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Reducing an arbitrary fullerene to the dodecahedron

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ABSTRACT

Viewing fullerenes as plane graphs with facial cycles being pentagonal and hexagonal only, it is shown how to reduce an arbitrary fullerene to the (graph of the) dodecahedron. This can be achieved by a sequence of eight reduction steps, seven of which are local operations and the remaining reduction step acts globally. In any case, the resulting algorithm has polynomial running time.

1. Introduction and preliminary discussion

All concepts not defined in this paper can be found in [1]. As for developments on the topic under consideration, we refer to [6]. As for the relation between [6] and the current article, see the final remarks at the end of this article. However, there is a considerable overlap of these two articles. The differences between them lie in a more formalistic approach in the current article, on the one hand (this article is aiming primarily at mathematicians). On the other hand, the current article includes additional reduction steps which permit a unified approach to the reduction of arbitrary fullerenes to the dodecahedron. As a consequence one obtains a single algorithm for reducing an arbitrary fullerene to the dodecahedron; or conversely, for constructing an arbitrary fullerene from the dodecahedron (in [6], Algorithm 1 uses only three types of reductions to reduce every fullerene except one C_{28}. Algorithms 2 and 3 are simplifications for practical use—see also the algorithmic considerations in Section 3 of this paper).

Next we give some definitions.

Definition 1. A fullerene is a plane cubic graph G all of whose face boundaries are pentagonal or hexagonal.

However, it has been shown in [3] that fullerenes are cyclically 5-edge-connected and thus are uniquely embeddable in the plane since they are 3-connected graphs. That is, a fullerene's face boundaries are uniquely determined. By unique embeddability in the plane we mean that if G_1, G_2 are two embeddings of G on the sphere, then G_2 can be obtained from G_1 by a topological transformation of the sphere. Consequently, the dual graph $D(G)$ of a fullerene G is uniquely determined. In fact, we shall consider G and $D(G)$ simultaneously in view of certain reduction steps. Therefore, we shall denote by F the face of G which corresponds to $f \in V(D(G))$. We also note that fullerenes have precisely 12 pentagonal face boundaries independent of the number of hexagonal face boundaries, and that fullerenes exist for any integer $n > 1$ of hexagonal face boundaries, [5].

For brevity's sake and because of fullerene's unique embeddability we shall not distinguish between faces and face boundaries. Correspondingly, we can just speak of pentagons and hexagons which are face boundaries.

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Definition 2. Let G be a graph having a 2-valent vertex x with $N_G(x) = \{u, v\}$. By suppressing the vertex x we mean the graph $(G - x) \cup \{uv\}$ (in case that $uv \in E(G)$ we double this edge).

When walking in a path $P(x, y) \subset G$ from x to y, where G is an embedded planar graph, then we can speak of the *left side, right side* respectively, of $P(x, y)$. Correspondingly, when considering $u \in V(P(x, y)) - \{x, y\}$ we can speak of edges incident to u as lying to the left (to the right) of u if these edges lie on the left side (on the right side) of $P(x, y)$.

Now we look at a path $P(x, y)$ in $D(G)$ where G is a plane graph. Suppose $P(x, y)$ contains a 6-valent vertex $v \neq x, y$. When traversing $P(x, y)$ from x to y we call v a *transient* vertex if two edges incident to v lie on the left side of $P(x, y)$ and two edges incident to v lie on the right side of $P(x, y)$. If, however, precisely one edge incident to v lies on the left side (right side) of $P(x, y)$, then we say $P(x, y)$ *deviates to the left (deviates to the right)* at v.

For a graph G, set $V_i(G) = \{v \in V(G) : d_G(v) = i\} \subseteq V(G)$.

In the special case where G is a fullerene, we consider $V_i(D(G))$: clearly,

$$V(D(G)) = V_5(D(G)) \dot{\cup} V_6(D(G)).$$

Let

$$D_5 := D(G) - V_6(D(G)) = D(G)[V_5(D(G))].$$

In what follows we restrict ourselves to the fullerenes.

A component $C^{(5)}$ of D_5 corresponds in G to a subgraph consisting of pentagons; such subgraph we call a *cluster* (of pentagons). More precisely, we call a cluster an i-cluster if it consists of at least i pentagons.

Next we consider special subgraphs of G which are parts of clusters (or clusters in itself).

- An edge $e = xy$ is said to be of *type I* if it belongs to two pentagons, F_5' and F_5'' say, and both x and y lie also in hexagons.
- A vertex x with $N(x) = \{x_1, x_2, x_3\}$ is said to be of *type Y* if xx_i belongs to two pentagons and x_i belongs to a hexagon, for every $i \in \{1, 2, 3\}$.
- An edge $e = xy$ with $N(x) - \{y\} = \{x_1, x_2\}$ and $N(y) - x = \{y_1, y_2\}$ is said to be of *type H* if x and y belong to pentagons only, whereas each of x_i, y_i, $i = 1, 2$, belongs to a hexagon as well.

The following is obvious.

- An edge e of type I corresponds to $I_5^* := D_5[\{f_5', f_5''\}]$ with $f_5'f_5'' \in E(D_5)$ satisfying $N_{D_5}(f_5') \cap N_{D_5}(f_5'') = \emptyset$.
- A vertex x of type Y corresponds in D_5 to an induced triangle $\Delta_5^* := D_5[\{f_5', f_5'', f_5'''\}]$ such that

$$N_{D_5}(f_5^{(i)}) \cap N_{D_5}(f_5^{(j)}) = \{f_5^{(k)}\} \text{ for } \{(i), (j), (k)\} = \{', '', '''\}.$$

- An edge e of type H corresponds to an induced subgraph $F_5^* := D_5[\{f_5', f_5'', f_5''', f_5^{iv}\}]$ where vertices are 'dashed' in cyclical order and with $f_5''f_5^{iv} \in E(F_5^*)$ corresponding to $\{e\} = F_5'' \cap F_5^{iv}$ (hence $f_5'f_5''' \notin E(F_5^*)$).

Correspondingly, we call I_5^*, Δ_5^*, F_5^* an *I^*-configuration*, *Y^*-configuration*, *H^*-configuration*, respectively, in D_5. Likewise, we call the subgraphs I_5, Δ_5, F_5 of G consisting of the pentagons which correspond to the vertices of I_5^*, Δ_5^*, F_5^* respectively, *I-configuration*, *Y-configuration*, *H-configuration* of G, respectively.

2. Various reduction steps and structural results

The first reduction steps are obvious.

(i) If G contains an I-configuration with $e = xy$ being of type I, then the cubic graph G^- homeomorphic to $G - xy$ is also a fullerene. The transition from G to G^- is called an *I-reduction*.
(ii) If G contains a Y-configuration with vertex x being of type Y, then we let G^- to be the cubic graph homeomorphic to $G - x$, and we speak of a *Y-reduction*; G^- is also a fullerene.
(iii) If G contains an H-configuration with $e = xy$ being of type H, then we denote by G^- the cubic graph homeomorphic to $G - \{x, y\}$; G^- is also a fullerene, and we speak of an *H-reduction*.

For $S \in \{I, Y, H\}$ it is clear how an S-reduction results in deriving $D_5^- = D(G^-) - V_6(D(G^-))$ from D_5. Note that some vertices $v \in V_6(D(G))$ are vertices in $V_5(D(G^-))$.

Next suppose that G does not admit any S-reduction for any $S \in \{I, Y, H\}$, but that D_5 has a non-trivial component. It follows that there is a pentagon P with four of its neighbors being pentagonal; the remaining neighbor, call it D, is either pentagonal or hexagonal. That is, we are faced with a configuration as depicted in Fig. 1. We also consider face Z placed diametrically opposite to D and adjacent to two of the neighbors of P. We consider vertices and edges of Fig. 1 as labeled there and focus on $e_1 = zu$, $e_2 = rv_1$, $e = v_iv_2$, $f = xr$, $g = ys$. Set $M_1 := \{e_1, e_2\}$, $M_2 := \{e, f, g\}$.

Suppose D has length $\ell(D) = 6$.

If $\ell(Z) = 6$, then the cubic graph G^- homeomorphic to $G - M_1$ is also a fullerene; the faces Z' and D' of G^- corresponding to Z and D, respectively, are pentagonal. In this case we speak of an *M_1-reduction* when transforming G into G^- (cf. Fig. 2a). Whence we need to consider the case $\ell(Z) = 5$.

If $\ell(X) = \ell(Y) = 6$ and $\ell(Z) = 5$, then the cubic graph G^- homeomorphic to $G - M_2$ has pentagonal faces D', X', Y' corresponding to the hexagonal faces D, X, Y in G (cf. Fig. 2b). Here we say that G^- results from G by an *M_2-reduction*.