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On Graph Irregularity Indices with Particular Regard to Degree Deviation

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Abstract. Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph of order n and size m, with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. A graph G is said to be regular if $d_1 = d_2 = \cdots = d_n$. Otherwise it is irregular. In many applications and problems it is important to know how irregular a given graph is. A quantity called degree deviation $S(G) = \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right|$ can be used as an irregularity measure. Some new lower bounds for $S(G)$ are obtained. A simple formula for computing $S(G)$ for connected bidegreed graphs is derived also. Besides, two novel irregularity measures are introduced.

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph with n vertices, m edges and a sequence of vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(v_i)$. With $i \sim j$ we denote the adjacency of vertices v_i and v_j in graph G.

A topological index, or a graph invariant, is a numerical quantity which is invariant under automorphisms of the graph. Topological indices are important and useful tools in mathematical chemistry, nanomaterials, pharmaceutical engineering, etc. used for quantifying information on molecules. Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph.

The first and the second Zagreb indices are vertex-degree-based graph invariants introduced in [25] and [26], respectively, and defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i \sim j} (d_i + d_j) \quad \text{and} \quad M_2(G) = \sum_{i \sim j} d_i d_j.$$

Both $M_1(G)$ and $M_2(G)$ were recognized to be a measure of the extent of branching of the carbon–atom skeleton of the underlying molecule.

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In [13] it was proven that for $M_1(G)$ holds the followig identity

$$M_1(G) = \sum_{i=1}^{n} t_i d_i\,,$$

where t_i stands for the average of degrees of vertices adjacent to v_i in G.

A modification of the first Zagreb index, defined as the sum of third powers of vertex degrees, that is

$$F(G) = \sum_{i=1}^{n} d_i^3 = \sum_{i\sim j} (d_i^2 + d_j^2)\,,$$

was encountered in [25] as well. However, for the unknown reasons, it did not attracted any attention until 2015 when it was reinvented in [19] and named the forgotten topological index.

The inverse degree of a graph G, with no isolated vertices, is defined in [17] as

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i\sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right).$$

The inverse degree first attracted attention through conjectures of the computer program Graffiti [17].

In [40] the modified first Zagreb index, ${}^{m}M_1(G)$, was defined as

$${}^{m}M_1(G) = \sum_{i=1}^{n} \frac{1}{d_i^2} = \sum_{i\sim j} \left(\frac{1}{d_i^3} + \frac{1}{d_j^3} \right).$$

Generalization of the second Zagreb index, reported in the [9], known as general Randić index, $R_\alpha(G)$, is defined as

$$R_\alpha(G) = \sum_{i\sim j} (d_i d_j)^\alpha\,,$$

where α is a real number. Some well known special cases are $R_{-1}(G)$ (general Randić index R_{-1}) and ordinary Randić index $R(G) = R_{-\frac{1}{2}}(G)$ [43].

A family of 148 discrete Adriatic indices was introduced and analyzed in [49] (see also [50]). The so-called inverse sum indeg index, was singled out in [50] as being a significantly accurate predictor of total surface area of octane isomers. It is defined as

$$ISI(G) = \sum_{i\sim j} \frac{d_i d_j}{d_i + d_j}\,.$$

More details about above mentioned indices can be found in the recent surveys [6, 10], where the mathematical properties of these indices have been summarized.

A graph G is regular if and only if $d_1 = d_2 = \cdots = d_n > 0$. A connected graph is called irregular if it contains at least two vertices with different degrees. A bidegreed graph $G(\Delta, \delta)$ is an irregular graph whose vertices have exactly two degrees, δ and Δ. A connected bipartite bidegreed graph $G(\Delta, \delta)$ is semiregular if every edge of G joins a vertex of degree δ to a vertex of degree Δ [31].

A topological index $IT(G)$ is a graph irregularity index if $IT(G) \geq 0$, and $IT(G) = 0$ if and only if G is a regular graph. In many applications and problems it is of importance to know how much a given graph deviates from being regular, i.e., how great its irregularity is. For this purpose, various quantitative measure of graph irregularity have been proposed. Some of these measures are in terms of vertex degrees, of which the Albertson index [5]

$$Alb(G) = \sum_{i\sim j} |d_i - d_j|\,,$$

and the Bell index [8]

$$Var(G) = \frac{1}{n}\sum_{i=1}^{n}\left(d_i - \frac{2m}{n}\right)^2 ,$$

are the most popular.

Trying to avoid the absolute value calculation in the Albertson index, the irregularity index $\sigma(G)$ was recently introduced in [3, 4, 22]. It is defined as

$$\sigma(G) = \sum_{i\sim j}(d_i - d_j)^2 .$$

In [39] Nikiforov suggested degree deviation, $S(G)$, defined as

$$S(G) = \sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right| ,$$

to be used as a measure of irregularity of G. It needs to be mentioned here that the degree deviation of G is actually n times the discrepancy of G [28, 29]. Some mathematical properties of the degree deviation can be found in the survey [41] and papers [33, 39].

In [20] Goldberg noticed that the simplest irregularity measure is $d(G) = \Delta - \delta$. It is really simple, but it is (completely) insensitive to the changes of parameter m when parameters d_1 and d_n remain unchanged. Thus, for example, if graph G_1 is obtained by adding edges to the graph G, while d_1 and d_n remain unchanged, then $d(G_1) = d(G)$. However, it is obvious that G deviates from regularity more than G_1. Therefore it is desirable that irregularity measure is sensitive to the changes of all basic graph parameters: n, m, d_1 and d_n. In [2] it was observed that most irregularity measures are mutually inconsistent. Namely, for any two irregularity indices $Ir_1(G)$ and $Ir_2(G)$, there exist pair of graphs G_1, G_2, such that $Ir_1(G_1) > Ir_2(G_1)$, but $Ir_1(G_2) < Ir_2(G_2)$. This means that there is no single parameter that can be used to measure the irregularity of graphs. A relevant list of papers concerned with various irregularity measures, but hardly exhaustive, would include [1, 5, 8, 10, 11, 15, 16, 21, 23, 24, 33, 34, 39, 41, 44–46].

In this paper we further investigate degree deviation, $S(G)$, and introduce two novel irregularity measures.

The rest of the paper is organized as follows. In section 2 we recall some discrete inequalities for real number sequences. Different lower bounds for $S(G)$ are derived in Section 3. A simple formula for computing $S(G)$ for connected bidegreed graphs is presented in Section 4. Finally, two novel irregularity indices are presented in Section 5.

2. Preliminaries

In this section we recall a few discrete analytical inequalities for real number sequences that will be often used in this paper.

Let $x = (x_i)$, $i = 1, 2, \ldots, n$, be a sequence of real numbers with the properties

$$\sum_{i=1}^{n} x_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} |x_i| = 1. \tag{1}$$

In the monograph [38, pp. 346] it was proven that for any real number sequence $a = (a_i)$, $i = 1, 2, \ldots, n$, holds

$$\left|\sum_{i=1}^{n} a_i x_i\right| \le \frac{1}{2}\left(\max_{1\le i\le n} a_i - \min_{1\le i\le n} a_i\right). \tag{2}$$

Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a sequence of nonnegative real numbers, and $a = (a_i)$, $i = 1, 2, \dots, n$, a sequence of positive real numbers. Then for any real r, $r \le 0$ or $r \ge 1$, holds [37]

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \ge \left(\sum_{i=1}^{n} p_i a_i\right)^r . \tag{3}$$

When $0 \le r \le 1$, the opposite inequality holds in (3). Equality is attained if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, for some t, $1 \le t \le n-1$.

Let $x = (x_i)$, $i = 1, 2, \dots, n$ be a sequence of non negative real numbers, and $a = (a_i)$, $i = 1, 2, \dots, n$, a sequence of positive real numbers. In [42] it was proved that for any real r, $r \ge 0$, holds

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^r} , \tag{4}$$

with equality holding if and only if $r = 0$, or $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

3. Lower bounds for S(G)

In the following theorem we determine a lower bound for $S(G)$ in terms of topological index $ID(G)$ and parameters n, m, Δ and δ.

Theorem 3.1. *Let G be a simple connected irregular graph, with $n \ge 3$ vertices and m edges. Then*

$$S(G) \ge \frac{2(2mID(G) - n^2)\Delta\delta}{n(\Delta - \delta)}. \tag{5}$$

Equality holds if and only if $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$ for some t, $1 \le t \le n-2$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$.

Proof. Let $x = (x_i)$, $i = 1, 2, \dots, n$, be real number sequence defined as $x_i = \dfrac{d_i - \frac{2m}{n}}{S(G)}$. Since

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \frac{d_i - \frac{2m}{n}}{S(G)} = 0 \quad \text{and} \quad \sum_{i=1}^{n} |x_i| = \sum_{i=1}^{n} \left| \frac{d_i - \frac{2m}{n}}{S(G)} \right| = \frac{S(G)}{S(G)} = 1,$$

this sequence satisfies identities (1). Now, for $a_i = \frac{1}{d_i}$, $i = 1, 2, \dots, n$, from (2) we get

$$\left| \sum_{i=1}^{n} \frac{d_i - \frac{2m}{n}}{d_i S(G)} \right| \le \frac{1}{2} \left(\max_{1 \le i \le n} \frac{1}{d_i} - \min_{1 \le i \le n} \frac{1}{d_i} \right),$$

that is

$$\left| n - \frac{2m}{n} ID(G) \right| \le \frac{1}{2} \frac{(\Delta - \delta)S(G)}{\Delta\delta}. \tag{6}$$

Based on the arithmetic–harmonic mean inequality, AM–HM inequality (see e.g. [38]), we have that

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{1}{d_i} \ge n^2,$$

i.e.

$$n^2 - 2mID(G) \le 0.$$

From the above and (6) it follows

$$(\Delta - \delta)S(G) \geq \frac{2\Delta\delta(2mID(G) - n^2)}{n}.$$

If G is regular, then equality occurs in the above inequality. Without loss of generality, we can assume that G is irregular. From the above inequality immediately follows (5). □

In the next corollary of Theorem 3.1 we establish lower bound for $S(G)$ in terms of $R_{-1}(G)$ and parameters n, m, Δ and δ.

Corollary 3.2. *Let G be a simple irregular graph, with $n \geq 3$ vertices and m edges. Then*

$$S(G) \geq \frac{2\Delta\delta \left|4mR_{-1}(G) - n^2\right|}{n(\Delta - \delta)}. \tag{7}$$

Proof. The following inequality was proven in [31]

$$ID(G) \geq 2R_{-1}(G), \tag{8}$$

as a part of one broader result. Equality in (8) holds if and only if G is regular.

Based on the identity

$$ID(G) = \sum_{i\sim j} \left(\frac{d_i + d_j}{d_i d_j}\right)^2 - 2R_{-1}(G),$$

in [35] it was proven that

$$ID(G) \geq \frac{n^2}{m} - 2R_{-1}(G), \tag{9}$$

with equality if and only if G is regular or semiregular graph.

The inequalities (8) and (9) are not comparable. As an example, consider two bidegreed graphs G_1 and G_2 depicted in Figure 1.

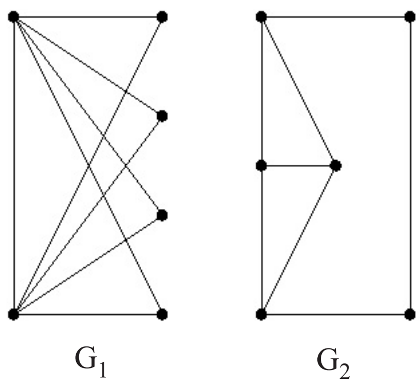

Figure 1. Bidegreed connected 6-vertex graphs.

When $G = G_1$, the inequality (9) is stronger than (8). However, when $G = G_2$, (8) is stronger than (9). Therefore we have that

$$ID(G) \geq \max\left\{2R_{-1}(G), \frac{n^2}{m} - 2R_{-1}(G)\right\},$$

with equality if and only if G is regular.

From the above and inequality (5) we have that

$$S(G) \geq \max\left\{ \frac{2\Delta\delta(4mR_{-1}(G) - n^2)}{n(\Delta - \delta)}, \frac{2\Delta\delta(n^2 - 4mR_{-1}(G))}{n(\Delta - \delta)} \right\},$$

from which (7) is obtained.

□

Denote by $U_{t,\Delta}^{k}$ a class of unicyclic graphs with $n = k + t(\Delta - 1)$ vertices, $k \equiv n \mod (\Delta - 1)$, from which t are of degree Δ, k of degree 2 and $t(\Delta - 2)$ of degree 1, as presented in Figure 2.

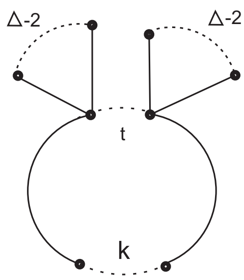

Figure 2.

In the next corollary of Theorem 3.1 we obtain a lower bound for $S(G)$ when $G \cong U$ is an arbitrary unicyclic connected graph.

Corollary 3.3. *Let U, $U \ncong C_n$, be unicyclic connected graph with $n \geq 4$ vertices. Then*

$$S(U) \geq \frac{2\Delta\delta(2ID(U) - n)}{\Delta - \delta}. \tag{10}$$

Equality holds if and only if $U \in U_{t,\Delta}^{k}$, $\Delta \geq 3$, $t \geq 1$ and $k \equiv n \mod (\Delta - 1)$.

Remark 3.4. *According to (10) we get that the largest lower bound for $S(G)$, when G is an arbitrary connected unicyclic graph, is*

$$S(U) = \frac{2(n-k)(\Delta - 2)}{\Delta - 1},$$

where $k \equiv n \mod (\Delta - 1)$.

In the following corollaries of Theorem 3.1 we consider lower bounds for $S(G)$ when G is an arbitrary tree, $G \cong T$.

Corollary 3.5. *Let T be a tree with $n \geq 3$ vertices. Then*

$$S(T) \geq \frac{2\Delta(2(n-1)ID(T) - n^2)}{n(\Delta - 1)}. \tag{11}$$

Equality holds if and only if T is a tree such that $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta = 1$ for some t, $1 \leq t \leq n-2$.

Proof. For $m = n - 1$ and $\delta = 1$ from (5) we arrive at (11). □

Corollary 3.6. *Let T be a tree with $n \geq 3$ vertices. Then*

$$S(T) \geq \frac{2(n-2)\Delta}{n(\Delta - 1)}. \tag{12}$$

Equality holds if $T \cong P_n$.

Proof. In [30] it is proven that for arbitrary tree T holds

$$ID(T) \geq \frac{n+2}{2},$$

with equality if and only if $T \cong P_n$. From the above and (11) we get (12). □

The proof of the next Theorem is fully analogous to that of Theorem 3.1, hence omitted.

Theorem 3.7. *Let G be a simple connected irregular graph, with $n \geq 3$ vertices and m edges. Then*

$$S(G) \geq \frac{2(nM_1(G) - 4m^2)}{n(\Delta - \delta)}. \tag{13}$$

Equality holds if and only if $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$ for some t, $1 \leq t \leq n-2$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$.

Remark 3.8. *In* [39] *it was proven that*

$$S(G) \geq \frac{nM_1(G) - 4m^2}{n^2}.$$

The inequality (13) *is stronger than the above one.*

Corollary 3.9. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$S(G) \geq \Delta - \delta.$$

Equality holds if $\Delta = d_1 = \cdots = d_n = \delta$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$.

Proof. In [36] the following inequality was proven

$$M_1(G) \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2,$$

with equality holding if and only if $\Delta = d_1 = \cdots = d_n = \delta$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$ (see [10, 32]). From the above and (13) we obtain the desired result. □

Corollary 3.10. *Let T be a tree with $n \geq 3$ vertices. Then*

$$S(T) \geq \frac{2(nM_1(T) - 4(n-1)^2)}{n(\Delta - 1)}. \tag{14}$$

Equality holds if and only if $T \cong P_n$.

Remark 3.11. *In* [30] *it is proven that for arbitrary tree T holds*

$$M_1(T) \geq 4n - 6,$$

with equality if and only if $T \cong P_n$. From the above inequality and (14) *it follows*

$$S(T) \geq \frac{4(n-2)}{n(\Delta - 1)}.$$

The inequality (12) *is stronger than the above one.*

Remark 3.12. *According to* (13) *it follows that*

$$S(G) \geq \frac{2(nM_1(G) - 4m^2)}{n(\Delta - \delta)} = \frac{2nVar(G)}{\Delta - \delta}.$$

The proofs of the following theorems are similar to that of Theorem 3.1.

Theorem 3.13. *Let G be a simple connected irregular graph, with $n \geq 3$ vertices and m edges. Then*

$$S(G) \geq \frac{2(F(G) - \frac{2m}{n}M_1(G))}{\Delta^2 - \delta^2}. \tag{15}$$

Equality holds if and only if $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$ for some t, $1 \leq t \leq n-2$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$.

Theorem 3.14. *Let G be a simple connected irregular graph, with $n \geq 3$ vertices and m edges. Then*

$$S(G) \geq \frac{2\Delta^2\delta^2(\frac{2m}{n}^m M_1(G) - ID(G))}{\Delta^2 - \delta^2}. \tag{16}$$

Equality holds if and only if $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$ for some t, $1 \leq t \leq n-2$, or $d_2 = d_3 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$.

Remark 3.15. *Equalities in* (13), (15) *and* (16) *are attained, among others, for tridegreed graphs containing one vertex of maximum degree Δ, one vertex of minimum degree δ, and $(n-2)$ vertices with degree $(\Delta+\delta)/2$. Studying the structure of such tridegreed graphs, it can be observed that there are infinitely many tridegreed graphs satisfying the equality. These graphs are the n-vertex lollipop graphs denoted by $Lo(n,k)$. Lollipop graphs are unicyclic graphs with degree set $(1,2,3)$. They are obtained by attaching a path to a k-cycle. Consequently, lollipop graphs have only one maximum degree 3, one minimum degree 1, and $(n-2)$ vertices with degree 2. Let us note that for every lollipop graph the equality $S(Lo(n,k)) = 2$ holds.*

Remark 3.16. *Lower bounds for $S(G)$ given by* (5), (13), (15) *and* (16) *are incomparable. To illustrate this, let us consider, for example, the graph $K_{n-1}+e$ obtained from the complete graph K_{n-1} by adding a new vertex connected to an arbitrary vertex, and graph $K_n - 2e$ obtained from the complete graph K_n by deleting two arbitrary adjacent edges. Lower bounds determined by* (5), (13), (15) *and* (16) *for graphs $K_{n-1}+e$ and $K_n - 2e$ when $n = 5, 10, 50, 100$ are given in Tables 1 and 2, respectively.*

n	$S(G)$	(5)	(13)	(15)	(16)
5	3.6	3.467	3.2	3.04	3.538
10	12.8	12.65	11.6	10.76	12.768
50	92.16	92.122	90.32	88.59	92.159
100	192.08	192.06	190.16	188.299	192.08

Table 1: Lower bounds of $S(G)$ for $K_{n-1}+e$

n	$S(G)$	(5)	(13)	(15)	(16)
5	3.2	2.667	2.8	2.867	2.608
10	5.6	4.25	4.4	4.475	4.177
50	7.52	5.642	5.68	5.7	5.225
100	7.76	5.820	5.84	5.85	5.81

Table 2: Lower bounds of $S(G)$ for $K_n - 2e$.

From Table 1 we conclude that lower bounds are given in the following hierarchical sequence (16) > (5) > (13) > (15), *and from Table 2 we have* (15) > (13) > (5) > (16). *This means that these bounds are mutually incomparable.*

4. Computing the degree deviation for connected bidegreedgraphs

In what follows it will be shown that the degree deviation $S(G)$ for connected bidegreed graphs can be computed using a simple formula. Denote by N_Δ and N_δ the number of vertices with degree Δ and δ, respectively.

Lemma 4.1. *Let $= G(\Delta, \delta)$ be a connected bidegreed graph with n vertices and m edges. Then*

$$S(G) = \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right| = \frac{2m}{n}(N_\delta - N_\Delta) + (\Delta N_\Delta - \delta N_\delta)\,. \tag{17}$$

Proof. Since

$$S(G) = N_\Delta \left(\Delta - \frac{2m}{n} \right) + N_\delta \left(\frac{2m}{n} - \delta \right),$$

it follows that

$$nS(G) = n\Delta N_\Delta - 2mN_\Delta + 2mN_\delta - n\delta N_\delta\,,$$

wherefrom (17) is obtained. □

Lemma 4.2. *Let $= G(\Delta, \delta)$ be a connected bidegreed graph with n vertices and m edges. Then*

$$\frac{2m}{n}(N_\delta - N_\Delta) + (\Delta N_\Delta - \delta N_\delta) = \frac{2N_\Delta N_\delta}{n}(\Delta - \delta)\,.$$

Proof. It suffices to show that

$$2m(N_\delta - N_\Delta) + n(\Delta N_\Delta - \delta N_\delta) = 2N_\Delta N_\delta(\Delta - \delta)\,.$$

One obtains that

$$\begin{aligned} 2m(N_\delta - N_\Delta) + n(\Delta N_\Delta - \delta N_\delta) &= (\Delta N_\Delta + \delta N_\delta)(N_\delta - N_\Delta) + \\ &+ (N_\Delta + N_\delta)(\Delta N_\Delta - \delta N_\delta) = \\ &= 2\Delta N_\Delta N_\delta - 2\delta N_\delta N_\Delta = 2N_\Delta N_\delta(\Delta - \delta)\,. \end{aligned}$$

□

From Lemma 4.1 and Lemma 4.2, the following result yields:

Theorem 4.3. *Let $= G(\Delta, \delta)$ be a connected bidegreed graph with $n = N_\Delta + N_\delta$ vertices. Then*

$$S(G) = \frac{2N_\Delta N_\delta}{n}(\Delta - \delta)\,.$$

Remark 4.4. *Using the above formula, the degree deviation $S(G)$ for various connected bidegreed graphs can be simply determined. Such bidegreed graphs are: paths, complete bipartite graphs, wheel graphs, windmill graphs, complete split graphs.*

Remark 4.5. *Let $= G(\Delta, \delta)$ be irregular bidegreed graph. Then*

$$S(G) = \frac{2nVar(G)}{\Delta - \delta} = \frac{2N_\Delta N_\delta}{n}(\Delta - \delta)\,.$$

5. Two novel graph irregularity indices

Define the graph irregularity indices $IR_1(G)$ and IR_2(G) as follows

$$IR_1(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i + d_j} \qquad \text{and} \qquad IR_2(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i d_j}\,.$$

In what follows some lower and upper bounds are established for irregularity indices $IR_1(G)$ and $IR_2(G)$.

Theorem 5.1. *Let G be a connected graph with n vertices. Then*

$$IR_1(G) \leq nVar(G)\,. \tag{18}$$

Equality holds if and only if G is regular or semiregular graph.

Proof. In [33] it was proven that

$$IR_1(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i + d_j} = M_1(G) - 4ISI(G)\,, \tag{19}$$

and in [18] that

$$ISI(G) \geq \frac{m^2}{n}\,. \tag{20}$$

Now, from the above and inequality (19) we obtain (18). Equality in (20), and consequently in (18), holds if and only if G is a regular or a semiregular graph. □

In the following theorems we determine upper bounds for $IR_1(G)$ for connected triangle-free graphs.

Theorem 5.2. *Let G be a connected triangle–free graph with n vertices. Then*

$$IR_1(G) \leq M_1(G) - 4\frac{M_2(G)}{n}\,. \tag{21}$$

Equality holds when $G \cong K_{p,q}$, $p + q = n$.

Proof. In [48] it was proven that for the connected triangle–free graph holds

$$d_i + d_j \leq n\,, \tag{22}$$

for any pair of adjacent vertices v_i and v_j. Thus, we have

$$ISI(G) = \sum_{i\sim j} \frac{d_i d_j}{d_i + d_j} \geq \sum_{i\sim j} \frac{d_i d_j}{n} = \frac{M_2(G)}{n}\,.$$

From the above and (19) we obtain (21). □

The next theorem reveals relationship between $IR_1(G)$ and $\sigma(G)$.

Theorem 5.3. *Let G be a connected triangle–free graph with n vertices. Then*

$$IR_1(G) \geq \frac{1}{n}\sigma(G)\,. \tag{23}$$

Equality holds if $G \cong K_{p,q}$, $p + q = n$.

Proof. According to (22) we have that

$$IR_1(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i + d_j} \geq \frac{1}{n} \sum_{i\sim j} (d_i - d_j)^2 = \frac{1}{n} \sigma(G)\,.$$

□

In the following theorems we establish relationships between $IR_1(G)$ and $IR_2(G)$ and Albertson index, $Alb(G)$.

Theorem 5.4. *Let G be a simple connected graph with n vertices. Then*

$$IR_1(G) \geq \frac{(Alb(G))^2}{M_1(G)}\,. \tag{24}$$

Equality holds if G is a regular or a semiregular graph.

Proof. For $r = 1$, $x_i : |d_i - d_j|$, $a_i := d_i + d_j$, with summation performed over all edges of G, from (4) the inequality (24) immediately follows. □

The next theorem can be proved analogously.

Theorem 5.5. *Let G be a simple connected graph with n vertices. Then*

$$IR_2(G) \geq \frac{(Alb(G))^2}{M_2(G)}\,.$$

Equality holds if G is a regular or a semiregural graph.

The next theorem gives a relation between $IR_2(G)$ and generalized Randić index $R_{-1}(G)$.

Theorem 5.6. *Let G be a connected graph with n vertices. Then*

$$IR_2(G) \leq (\Delta - \delta)^2 R_{-1}(G)\,. \tag{25}$$

Equality holds if and only if G is regular or semiregular graph.

Proof. It is easy to see that

$$IR_2(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i d_j} \leq (\Delta - \delta)^2 \sum_{i\sim j} \frac{1}{d_i d_j}\,, \tag{26}$$

from which (25) is obtained. Equality in (26), and consequently in (25), holds if and only if G is regular or semiregular graph. □

In the next theorem we establish a lower bound on $IR_2(G)$ that depends on $M_1(G)$ and $M_2(G)$.

Theorem 5.7. *Let G be a connected graph with m edges. Then*

$$IR_2(G) \geq \frac{M_1(G)^2}{M_2(G)} - 4m\,. \tag{27}$$

Equality holds if and only if G is regular or semiregular graph.

Proof. In [33] it was proven that

$$IR_2(G) = \sum_{i\sim j} \frac{(d_i - d_j)^2}{d_i d_j} = SDD(G) - 2m\,, \tag{28}$$

where $SDD(G)$ is the symmetric division deg index introduced in [50]. On the other hand, in [14] it was proven that

$$SDD(G) \geq \frac{M_1(G)^2}{M_2(G)} - 2m\,,$$

with equality if and only if G is regular or semiregular graph. From the above and inequality (28) we obtain (27). □

Theorem 5.8. *Let G be a simple connected graph with $n \geq 2$ vertices. Then*

$$IR_2(G) \leq \sqrt{(F(G) - 2M_2(G))(ID(G) - 2R_{-1}(G))}\,. \tag{29}$$

Equality holds if G is a regular or a semiregular graph.

Proof. From the definitions of $ID(G)$ and $R_{-1}(G)$, we have that

$$ID(G) - 2R_{-1}(G) = \sum_{i\sim j}\left(\frac{1}{d_i^2} + \frac{1}{d_j^2}\right) - \sum_{i\sim j}\frac{2}{d_i d_j} = \sum_{i\sim j}\frac{\left(\frac{(d_i-d_j)^2}{d_i d_j}\right)^2}{(d_i - d_j)^2}\,. \tag{30}$$

On the other hand, for $r = 1$, $x_i := \frac{(d_i-d_j)^2}{d_i d_j}$, $a_i := (d_i - d_j)^2$, with summation performed over all edges of G, the inequality (4) becomes

$$\sum_{i\sim j}\frac{\left(\frac{(d_i-d_j)^2}{d_i d_j}\right)^2}{(d_i - d_j)^2} \geq \frac{\left(\sum_{i\sim j}\frac{(d_i-d_j)^2}{d_i d_j}\right)^2}{\sum_{i\sim j}(d_i - d_j)^2} = \frac{(IR_2(G))^2}{F(G) - 2M_2(G)}\,. \tag{31}$$

By combining (30) and (31) we obtain

$$ID(G) - 2R_{-1}(G) \geq \frac{(IR_2(G))^2}{F(G) - 2M_2(G)}\,,$$

wherefrom (29) immediately follows.

Equality in (31) holds if and only if $d_i d_j$ is a constant for all pairs of adjacent vertices v_i and v_j of G, which implies that equality in (29) holds if G is a regular of a semiregular graph. □

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