric character of the model which is induced to a great extent by the regularity of the underlying lattice graphs. For this reason, we base our computations on a variant of the original model (48) which takes into account certain symmetries inherent to the model formulation. These symmetries can be broken to a considerable extent by fixing selected HP string elements on adequate lattice vertices. However, this approach is only practicable in cases where the lattice graph is chosen large enough in order to allow at least one potentially optimal solution after the fixation of string elements has been performed. Typically, the two mid elements of the HP string are fixed in the center of the lattice graph. However, the choice of the fixation can have a significant impact on the efficiency of the solution process. For a thorough discussion of this issue, we refer to [16].

In the following, we show how we use our insights into the polytopes $P^{(n)}$ in the form of cutting planes in order to furthermore enhance the solution process. We use a strengthened formulation of (48) by lifting the contiguity constraints (4) as stated in [9]:

$$(49) \quad x_v^{s-1} + x_v^{s+1} \leq \sum_{w \in \delta_G(v)} x_w^s, \quad \forall v \in V, s \in S^{(n)} \setminus \{0, n-1\}.$$

A further strengthening of (48) can be accomplished, in principle, by adding all inequalities defining the facets of the SAW- n polytope. However, even for the smallest length (i.e., $n = 2$) their number is too high to add them all in the beginning. Hence we resort to a cutting plane approach, i.e., we solve the LP relaxation of (48) and then separate over a class of cutting planes which are obtained either from the SAW-2 polytope or the submonotone SAW- k polytope for an appropriate k with $2 \leq k \leq n$. We add violated inequalities, if available, to the root LP relaxation and iterate. If the LP relaxation is still fractional after completion of this cutting plane phase, we continue with a branch-and-bound scheme. The separation of SAW-2 inequalities is done by means of an exact polynomial-time procedure, whereas submonotone SAW- k inequalities are separated by a heuristic polynomial-time routine. For the technical details of the respective cutting plane separation procedures, we refer to [16]. In the sequel, we focus on some issues on the use of cutting planes found.

In order to use an SAW-2 inequality (10) with left-hand side $L \subseteq V^{(2)}$ for a polytope describing SAWs of length $n > 2$, we choose $t \in \{0, \dots, n-2\}$ and consider the inequality

$$(50) \quad \sum_{(v,s) \in L} x_v^{t+s} \leq \sum_{(w,1-s) \in \delta_{G^{(2)}}(L)} x_w^{t+1-s}$$

which we call the *embedding* of (10) into $P^{(n)}$ at position t . A set $T \subseteq \{0, \dots, n-2\}$ of values for t within a cutting plane cycle defines the positions of SAW segments of length two for which a violated SAW-2 inequality is sought. For the choice of T , we identify several possibilities. The most dense one corresponds to the choice of $T = \{0, \dots, n-2\}$ and can be imagined as a covering of the SAW by overlapping segments of length two. For our purposes, we introduce a parameter d_{cut} which describes the distance between two positions at which separation is to be applied, such that $T = \{d_{\text{cut}}j \mid 0 \leq j \leq \lfloor (n-2)/d_{\text{cut}} \rfloor\}$. The overlapping cover described before is then given by $d_{\text{cut}} = 1$. For $d_{\text{cut}} = 2$, we deal with a (non-overlapping) partition of the SAW into segments of length two. For any $d_{\text{cut}} > 2$, we have a distribution of segments of length two leaving some elements uncovered. The value of d_{cut} can be used to control the number of cuts added. This is

relevant since there is a trade-off between a high number of cuts that improve the LP relaxation, and the computing time required to solve it. For our computations, we select the parameter d_{cut} individually for each instance by numerical experiments. In the tables below, we indicate the usage of SAW-2 cuts by “C2”. Eventually, we remark that for any SAW-2 inequality a lifting step can be applied yielding inequalities similar to the lifted contiguity constraints (49). For the computations presented below, we therefore use embeddings of lifted SAW-2 inequalities as cutting planes. For $s = 0$, these inequalities are of the form

$$(51) \quad \sum_{v \in V_L} (x_v^t + x_v^{t+2}) \leq \sum_{w \in \delta_G(V_L)} x_w^{t+1},$$

and for $s = 1$, they read

$$(52) \quad \sum_{v \in V_L} (x_v^{t+1} + x_v^{t-1}) \leq \sum_{w \in \delta_G(V_L)} x_w^t.$$

The embedding of submonotone SAW- k inequalities into $P^{(n)}$ can be accomplished along the lines of the SAW-2 case. Given a submonotone SAW- k inequality (26) and some $t \in \{0, \dots, n - k\}$, we call

$$(53) \quad \sum_{a=1}^{\alpha} a \cdot \sum_{(v,s) \in V_a} x_v^{t+s} \leq \alpha$$

the *embedding* of (26) into $P^{(n)}$ at position t . The parameter d_{cut} is used just as described above. In the tables below, we indicate the usage of submonotone SAW- k cuts by “ S_k ”.

As a first example, we consider the HP string `pphpphpppphpppphpppphh` of length 25 which is taken from [26]. An optimal fold features a compact 3×3 hydrophobic core. The maximum number of hydrophobic contacts thus is 8. We choose the 12×12 square lattice, and we fix the two mid HP string elements in its center. This instance was solved to optimality without addition of SAW-2 and submonotone SAW- k cuts. The computation required 166 branch-and-bound nodes and 90.49 seconds of cpu time. Figure 8 shows the solution. Subsequently, we solved the same

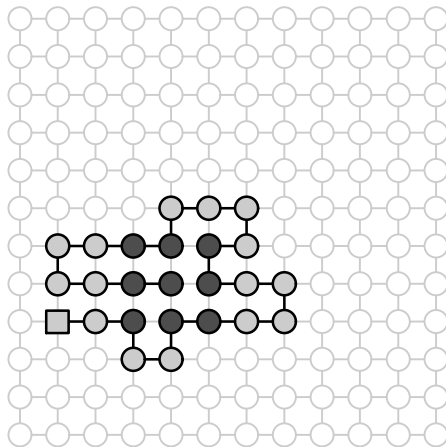


FIGURE 8. Optimal fold for the HP string `pphpphpppphpppphpppphh` on the 12×12 square lattice with the two middle string elements fixed in the center of the lattice

instance including the separation of cutting planes. The results of the computations are listed in Tables 1 and 2. We observe that the choice of the parameters d_{cut} and, where applicable, k , causes a great variation in the number of cuts that have been added. In turn, the number of cuts has a profound impact on the efficiency of the solution process; in particular, too many cuts added cause an increase in the cpu time. This behavior becomes obvious in Table 1. The best result w.r.t

both the number of branch-and-bound nodes and the computing time is achieved with $d_{\text{cut}} = 6$, where 15 SAW-2 cuts have been added. In contrast, with $d_{\text{cut}} = 2$, as many as 313 SAW-2 cuts are added, which causes the computing time to be nearly four times the time needed for the run without cutting plane separation, even though the number of processed branch-and-bound nodes is slightly lower. However, we also observe that with $d_{\text{cut}} = 7$, causing the addition of 8 SAW-2 cuts, the number of branch-and-bound nodes increases significantly, and so does the need for computing time. From these facts, we deduce the necessity of having a criterion for the rating of

cuts	d_{cut}	#cuts	#nodes	cpu time
–	–	0	166	90.49
C2	2	313	121	336.54
C2	3	359	19	259.35
C2	4	58	31	51.66
C2	5	40	44	62.53
C2	6	15	20	34.79
C2	7	8	439	230.49
C2	8	26	114	81.29
C2	9	12	274	222.85
C2	10	28	39	57.79
C2	11	4	36	44.4

TABLE 1. SAW-2 cuts for pphpphhpppphhpppphhpppphh on the 12×12 square lattice

cuts which brings about a decision whether to add the respective inequality to the LP relaxation or not. We suppose that there is a correlation between the HP sequence and the optimal choice of a cutting plane distance (which in general should not be chosen constant). In the present example, we recognize $d_{\text{cut}} = 6$ as a preferable cutting plane distance which is substantially independent of the type of the separated cutting planes. The present instance features three blocks of four subsequent p elements, separated each by two h elements. Thus there are three identical subsequences of length six which coincides with the optimal value for d_{cut} . However, at this point no precise statements can be given regarding the character of a potential interrelation, which indeed constitutes a topic subject to further research activities.

cuts	d_{cut}	#cuts	#nodes	cpu time
–	–	0	166	90.49
S2	2	28	154	150.14
S2	5	28	154	149.14
S2	10	28	154	145.57
S3	2	5	118	76.34
S3	3	9	41	45.31
S3	4	5	118	73.76
S3	8	5	118	74.44
S3	9	9	41	45.49
S4	2	121	40	202.83
S4	3	8	69	46.42
S4	4	10	44	46.82
S4	6	8	69	46.27
S4	7	5	76	52.56
S4	8	10	44	46.46
S5	2	24	20	36.12
S5	3	5	18	29.51
S5	5	8	10	16.98
S5	6	5	18	28.89
S5	7	254	19	552.18
S6	2	54	90	106.61
S6	3	134	23	151.02
S6	4	9	6	18.12
S6	5	13	131	99.65
S6	6	176	5	312.54
S7	2	119	214	265.64
S7	3	60	60	84.08
S7	4	149	53	183.90
S7	5	105	44	148.75
S7	6	3	40	39.31
S8	2	53	35	68.25
S8	3	26	43	55.49
S8	4	22	27	29.83
S8	5	32	32	66.75
S9	2	5	21	24.14
S9	3	15	40	48.23
S9	4	3	21	25.30
S10	2	8	30	33.32
S10	3	4	21	27.90
S11	2	3	22	26.46

TABLE 2. Submonotone SAW- k cuts for ppphhpppphhpppphhpppphh on the 12×12 square lattice

The next example is given by the HP string `ppphpphpppppphhhhhhpphpppphpphpp` of length 36 which we also obtained from [26]. Here we are interested in an optimal *compact* fold, i.e., a fold on a lattice graph whose number of vertices equals the length of the HP string. For this type of instances, fixing of HP string elements for the purpose of symmetry breaking is not applicable in the same way as for unrestricted folds. For this reason, we perform the computations without fixing of elements. We choose the 6×6 square lattice. Without separation of SAW-2 and submonotone SAW- k cuts, this instance was solved to optimality within 394.92 seconds of cpu time processing 224 branch-and-bound nodes. Figure 9 shows the solution which features a compact 4×4 hydrophobic core with 14 hydrophobic contacts. The results of the computations using cutting plane separation

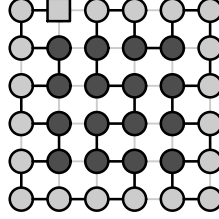


FIGURE 9. Optimal fold for the HP string `ppphpphpppppphhhhhhpphpppphpphpp` on the 6×6 square lattice

are listed in Tables 3 and 4. Concerning the influence of the number of cutting planes on the runtime of the solution procedure, we observe a similar behavior as in the above example. In principle, it is essential to use a suitable selection of cutting planes in order to achieve an enhancement in the solution process. This becomes obvious considering Table 3, where with the parameter $d_{\text{cut}} = 7$, the instance can be solved after processing 7 branch-and-bound nodes after addition of 9 SAW-2 cuts, whereas for $d_{\text{cut}} = 9$ with 26 SAW-2 cuts added, 245 nodes were necessary. Even worse, setting $d_{\text{cut}} = 2$ leads to the addition of 378 SAW-2 cuts which significantly increases the number of branch-and-bound nodes and almost triples the computing time. Table 4 demonstrates that

cuts	d_{cut}	#cuts	#nodes	cpu time
-	-	0	224	394.92
C2	2	378	344	1126.53
C2	3	285	13	452.19
C2	4	191	2	319.98
C2	5	106	331	732.38
C2	6	54	240	553.79
C2	7	9	7	103.33
C2	8	12	14	131.77
C2	9	26	245	411.04
C2	10	10	8	107.44
C2	11	22	135	343.25

TABLE 3. SAW-2 cuts for `ppphpphpppppphhhhhhpphpppphpphpp` on the 6×6 square lattice

even a low number of submonotone SAW- k cuts may lead to a decline in efficiency of the solution procedure. When separating submonotone SAW-7 cuts (S7) with distance $d_{\text{cut}} = 3$, only three violated inequalities are added, however, both the number of branch-and-bound nodes and the computing time are about doubled compared to the run without cutting plane separation, which is one of the worst results listed in the table. In contrast, separation of SAW-7 cuts with distance $d_{\text{cut}} = 5$ causes the addition of 5 violated inequalities, which leads to the best result in which the

cuts	d_{cut}	#cuts	#nodes	cpu time
–	–	0	224	394.92
S2	2, ..., 10	0	224	377.48
S3	2, ..., 9	3	383	609.45
S4	2, ..., 8	9	18	132.97
S5	2	14	289	541.49
S5	3, ..., 7	8	281	442.13
S6	2	10	102	232.69
S6	3	32	18	176.10
S6	4, ..., 6	8	15	117.49
S7	2	7	220	269.87
S7	3	3	463	689.51
S7	4	8	370	431.43
S7	5	5	13	106.38
S8	2	12	468	599.67
S8	3	10	179	302.27
S8	4	8	509	822.89
S9	2	98	12	291.14
S9	3	42	83	307.16
S10	2	36	320	530.05

TABLE 4. Submonotone SAW- k cuts for ppphhpphppppphhhhhhhpphhpppphhpppp on the 6×6 square lattice

solution is obtained after processing only 13 nodes in about a quarter of the cpu time spent for the solution of the instance without cutting plane separation.

The above discussion shows that it is really instance dependent how to choose the parameters appropriately. And we are currently far away from having some default strategy at hand that solves most of the instances in reasonable time. However, Table 6 finally gives an impression of the potential of our approach when choosing the parameters in the best way. It shows the computational benefit drawn from cutting plane generation for three selected instances, each specified by an HP string $S^{(N)}$ of length N and a lattice graph G . The instances are listed in Table 5, and Figures 10, 11, and 12 show associated optimal solutions. We note that the optimal solutions have been obtained by combining cutting plane generation with certain slight extensions and/or modifications to the binary program (48), such as the introduction of additional variables or the fixing of selected string elements. For a detailed discussion concerning these topics, we refer to [16].

instance	S	N	G
1	(php) ¹²	36	16×15 square
2	hppppphhhhhhhppphhhhhhhpppphphpphpppphphpphphpp	49	7×7 square
3	hhpphphpphphpphphpphphpphphpphh	30	12×12 triangular

TABLE 5. Selected instances demonstrating the computational benefit of SAW-2 cuts and submonotone SAW- k cuts for the computation of optimal solutions

6. CONCLUSION

In this article, we investigated a polyhedral description of self-avoiding walks on regular lattice graphs. We studied the polytopes $P_G^{(N)}$ associated to feasible solutions which are determined by N -step self-avoiding walks on a given lattice G . By the investigation of appropriate substructures of $P_G^{(N)}$, we derived two classes of cutting planes. First, we considered the sub-polytope $P^{(2)}$ related

instance	cuts	d_{cut}	#cuts	#nodes	cpu time
1	–	–	–	15000	77029
1	C2	3	57	5746	42618
2	–	–	–	531	5762
2	C2	6	101	136	2486
2	C2	8	173	70	3177
2	C2	10	104	18	1613
2	S3	5	8	8	551
3	–	–	–	675	11031
3	S14	1	3	185	2712

TABLE 6. Computational benefit of the separation of SAW-2 cuts and submonotone SAW- k cuts for the solution of selected instances

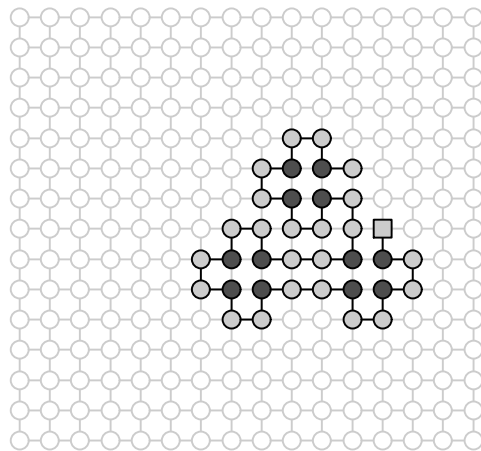


FIGURE 10. Optimal fold for instance 1 ((php)¹² on the 16×15 square lattice)

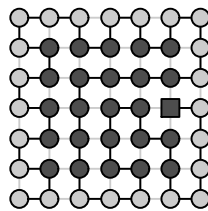


FIGURE 11. Optimal fold for instance 2 (hppppphhhhhhhppphhhhhhhpppphphpphppphpphphpph on the 7×7 square lattice)

to the contiguity constraints. For this 0/1 polytope, we gave a complete outer description by linear equations and facet-defining inequalities. Embedding these inequalities into the original polytope $P_G^{(N)}$ leads to the class of chain-2 cutting planes. Moreover, we studied the family of polytopes $P^{(k)}$ related to k -step self-avoiding walks on G with $2 \leq k \leq N$. We investigated the facial structure of the down-monotonization $P^{(k;\leq)}$ of $P^{(k)}$ from which we derived the class of submonotone chain- k cutting planes.

We implemented the binary linear program for the HP model using the ILOG Concert Technology C++ API in combination with ILOG CPLEX as the underlying IP solver. The implementation enables the use of various lattices and the specification of arbitrary fixings of HP string elements

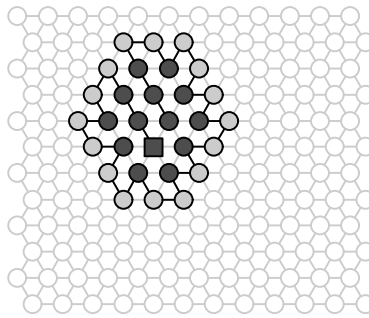


FIGURE 12. Optimal fold for instance 3 (hhhp p p p p p p p p p p p p p p p p h h h h on the 12×12 triangular lattice)

on lattice vertices. We extended the provided branch-and-cut framework by the implementation of a callback function for cutting plane generation. Cutting plane generation can be applied for SAW-2 cuts or for submonotone SAW- k cuts. The number of cuts added to the model is controlled by the specification of a cutting plane distance d_{cut} . For submonotone SAW- k cuts, the parameter k specifies the cutting plane wingspan.

We evaluated the performance of the branch-and-cut procedure for selected test instances with different parameter settings, where we put the focus on folds on 2-D square lattices. We observe that the separation of either SAW-2 cuts or submonotone SAW- k cuts with adequate parameter settings tends to result in an enhancement of the solution process regarding the number of branch-and-bound nodes as well as the computing time. This behavior occurs for instances with sufficiently large lattices that allow arbitrarily shaped folds and for which symmetry breaking is applied as well as for instances forcing the fold into a compact shape prescribed by the lattice where symmetry breaking is neglected.

Furthermore, we observe that the tractability of an instance and in particular the usefulness of cutting planes strongly depends on the sequence of **h** and **p** elements within the HP string. This fact gives rise to further research activities. In this connection, a topic of significant interest is the selection of HP string elements to be fixed and the choice of the settings for cutting plane generation, such as cutting plane distance and, if applicable, wingspan.

A further aspect concerns the impact of fixed HP string elements on the SAW- n polytopes $P^{(n)}$. Since any fixing reduces the dimension of the polytope, the inequalities derived for the original problem have to be adapted in a suitable way. To this end, the investigation of the facial structure of the polytopes associated with a given set of fixed HP string elements is necessary in order to obtain efficient cutting planes when solving the respective instances.

We arrive at the conclusion that the skillful application of the cutting planes presented above and the appropriate setting of the associated parameters is essential in order to obtain satisfactory results. The results of this article can be seen as a basis for the analysis of the polyhedral structure of combinatorial optimization problems associated with self-avoiding walks. They potentially provide the fundamentals for the development of new approaches that, in combination with standard methods, may lead to further progress in a more general context than protein structure prediction.

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