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ON A CONJECTURE ABOUT DEGREE DEVIATION MEASURE OF GRAPHS

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ABSTRACT. Let G be an n -vertex graph with m edges. The degree deviation measure of G is defined as $s(G) = \sum_{v \in V(G)} |deg_G(v) - \frac{2m}{n}|$, where n and m are the number of vertices and edges of G , respectively. The aim of this paper is to prove the Conjecture 4.2 of [J. A. de Oliveira, C. S. Oliveira, C. Justel and N. M. Maia de Abreu, Measures of irregularity of graphs, *Pesq. Oper.*, **33** (2013) 383–398]. The degree deviation measure of chemical graphs under some conditions on the cyclomatic number is also computed.

1. Introduction

Throughout this paper all graphs are assumed to be simple and undirected. If G is such a graph, then the vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The *degree* of a vertex v is denoted by $deg_G(v)$ (or $deg(v)$ for short), $N[v, G]$ is the set of all vertices adjacent to v and $H(n)$ denotes the set of all connected n -vertex graphs.

A *clique* of a graph G is a subset of vertices such that its induced subgraph is a complete subgraph of G and a *stable set* in G is a subset of vertices no two of which are adjacent. Let k and n be integers such that $0 \leq k \leq n$. A graph $S(n, k)$ is a *split graph* if there is a partition of its vertex set into a clique of order k and a stable set of order $n - k$. A *complete split graph*, $CS(n, k)$, is a split graph such that each vertex of the clique is adjacent to each vertex of the stable set [6].

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A graph in which all vertices have the same degree is said to be *regular*. Suppose α is a function from the set of all graphs into non-negative real numbers. If $\alpha(G) = 0$ if and only if G is regular, then the function α is called a *measure of regularity*. It is merit to mention here that for a graph H , the graph invariant $\Omega(H) = M_1(H)^2 - 4mM_2(H)$, proposed by Réti and Drégelyi-Kiss [8] is zero not only for every regular graph but it is zero also for the non-regular graphs J_1 and J_2 , where m is the size of H , $M_1(H) = \sum_{v \in V(H)} \deg_H(v)^2$ and $M_2(H) = \sum_{uv \in E(H)} \deg_H(u)\deg_H(v)$ [5]. The graphs J_1 and J_2 in Figure 1 which are taken from [8] explains the reason that in definition of a measure of irregularity we force the invariant α to be zero only for regular graphs.

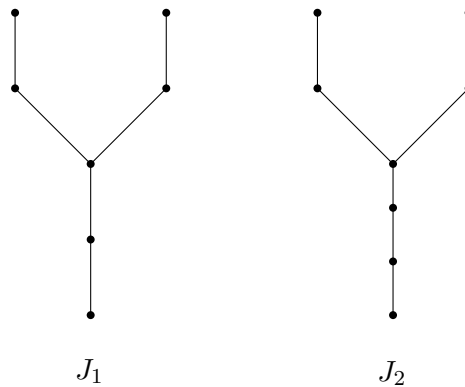


FIGURE 1. The graphs J_1 and J_2 .

Albertson [1] introduced a measure of irregularity for graphs as $irr(G) = \sum_{xy \in E(G)} |deg(x) - deg(y)|$ and determined the maximum irregularity of various classes of graphs. As a consequence of his results, the irregularity of an n -vertex graph is less than $\frac{4n^3}{27}$, and the bound is tight. Abdo et al. [3] proposed an extended version of the irregularity measure of Albertson which is called the *total irregularity*. It is defined as $irr_t(G) = \frac{1}{2} \sum_{u,v \in V(G)} |deg(u) - deg(v)|$. They obtained all graphs with maximal total irregularity and proved that among all trees of the same order the star has the maximal total irregularity.

Following Nikiforov [7], the *degree deviation measure* of G is defined as

$$s(G) = \sum_{v \in V(G)} \left| deg_G(v) - \frac{2m}{n} \right|,$$

where n and m are the number of vertices and edges of G , respectively. Let G be a graph with maximum eigenvalue $\mu(G)$. The well-known result of Euler which states that $\sum_{v \in V(G)} deg_G(v) = 2|E(G)|$ implies that the degree deviation measure $s(G)$ is a measure of irregularity. Nikiforov proved that

$$\frac{s^2(G)}{2n^2\sqrt{2m}} \leq \mu(G) - \frac{2m}{n} \leq \sqrt{s(G)}$$

and these inequalities are tight up to a constant factor.

de Oliveira et al. [6] investigated four distinct graph invariants used to measure the irregularity of a graph and proved the following theorem:

Theorem 1.1. *Let $k \in \mathbb{N}$ and $0 \leq k \leq n$. If $G = CS(n, k)$ is a complete split graph then $s(G) = \frac{n}{2}k(n - k)(n - 1 - k)$. Besides, among all complete split graphs, the most irregular one by $s(G)$ has to attend the following conditions on k :*

$$k = \begin{cases} \frac{n}{3} & 3 \mid n \\ \frac{n-1}{3} & 3 \mid n - 1 \\ \frac{n-2}{3} \text{ and } \frac{n+1}{3} & 3 \mid n - 2 \end{cases} .$$

They conjectured that

Conjecture 1.2. *Let $H(n)$ be the set of all connected graphs G with n vertices. Then $\max_{G \in H(n)} s(G) = s(CS(n, k))$, where*

$$k = \begin{cases} \frac{n}{3} & 3 \mid n \\ \frac{n-1}{3} & 3 \mid n - 1 \\ \frac{n-2}{3} \text{ and } \frac{n+1}{3} & 3 \mid n - 2 \end{cases}$$

The aim of this paper is to prove Conjecture 1.2 and then compute the degree deviation measure of a chemical graph G under some conditions on its cyclomatic number. We refer to [4] for some mathematical properties of vertex degrees in graphs.

2. Proof of the Conjecture

In this section, we will present a proof for Conjecture 1.2. To do this, we need some notations as follows:

$$\begin{aligned} V^\downarrow(G) &= \{v \in V(G) \mid \deg_G(v) \leq \frac{2m}{n}\}, \\ V^\uparrow(G) &= \{v \in V(G) \mid \deg_G(v) > \frac{2m}{n}\}, \\ E^\downarrow(G) &= \{uv \in E(G) \mid \{u, v\} \subseteq V^\downarrow(G)\}, \\ \overline{E}^\uparrow(G) &= \{\{u, v\} \subseteq V^\uparrow(G) \mid uv \notin E(G)\}. \end{aligned}$$

The well-known result of Euler which states that $\sum_{v \in V(G)} \deg_G(v) = 2|E(G)|$ lead us to the following useful lemma:

Lemma 2.1. *Let $F(n, m)$ denote the family of all connected graphs with n vertices and m edges. Then,*

- (1) $\{G \in F(n, m) \mid V^\downarrow(G) = V(G)\} = \{G \in F(n, m) \mid G \text{ is } \frac{2m}{n} - \text{regular}\},$
- (2) $\{G \in F(n, m) \mid V^\uparrow(G) = V(G)\} = \emptyset.$

Lemma 2.2. *Let G be a connected n -vertex irregular graph, $n \geq 3$, and $e = uv \in E^\downarrow(G)$ is not a cut edge of G . If $G^- = G - e$ then $s(G) < s(G^-)$.*

Proof. Let $V_1^\downarrow(G) = \{v \in V^\downarrow(G) : \text{deg}_G(v) > \frac{2m-2}{n}\}$. By definition,

$$\begin{aligned} s(G^-) - s(G) &= \frac{2m-2}{n} - \text{deg}_G(u) + 1 + \frac{2m-2}{n} - \text{deg}_G(v) + 1 \\ &- \left[\frac{2m}{n} - \text{deg}_G(u) + \frac{2m}{n} - \text{deg}_G(v) \right] + \sum_{w \in V_1^\downarrow(G)} 2 \left[\text{deg}_G(w) - \frac{2m-1}{n} \right] \\ &- \sum_{w \in V^\downarrow(G) \setminus (V_1^\downarrow(G) \cup \{u,v\})} \frac{2}{n} + \sum_{v \in V^\uparrow(G)} \frac{2}{n} \\ &\geq 2 - \frac{2}{n} \left[\left| V^\downarrow(G) \setminus V_1^\downarrow(G) \right| - \left| V^\uparrow(G) \right| \right] > 0, \end{aligned}$$

proving the lemma. □

Lemma 2.3. *Let G be a connected irregular n -vertex graph, $n \geq 3$, and $\{w, z\} \in \overline{E}^\uparrow(G)$. If $G^+ = G + f$, $f = wz$, then $s(G) < s(G^+)$.*

Proof. Let $V_1^\uparrow(G) = \{v \in V^\uparrow(G) : \text{deg}_G(v) \leq \frac{2m+2}{n}\}$. By definition,

$$\begin{aligned} s(G^+) - s(G) &= \text{deg}_G(u) + 1 - \frac{2m+2}{n} + \text{deg}_G(v) + 1 - \frac{2m+2}{n} \\ &- \left[\text{deg}_G(u) - \frac{2m}{n} + \text{deg}_G(v) - \frac{2m}{n} \right] + \sum_{w \in V_1^\uparrow(G)} 2 \left[\frac{2m+1}{n} - \text{deg}_G(w) \right] \\ &+ \sum_{w \in V^\downarrow(G)} \frac{2}{n} - \sum_{w \in V^\uparrow(G) \setminus (V_1^\uparrow(G) \cup \{u,v\})} \frac{2}{n} \\ &\geq 2 - \frac{2}{n} \left[\left| V^\uparrow(G) \setminus V_1^\uparrow(G) \right| - \left| V^\downarrow(G) \right| \right] > 0, \end{aligned}$$

proving the lemma. □

Suppose G is a connected irregular graph with a cut edge $e = uv \in E^\downarrow(G)$. It is clear that there exists a vertex $w \in V^\uparrow(G)$ such that at least one of the graphs $G - uv + uw$ and $G - uv + vw$ is connected. Without loss of generality, we assume that $G - uv + uw$ is connected. Then the edge uw is called a *connectedness factor* of $G - e$ with respect to $V^\downarrow(G)$ and $V^\uparrow(G)$.

Lemma 2.4. *Let G be a connected irregular n -vertex graph, $n \geq 3$, and $e = uv \in E^\downarrow(G)$ is an cut edge of G . If $w \in V^\uparrow(G)$, $G^* = G - uv + uw$ and uw is a connectedness factor of $G - uv$ with respect to $V^\downarrow(G)$ and $V^\uparrow(G)$, then $s(G) < s(G^*)$.*

Proof. By definition,

$$\begin{aligned} s(G^*) - s(G) &= \frac{2m}{n} - (\text{deg}_G(v) - 1) + \text{deg}_G(w) + 1 - \frac{2m}{n} \\ &- \left[\frac{2m}{n} - \text{deg}_G(v) + \text{deg}_G(w) - \frac{2m}{n} \right] \\ &= 2, \end{aligned}$$

as desired. □

Lemma 2.5. Suppose G is a connected irregular n -vertex graph such that $V^\uparrow(G) = \{u_1, \dots, u_k\}$ is a clique, $V^\downarrow(G) = \{v_1, \dots, v_{n-k}\}$ is a stable set and $\sum_{i=1}^{n-k} \deg_G(v_i) < |V^\downarrow(G)|k$. Let $N[G, v_i] = \{u_{i_1}, \dots, u_{i_{\deg_G(v_i)}}\}$, for $1 \leq i \leq n - k$.

- (1) If $|V^\downarrow(G)| > |V^\uparrow(G)|$ and $G^\ddagger = G + \{v_i u_j : 1 \leq i \leq n - k \text{ and } u_j \in V^\uparrow(G) \setminus N[v, G]\}$, then $s(G) < s(G^\ddagger)$.
- (2) If $|V^\downarrow(G)| \leq |V^\uparrow(G)|$ and $G^\top = G - \{v_i u_{i_j} : 1 \leq i \leq n - k \text{ and } 2 \leq j \leq \deg_G(v_i)\}$, then $s(G) \leq s(G^\top)$.

Proof. Let $\alpha = |\{v_i u_j : 1 \leq i \leq n - k \text{ and } u_j \in V^\uparrow(G) \setminus N[v, G]\}|$. To prove (1), we note that:

$$\begin{aligned} s(G^\ddagger) - s(G) &= k(k-1) + (n-k)k - \frac{2m+\alpha}{n}|V^\uparrow(G)| + \frac{2m+\alpha}{n}|V^\downarrow(G)| - (n-k)k \\ &\quad - \left[k(k-1) + (n-k)k - \alpha - \frac{2m}{n}|V^\uparrow(G)| + \frac{2m}{n}|V^\downarrow(G)| - (n-k)k + \alpha \right] \\ &= \frac{\alpha}{n}|V^\downarrow(G)| - \frac{\alpha}{n}|V^\uparrow(G)| > 0, \end{aligned}$$

as desired. Part (2) follows from definition, above discussion and the fact that, $s(G^\top) - s(G) = \frac{\alpha}{n}|V^\uparrow(G)| - \frac{\alpha}{n}|V^\downarrow(G)| \geq 0$. □

Let $S^1(n, k)$ be a split graph such that all vertices in its stable set are of degree one. Define:

$$\begin{aligned} H(n, 1) &:= \{G \in H(n) : \text{for one } 1 \leq k \leq n - 1, G \cong S^1(n, k)\}, \\ CH(n) &:= \{G \in H(n) : \text{for one } 1 \leq k \leq n - 2, G \cong CS(n, k)\}. \end{aligned}$$

Lemma 2.6. Let $k \in N$ and $1 < k < n - 1$. Then $\max_{G \in H(n, 1)} s(G) = s(S^1(n, k))$, where

$$k = \begin{cases} \frac{2}{3}n & 3 \mid n \\ \frac{2}{3}(n-1) & 3 \mid n-1 \\ 1 \text{ and } 2 & n = 5 \\ \frac{2}{3}(n+1) & n \neq 5 \text{ and } 3 \mid n-2 \end{cases}.$$

Proof. By definition $s(S^1(n, k)) = \frac{2}{n}(3k - k^2 - n)(n - k)$. For a given n , define $g(k) = \frac{2}{n}(3k - k^2 - n)(n - k)$. By a simple calculation the maximal value of $g(k)$ is obtained by $k = \frac{2}{3}n$. Since k is an integer, we have to determine $\lceil k \rceil$ and $\lfloor k \rfloor$ and then comparing $g(\lceil k \rceil)$ and $g(\lfloor k \rfloor)$ in all previous cases give the our result. □

Lemma 2.7. Let $k \in N$ and $1 < k < n - 1$. Then $\max_{G \in H(n, 1)} s(G) < \max_{G \in CH(n)} s(G)$.

Proof. Let $\max_{G \in CH(n)} s(G) = \lambda$ and $\max_{G \in H(n, 1)} s(G) = \mu$. By Theorem 1.1 and Lemma 2.6,

$$\lambda - \mu = \begin{cases} \frac{2}{9}n & 3 \mid n \\ \frac{2}{9} \frac{(n+2)^2 - 18}{n} & 3 \mid n - 1 \\ \frac{2}{9} \frac{(n+4)(n-2)}{n} & 3 \mid n - 2 \end{cases},$$

as desired. □

We are now ready to prove Conjecture 1.2.

Theorem 2.8. *Let $H(n)$ be the set of all connected graphs G with n vertices. Then, $\max_{G \in H(n)} s(G) = s(CS(n, k))$, where*

$$k = \begin{cases} \frac{n}{3} & 3 \mid n \\ \frac{n-1}{3} & 3 \mid n-1 \\ \frac{n-2}{3} \text{ and } \frac{n+1}{3} & 3 \mid n-2 \end{cases} .$$

Proof. Suppose G is not a regular graph. Then by repeated applications of Lemmas 2.2, 2.3 and 2.4, we obtain a connected split graph $H = S(n, k)$ such that $s(G) \leq s(H)$. Now by repeated applications of Lemmas 2.5 on graph H , we obtain a $F = S^1(n, k)$ or $F = CS(n, k)$ such that $s(G) \leq s(H) \leq s(F)$ with equality if and only if $G \cong S^1(n, k)$ or $G \cong CS(n, k)$. The proof follows from Theorem 1.1 and Lemmas 2.6, 2.7. \square

3. Connected Chemical Graphs

The aim of this section is to continue the interesting paper [2] by computing the degree deviation measure of chemical graphs under some conditions on the cyclomatic number.

Suppose $n_i = n_i(G)$ is the number of vertices of degree i in a graph G . It can be easily seen that $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$. If the graph G has exactly n vertices, m edges and k components, then $c = m - n + k$ is called the *cyclomatic number* of G . A *chemical graph* is a graph with the condition that all vertex degrees are less than or equal to 4. A connected chemical graphs with exactly n vertices and cyclomatic number c is called (n, c) -*chemical graph*.

Lemma 3.1. [4] *Let G be an (n, c) -chemical graph. Then*

$$n_1(G) = 2 - 2c + n_3 + 2n_4 \quad \text{and} \quad n_2(G) = 2c + n - 2 - 2n_3 - 3n_4 .$$

Lemma 3.2. *Let T be a chemical tree with n vertices. Then*

$$s(T) = \frac{4(n-2)}{n} + \frac{n-2}{n} [2n_3(T) + 4n_4(T)] .$$

Proof. Since $|E(T)| = n - 1$,

$$\begin{aligned} s(T) &= n_1(T) \left[\frac{2(n-1)}{n} - 1 \right] + n_2(T) \left[2 - \frac{2(n-1)}{n} \right] + n_3(T) \left[3 - \frac{2(n-1)}{n} \right] \\ &+ n_4(T) \left[4 - \frac{2(n-1)}{n} \right] \\ &= \frac{n-2}{n} n_1(T) + \frac{2}{n} n_2(T) + \frac{n+2}{n} n_3(T) + \frac{2n+2}{n} n_4(T) . \end{aligned}$$

We now apply Lemma 3.1 to deduce that $s(T) = \frac{4(n-2)}{n} + \frac{n-2}{n} [2n_3(T) + 4n_4(T)]$, proving the lemma. \square

Corollary 3.3. *Let T be a chemical tree with n vertices. Then $s(T) \geq \frac{4(n-2)}{n}$, with equality if and only if $T \cong P_n$.*

Lemma 3.4. *Let G be an $(n, 1)$ -chemical graph. Then $s(G) = 2n_3(G) + 4n_4(G)$.*

Proof. Since $|E(G)| = n$,

$$\begin{aligned} s(G) &= n_1(G)[2 - 1] + n_2(G)[2 - 2] + n_3(G)[3 - 2] + n_4(G)[4 - 2] \\ &= n_1(G) + n_3(G) + 2n_4(G), \end{aligned}$$

and by Lemma 3.1, $s(G) = 2n_3(G) + 4n_4(G)$, as desired. □

Theorem 3.5. *Let G be an (n, c) -chemical graph such that $c \geq 2$.*

(1) *If $n > 2c - 2$, then*

$$s(G) = \frac{1}{n} \left[(2n - 4c + 4)n_3(G) + (4n - 4c + 4)n_4(G) \right].$$

(2) *If $n \leq 2c - 2$, then $s(G) = \frac{4(n-c+1)}{n}n_4(G)$.*

Proof. By definition, $|E(G)| = n + c - 1$.

(1) $n > 2c - 2$. Then,

$$\begin{aligned} s(G) &= n_1(G) \left[\frac{2(n+c-1)}{n} - 1 \right] + n_2(G) \left[\frac{2(n+c-1)}{n} - 2 \right] \\ &+ n_3(G) \left[3 - \frac{2(n+c-1)}{n} \right] + n_4(G) \left[4 - \frac{2(n+c-1)}{n} \right] \\ &= \frac{n+2c-2}{n}n_1(G) + \frac{2c-2}{n}n_2(G) + \frac{n-2c+2}{n}n_3(G) + \frac{2n-2c+2}{n}n_4(G), \end{aligned}$$

and by Lemma 3.1

$$s(G) = \frac{1}{n} \left[(2n - 4c + 4)n_3(G) + (4n - 4c + 4)n_4(G) \right].$$

(2) $n \leq 2c - 2$. By the well-known result of Euler, $2|E(G)| = \sum_{v \in V(G)} \deg_G(v) \leq \sum_{v \in V(G)} 4 = 4n$. Therefore, $c = |E(G)| - n + 1 \leq n + 1$. Thus $2c - 2 \leq 2n$ and

$$\begin{aligned} s(G) &= n_1(G) \left[\frac{2(n+c-1)}{n} - 1 \right] + n_2(G) \left[\frac{2(n+c-1)}{n} - 2 \right] \\ &+ n_3(G) \left[\frac{2(n+c-1)}{n} - 3 \right] + n_4(G) \left[4 - \frac{2(n+c-1)}{n} \right] \\ &= \frac{n+2c-2}{n}n_1(G) + \frac{2c-2}{n}n_2(G) + \frac{2c-2-n}{n}n_3(G) + \frac{2n-2c+2}{n}n_4(G), \end{aligned}$$

and by Lemma 3.1, $s(G) = \frac{4(n-c+1)}{n}n_4(G)$.

Hence the result. □

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