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Fullerene Graphs of Small Diameter

Diego Nicodemos[*1], **Matěj Stehlík**[†2]

[1] *Colégio Pedro II, COPPE/Sistemas, Universidade Federal do Rio de Janeiro, Brazil,*
nicodemos@cos.ufrj.br
[2] *Laboratoire G-SCOP, Université Grenoble Alpes, France,*
matej.stehlik@grenoble-inp.fr

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Abstract

A fullerene graph is a cubic bridgeless plane graph with only pentagonal and hexagonal faces. We construct, for infinitely many values of n, a fullerene graph on n vertices of diameter at most $\sqrt{4n/3}$. This disproves a conjecture of Andova and Škrekovski [MATCH Commun. Math. Comput. Chem. 70 (2013) 205–220], who conjectured that every fullerene graph on n vertices has diameter at least $\lfloor\sqrt{5n/3}\rfloor - 1$.

1 Introduction

Fullerene graphs are cubic bridgeless plane graphs with only pentagonal and hexagonal faces. Their beautiful structure—along with the fact that they can serve as models for fullerene molecules—have attracted many researchers, and there is now a wide body of literature on the various properties and parameters of fullerene graphs.

One parameter that has received relatively little attention is the *diameter*, defined for a graph G as the maximum distance between two vertices of G, and denoted by $\mathrm{diam}(G)$. Andova et al. [2] have shown that if G is a fullerene graph on n vertices, then $\mathrm{diam}(G) \geq \sqrt{2n/3 - 5/18} - \frac{1}{2}$. In a subsequent paper, Andova and Škrekovski [3] studied the diameter of fullerene graphs with full icosahedral symmetry. Believing that these fullerene graphs minimise the diameter, they proposed the following conjecture.

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Conjecture 1 (Andova and Škrekovski [3]). *If G is any fullerene graph on n vertices, then* $\mathrm{diam}(G) \geq \lfloor\sqrt{5n/3}\rfloor - 1$.

The conjecture bears a striking resemblance to a famous conjecture in differential geometry due to Alexandrov [1], which states that $D \geq \sqrt{2A/\pi}$, for any closed orientable surface of area A and intrinsic diameter D. The bound in Alexandrov's conjecture is attained by the doubly-covered disk, a degenerate surface formed by gluing two discs along their boundaries.

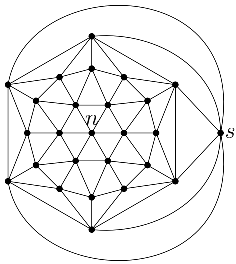
By a deep theorem of Alexandrov (see e.g. [5, Theorem 23.3.1] or [7, Theorem 37.1]), any fullerene graph can be embedded in the surface ∂P of a convex (possibly degenerate) polyhedron $P \subset \mathbb{R}^3$ so that every face is isometric to a regular pentagon or a regular hexagon with unit edge length, and this polyhedron is unique up to isometry of $\mathbb{R}^3$. (We should stress that the edges of the polyhedron may not correspond to the edges of the graph.) This allows us to view fullerene graphs as geometric objects, and to talk about the 'shape' of a fullerene graph.

The fullerene graphs with full icosahedral symmetry investigated by Andova and Škrekovski [3] have a rather 'spherical' shape. However, since the minimisers in Alexandrov's conjecture are doubly-covered discs, it seems that fullerene graphs which minimise the diameter, for a given number of vertices, ought to resemble a disc. This led us to study the class of fullerene graphs which were called *nanodiscs* by Graver and Monacino [6]. We were able to show that they have diameter at most $\sqrt{4n/3}$, thus disproving Conjecture 1. (The smallest counterexample we found has 300 vertices.)

Theorem 1. *For every $r \geq 2$ and every $1 \leq t \leq r-1$, there exists a fullerene graph $D_{r,t}$ on $12r^2$ vertices of diameter at most $4r$. In particular,* $\mathrm{diam}(D_{r,t}) \leq \sqrt{4n/3}$.

The graph $D_{r,t}$ is best defined using the planar dual graph. Let T be the (infinite) 6-regular planar triangulation. Fix a vertex $u \in V(T)$, and let $T_r(u)$ be the subgraph of T induced by all the vertices at distance at most r from u. Let $C = (u_1, u_2, \dots, u_{6r})$ be the outer cycle of $T_r(u)$; clearly, C has six vertices of degree 3 (say u_{kr}, for $1 \leq k \leq 6$), and the other vertices u_i all have degree 4.

Let r and t be integers such that $r \geq 2$ and $1 \leq t \leq r-1$. Take two copies $T_r(n)$ and $T_r(s)$ of the graph defined above (one with centre n and the other with centre s), and suppose $u_1, \dots, u_{6r}$ is the outer cycle of $T_r(n)$ and $v_1, \dots, v_{6r}$ is the outer cycle of $T_r(s)$. The graph $D^*_{r,t}$ is obtained from the disjoint union of $T_r(n)$ and $T_r(s)$ by identifying the vertex u_i and v_{i+t}, for all $1 \leq i \leq 6r$ (the indices are taken modulo $6r$).



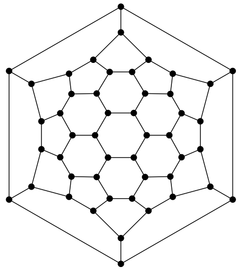


Figure 1: The plane triangulation $D^*_{2,1}$ and its dual fullerene graph $D_{2,1}$.

Clearly, $D^*_{r,t}$ is a planar triangulation, with all vertices of degree 5 and 6, so the planar dual $D_{r,t}$ is a fullerene graph. The graphs $D^*_{2,1}$ and $D_{2,1}$ are shown in Figure 1.

2 The proof

Our graph-theoretic terminology is standard and follows [4]. To prove Theorem 1, we will make use of the following simple lemma, which relates distances in a fullerene graph to distances in its dual graph.

Lemma 2. *Let G be a fullerene graph and G^* its dual graph. Fix any pair of vertices $A, B \in V(G)$, and let u and v be faces of G incident to A and B, respectively. Then* $\operatorname{dist}_G(A,B) \le 2\operatorname{dist}_{G^*}(u,v) + 3$.

Proof. Let $k = \operatorname{dist}_{G^*}(u,v)$, and let P^* be a path of length k between u and v in the dual graph G^*. So $P^* = u_0, u_1, \ldots, u_k$, where $u_0 = u$ and $u_k = v$. Let $\delta(P^*)$ be the edges of G^* with precisely one end vertex in $V(P^*)$. Since the vertices in G^* have degree at most 6, $|\delta(P^*)| \le 6 + 4k$. Therefore, the dual edges to the cut $\delta(P^*)$ form a cycle in G of length at most $6 + 4k$ containing the vertices A and B. Hence, $\operatorname{dist}_G(A,B) \le 2k + 3$. □

Recall that the graph $D^*_{r,t}$ has two special vertices n and s, which can be thought of as the north and south poles. To continue the analogy with geography, we shall define the *latitude* $\varphi(u)$ of a vertex $u \in V(D^*_{r,t})$ as

$$\varphi(u) = \begin{cases} r - \operatorname{dist}(n,u) & \text{if } \operatorname{dist}(n,u) \le r \\ -r + \operatorname{dist}(s,u) & \text{if } \operatorname{dist}(s,u) \le r. \end{cases}$$

In particular, n has latitude r, s has latitude $-r$, and vertices at distance r from n and s have latitude 0, i.e., they lie on the 'equator'.

Proof of Theorem 1. Fix any pair of vertices $A, B \in V(D_{r,t})$. Our goal is to show that $\mathrm{dist}_{D_{r,t}}(A, B) \leq 4r$. To simplify notation, we shall denote the faces in the dual triangulation $D^*_{r,t}$ by the vertices they are incident to (we consider $D^*_{r,t}$ as a simplicial complex). The vertices A, B correspond to faces $A = \{u_1, u_2, u_3\}$ and $B = \{v_1, v_2, v_3\}$ in $D^*_{r,t}$. Note that every face of $D^*_{r,t}$ is incident to two vertices at the same latitude, and another vertex at a different latitude. Assume without loss of generality that $\varphi(u_1) \neq \varphi(u_2)$, and $\varphi(v_1) \neq \varphi(v_2) = \varphi(v_3)$. Furthermore, let $B' = \{v'_1, v_2, v_3\}$ be the (unique) face incident to $\{v_2, v_3\}$ which is different from B.

There exists a path P_u of length $2r$ from n to s containing the subpath u_1, u_2, and a path P_v of length $2r$ from n to s containing the subpath v_1, v_2, v'_1. (To see this, it is enough to note that every vertex $v \in V(D^*_{r,t}) \setminus \{n, s\}$ has a 'northern' neighbour v_N of latitude $\varphi(v_N) = \varphi(v) + 1$ and a 'southern' neighbour v_S of latitude $\varphi(v_S) = \varphi(v) - 1$.) The union $P_u \cup P_v$ is a closed walk W of length $4r$, which must contain two subwalks W_1, W_2 from $\{u_1, u_2\}$ to $\{v_1, v'_1\}$, of length ℓ_1, ℓ_2, respectively. Without loss of generality assume that $\ell_1 \leq \ell_2$. Since $\ell_1 + \ell_2 \leq 4r - 3$, it follows that $\mathrm{dist}_{D^*_{r,t}}(\{u_1, u_2\}, \{v_1, v'_1\}) \leq \ell_1 \leq \lfloor \frac{1}{2}(4r - 3) \rfloor = 2r - 2$.

If $\mathrm{dist}_{D^*_{r,t}}(\{u_1, u_2\}, v_1) \leq 2r - 2$, then $\mathrm{dist}_{D_{r,t}}(A, B) \leq 4r - 1$ by Lemma 2. If $\mathrm{dist}_{D^*_{r,t}}(\{u_1, u_2\}, v'_1) \leq 2r - 2$, then $\mathrm{dist}_{D_{r,t}}(A, B') \leq 4r - 1$ by Lemma 2 again, but then clearly $\mathrm{dist}_{D_{r,t}}(A, B) \leq 4r$. This completes the proof. □

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