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Unimodularity of the Clar number problem

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Abstract

We study the generalization to bipartite and 2-connected plane graphs of the Clar number, an optimization model proposed by Clar [E. Clar, The Aromatic Sextet, John Wiley & Sons, London, 1972] to compute indices of benzenoid hydrocarbons. Hansen and Zheng [P. Hansen, M. Zheng, The Clar number of a benzenoid hydrocarbon and linear programming, J. Math. Chem. 15 (1994) 93–107] formulated the Clar problem as an integer program and conjectured that solving the linear programming relaxation always yields integral solutions. We establish their conjecture by proving that the constraint matrix of the Clar integer program is always unimodular. Interestingly, in general these matrices are not totally unimodular. Similar results hold for the Fries number, an alternative index for benzenoids proposed earlier by Fries [K. Fries, Uber Byclische Verbindungen und ihren Vergleich mit dem Naphtalin, Ann. Chem. 454 (1927) 121–324].
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1. Introduction

The Clar and Fries numbers are two optimization models defined for 2-connected subgraphs of the hexagonal lattice. These models are used in chemical graph theory to compute indices of benzenoid hydrocarbons. In this paper, we extend these two models to the class of bipartite

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and 2-connected plane graphs and apply linear algebra tools to study their properties. For further background on the Clar and Fries models, we recommend the articles by Hansen and Zheng [6,7] and the bibliography therein.

Integer programming formulations for the Clar and Fries numbers were proposed by Hansen and Zheng [6,7]. In particular, their computational results led them to conjecture that the linear programming relaxation of the Clar integer program yields integer solutions for all benzenoid graphs. We establish here their conjecture by proving that the constraint matrix of the Clar integer program is always unimodular, though it is not in general totally unimodular. In our case, unimodularity is sufficient to assure the integrality property since the constraints are equations. We also obtain an analogous result for the Fries number. Thus, the Clar and Fries indices can be computed in polynomial time using linear programming methods.

The paper is organized as follows. We provide essential definitions in Section 2 and also present integer programming formulations for the Clar and Fries problems. In Section 3 we establish the unimodularity of the constraint matrices of the Clar integer programs. For the sake of brevity we omit the unimodularity proof of the Fries matrix since it is similar to the Clar case. The results in this paper appeared in the extended abstracts [1,2] and in the dissertation by Atkinson [3].

2. Definitions and formulations

Throughout this paper (V, E, F) will denote a bipartite and 2-connected plane graph with node set V, edge set E, and set of bounded faces F. We assume that V is partitioned into a set of black nodes V_1 and a set of white nodes V_2, so that all edges connect nodes of different color. We consider two faces of (V, E, F) to be node-disjoint if their boundaries have no nodes in common. We refer the reader to [12] for the undefined terminology and results we utilize from graph theory.

Since the graph $G = (V, E)$ is bipartite and 2-connected, the boundary of each face $f \in F$ is an even cycle which can be perfectly matched in two different ways. Each of these two possible perfect matchings of the boundary cycle is called here a *frame* of the face. A frame of a face f is *clockwise oriented* if each frame edge is drawn from a black node to a white node in a clockwise direction along the boundary of f. Otherwise, the frame is *counterclockwise oriented*. A *framework* for (V, E, F) is a mapping $\varphi : F \mapsto 2^E$ such that $\varphi(f)$ is a frame of f, for each $f \in F$. An *oriented* framework has all frames with the same orientation. A framework $\varphi(f)$ is *simple* if each edge belongs to at most one frame. It follows that an oriented framework is simple.

We call a set of pairwise node-disjoint faces $F' \subseteq F$ a *Clar set* for (V, E, F) if there exists a perfect matching for $G = (V, E)$ that contains a frame of each face in F'. The cardinality of a Clar set with maximum number of faces is the *Clar number* of (V, E, F) and will be denoted here as $\mathrm{Clar}(V, E, F)$. We remark that any given Clar set is supported by different perfect matchings, obtained by exchanging a frame with its oppositely oriented counterpart for one or more faces in the Clar set. The Clar number was originally proposed by Clar [4] in the context of benzenoid systems, but here we extend this optimization model to the entire class of bipartite and 2-connected plane graphs.

The Clar number can be formulated as a node set partitioning problem, where each node of the plane graph (V, E, F) must be covered exactly once by either an edge in E or by the cycle boundary of a face in F. Identifying faces with their boundaries, the objective is to maximize the number of faces in the partition. This approach is represented by the following integer program for the Clar number that we refer to as IP1:

$$\max\{1^{\mathrm{T}} y : \; Kx + Ry = 1, \; x \in Z_{+}^{E}, \; y \in Z_{+}^{F}\},$$

where K is the $V \times E$ node-edge incidence matrix of $G = (V, E)$, R is the $V \times F$ node-face incidence matrix of (V, E, F), and Z_+^E and Z_+^F denote the sets of nonnegative integer vectors indexed by the elements of E and F, respectively. This formulation was originally proposed by Hansen and Zheng [6] to compute the Clar number of a benzenoid system.

A framework φ for a plane graph (V, E, F) can be represented by an $E \times F$ edge-face incidence matrix U where, for each face $f \in F$, its corresponding column in U is the incidence vector of edges in the frame $\varphi(f)$. The following result shows that the incidence matrix of a framework can be used to factor the node-face incidence matrix R.

Lemma 2.1. *Let K be the node-edge incidence matrix of $G = (V, E)$, let R be the node-face incidence matrix of (V, E, F), and let U be the edge-face incidence matrix of a framework for (V, E, F). Then $R = KU$.*

Proof. Let K^v be the row of K indexed by vertex v, let U_f be the column of U corresponding to face f, and let R_f^v be the entry of matrix R indexed by v and f. We must prove $R_f^v = K^v U_f$. If $R_f^v = 1$, then v belongs to the boundary of f and has precisely two incident edges that are also in the boundary of f. Since exactly one of these two edges belongs to $\varphi(f)$, we conclude that $K^v U_f = 1$. Alternatively, if $R_f^v = 0$, then v does not belong to the boundary of f and $K^v U_f = 0$ since the supports of vectors K^v and U_f are disjoint. □

Based on Lemma 2.1, we formulate an alternative integer program to compute the Clar number that we refer to as IP2:

$$\max\{1^{\mathrm{T}} y : \ Kz = 1, \ x + Uy = z, \ x \in Z_+^E, \ y \in Z_+^F, \ z \in Z_+^E\}.$$

All feasible solutions to this integer program are necessarily binary vectors. Hence, constraints $Kz = 1$ express that z is the incidence vector of a perfect matching for G. Constraints $x + Uy = z$ partition the edges in the perfect matching represented by z into those in the frames of faces in a Clar set identified by the vector y, and a set of remaining edges identified by x that complete the perfect matching.

If we eliminate from the definition of a Clar set the requirement that the faces be pairwise node-disjoint, we obtain the definition of a *Fries set* for the plane graph (V, E, F). The *Fries number* of (V, E, F) is then the cardinality of a maximum Fries set and will be denoted by Fries (V, E, F), since it was Fries [5] who proposed this index for benzenoid molecules. We provide below an integer programming model for Fries (V, E, F) that was originally formulated by Hansen and Zheng [7] in the context of benzenoid systems. In this model, U and W denote the incidence matrices of the clockwise and counterclockwise frameworks of (V, E, F), respectively.

$$\max\{1^{\mathrm{T}} y + 1^{\mathrm{T}} \tilde{y} : \ Kz = 1, \ Uy \leqslant z, \ W\tilde{y} \leqslant z, \ y, \tilde{y} \in Z_+^F, \ z \in Z_+^E\}.$$

For motives that will become evident in the next section, we will consider instead the following formulation for Fries(V, E, F), which will be referred to as IP3, obtained after introducing slack variables x and $\tilde{x}$:

$$\max\{1^{\mathrm{T}} y + 1^{\mathrm{T}} \tilde{y} : \ Kz = 1, \ Uy + x = z, \ W\tilde{y} + \tilde{x} = z, \ z, x, \tilde{x} \in Z_+^E, \ y, \tilde{y} \in Z_+^F\}.$$

3. Unimodularity results

In this section we prove that the constraint matrices of the integer programs for computing the Clar and Fries numbers are unimodular. These matrix properties imply that the linear relaxations of these optimization models have integral polytopes and, therefore, that the Clar and Fries numbers can be computed as linear programs.

We begin with some definitions from matrix theory. A *basis* of a matrix is a maximal linearly independent column submatrix. An integer matrix of rank r is called *unimodular* if, for each basis, the determinants of its $r \times r$ submatrices are relatively prime [8,11,10]. A matrix is *totally unimodular* if the determinant of every square submatrix is 0, 1, or -1. Totally unimodular matrices are unimodular, but the converse is not true in general. Our development assumes familiarity with properties of totally unimodular matrices such as can be found in [10] or [9].

A polyhedron is *integral* if each of its faces contains an integer vector. The relationship between unimodular matrices and integral polyhedra was explored by Hoffman and Kruskal [8], who showed the following result.

Theorem 3.1 [8]. *An integer matrix A is unimodular if and only if the polyhedron $\{x{:}Ax = b,\ x \geqslant 0\}$ is integral for each integer vector b.*

An integer matrix M is called *column eulerian* if the sum of its columns is a vector with all entries even: $M\mathbf{1} = \mathbf{0}$ (mod 2). Truemper [11] gave the following sufficient condition for a matrix to be unimodular.

Theorem 3.2 [11]. *An integer matrix A is unimodular if the following two conditions hold*:

(a) $A = BC$, *with B a unimodular basis of A and each entry of C is* 0, 1, *or* -1.
(b) *No column eulerian column submatrix of A is linearly independent.*

The following property of simple frameworks will be useful for our developments.

Lemma 3.3. *Let U be the incidence matrix of a simple framework for (V, E, F). Then, each row of U has at most one entry of* 1.

We show next that the constraint matrix of integer program IP2 is unimodular whenever U is the incidence matrix of a simple framework.

Theorem 3.4. *Let U be the incidence matrix of a simple framework for (V, E, F). Then, the following matrix is unimodular*:

$$\begin{bmatrix} 0 & 0 & K \\ I & U & -I \end{bmatrix}.$$

Proof. Since unimodularity is preserved when rows and columns are multiplied by -1, it is equivalent to show that the following matrix is unimodular:

$$A = \begin{bmatrix} 0 & 0 & K \\ I & U & I \end{bmatrix}.$$

We prove first that matrix A satisfies condition (a) of Theorem 3.2. Let T be the edge set of a spanning tree for $G = (V, E)$. We consider the following column submatrix of A:

$$B = \begin{bmatrix} 0 & K_T \\ I & I_T \end{bmatrix},$$

where K_T and I_T are the column submatrices of K and I that correspond to the edges in T. Since G is bipartite, K_T is a basis of K and, thus, B is a basis of A. Also, since G is bipartite, K is totally unimodular. This implies that B is totally unimodular and, in particular, that B is unimodular.

Next, let C be the unique matrix that satisfies $A = BC$ and let $T^c = E \setminus T$. For each $e \in T^c$, let K_e be its corresponding column in matrix K and let the vector λ_e be the solution to $K_T\lambda_e = K_e$. It is well known that the entries of λ_e must all be 0, 1 or -1. Let Λ be the $T \times T^c$ matrix whose columns are the λ_e vectors indexed by the edges in T^c. We may assume that the edges in E are ordered so that matrices K and I can be partitioned as $K = [K_T\, K_{T^c}]$ and $I = [I_T\, I_{T^c}]$. Then, the following factorization of A holds:

$$A = \begin{bmatrix} 0 & 0 & K_T & K_{T^c} \\ I & U & I_T & I_{T^c} \end{bmatrix} = \begin{bmatrix} 0 & K_T \\ I & I_T \end{bmatrix} \begin{bmatrix} I & U & 0 & I_{T^c} - I_T\Lambda \\ 0 & 0 & I & \Lambda \end{bmatrix} = BC.$$

Since the columns of I_{T^c} and I_T are mutually orthogonal, and the entries Λ are all 0, 1 or -1, it follows that all entries of $I_{T^c} - I_T\Lambda$ are also 0, 1 or -1. Thus, condition (a) of Theorem 3.2 holds.

We now prove that condition (b) of Theorem 3.2 is also satisfied. Let A' be a column eulerian column submatrix of A. Then

$$A' = \begin{bmatrix} 0 & 0 & K_{E'} \\ I_{D'} & U_{F'} & I_{E'} \end{bmatrix},$$

where $D' \subseteq E$, $E' \subseteq E$ and $F' \subseteq F$ are edge and face subsets whose elements index the columns of A'. Since A' is column eulerian and, by Lemma 3.3, each row of U has at most one entry of 1, it follows that the nonzero rows of $[I_{D'}\ U_{F'}\ I_{E'}]$ have exactly two entries of 1. To prove that A' is linearly dependent, we must show there are vectors $u \in R^{D'}$, $v \in R^{F'}$, and $w \in R^{E'}$, not all zero, such that

$$\begin{bmatrix} 0 & 0 & K_{E'} \\ I_{D'} & U_{F'} & I_{E'} \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0. \tag{1}$$

If E' is empty, we can set all entries of u equal to 1 and all entries of v equal to -1. Otherwise, let $G' = (V', E')$ be the subgraph of $G = (V, E)$ induced by E' and let $(V', E', \tilde{F})$ denote the plane graph determined by the original embedding (V, E, F). The graph $G' = (V', E')$ is of course bipartite, but may be disconnected. Since $K_{E'}$ is column eulerian, all nodes of G' have even degree. Thus, the components of the boundary of each face of $(V', E', \tilde{F})$ (bounded or unbounded) are even closed walks. Furthermore, the even degree of the nodes implies that the faces of $(V', E', \tilde{F})$ are 2-colorable (see, e.g., [12] for the case where G' is eulerian, the extension of this result to disconnected graphs is straightforward). Henceforth, we assume that we have a 2-coloring where all faces of $(V', E', \tilde{F})$, including the unbounded one, are painted either red or blue. Therefore, each edge in E' belongs to the boundary of two differently colored faces.

We now assign values to the vector w. Let e be an edge in E' and let us consider the blue face that has e in its boundary. If e is drawn from a black node to white node in a clockwise direction along the boundary of this blue face we assign $w_e = 1$, otherwise we set $w_e = -1$. Of course the same assignment of values to w can be obtained by focusing instead on the red faces. In this case, we assign $w_e = 1$ if e is drawn from a black node to a white node in a counterclockwise direction along the boundary of a red face and let $w_e = -1$ otherwise.

Let φ be the simple framework represented by U and let $f \in F$ be a bounded face of the plane graph (V, E, F). We claim that all frame edges of f that are also in the subgraph G' were assigned the same value in the vector w. That is, $w_e = w_{e'}$ for all pairs of edges e and e' in $\varphi(f) \cap E'$. To prove this claim, we note that the face f must be topologically contained in a (bounded or unbounded) face f' of $(V', E', \tilde{F})$. Without loss of generality, we may assume that f has a clockwise frame and that f' is a blue face. Let e be an edge in $\varphi(f) \cap E'$. Then e is drawn from a black node to a white node in a clockwise direction along the boundary of f' and $w_e = 1$.

We now proceed to assign values to the entries of u and v. For each $f \in F'$, if $\varphi(f) \cap E' \neq \emptyset$, we let $v_f = -w_e$ for all $e \in \varphi(f) \cap E'$. The claim we just proved shows that v_f is well defined. Otherwise, if $\varphi(f) \cap E' = \emptyset$, v_f can be chosen arbitrarily, say $v_f = 1$. Finally for each $e \in D'$, either $e \in E'$ or $e \in \varphi(f)$ for some $f \in F'$. In the first case, we assign $u_e = -w_e$ and, in the second case, we let $u_e = -v_f$. It can now be easily checked that the vectors u, v, and w we have defined are a solution to the homogeneous system (1). Thus, the columns of A' are linearly dependent. □

Theorems 3.1 and 3.4 imply that IP2 has the integrality property when the framework used in the formulation is simple. We now establish that [*KR*], the constraint matrix of the integer program IP1, is also unimodular. This result, combined with Theorem 3.1, proves that IP1 also has the integrality property, as was conjectured by Hansen and Zheng [6].

Theorem 3.5. *Let K be the node-edge incidence matrix of (V, E) and let R be the node-face incidence matrix of (V, E, F). Then the matrix $[KR]$ is unimodular.*

Proof. Let U be the incidence matrix of a simple framework for (V, E, F) and let $P_1(b)$ and $P_2(b)$ denote the following polyhedra:

$$P_1(b) = \{Kx + Ry = b,\ x \geqslant 0,\ y \geqslant 0\},$$
$$P_2(b) = \{Kz = b,\ x + Uy - z = 0,\ x \geqslant 0,\ y \geqslant 0,\ z \geqslant 0\}.$$

Let b be an integer vector such that $P_1(b)$ is not empty. Lemma 2.1 implies that (x, y) belongs to $P_1(b)$ if (x, y, z) belongs to $P_2(b)$. Conversely, let $(x, y) \in P_1(b)$ and define z by $z = x + Uy$. The nonnegativity of x, y and of the entries of matrix U implies that z is also nonnegative. It follows that $(x, y, z) \in P_2(b)$ and, thus, $P_1(b)$ is the projection of the polyhedron $P_2(b)$ onto the space of variables (x, y). By Theorems 3.1 and 3.4, $P_2(b)$ is an integral polyhedron. Since $P_1(b)$ is the projection of $P_2(b)$, we conclude that $P_1(b)$ is also integral. Invoking Theorem 3.1 again, we conclude that matrix $[KR]$ is unimodular. □

Similar to Theorem 3.4, the constraint matrix of the Fries integer program IP3 can also be shown to be unimodular. We avoid providing a proof since essentially the same arguments used in Theorem 3.4 can be applied again to this case.

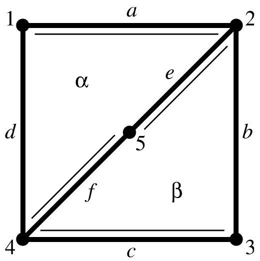
Theorem 3.6. *Let U and W be the incidence matrices of the clockwise and counterclockwise frameworks for (V, E, F), respectively. Then the following matrix is unimodular:*

$$\begin{bmatrix} 0 & 0 & 0 & 0 & K \\ U & I & 0 & 0 & -I \\ 0 & 0 & W & I & -I \end{bmatrix}.$$

Counterexample

The example below shows that the constraint matrices of formulations IP1, IP2, and IP3 may fail to be totally unimodular. Consider a plane bipartite graph (V, E, F) where $V = \{1, \ldots, 5\}$, $E =$

$\{a, \ldots, f\}$, and $F = \{\alpha, \beta\}$. The planar embedding is shown in the figure. Identifying faces with the nodes on their boundary, the set of faces F consists of $\alpha = \{1, 2, 4, 5\}$ and $\beta = \{2, 3, 4, 5\}$. An oriented framework U is represented in the figure by double edges along the boundary of each face. Matrix [*KR*] is from model IP1. The second one is a submatrix of matrix A, as defined in Theorem 3.4, formed by its last two column blocks.



$$[KR] = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{cccccccc} a & b & c & d & e & f & \alpha & \beta \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix} \end{array}$$

$$\begin{bmatrix} K & 0 \\ I & U \end{bmatrix} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ a \\ b \\ c \\ d \\ e \\ f \end{array} \begin{array}{c} \begin{array}{cccccccc} a & b & c & d & e & f & \alpha & \beta \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

The 3×3 submatrix of [*KR*] formed by rows 2, 3, 4 and columns a, c, α has exactly two entries of 1 per row and column. Thus, its determinant has absolute value equal to 2, implying that [*KR*] is not totally unimodular.

For the second matrix, the 5×5 submatrix corresponding to rows 2, 3, 4, a, f and columns a, b, c, f, α again has exactly two entries of 1 per row and column, implying that the constraint matrix of model IP2 is not totally unimodular. Finally, since the constraint matrix of IP2 appears as a submatrix in model IP3, the same example shows that the matrices of model IP3 are not totally unimodular matrix in general.

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