Graph Irregularity and a Problem Raised by Hong

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Abstract: Starting with the study of the Collatz-Sinogowitz and the Albertson graph irregularity indices the relationships between the irregularity of graphs and their spectral radius are investigated. We also use the graph irregularity index defined as $Ir(G) = \Delta - \delta$, where Δ and δ denote the maximum and minimum degrees of G. Our observations lead to the answer for a question posed by Hong in 1993. The problem concerning graphs with the smallest spectral radius can be formulated as follows: If G is a connected irregular graph with n vertices and m edges, and G has the smallest spectral radius, is it true that $Ir(G) =1$? It will be shown that the answer is negative; counterexamples are represented by several cyclic graphs. Based on the previous considerations the problem proposed by Hong can be reinterpreted (refined) in the form of the following conjecture: If G is a connected irregular graph with n vertices and m edges, and G has the smallest spectral radius, then $Ir(G)=1$ if such a graph exists, and if not, then $Ir(G)=2$. Considering the family of unicyclic graphs for which $Ir(G) \geq 2$, we prove that among n-vertex irregular unicyclic graphs the minimal spectral radius belongs to the uniquely defined short lollipop graphs where a pendent vertex is attached to cycle C_{n-1}. Moreover, it is verified that among n-vertex graphs there exists exactly one irregular graph J_n having a maximal spectral radius and an irregularity index of $Ir(J_n)=1$. Finally, it is also shown that by using the irregularity index $Ir(G)$ a classification of n-vertex trees into (n-2) disjoint subsets can be performed.

Keywords: irregularity indices; spectral radius; unicyclic graphs; lollipop

1   Introduction

For a graph G with n vertices and m edges, V(G) and E(G) denote the set of vertices and edges, respectively. Let d(u) be the degree of vertex u in G, and denote by uv an edge of G connecting vertices u and v. Denote by Δ and δ the maximum and minimum degree of G.

We use the standard terminology in graph theory, for notations not defined here we refer the reader to [1, 2, 3]. A graph is called regular, if all its vertices have the

same degree. A non-regular connected graph G is said to be irregular. Let $\rho(G)$ be the spectral radius of G and denote by $Cy = m - n + 1$ the cyclomatic number of a graph G. Because a tree graph is acyclic, its cyclomatic number is equal to zero. A connected graph G having $Cy(G) = k \geq 1$ cycles is said to be a k-cyclic graph.

A connected bidegreed bipartite graph $G(\Delta, \delta)$ is called semiregular if each vertex in the same part of bipartition has the same degree. An n-vertex unicyclic graph is a connected graph obtained by attaching a finite number of trees at vertices of a cycle. Because m = n for unicyclic graphs, their cyclomatic number equals one. The only regular unicyclic graphs are the cycles. By definition, let C(n,m) be the family of connected irregular graphs with n vertices and m edges, respectively. Consequently, C(n,n-1) denotes the set of trees, and C(n,n) denotes the set of irregular unicyclic graphs. It is immediate that for any connected irregular n-vertex graph, $1 \leq \Delta - \delta \leq n-2$. By definition, an n-vertex graph G is said to be *maximally irregular graph* if Ir(G) = n-2, and *weakly irregular graph* (WIR graph) if Ir(G) = 1. It is obvious that any connected WIR graph is a bidegreed graph.

The organization of this paper is as follows. In Section 2, we review some known irregularity indices, and their relations with the spectral radius of acyclic and various cyclic graphs. In Section 3, the Hong's problem is investigated with particular regard to unicyclic graphs. In Section 4, inequalities characterizing the irregularity of lollipop graphs are presented. In Section 5, it is proved that among n-vertex graphs there exists an irregular graph J_n having a maximal spectral radius and an irregularity index of Ir(J_n)=1. Moreover, a sharp upper bound is given for the spectral radius of n-vertex connected irregular graphs. In Section 6, it is shown that by using the irregularity index Ir(G) a classification of n-vertex trees into (n-2) disjoint subsets can be performed.

2 Relations between Graph Irregularity Indices and the Spectral Radius

By definition, a topological invariant IT(G) is called an irregularity index of a graph G if IT(G) $\geq$ 0 and IT(G)=0 if and only if G is a regular graph. The majority of irregularity indices are degree-based, but there exist eigenvalue-based irregularity indices as well [6-19]. Widely used topological invariants are the Collatz–Sinogowitz irregularity index [6]

$$\varepsilon(G) = \rho(G) - \frac{2m}{n}$$

and the Albertson irregularity index [7],

$$AL(G) = \sum_{uv \in E} |d(u) - d(v)|$$

Among the degree-based irregularity indices, $Ir(G) = \Delta - \delta$ is one of the simplest topological graph invariants [8]. It is easy to see that for any m-edge connected graph

$$AL(G) = \sum_{uv \in E} |d(u) - d(v)| \leq mIr(G)$$

and equality holds if graph G is a regular or semiregular.

Weakly irregular graphs play a central role in the mathematical chemistry. Benzenoid graphs are bidegreed graphs composed of finite number hexagons (except C_6 cycle) [4]. They form a subset of WIR graphs because $\Delta=3$ and $\delta=2$ hold for them. The dual graphs of traditional trivalent fullerene graphs contain only vertices with degrees 5 and 6, consequently all dual fullerene graphs are WIR graphs with $\Delta - \delta = 6 - 5 = 1$ [5]. It is worth noting that semiregular WIR graphs with $\Delta=3$ and $\delta=2$ can be easily generated by performing a subdivision operation on edges of arbitrary 3-regular graphs. Complete bipartite graphs $K_{p,q}$ where $p \geq 1$ and $q=p+1$ are also semiregular WIR graphs with $n=2p+1$ vertices and $m=p(p+1)$ edges. This observation implies that for any $n \geq 3$ odd integer there is an n-vertex WIR graph isomorphic to an n-vertex complete bipatite graph.

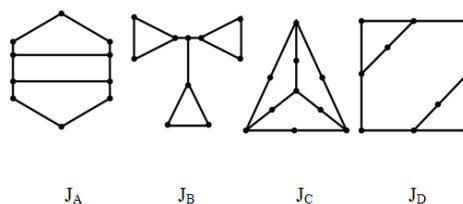As an example, in Fig.1, tricyclic WIR graphs with $\Delta=3$ and $\delta=2$ are depicted.

Figure 1
WIR graphs having identical vertex degree sequence

As can be seen, graphs J_C and J_D are semiregular, and J_C is generated by using a subdividing operation on the edges of K_4 complete graph.

The Collatz–Sinogowitz irregularity index has been extensively studied during the last two decades [10-19]. As can be seen, $\varepsilon(G)$ is a linear function of the spectral radius, consequently among graphs with n vertices and m edges the maximal irregularity index $\varepsilon(G)$ belongs to graphs with maximal spectral radius, and the minimal irregularity index $\varepsilon(G)$ belongs to graphs with minimal spectral radius. Similar phenomenon can be observed for some particular classes of graphs which are characterized by the irregularity index Ir(G.

2.1   Acyclic Graphs with Extremal Irregularity

Denote by P_n and $K_{1,n-1}$ the n-vertex paths and stars, respectively.

Lemma 1 Let T_n be an (n≥3)-vertex tree. Then $Ir(P_n)=1$ and $Ir(K_{1,n-1})=n-2$, consequently,

$1 = Ir(P_n) \le Ir(T_n) \le Ir(K_{1,n-1}) = n-2$.

In other words, the lower bounds are attained if T_n is the path P_n, and the upper bounds if T_n is the star $K_{1,n-1}$. Based on the Lemma 1 and using the known formulas published in Ref. [3] the following proposition is obtained:

Proposition 1 Let T_n be an n-vertex tree with $n \ge 3$ vertices. Then

$$\rho(T_n) \ge \rho(P_n) = 2\cos\left(\frac{\pi}{n+1}\right) \ge \sqrt{2} > Ir(P_n) = 1,$$

$$\rho(T_n) \le \rho(K_{1,n-1}) = \sqrt{\Delta(K_{1,n-1})} = \sqrt{n-1} = \sqrt{Ir(K_{1,n-1})+1},$$

$$1 = Ir(P_n) < \rho(T_n) \le \sqrt{Ir(K_{1,n-1})+1} = \sqrt{n-1}.$$

2.2   Maximally Irregular Cyclic Graphs

In what follows methods for constructing maximally irregular n-vertex cyclic graphs with Ir(G)=n-2 are presented.

Proposition 2 For any $n \ge 4$ positive integer there exists a maximally irregular n-vertex graph G_n with m=(n-1)(n-2)/2 +1 edges having one vertex of degree 1, one vertex of degree n-1, and n-2 vertices of degree n-2.

Proof: Let K_{n-1} be a complete graph with n-1 vertices, where n≥ 4. By attaching one pendent edge to K_{n-1} we obtain the n-vertex graph G_n belonging to the family of kite graphs [30]. It is easy to see that the kite graph G_n has one vertex of degree 1, one vertex of degree n-1, and n-2 vertices of degree n-2.

Proposition 3 Denote by $G_n^{(k,p)}$ an n-vertex and k-cyclic graph composed of k triangles and p=n-k-2 ≥ 1 pendent edges. Let us assume that k triangles have a sole common vertex u and all pendent edges are attached to vertex u. Then, $Ir(G_n^{(k,p)}) = k+p = n-2$

Proof: Consider the n-vertex cyclic graphs depicted in Fig. 2.

Figure 2
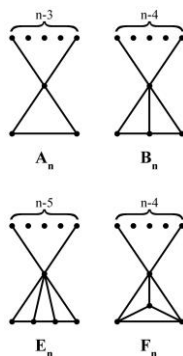
Four n-vertex and k-cyclic graphs with k= 1, 2 and 3

In Fig. 2 graphs A_n are unicyclic, B_n are bicyclic graphs, while E_n and F_n are non-isomorphic 3-cyclic graphs, respectively. It is easy to see that graphs denoted by A_n, B_n and E_n form subsets of $G_n^{(k,p)}$ graphs. Because k+p=n-2 is fulfilled, this implies that, $A_n = G_n^{(1,n-3)}$, $B_n = G_n^{(2,n-4)}$, and $E_n = G_n^{(3,n-5)}$.

Remark 1 According to results published in [25] a fundamental property of graphs A_n, B_n and F_n is that all of them have maximal spectral radius among n-vertex unicyclic, bicyclic and tricyclic connected graphs, respectively. From this observation it can be concluded that tricyclic graphs F_n have a larger spectral radius than graphs E_n.

Remark 2 It is interesting to note that among 6-vertex connected graphs there exist two non-isomorphic 3-cyclic graphs having identical minimal spectral radius of 2,732 and identical minimal irregularity index Ir=3-2=1.

2.3   Irregularity of Unicyclic Graphs

Structural properties of unicyclic graphs have been characterized in several papers [20-31]. As an example, consider the n-vertex sun graphs denoted by SG_n where n≥6 even integer. A sun graph SG_n is the graph on n=2k vertices obtained by attaching k pendent edges to a cycle C_k. [42]. (See Fig. 3)
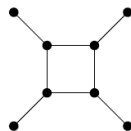

Figure 3

Sun graph SG_8

Sun graphs represent a particular subset of unicyclic graphs where $\Delta=3$ and $\delta=1$ hold [42]. For these graphs

$$\rho(SG_n) = 1 + \sqrt{2} = 1 + \sqrt{\Delta - \delta} = 1 + \sqrt{Ir(SG_n)}.$$

As can be seen, the spectral radius and the irregularity index of sun graphs are constant numbers; they are independent of the vertex number and the graph diameter.

For the spectral radius of unicyclic graphs various upper bounds have been deduced [20-31].

Proposition 4 Let U be a unicyclic graph different from a cycle. Then

$$\rho(U) < 2\sqrt{\Delta - \delta} = 2\sqrt{Ir(U)}.$$

Proof: Hu in [20] verified that for a unicyclic graph with maximum degree Δ the inequality $\rho(G) \leq 2\sqrt{\Delta - 1}$ is valid, and equality holds if and only if G is a cycle. Because any unicyclic graph different from a cycle contains one or more pendent vertices, from this observation the result follows.

Hong in 1986 [40] and, independently Brualdi and Solheid [25] obtained a sharp upper bound for the spectral radius of unicyclic graphs.

Proposition 5 [40, 25]: Let U_n be an n-vertex unicyclic graph different from cycle C_n. Then

$$\rho(U_n) \leq \rho(S_n^3),$$

where S_n^3 denotes the graph obtained by joining any two vertices of degree one of the star $K_{1,n-1}$ by an edge. The upper bound is attained only when U_n is the graph S_n^3.

Remark 3 It should be noted that the set of S_n^3 graphs is identical to the family of unicyclic graphs A_n depicted in Fig. 2.

In 1993, Hong asked the following question (his Problem 3) [31]: *Let G be a simple irregular connected graph with n vertices and m edges. If G has the smallest spectral radius, is it true that $\Delta - \delta = Ir(G) = 1$?*

3   Investigating the Hong's Problem

Concerning the Hong's problem, it is easy to see that a necessary condition for the fulfillment of equality $Ir(G) = \Delta - \delta = 1$ is that the connected graph G must be a WIR graph. It is known that in the set C(n,n-1) of trees there is exactly one tree

(path P_n) which is a WIR graph. Moreover, paths P_n have minimal spectral radius among n-vertex trees. Unicyclic graphs other than cycles contain at least one pendent vertex of degree 1 and at least one vertex of degree not smaller than 3. As a consequence:

Proposition 6 For any irregular unicyclic graph $Ir(G) = \Delta - \delta \geq 2$ holds.

It is easy to show that there exist M and N, M > N positive integers such that all graphs in C(N,M) are not WIR graphs (that is $Ir(G) = \Delta - \delta \geq 2$ is fulfilled). This observation is demonstrated by simple examples.

Proposition 7 If N=6 and M=12, then the set C(6,12) of connected irregular graphs does not contain WIR graphs.

Proof: Set C(6,12) contains exactly 4 irregular graphs with cyclomatic number C_y=12-6+1=7. They are denoted by H_A, H_B, H_C, and H_D and are characterized by the following properties:

Degree sequence of H_A is [5,5,4,4,4,2] and $Ir(H_A)$ =5 − 2 = 3

Degree sequence of H_B is [5,5,5,3,3,3] and $Ir(H_B)$= 5 − 3 = 2

Degree sequence of H_C is [5,5,4,4,3,3] and $Ir(H_C)$ =5 − 3 = 2

Degree sequence of H_D is [5,4,4,4,4,3] and $Ir(H_D)$ =5 − 3 = 2

The minimal spectral radius belongs to graph H_D, namely $\rho(H_D)$ = 4,067. In Fig. 4 these graphs taken from [32] are depicted.
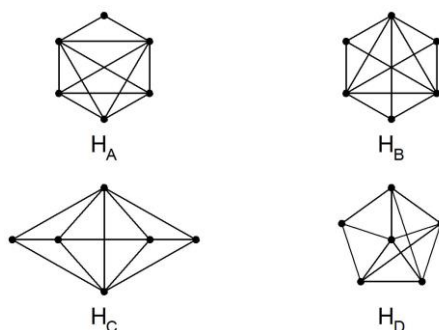

Figure 4
The four 6-vertex graphs from set C(6,12)

Proposition 8 If N=6 and M=9, then the set C(6,9) does not contain WIR graphs.

Proof: Set C(6,9) contains 18 irregular graphs with cyclomatic number C_y=9-6+1=4. None of them are WIR graphs. Among these 18 graphs the graph H_E depicted in Fig. 5 has the minimal spectral radius, $\rho(H_E)$ = 3,086. The corresponding degree sequence is [4,3,3,3,3,2], so $Ir(H_E)$ = 2.

Figure 5

The 9-edge graph H_E from set C(6,9)

In what follows we deal with the construction of n-vertex irregular unicyclic graphs having minimal spectral radius. To do this, the introduction of some definitions and two lemmas are needed.

Lemma 2 [3, 33]: If H is a (not necessarily induced) subgraph of a graph G, that is $H \subset G$, then $\rho(H) < \rho(G)$.

Hoffman and Smith [34] defined *an internal path* of graph G as a walk $v_0, v_1, \ldots v_k$ ($k \geq 1$) such that the vertices $v_1, \ldots, v_k$ are distinct (v_0, v_k do not need to be distinct), $d(v_k) > 2$, and $d(v_i) = 2$ whenever $0 < i < k$, holds.

Lemma 3 [30, 33]: Let uv be an edge of the n-vertex connected graph G and let G_{uv} be obtained from G by subdividing the edge uv of G. Let W_n, with $n \geq 6$ be the double-snake depicted in Fig. 6. If uv belongs to an internal path of G, and $G \neq W_n$, then $\rho(G_{uv}) < \rho(G)$.
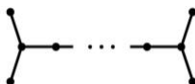

Figure 6

The double-snake graph W_n ($n \geq 6$)

The lollipop graphs are a subset of unicyclic graphs [30, 35-38]. A *lollipop Lo(n,k)* with $3 \leq k \leq n$ is a graph obtained from a cycle C_k and a path P_{n-k} by adding an edge between a vertex from the cycle and the endpoint from the path. Lollipop Lo(n,n-1) is called the short lollipop, while Lo(n,n) is the cycle C_n [36].

Proposition 9 The minimal spectral radius of an n-vertex unicyclic graph different from a cycle C_n belongs to uniquely defined short lollipop Lo(n,n-1) obtained by appending a cycle C_{n-1} ($n \geq 4$) to a pendent vertex u.

Proof: It is based on the application of two different graph transformation operations. A common feature of these transformations is that both of them decrease the spectral radii of unicyclic graphs.

　　i)　Denote by $\Omega(n,k)$ the class of n-vertex irregular unicyclic graphs including a k-edge cycle C_k, where $3 \leq k \leq n-1$. Let $G_1 \in \Omega(n,k)$ be an arbitrary n-vertex unicyclic graph. Consider the finite sequence of unicyclic graphs $G_1 \supset G_2, \ldots, \supset G_j, \ldots \supset G_J$ obtained by deleting step-by-step pendent edges, in such a way, that $G_{j+1} = G_j - e$, where e is an

arbitrary pendent edge of G_j. According to Lemma 2, $G_{j+1} \subset G_j$ holds, consequently, as a result of consecutive edge-deleting operations $\rho(G_{j+1}) < \rho(G_j)$ is fulfilled. Because in the final step the corresponding vertex number is equal to k+1, we get the short lollipop graph Lo(k+1,k) composed of a k-edge cycle C_k and one pendent edge attached to C_k.

ii) In order to identify the n-vertex unicyclic graph with a minimal spectral radius, the lollipop graph Lo(k+1,k) must be further transformed. For this purpose, based on the concept outlined in Lemma 3, we have to create a sequence of subdividing transformations on the cycle C_k by increasing step-by-step the edge number of C_k until we obtain the lollipop graph Lo(n,n-1). (The final step of transformations is characterized by the case of k=n-1.) It is clear that in each step, our subdividing transformations are always performed on an edge belonging to an internal path of cycles considered. Moreover, from Lemma 3 it follows that as a result of subsequent subdividing operations we get a sequence of lollipop graphs with increasing vertex numbers and decreasing spectral radii, simultaneously. It is easy to see that the short lollipop graph Lo(n,n-1) obtained at the final step has the minimal spectral radius among all n-vertex irregular unicyclic graphs.

Remark 4 From the previous considerations it follows that for short lollipops Lo(n,n-1) having the minimal spectral radius the equality $\Delta - \delta = 3 - 1 = 2$ holds.

In Fig. 7, the concept for constructing n-vertex unicyclic graphs with the minimal spectral radius is demonstrated.
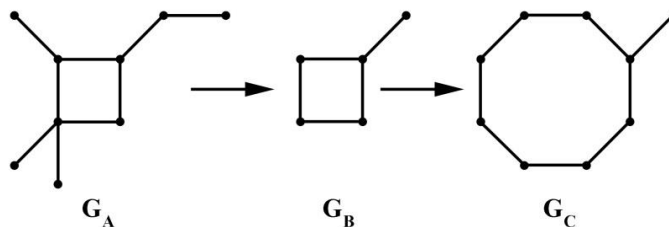

Figure 7
Transformations used for obtaining a unicyclic graph with the smallest spectral radius

Considering the three graphs shown in Fig. 7 it can be concluded that

i) graph G_A is a 9-vertex unicyclic graph with a spectral radius

$\rho(G_A) = 2{,}456$

ii) the 5-vertex lollipop graph G_B obtained from unicyclic G_A has the spectral radius $\rho(G_B) = \sqrt{(5 + \sqrt{17})/2} = 2{,}1358$,

iii) the short lollipop graph G_C obtained from G_B represents the unique unicyclic graph having the minimal spectral radius $\rho(G_C) = 2,084$ among all 9-vertex unicyclic graphs.

Remark 5 In the family of n-vertex, non-isomorphic unicyclic graphs there are graphs having cycles C_k with different $k \geq 3$ edge numbers. The characteristic feature of the method used for identifying the n-vertex unicyclic graph with minimal spectral radius is that independently from the topological structure of graph G_1, in the final step we always obtain the same uniquely defined extremal lollipop graph Lo(n,n-1).

4   Some Considerations Related to Lollipop Graphs

Lemma 4 Boulet and Jouve in [37] verified that for the spectral radius of lollipop graphs Lo(n,k) the following universal upper bound holds

$$\rho(Lo(n,k)) < \sqrt{5} = 2,236068$$

The value $\sqrt{5}$ seems to be the best upper bound for lollipop graphs. This claim is confirmed by computational results as well. For example, for lollipop Lo(8,3) one obtains that $\rho(Lo(8,3))= 2,2350$. (See computed spectral radii of 8-vertex unicyclic graphs summarized in [22]).

Remark 6 Let $k \geq 2$ a positive integer. It is easy to show that there exist infinitely many unicyclic graphs H_k with vertex number n=3k for which

$$\rho(H_k) = \sqrt{5} = 2,236068 \text{ holds.}$$

Consider the infinite sequence of unicyclic graphs H_k depicted in Fig. 8. Graphs H_k having an identical degree set {1,2,3} and an arbitrary large diameter. They belong to the family of bipartite pseudo-semiregular graphs [48].
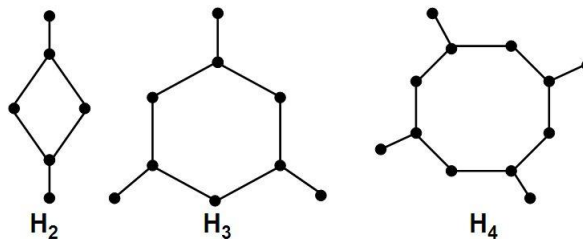

Figure 8

Unicyclic graphs H_k for k=2, 3, 4, with vertex number 6, 9, 12, ..

It is likely that there is no simple closed formula for computing the spectral radius of short lollipop graphs Lo(n,n-1). Supposing that a closed formula exists, this will be very complicated. As an example, consider the smallest lollipop graph Lo(4,3), having only 4 vertices.

In [39] the formula for calculating the spectral radius of the smallest lollipop graph Lo(4,3) is given. Namely, $\rho(Lo(4,3)) = \theta_1 = 2{,}17009$ where θ_1 is one of the three roots of the polynomial defined by $\theta^3 - \theta^2 - 3\theta + 1 = 0$.

Woo and Neumayer [33] studied the structural properties of a particular class of unicyclic graphs called closed quipus. By definition, a *closed quipu* is a unicyclic graph G of maximum degree 3 such that all vertices of degree 3 lie on a cycle [30, 33]. This implies the following proposition:

Proposition 10 Because lollipop graphs form a subset of closed quipus it follows that in the family of n-vertex closed quipus the short lollipop Lo(n,n-1) has the smallest spectral radius.

Based on the previous considerations, the problem suggested by Hong can be modified (refined) in the form of the following conjecture: *If G is a connected irregular graph with n vertex and m edges, and G has the smallest spectral radius, then Ir(G)=1 if such a graph exists, and if not, then Ir(G)=2.*

Remark 7 From the relations between the spectral radius of unicyclic graphs and the corresponding Collatz-Sinogowitz irregularity index the following inequalities yield. For any n-vertex unicyclic graph U_n

$$\varepsilon(U_n) = \rho(U_n) - \frac{2m}{n} \geq \rho(Lo(n, n-1)) - 2 > \rho(Lo(n, n)) - 2 = 0 \cdot$$

Furthermore, from Lemma 4, one obtains that

$$\varepsilon(Lo(n, k)) = \rho(Lo(n, k)) - \frac{2m}{n} < \sqrt{5} - 2 = 0{,}236068 \cdot$$

5   WIR Graphs with Maximal Spectral Radius

The Hong'problem concerns WIR graphs. On the analogy of Hong's problem the following question can be asked: *Let G be a simple irregular connected graph with n vertices and m edges. If G has the maximal spectral radius, is it true that Δ − δ = Ir(G) = n-2 ?*

The answer is negative. It is easy to show that for any $n \geq 4$ positive integer there always exists an n-vertex irregular graph J_n possessing the following properties: $Ir(J_n)=1$ and J_n has a maximal spectral radius among n-vertex irregular graphs.

Consider the unambiguously defined n-vertex irregular graph J_n obtained as $K_n - e$, where K_n is the n-vertex complete graph and e is an arbitrary edge of K_n. From the definition of graph J_n the following proposition is obtained:

Proposition 11 The n-vertex irregular graph J_n is characterized by the following properties:

   i) J_n is the only n-vertex irregular graph having the maximal edge number equal to $m^* = n(n-1)/2 - 1$. This implies that J_n is the sole graph in the set $C(n, m^*)$.

   ii) Because $\Delta(J_n)= n-1$ and $\delta(J_n)=n-2$, this implies that $Ir(J_n)=1$.

   iii) J_n has the maximal spectral radius among n-vertex irregular graphs [49].

   iv) Using the formula published by Hong et al. [41], for the spectral radius of a connected irregular graph G one obtains that

$$\rho(G) \leq \frac{n-3+\sqrt{n^2+2n-7}}{2},$$

and equality is fulfilled if and only if G is isomorphic to J_n.

Remark 8 Cioabă [43] proved that for a connected R-regular graph $G_{R,n}$ with n vertices

$$\frac{2}{n} > \Delta - \rho(G_{R,n} - e) > \frac{1}{nD}$$

holds. If $G_{R,n}$ is isomorphic to K_n then $\Delta(K_n) = \Delta(J_n) = n-1$. Because $D(J_n) = 2$, it follows that

$$\frac{2}{n} > n - 1 - \rho(J_n) > \frac{1}{2n}.$$

Remark 9 Let G be a connected graph with n vertices and m edges. If $n \geq 4$ and $m^* = n(n-1)/2 - 1$ then the known Hong's bound [44] represented by $\rho(G) \leq \sqrt{2m-n+1}$ slightly overestimates the spectral radii of graphs J_n:

$$\sqrt{2m^* - n + 1} = \sqrt{n^2 - 2n - 1} > \left(n - 3 + \sqrt{n^2 + 2n - 7}\right)/2 = \rho(J_n).$$

Remark 10 For example, if $J_4 = K_4 - e$, then for the spectral radius of the "diamond graph" J_4 one obtains that $\rho(J_4) = (1 + \sqrt{17})/2$.

6   Additional Considerations

The next inequalities represent some results relating to irregularity indices. Cioabă and Gregory have proved the following inequality [45]: Let G be a non-regular graph with n vertices and m edges having maximum degree Δ. Then

$$\varepsilon(G) = \rho - \frac{2m}{n} \geq \frac{(\Delta - \delta)^2}{4n\Delta} = \frac{\mathrm{Ir}^2(G)}{4n\Delta}.$$

An interesting conjecture has been posed in [46]: For any connected non-regular graph G with n vertices

$$\Delta - \rho > \frac{\sqrt{\Delta - \delta}}{nD} = \frac{\sqrt{\mathrm{Ir}(G)}}{nD}.$$

By a computer search the conjecture is verified for all connected graphs of order at most 8 [46].

Proposition 12 Let G be a connected graph. Then $2n\mathrm{Var}(G) \geq \mathrm{Ir}^2G) \geq 4\mathrm{Var}(G)$ where

$$\mathrm{Var}(G) = \frac{1}{n}\sum_{u \in V} d^2(u) - \left(\frac{2m}{n}\right)^2 \geq 0$$

is the degree-variance irregularity index proposed by Bell [9]. In the above formula equalities hold in both sides if and only if G is a regular graph.

Proof. In [47] Izumino et al. have proved that for a connected non-regular graph G with n vertices and m edges

$$\mathrm{Ir}^2G) = (\Delta - \delta)^2 \geq 4\mathrm{Var}(G)$$

Moreover, in [50] Gutman et al. verified that

$$\mathrm{Ir}^2G) = (\Delta - \delta)^2 \leq 2n\mathrm{Var}(G).$$

Proposition 13 Let G be a connected irregular graph with n vertices and m edges.

According to [19] consider the graph irregularity index IRF(G) defined by

$$\mathrm{IRFG}) = \sum_{uv \in E} \big(d(u) - d(v)\big)^2$$

Then

$$\mathrm{Ir}^2G) \geq \frac{1}{m}\mathrm{IRF}(G) = \frac{1}{m}\big(F(G) - 2M_2(G)\big).$$

where

$$F(G) = \sum_{u \in V} d^3(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E} d(u)d(v),$$

and equality is valid if G is regular or semiregular.

Proof. In [19] it was shown that $IRF(G) = F(G) - 2M_2(G)$. This implies that

$$IRFG) = F(G) - 2M_2(G) = \sum_{uv \in E}(d(u) - d(v))^2 \leq m(\Delta - \delta)^2 \text{ where equality holds}$$

if G is regular or semiregular.

Using the irregularity index Ir(G) a classification of n-vertex trees into (n-2) disjoint subsets can be performed.

Proposition 14 Let n ≥ 4 and 2 ≤ q ≤ n-1 be positive integers. There exists at least one n-vertex tree T_q for which Ir(T_q)=q-1 holds.

Proof. The concept of generating the proper sequence of n-vertex trees T_q is based on the ordering of trees according to their maximum vertex degrees.
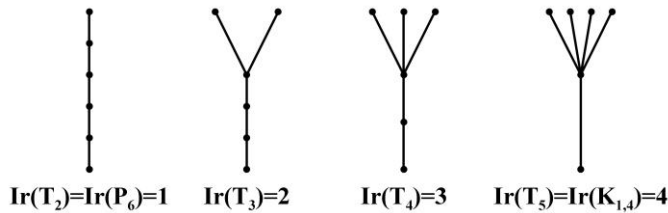

Ir(T_2)=Ir(P_6)=1   Ir(T_3)=2   Ir(T_4)=3   Ir(T_5)=Ir($K_{1,4}$)=4

Figure 9

The sequence of T_q graphs with increasing irregularity (case of n=6)

As it is demonstrated in Fig. 9, for constructing the sequence of n-vertex trees T_q a simple graph transformation is used by which only the irregularity changes, but the vertex number n remains the same. Starting with path $T_2=P_n$, as a result of consecutive transformation steps, the maximum degree increases as $\Delta(T_{q+1})$ =$\Delta(T_q)$+1, and simultaneously the graph irregularity also increases according to Ir(T_{q+1}) = Ir(T_q)+1.

Based on previous considerations, the following conjecture is posed: *Let n ≥ 4 and 2 ≤ q ≤ n-1 be positive integers. There exists at least one n-vertex cyclic graph G_q for which Ir(G_q)=q-1 holds, except for unicyclic graphs with q=2.*

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