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The complexity of the Clar number problem and an FPT algorithm

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Abstract

The Clar number of a (hydro)carbon molecule, introduced by Clar [E. Clar, *The aromatic sextet*, (1972).], is the maximum number of mutually disjoint resonant hexagons in the molecule. Calculating the Clar number can be formulated as an optimization problem on 2-connected planar graphs. Namely, it is the maximum number of mutually disjoint even faces a perfect matching can simultaneously alternate on. It was proved by Abeledo and Atkinson [H. G. Abeledo and G. W. Atkinson, *Unimodularity of the clar number problem*, Linear algebra and its applications **420** (2007), no. 2, 441–448] that the Clar number can be computed in polynomial time if the plane graph has even faces only. We prove that calculating the Clar number in general 2-connected plane graphs is NP-hard. We also prove NP-hardness of the maximum independent set problem for 2-connected plane graphs with odd faces only, which may be of independent interest. Finally, we give an FPT algorithm that determines the Clar number of a given 2-connected plane graph. The parameter of the algorithm is the length of the shortest odd join in the planar dual graph. For fullerenes this is not yet a polynomial algorithm, but for certain carbon nanotubes it gives an efficient algorithm.

Keywords: Clar number, fullerene, complexity, planar graph, graph algorithm

1 Introduction

1.1 Previous work

Our research is motivated by problems in chemical graph theory. Some molecules, for example polycyclic aromatic hydrocarbon (PAH) molecules, benzenoid hydrocarbon

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molecules, or fullerene molecules can be represented as a 2-connected plane graph. In this representation only carbon atoms are depicted, while hydrogen atoms are omitted. Several of the chemical properties of these molecules (e.g. chemical stability) are closely related to some parameters of the underlying graph. In this note we will be concerned with a parameter called the Clar number, which we will define in Subsection 1.2. The Clar number was introduced by Clar in [3] as an indicator of stability of a (hydro)carbon molecule. Since its definition, it was investigated for several molecule classes.

A subclass of PAHs, the benzenoid PAHs have the special property that every bounded face in their representing plane graph is a hexagon, in particular, every face has an even number of nodes. One can see that such a 2-connected plane graph is also bipartite. Hansen and Zheng formulated the Clar number for this graph class with integer programming [6], later, applying this formulation Shalem and Abeledo proved that this problem can be computed in polynomial time [11]. Abeledo and Atkinson gave a combinatorial minmax characterization for the problem [2]. A combinatorial algorithm was also given by Erdős, Frank and Kun [4].

Fullerenes are carbon molecules with a hollow cage-like structure. The first fullerene molecule to be discovered, and the family's namesake, buckminsterfullerene (C_{60}), was prepared in 1985 by Richard Smalley, Robert Curl, James Heath, Sean O'Brien, and Harold Kroto at Rice University [7]. The graph representing a fullerene molecule contains exactly 12 pentagon faces, and the rest of the faces are hexagons (the number of hexagons can be arbitrarily large). Zhang Ye and Yunrui [14] proposed a method applying the Clar number, along with other parameters, for ordering fullerene molecules according to their stability. For the Clar number of fullerenes Ye and Zhang gave an upper bound of $\lfloor \frac{n-12}{6} \rfloor$ [13]. Later they characterized the fullerenes achieving this bound [12]. M.Ghorbani, E.Naserpour presented exact solutions for certain nanotube classes [5].

Our motivation was to determine the Clar number of fullerene molecules in polynomial time. Note that former results for benzenoid molecules cannot be applied, because the underlying graph of a fullerene is not bipartite. One of our main contributions is to show that determining the Clar number of a general 2-connected plane graph is NP-hard (see Section 2). Our second contribution is an algorithm that determines the Clar number of a 2-connected plane graph, and has good running time, provided that the odd faces are "not too far from each other"(see Section 3). More precisely, our algorithm is fixed parameter tractable (FPT) where the parameter is the length of the shortest odd join in the planar dual graph. In Section 3 we also explain that for a subclass of fullerenes called carbon nanotubes our algorithm efficiently computes the Clar number.

1.2 Problem Definition

By a **plane graph** we mean a planar graph with a fixed planar embedding. Let $G = (V, E)$ denote a 2-connected plane graph which has a perfect matching. For a perfect matching M of G let F_M denote the set of those faces which alternate with respect to M. Note that faces in F_M are even. A pairwise vertex disjoint subset of

F_M is a **Clar set with respect to** M. A subset C of the faces is a **Clar set** if there exists a perfect matching M for which C is a Clar set with respect to M. Note that a set of pairwise vertex disjoint even faces is a Clar set if and only if deleting all (the nodes of) these even faces the remaining graph still has a perfect matching. The **Clar number** of G, denoted by $Cl(G)$ is the maximum size of a Clar set. For sake of simplicity we allow the unbounded face in a Clar set as well, but there are no difficulties if we want to exclude it.

2 Hardness of the Clar number problem

Our first result is the following theorem.

Theorem 2.1. *It is NP-hard to calculate the Clar number of a 2-connected planar graph (given with a fixed planar embedding).*

In this section we prove Theorem 2.1. Our reduction will be based on a special case of the Independent Set Problem. Let us start with defining this problem.

Definition 2.2. Given a graph $G = (V, E)$, a subset $U \subseteq V$ is said to be **independent** if there is no edge of G between two nodes of U. Let $\alpha(G)$ denote the maximum size of an independent set in G.

Problem 1. *Given a 2-connected planar cubic graph G and a positive integer K, does G contain an independent set of size K?*

Theorem 2.3 (Mohar, Theorem 4.1 in [8])**.** *Problem 1 is NP-complete.*

Problem 2. *Given a 2-connected plane graph G with odd faces only, and a positive integer K, does G contain an independent set of size K?*

Lemma 2.4. *Problem 2 is NP-hard.*

Proof. According to Theorem 2.3, the independent set problem is also NP-complete for 2-connected planar graphs. Let $G = (V, E)$ denote an instance of this problem, and let us fix a planar embedding of G. If G has an even face F, let G_F denote the planar graph obtained from G by the following operation. We add three vertices a, b, c inside F and edges ab, bc, ca, au, bu, bv where u and v form an edge of F (see Figure 1).

Claim 2.5. $\alpha(G_F) = 1 + \alpha(G)$.

Proof. First, for an independent set I of G, clearly $I \cup \{c\}$ is independent in G_F and hence $\alpha(G_F) \geq 1 + \alpha(G)$. Second, an independent set I_F in G_F can contain at most one vertex from the set $\{a, b, c\}$. Since $I_F \setminus \{a, b, c\}$ is independent in G we get that $\alpha(G) \geq \alpha(G_F) - 1$. □

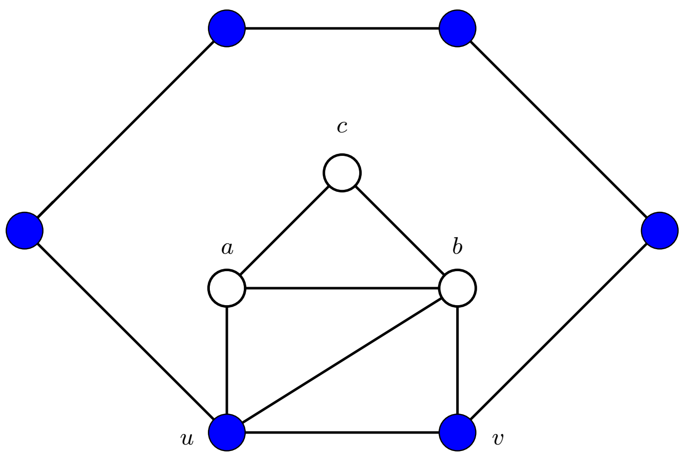

Figure 1: Eliminating even faces.

Note that the number of even faces of G_F is one less than that of G, and G_F is also 2-connected. Let $\mathbb{F}$ denote the set of even faces of G. By consecutively applying the above operation on every member of $\mathbb{F}$ we get another graph $G_{\mathbb{F}}$ for which $\alpha(G_{\mathbb{F}}) = \alpha(G) + |\mathbb{F}|$ and which has odd faces only. Hence we reduced Problem 1 to Problem 2, which proves Lemma 2.4. $\square$ $\square$

We are now ready to prove the hardness of the Clar number problem.

Proof of Theorem 2.1. We prove the theorem by reducing Problem 2 to the Clar number problem. Let $G = (V, E)$ denote an instance of this problem. We construct graph G' the following way: for every edge of G we add two vertices to G'. Let $uv \in E$ be an edge of G and let F_1 and F_2 denote the faces that uv is incident to. We add vertices x_{uv,F_1} and x_{uv,F_2} to G' along with the edge $x_{uv,F_1}x_{uv,F_2}$. For every pair of edges uv and vw that have a common face F we add edge $x_{uv,F}x_{vw,F}$ to G'. It is easy to see that G' is planar (see Figure 2). Informally, G' is obtained from the planar dual graph G^* of G by "blowing a circuit" into each vertex of G^*. Every face of G' either corresponds to a face of G, or to a vertex of G, and since G has odd faces only, all the even faces of G' are the ones corresponding to vertices of G. Note that G' trivially has a perfect matching M consisting of the edges of the form $x_{uv,F_1}x_{uv,F_2}$, for every $uv \in E$. Since M is alternating on every even face of G', corresponding to a vertex of G, for this graph the Clar number equals the maximum size of a Clar set with respect to M. The Clar sets of G' and the independent sets of G have a one to one correspondence, proving the theorem. $\square$ $\square$

Corollary 2.6. *It is also NP-hard to find a maximum cardinality Clar set with respect to a fixed perfect matching.*

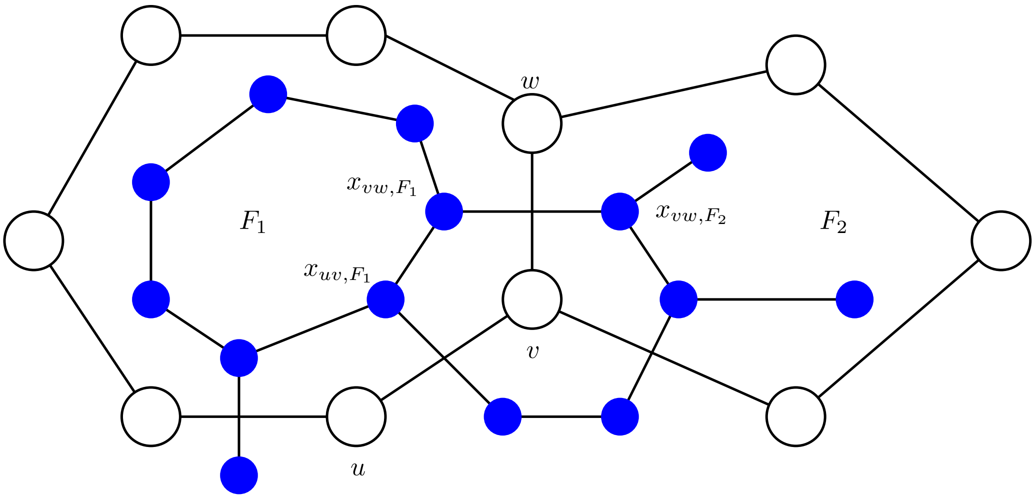

Figure 2: Reduction of the Independent Set Problem to the Clar number problem

3 An FPT algorithm for determining the Clar number

In this section we present an algorithm that determines the Clar number of a 2-connected plane graph, and has a good running time, unless the odd faces are "far from each other" in the planar representation. The idea is the following. Consider a 2-connected plane graph that has only 2 odd faces in its (fixed) planar representation, and take a shortest path (in the planar dual graph) between these odd faces. An optimal Clar set might use some of the even faces that lie on this shortest path. Our algorithm takes an arbitrary subset of even faces along this shortest path and tries to extend this subset into a Clar set. This is repeated for every possible subset of even faces along the shortest path. We will generalize this for plane graphs having more than 2 odd faces below. First we need a definition and a theorem.

Definition 3.1. Given a graph $G = (V, E)$ and a subset $T \subseteq V$ of even size, a T**-join** is a subset of edges $J \subseteq E$ so that the number of edges of J incident to a node $v \in V$ is odd if and only if $v \in T$. An **odd-join** of G is a T-join where T is the set of nodes having odd degree in G.

Theorem 3.2 (See e.g. [10], Chapter 29)**.** *Given a graph $G = (V, E)$, a subset $T \subseteq V$ of even size, and edge-lengths $c : E \to \mathbb{R}_+$, a shortest T-join can be found in polynomial time.*

Given a 2-connected plane graph $G = (V, E)$, let $G^* = (V^*, E^*)$ denote its planar dual. Let $J^* \subseteq E^*$ be a shortest odd-join in G^*, where each edge of G^* has length 1. We give an algorithm determining the Clar number of G that runs in $O(3^{|J^*|}p(|V|))$ for some polynomial p.

Let $J \subseteq E$ be the set of edges corresponding to J^*. Let F_{even} be the set of even faces of G and let $F_J \subseteq F_{even}$ be the set of even faces that have some edge of J in their boundary. Let $G' = (V + U, E - J + J')$ be the 2-connected bipartite plane graph that is obtained from G by subdividing each edge of J with a new node, where the set of these subdivision nodes is U and the set of subdivided edges is J'. Observe that $|U| = |J|$ and $|J'| = 2|J|$. Note that G' is indeed bipartite, since every face is even in its planar embedding.

Let K' be the node-edge incidence matrix of G', and R' be the node-face incidence matrix of G'. Let R^* be obtained from R' by deleting the columns corresponding to odd faces of G, and let K^* be obtained from K' by deleting the columns corresponding to J'.

Our algorithm determines integer optimums of some LP formulations related to matrices R^*, K^*. In order to show that an integer optimum exist we use the notion unimodularity.

Definition 3.3. An $m \times n$ matrix A of full row rank is **unimodular**, if it is integer and every submatrix of size $m \times m$ has determinant 0, 1 or -1.

Theorem 3.4 (See e.g. [9], Theorem 19.2)**.** *Let A be an integral matrix of full row rank. Then the polyhedron $\{x|x \geq 0; Ax = b\}$ is integral for each integral vector b if and only if A is unimodular.*

Lemma 3.5. *The matrix $[R^*, K^*]$ is unimodular.*

Proof. We apply a result from [1] on the unimodularity of a special matrix of bipartite 2-connected plane graphs.

Lemma 3.6 (Abeledo, Atkinson, Theorem 3.5 of [1])**.** *Let (V, E, F) denote a bipartite 2-connected plane graph with node, edge and face sets V, E and F, respectively. 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.*

Applying that the matrix $[R', K']$ is unimodular by Lemma 3.6, and deleting some columns of a unimodular matrix also gives a unimodular matrix, we get Lemma 3.5. □ □

After these preliminaries we present the pseudocode of our algorithm that calculates the Clar number of a 2-connected plane graph. The basic idea of the algorithm is the following. Determining the Clar number of G means that we want to choose pairwise node disjoint even faces and edges, so that every node is contained in exactly one of the chosen objects, and we want to maximize the number of faces chosen. Given a feasible solution consisting of a set F_1 of even faces of G and a set E_1 of edges of G, let F_1' be the set of even faces of G' corresponding to faces in F_1, and similarly let E_1' be set of edges of G' corresponding to edges in E_1 (if an edge $e \in J$ is in E_1 then we add both edges obtained from the subdivision of e into E_1'). Every subdivision node (that is, node in U) is then incident to either $0, 1$ or 2 objects in $F_1' \cup E_1'$. If someone tells us these $0, 1, 2$ values for every $u \in U$ then we can reconstruct E_1 and F_1 using these numbers, see Lemma 3.7 below. Therefore what we do is that we try every possible vector in $\{0, 1, 2\}^U$ to find the one giving the best solution.

Algorithm Clar_Number

begin

INPUT: a 2-connected plane graph $G = (V, E)$

OUTPUT: the Clar number of G

1.1. Find a shortest odd-join in G^*, where each edge of G^* has length 1 (G^* is the planar dual of G, and we will use more notations that were introduced above in this section).

1.2. For every vector $b_U \in \{0, 1, 2\}^U$

1.3. Let $b = \begin{pmatrix} 1_V \\ b_U \end{pmatrix} \in \{0, 1, 2\}^{V+U}$.

1.4. For every $e \in J'$

1.5. Let $z_e = 1$ if e is incident with a node $u \in U$ with $b_U(u) = 2$, and let $z_e = 0$ otherwise.

1.6. Take the integer optimum of the LP Problem (1)-(2) (see Lemma 3.7).

$$\max\{1y : y \in \mathbb{R}_+^{F_{even}}, x \in \mathbb{R}_+^{E-J+J'}, \tag{1}$$

$$R^*y + K'x = b, x_e = z_e \text{ for every } e \in J'.\} \tag{2}$$

1.7. Output the best of the candidates obtained in Step 1.6.

end

Lemma 3.7. *The LP problem* (1)-(2) *has an integer optimum.*

Proof. After eliminating the variables x_e for $e \in J'$ we obtain an LP Problem of the form $\max\{1y : y \in \mathbb{R}_+^{F_{even}}, x \in \mathbb{R}_+^{E-J}, R^*y + K^*x = b\}$. The polyhedron in this problem is integral by Lemma 3.5 and Theorem 3.4. □ □

Lemma 3.8. *There is a one to one correspondence between the Clar sets of G and the integer solutions of LP problems formulated during the algorithm.*

Proof. Let $C \subset F$ be a Clar set of G with respect to perfect matching M, and let N denote the edges of M not incident to faces in C. For a node $v \in U$ define $b_U(v) = 1$ if v is on a face in C and let $b_U(v) = 2$ if the edge in E subdivided by v is in N. Finally, let $b_U(v) = 0$ otherwise. Let $\chi_C \in \mathbb{R}_+^{F_{even}}$ denote the characteristic vector of C and let $\chi_N \in \mathbb{R}_+^{E-J}$ denote the characteristic vector of N on $E - J$. Let $x \in \mathbb{R}_+^{E-J+J'}$ be the vector which is χ_N on $E - J$ and z on J'. Then vectors χ_C and x give an integer solution of the LP problem defined by vector b_U, moreover, the objective value of the LP is $|C|$. This shows that every Clar set corresponds to an integer solution. For the other direction of the theorem, given an integer solution for an LP problem of the algorithm, one can construct Clar set and perfect matching M analogously. □ □

Note that the LP problem (1)-(2) will not necessarily be feasible for every choice of b_U. We could be more careful in choosing only those vectors in Step 1.2 of the algorithm that make the LP feasible. However the algorithm is easier described this way. The running time is clearly $O(3^{|J^*|}p(|V|))$ for some polynomial p.

For certain fullerenes the method above gives an efficient algorithm. Carbon nanotubes are fullerenes with a cylindrical nanostructure, with two 'half-fullerene' caps on both ends. Six pentagonal faces are in both caps, forming three short pairs in the odd-join. So for this class of fullerenes the parameter of our FPT algorithm is relatively small, giving an efficient method to determine the Clar number.

4 Open questions

We have proved the NP-hardness of the Clar number problem for a general 2-connected plane graph G. The problem is motivated by the problem of determining the Clar number of fullerene graphs, when G has exactly twelve pentagonal faces and every other face is a hexagon. This problem is however left open, since our NP-hardness reduction involves creating a lot of odd faces. An FPT algorithm with the number of odd faces as parameter would yield a polynomial time algorithm for all fullerenes.

Another line of research would be to show that determining the Clar number is NP-hard even for some restricted class of 2-connected plane graphs, too. If we were able to specialize the Independent Set problem further to 3-regular plane graphs with odd faces, then our techniques would yield that the Clar number is NP-hard for graphs with only hexagonal even faces.

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