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Bipartite Edge Frustration and Maximum Independent Set Problems on Fulleroids-$(3, 4, 6)$

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Abstract

Fulleroid-$(3, 4, 6)$ graphs are planar, cubic, 3-connected graphs with faces of size 3, 4 or 6. Let G be a graph. Determining $\tau_{odd}(G)$ - the smallest number of edges to be deleted from G in order to obtain a bipartite spanning subgraph - is known in the literature as BIPARTITE EDGE FRUSTRATION problem. We studied the BIPARTITE EDGE FRUSTRATION and the MAXIMUM INDEPENDENT SET problems on fulleroid-$(3, 4, 6)$ graphs, obtaining the tight bounds $\tau_{odd}(G) \leq \sqrt{\frac{4}{3}n}$ and $\alpha(G) \geq n/2 - \sqrt{n/3}$, where $\alpha(G)$ is the independence number of G. In order to prove these bounds we use some combinatorial optimization tools.

1 Introduction

In 1985 the scientific community witnessed the discovery of a new molecule formed exclusively by carbon atoms, called *fullerene molecules*.

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The high stability and symmetry of these molecules boosted the study of its chemical, physical and consequently mathematical properties. Each fullerene molecule is modeled by a graph as follows: the atoms of the molecule are represented by the vertices of the graph and the bonds between the atoms correspond to the edges of the graph. This graph modelling the fullerene molecule, is called fullerene graph. A *fullerene graph* is planar, cubic, 3-connected, such that each face has size 5 or 6.

According to Došlić e Vukičević [2], if $G = (V, E)$ is a graph, then an edge $e \in E$ is *frustrated* with respect to a given bipartition (V_1, V_2) of V if both endpoints of e belong to the same set of the bipartition. Let G be a graph. Determining $\tau_{odd}(G)$ - the smallest number of edges to be deleted from a graph G in order to obtain a resulting bipartite spanning subgraph - is known in the literature as BIPARTITE EDGE FRUSTRATION problem.

The fulleroid-$(3,4,6)$ graphs extend fullerene graphs. A *fulleroid*-$(3,4,6)$ graph (or simply fulleroid-$(3,4,6)$) is a planar, cubic, 3-connected graph with all faces of size 3, 4, or 6. From the equation of Euler it is known that every fulleroid-$(3,4,6)$ graph has at most 4 triangular faces (faces of size 3). The central result of this work, Theorem 1.1, provides an upper bound for the bipartite edge frustration problem on fulleroid-$(3,4,6)$ graphs.

Theorem 1.1. *If G is a fulleroid-$(3,4,6)$ graph on n vertices, then $\tau_{odd}(G) \leq \sqrt{\frac{4}{3}n}$ with equality if and only if all faces have size 3, $n = 12k^2$ for some $k \in \mathbb{N}$, and $Aut(G) \cong T_d$.*

The rest of the paper is organized as follows. In Section 2, we discuss specific concepts for the BIPARTITE EDGE FRUSTRATION problem and introduce the concept of moats. In Section 3, we prove a dual version for BIPARTITE EDGE FRUSTRATION problem, after we introduce the Theorem 1.1 and as a consequence we get a result for INDEPENDENT SET problem to fulleroid-$(3,4,6)$ graphs.

2 Preliminary and Moat Concept

All definitions used in this paper are standard and can be found at [3].

According to Bondy and Murty [3], given a plane graph G the dual graph of G, denoted by G, is a graph defined as follows: to each face f of G there is a vertex f^* of G^* and to each edge e of G there is an edge e^* of G^* such that two vertices f^* and g^* are joined by the edge e^* in G^* if and only if their corresponding faces f and g are separated by the edge e in G. As consequence of this definition, the dual graph of a fulleroid-$(3, 4, 6)$ graph is a planar triangulation with no loop or multiple edge, and all its vertices have degree 3, 4 or 6. In the dual of a fulleroid-$(3, 4, 6)$ those vertices of degree 3 or 4 are called by *defective vertices*.

Let G be a planar triangulation with all vertices of degree 3, 4 or 6 and $T \subseteq V(G)$ a set of vertices such that $|T|$ is even. A *T-join* of G is a subset $J \subseteq E(G)$ such that T is the set of odd degree vertices in $G[J]$. It is easy to see that if T is the set of odd degree vertices in G and J is a T-join of G then $|T|$ is even and each vertex belonging to $G - J$ has even degree. The size of the smallest T-join of G is denoted by $\tau(G, T)$.

Let G be a planar triangulation with all vertices of degree 3, 4 or 6 and let $\delta_G(X)$ be the set of edges with exactly one vertex in $X \subseteq V(G)$. A set C of edges of G is an *edge cut* of G if $C = \delta_G(X)$, for some $X \subseteq V(G)$. Let $X \subseteq V(G)$ and T be the set of odd degree vertices of G. A *T-cut* is an edge cut $\delta(X)$ such that $|T \cap X|$ is odd.

A *packing* of T-cuts of G is a disjoint collection $\delta(\mathcal{F}) = \{\delta(X) \mid X \in \mathcal{F}\}$ of T-cuts of G. If T is the set of odd degree vertices in G, then we denote by $\nu(G, T)$ the maximum size of a packing of T-cuts of G. An inclusion-wise minimal is a set obtained from a collection of sets that does not contain any set of this collection. Given a packing of T-cuts, a T-cut $\delta_G(X)$ is an *inclusion wise minimal* when $\delta_G(X)$ contains no T-cut of packing of T-cuts. A family of sets $\mathcal{F}$ is said to be *laminar* if for every pair $X, Y \in \mathcal{F}$, we have $X \subseteq Y$, $Y \subseteq X$, or $X \cap Y = \emptyset$.

Let $X \subset V(G)$ and $G[X]$ be a subgraph 2-connected of G such that all faces of $G[X]$, except possibly the outer face, are triangular faces. A *moat* of width k in G surrounding $G[X]$ is a subset of $E(G)$ defined as:

$$\boxed{\delta_G^k(X) = \bigcup_{i=0}^{k-1} \delta_G\left(N^i[X]\right)}$$

Note that, $\delta_G^1(X) = \delta_G(X)$. If $\sum_{v \in X}(6 - d(v)) = d$, then $\delta_G^k(X)$ is a *d-moat* of width k, see Figure 1.

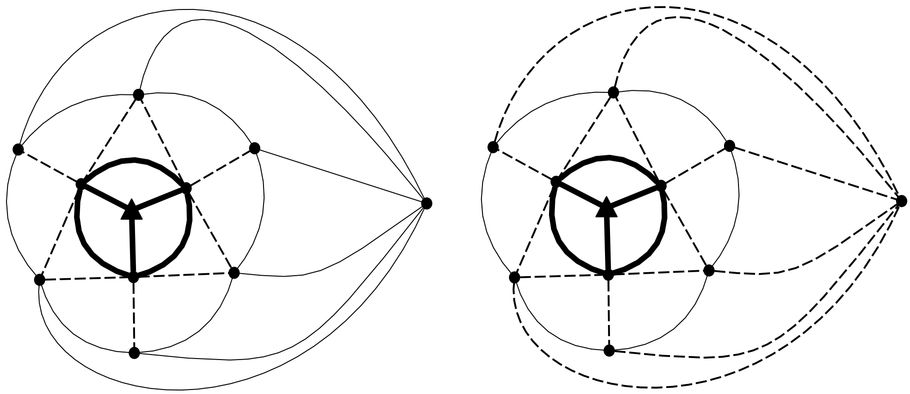

Figure 1: In both figures the thick edges represent $G[X]$. On the left, dashed edges represent a 3-moat of width 1, and on the right, dashed edges represent a 3-moat of widht 2.

Note that for each moat $\delta_G^k(X)$ there exists a set $|\delta_G^k(X)|$ of triangular faces, it means that there exists a one-to-one correspondence between the number of edges in a moat and the number of faces belonging to this moat. We say that the incident faces to at least one edge of $\delta_G^k(X)$ are *spanned* by the moat $\delta_G^k(X)$. If G is a fulleroid-$(3,4,6)$, then the number of edges in a 3-moat of G^* is easily determined by the Lemma 2.1.

Lemma 2.1. *Let G be a fulleroid-$(3,4,6)$ graph, G^* its dual and D the set of defective vertices of G^*. If $d_{G^*}(u) = 3$, and no edge of $\delta^{k-1}(u)$ is incident to a vertex of the set $D - \{u\}$, then $\left|\delta_{G^*}^k(u)\right| = 3k^2$.*

Proof. Note that $\left|\delta(N^i[u])\right| = 3(2i+1)$. Therefore,

$$\left|\delta^k(u)\right| = \sum_{i=0}^{k-1} \left|\delta(N^i[u])\right| = 3\sum_{i=0}^{k-1}(2i+1) = 3k^2.$$

■

3 Main Results

Let G be the dual of a fulleroid-$(3,4,6)$ graph. The graph G is not bipartite, because all its faces are triangular. The graph G', obtained subdividing the edges of G, is bipartite, because all its faces have size 6. Consider $G^{\triangle}$ the graph obtained from G', adding three new edges inside each faces of G', incident to each pair of the 3 vertices of degree 2. The graph $G^{\triangle}$ is said a *refinament* of G. All vertices in $V(G^{\triangle}) - V(G)$ have degree 6 in $G^{\triangle}$, so if D is the set of defective vertices in G, then D is also the set of defective vertices in $G^{\triangle}$. Moreover note that in G there exist only packings of 3-moats for the following reasons: the packings of 5-moats of G would be generated by one vertex of degree 3 and by one vertex of degree 4. Since we want to generate fulleroid-$(3,4,6)$ graphs with arbitrary number of vertices, we should ensure that the vertices of degree 3 are closer together than their distance to any vertex of degree 4. In this way, there is no packing of 5-moats in G.

The Lemma 3.1 has been proved by Klein, Faria and Stehlǐk [4].

Lemma 3.1. *For all planar triangulation G and each subset $T \subseteq V(G)$ such that $|T|$ is even, $\tau(G,T) = \frac{1}{2}\nu(G^{\triangle},T)$. Moreover, there exists an optimal laminar packing of inclusion-wise minimal of T-cuts in $G^{\triangle}$.*

Initially we will study the dual version of the bipatite edge frustration problem for fulleroid-$(3,4,6)$ graphs.

Lemma 3.2. *Let G be a planar triangulation whose vertices have degrees 3, 4 or 6. If f is the number of faces of G and T is the set of odd* *degree vertices of G, then $\tau(G,T) \leq \sqrt{4f/3}$. Equality holds if and only if $f = 12k^2$, for some $k \in \mathbb{N}$, and $Aut(G) \cong T_d$.*

Proof. Let $G^{\triangle}$ be the refinament of G. So $G^{\triangle}$ is a planar triangulation on $4f$ faces and all its vertices have degree 3, 4 or 6. By Lemma 3.1, there exists an optimal laminar packing of inclusion-wise minimal of T-cuts in $G^{\triangle}$. Let m_3 be the number of edges in a 3-moat of $\delta_{G^{\triangle}}(\mathcal{F})$. The incidence vector $\vec{s} \in \mathbb{R}^{|T|}$ is defined as follows: for each vertex $u \in T$ the width of a 3-moat surrounding u is denoted by s_u.

We define *the inner product* in $\mathbb{R}^{|T|}$ by $\left\langle \vec{a}, \vec{b} \right\rangle = \sum_{u \in T} a_u b_u$ and this inner product induces the *norm* $\|\cdot\|$ given by $\|\vec{a}\|^2 = \langle \vec{a}, \vec{a} \rangle$.

It is not difficult to see that $\tau(G^*,T) = \frac{1}{2}\left\langle \vec{r}, \vec{1} \right\rangle$, where the vector $\vec{1} \in \mathbb{R}^{|T|}$ has all coordinates equal to 1.

By Lemma 2.1, $\left|\delta^{s_u}_{G^{\triangle}}(u)\right| = 3s_u^2$. Adding over all 3-moats,

$$m_3 = 3\sum_{u \in T} s_u^2 = 3\|\vec{s}\|^2. \tag{1}$$

The graph $G^{\triangle}$ has $4f$ triangular faces and the 3-moats of $G^{\triangle}$ are spanned by m_3 triangular faces in $G^{\triangle}$. These faces are mutually disjoints.

Using (1), we obtain,

$$4f \geq m_3 \geq 3\|\vec{s}\|^2.$$

Thus,

$$\sqrt{\tfrac{4f}{3}} \geq \|\vec{s}\|\,. \tag{2}$$

Therefore, by (2) and Cauchy-Schwarz inequality,

$$\tau(G^*,T) = \tfrac{1}{2}\left\langle \vec{s}, 1 \right\rangle \leq \tfrac{1}{2}\,\|\vec{s}\|\,\|1\|. \tag{3}$$

Since $\vec{1} = (1,..,1,1)$, then $\|\vec{1}\| \leq \sqrt{4} = 2$ and,

$$\tau(G^*,T) \leq \frac{1}{2}\|\vec{s}\|\,\|1\| = \|\vec{s}\|\,.$$

Finally,

$$\tau(G^*,T) \leq \sqrt{\frac{4f}{3}}.$$

To the last part of Lemma 3.2, supose that $\tau(G,T) = \sqrt{\frac{4}{3}f}$. Consequently the entries of the vector $\vec{s}$ must all be equal, let's say equal to s_u, for all $u \in T$ and $\sqrt{\frac{4f}{3}} = ||\vec{s}||$. Therefore, $4f = 3||\vec{s}||^2$ and $4f = 3 \cdot 4s_u^2$. Since f is even, then $s_u = 2k$ and $f = 12k^2$, for some $k \in \mathbb{N}$. To see that $Aut(G) \cong T_d$, note that the graph G can be obtained from the regular tetrahedron by inserting into each face of a 3-patch of the form $G[N^k[u]]$. Conversely, if G is a plane triangulation with $f = 12k^2$ faces, all vertices of degree 3, 4 or 6, and $Aut(G) \cong T_d$, then G may be constructed from the regular tetrahedron by inserting into each face a 3-patch of the form $G^*[N^k[u]]$. Therefore, $dist(u,v) \geq 2k$, for each pair of distinct vertices in T, so $\tau(G,T) \geq 4k = \sqrt{\frac{4}{3}f}$.

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Theorem 3.1 provides an upper bound to bipartite edge frustration problem for fulleroids-$(3,4,6)$ and is a consequence from Lemma 3.2.

Theorem 3.1. *If G is a fulleroid-$(3,4,6)$ graph on n vertices, then $\tau_{odd}(G) \leq \sqrt{\frac{4}{3}n}$. Equality holds if and only if $n = 12k^2$, for some $k \in \mathbb{N}$, e $Aut(G) \cong T_d$.*

As a consequence of Theorem 3.1 we have the following corollary.

Corollary 3.2. *If G is a fulleroid-$(3,4,6)$ on n vertices, then $\alpha(G) \geq n/2 - \sqrt{n/3}$. Equality holds if and only if $n = 12k^2$, for some $k \in \mathbb{N}$, e $Aut(G) \cong T_d$.*

Figure 3 shows a sharp example for bipartite edge frustration and maximum independent set on a fulleroid-$(3,6)$.

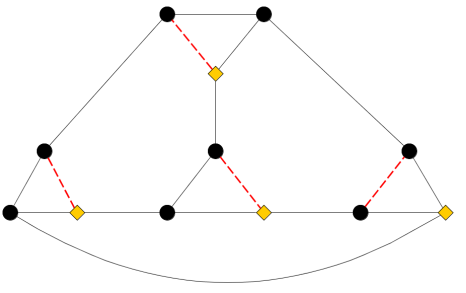

Figure 2: A fulleroid-$(3,4,6)$ G, such that $\tau_{odd}(G) = 4$, $\alpha(G) = 4$.

4 Conclusion

We establish bounds for bipartite edge frustration and maximum independent set on fulleroid-$(3,4,6)$ graphs and we provide an example of a fulleroid-$(3,4,6)$ that is sharp for both bounds..

In future works, we intend to find a solution for bipartite edge frustration and maximum independent set problems for more general fulleroid graphs.

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