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Irregularity of Graphs

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Abstract

The irregularity of a graph is the sum of the absolute values of the differences of degrees of pairs of adjacent vertices. The extremal graph with minimal irregularity among trees of order n with maximum degree Δ and the second maximum degree Δ_1 are determined, as well as unicyclic graphs of order n with girth g and maximum degree Δ. Lower and upper bounds are established on irregularity. Furthermore, the inverse problem for the irregularity of maximally irregular graphs is solved.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The order of G is denoted by n. Denote by $d_G(u)$ the degree of the vertex $u \in V(G)$. The maximum degree of G is denoted by Δ. A pendent vertex is a vertex of degree one. A tree of order n with maximum degree 2 is called a path and denoted P_n. Denote by C_g a cycle of length g. A

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graph is said to be unicyclic if it is connected and contains exactly one cycle. The girth of a unicyclic graph is the length of its cycle.

A graph is *regular* if all its vertices have equal degrees. In mathematical chemistry, the importance of regular graphs has much increased after the discovery of fullerenes and nanotubes. A graph that is not regular is said to be *irregular*. In various applications of graph theory (including chemical applications), it is necessary to know that how irregular a given graph is. In other words, there is a need to have a measure of irregularity.

The imbalance of an edge $xy \in E(G)$ is denoted by $imb_G(xy)$ and is defined as $|d_G(x) - d_G(y)|$ [6, 10]. Albertson [5] defined the *irregularity a graph G* as

$$irr = irr(G) = \sum_{xy \in E(G)} imb_G(xy)\,.$$

If the number of distinct elements in the degree sequence of a connected graph G is equal to the maximum degree, then G is said to be *maximally irregular*. In other words, a graph is maximally irregular if it possesses vertices of degree i, for all $i = 1, 2, \ldots, \Delta$. Properties of maximally irregular graphs were studied in [20, 23, 25].

For general graphs of order n, Albertson [5] obtained an asymptotically tight upper bound on irr. He also found sharp upper bounds on irr for bipartite and triangle-free graphs. Abdo et al. [1] solved the analogous problem for all graph with a given order. Hansen and Melot [18] characterized the graphs of order n and size m that have maximal irr-value. The irregularity of trees and unicyclic graphs was studied in [12] and [26], respectively. Recently, Lin et al. [22] introduced the general Albertson irregularity index of a connected graph and presented lower and upper bounds on this index. For more results on irregularity, Albetson index, and related measures, we refer the reader to [2–4, 7, 9, 11, 13–17, 19, 24, 27–32] and the references cited therein.

In this paper, we determine the extremal graphs with minimal irregularity among all trees of order n with maximum degree Δ and second maximum degree Δ_1. Also, we characterize the extremal graphs with minimal irregularity among all unicyclic graphs of order n with girth g and maximum degree Δ. Furthermore, we establish two lower bounds on irregularity in terms of maximum degree and the number of pendent vertices. Finally, we give bounds and solve the inverse problem for irregularity of maximally irregular graphs.

2 Graphs with minimal irregularity

A tree is said to be starlike if it has exactly one vertex of degree greater than two. This maximum degree vertex is called the center of the starlike tree. Denote by $\mathcal{S}_{n,\Delta}$ the set of all starlike trees of order n with maximum degree Δ. Let $\mathcal{S}_{n,\Delta,\Delta_1}$ be the set of trees of order n obtained by adding a new edge between the centers of two starlike trees with maximum degrees Δ and Δ_1. If $\Delta_1 \leq 2$ then $\mathcal{S}_{n,\Delta,\Delta_1} \equiv \mathcal{S}_{n,\Delta}$.

Let $u_0 u_1 \cdots u_t$ be a path in G which will be denoted by (u_0, u_t). Let (u, v) be a path in G. If $d_G(u) \geq 3$, $d_G(v) = 1$ and all internal vertices of (u, v) are of degree two, then it is called a pendent path.

We define the imbalance of the path (u_0, u_t) in G as

$$imb_G(u_0, u_t) = \sum_{i=0}^{t-1} \left| d_G(u_i) - d_G(u_{i+1}) \right|.$$

The following lemma is useful for characterizing graphs with minimal irregularity.

Lemma 1. *Let $(u_0, u_t) = u_0 u_1 \cdots u_t$ be a path in a graph G. Then $imb_G(u_0, u_t) \geq |d_G(u_0) - d_G(u_t)|$ with equality holding if and only if the sequence $d_G(u_0), d_G(u_1), \ldots, d_G(u_t)$ is monotonic.*

Proof. By the property of subadditivity of the absolute value, we have

$$\begin{aligned} imb_G(u_0, u_t) &= \sum_{i=0}^{t-1} |d_G(u_i) - d_G(u_{i+1})| \geq \left| \sum_{i=0}^{t-1} (d_G(u_i) - d_G(u_{i+1})) \right| \\ &= |d_G(u_0) - d_G(u_t)| \end{aligned}$$

with equality holding if and only if the sequence $d_G(u_0), d_G(u_1), \ldots, d_G(u_t)$ is monotonic. ■

A set of paths of a graph G is edge-disjoint if every two paths have no edges in common.

Theorem 1. *Let T be a tree of order n with maximum degree Δ and second maximum degree Δ_1. Then $irr(T)$ is minimum in the class of trees of order n with maximum degree Δ and second maximum degree Δ_1 if and only if $T \in \mathcal{S}_{n,\Delta,\Delta_1} \cup P_n$.*

Proof. If $T \in \mathcal{S}_{n,\Delta,\Delta_1} \cup P_n$, then one can easily check that $irr(T) = (\Delta-1)^2 + (\Delta_1-1)^2 + \Delta - \Delta_1$. Therefore, it is sufficient to prove that

$$irr(G) \geq (\Delta-1)^2 + (\Delta_1-1)^2 + \Delta - \Delta_1 \tag{1}$$

with equality holding if and only if $T \in \mathcal{S}_{n,\Delta,\Delta_1} \cup P_n$.

If $\Delta = 2$, then $\Delta_1 = 2$ or $\Delta_1 = 1$. Then T is isomorphic to P_n and the equality in (1) holds. Therefore, we suppose that $\Delta > 2$.

Let w be a maximum degree vertex and u be a second maximum degree vertex of T. Then there exist $\Delta-1$ edge-disjoint paths (w, w_i), $1 \leq i \leq \Delta-1$ and Δ_1-1 edge-disjoint paths (u, u_i), $1 \leq i \leq \Delta_1-1$, such that $d_T(w_i) = 1$ and $d_T(u_i) = 1$. Note that the path (w, u) is edge-disjoint with regard to all the above mentioned paths. Then by the definition of irregularity and Lemma 1, we get

$$\begin{aligned} irr(T) &\geq \sum_{i=1}^{\Delta-1} imb_T(w, w_i) + \sum_{i=1}^{\Delta_1-1} imb_T(u, u_i) + imb_T(w, u) \\ &\geq \sum_{i=1}^{\Delta-1} |d_T(w) - d_T(w_i)| + \sum_{i=1}^{\Delta_1-1} |d_T(u) - d_T(u_i)| + |d_T(w) - d_T(u)| \\ &= (\Delta-1)^2 + (\Delta_1-1)^2 + \Delta - \Delta_1 \,. \end{aligned}$$

If $T \in \mathcal{S}_{n,\Delta,\Delta_1}$, then one can easily check that equality holds in (1). Suppose that $T \notin \mathcal{S}_{n,\Delta,\Delta_1}$ and that the equality in (1) holds. If $d_T(w, u) \geq 2$ and the number of all pendent paths in T is exactly $\Delta + \Delta_1 - 2$ then $imb_T(w, u) > |d_T(w) - d_T(u)|$ by Lemma 1 and a contradiction. Therefore since $T \notin \mathcal{S}_{n,\Delta,\Delta_1}$, there exists a pendent path (v, v_1), such that $v \neq w, u$ and $v \neq w_i, u_j$ for all $1 \leq i \leq \Delta-1, 1 \leq j \leq \Delta_1-1$. Then by the definition of irregularity and Lemma 1, we have

$$\begin{aligned} irr(T) &= irr(T') + imb_T(v, v_1) \geq irr(T') + |d_T(v) - d_T(v_1)| \\ &\geq irr(T') + 2\,, \end{aligned} \tag{2}$$

where T' is a tree of order less than n that has maximum degree Δ and second maximum degree Δ_1. Thus, $irr(T') \geq (\Delta-1)^2+(\Delta_1-1)^2+\Delta-\Delta_1$ and from (2) it follows that $irr(T) \geq (\Delta-1)^2+(\Delta_1-1)^2+\Delta-\Delta_1+2$. This contradicts the fact that the equality in (1) holds and therefore all paths (w, w_i), (u, u_j), $1 \leq i \leq \Delta-1, 1 \leq j \leq \Delta_1-1$ are pendent. It is easy to check that the length of the path (w, u) is one. This completes the proof. ■

Corollary 1. *Let n and Δ be positive integers greater than one and T be a tree. Then $irr(T)$ is minimum in the class of trees of order n with maximum degree Δ if and only if $T \in \mathcal{S}_{n,\Delta} \cup P_n$.*

Proof. Let Δ_1 be the second maximum degree of T. Then by Theorem 1,

$$irr(T) \geq (\Delta-1)^2+(\Delta_1-1)^2+\Delta-\Delta_1\,.$$

Consider the function $f(x) = (\Delta-1)^2+(x-1)^2+\Delta-x$. It is easy to see that $f(x)$ is increasing on $x \geq 2$. Therefore,

$$\begin{aligned} irr(T) &\geq (\Delta-1)^2+(\Delta_1-1)^2+\Delta-\Delta_1 \\ &= f(\Delta_1) \geq \min(f(1), f(2)) = \Delta(\Delta-1) \end{aligned}$$

with equality holding if and only if $T \in \mathcal{S}_{n,\Delta} \cup P_n$. This completes the proof. ■

Corollary 2. [33] *Let T be a tree of order $n > 2$. Then $irr(T) \geq 2$ with equality holding if and only if T is isomorphic to P_n.*

The following classes of graphs were defined in [21]. Denote by $\mathcal{A}_n(g, \Delta)$ the set of graphs of order n obtained by attaching $\Delta-2$ paths to one vertex of C_g. In addition, $\mathcal{B}_n(g, \Delta)$ denotes the set of unicyclic graphs obtained by identifying a pendent vertex of a starlike tree in $\mathcal{S}_{n-g+1,\Delta}$

with one vertex of C_g. If $G \in \mathcal{A}_n(g,\Delta)$, then $irr(G) = (\Delta-2)(\Delta-1) + 2(\Delta-2) = \Delta^2 - \Delta - 2$. Let $G \in \mathcal{B}_n(g,\Delta)$ and ℓ be the length of the shortest path from the maximum degree vertex to the cycle of G. If $\ell = 1$, then $irr(G) = (\Delta-1)^2 + (\Delta-3) + 2 = \Delta^2 - \Delta$. If $\ell > 1$, then $irr(G) = (\Delta-1)^2 + (\Delta-2) + 3 = \Delta^2 - \Delta + 2$. This implies the following lemma.

Lemma 2. *Let G be a unicyclic graph of order n with maximum degree Δ and girth g. Let ℓ be the length of the shortest path from the maximum degree vertex to the cycle of G. Then*

$$irr(G) = \begin{cases} \Delta^2 - \Delta - 2, & \text{if } \ G \in \mathcal{A}_n(g,\Delta) \\ \Delta^2 - \Delta, & \text{if } \ G \in \mathcal{B}_n(g,\Delta), \quad \ell = 1 \\ \Delta^2 - \Delta + 2, & \text{if } \ G \in \mathcal{B}_n(g,\Delta), \quad \ell \geq 2\,. \end{cases}$$

We now give a sharp upper bound on the irregularity for this class of graphs and characterize the corresponding extremal graphs.

Theorem 2. *Let G be a unicyclic graph of order n with maximum degree Δ and girth g. Then $irr(G)$ is minimum in the class of unicyclic graphs of order n with maximum degree Δ and girth g if and only if $G \in \mathcal{A}_n(g,\Delta)$.*

Proof. Bearing in mind Lemma 2 , it is sufficient to prove that

$$irr(G) \geq \Delta^2 - \Delta - 2 \tag{3}$$

with equality holding if and only if $G \in \mathcal{A}_n(g,\Delta)$.

Let w be the maximum degree vertex of G and v be the nearest vertex from w which lies on the cycle. Also, let x and y be the neighbor vertices of v on the cycle. If $d_G(x) \geq 3$, then there exist $d_G(x) - 2$ edge-disjoint paths (x, x_i), $1 \leq i \leq d_G(x) - 2$ in G such that $d_G(x_i) = 1$ and each path does not contain any edge of the cycle. Similarly, if $d_G(y) \geq 3$, then there exist $d_G(y) - 2$ edge-disjoint paths (y, y_i), $1 \leq i \leq d_G(y) - 2$ in G such that $d_G(y_i) = 1$ and each path does not contain any edge of the cycle. Let ℓ be the length of the shortest path from w to the vertex v. Then we distinguish the following two cases.

Case (i): $\ell \geq 1$. Then there exist at least $\Delta - 1$ edge-disjoint paths, say (w, w_i), $1 \leq i \leq \Delta - 1$, that are all edge-disjoint from the path (w, v) and $d_G(w_i) = 1$. From the definition of the irregularity and Lemma 1, we have

$$\begin{aligned}
irr(G) &\geq \sum_{i=1}^{\Delta-1} imb_G(w, w_i) + \sum_{i=1}^{d_G(x)-2} imb_G(x, x_i) + \sum_{i=1}^{d_G(y)-2} imb_G(y, y_i) \\
&+ imb_G(w, v) + imb_G(vx) + imb_G(vy) \\
&\geq \sum_{i=1}^{\Delta-1} |d_G(w) - d_G(w_i)| + \sum_{i=1}^{d_G(x)-2} |d_G(x) - d_G(x_i)| \\
&+ \sum_{i=1}^{d_G(y)-2} |d_G(y) - d_G(y_i)| + |d_G(w) - d_G(v)| \\
&+ |d_G(v) - d_G(x)| + |d_G(v) - d_G(y)| \\
&= (\Delta - 1)^2 + (d_G(x) - 2)(d_G(x) - 1) + (d_G(y) - 2)(d_G(y) - 1) \\
&+ \Delta - d_G(v) + |d_G(v) - d_G(x)| + |d_G(v) - d_G(y)| \\
&\geq (\Delta - 1)^2 + (d_G(x) - 2)(d_G(x) - 1) + (d_G(y) - 2)(d_G(y) - 1) \\
&+ \Delta - d_G(v) + (d_G(v) - d_G(x)) + (d_G(v) - d_G(y)) \\
&= \Delta^2 - \Delta + (d_G(x) - 2)^2 + (d_G(y) - 2)^2 + d_G(v) - 3 \\
&\geq \Delta^2 - \Delta
\end{aligned}$$

since $d_G(x) \geq 2$, $d_G(y) \geq 2$, and $d_G(v) \geq 3$.

Case (ii): $\ell = 0$, i.e., $v \equiv w$. Then there exist $\Delta - 2$ edge-disjoint paths, say (w, w_i), $1 \leq i \leq \Delta - 2$, that are all edge-disjoint from the cycle of G and $w_1, w_2, \ldots, w_{\Delta-2}$ are pendent vertices. From the definition and Lemma 1, we have

$$\begin{aligned}
irr(G) &\geq \sum_{i=1}^{\Delta-2} imb_G(w, w_i) + \sum_{i=1}^{d_G(x)-2} imb_G(x, x_i) + \sum_{i=1}^{d_G(y)-2} imb_G(y, y_i) \\
&+ imb_G(wx) + imb_G(wy)
\end{aligned}$$

$$
\begin{aligned}
&\geq && \sum_{i=1}^{\Delta-2} |d_G(w) - d_G(w_i)| + \sum_{i=1}^{d_G(x)-2} |d_G(x) - d_G(x_i)| \\
&+ && \sum_{i=1}^{d_G(y)-2} |d_G(y) - d_G(y_i)| + |d_G(w) - d_G(x)| + |d_G(w) - d_G(y)| \\
&= && (\Delta - 2)(\Delta - 1) + (d_G(x) - 2)(d_G(x) - 1) \\
&+ && (d_G(y) - 2)(d_G(y) - 1) + \Delta - d_G(x) + \Delta - d_G(y) \\
&= && \Delta^2 - \Delta - 2 + (d_G(x) - 2)^2 + (d_G(y) - 2)^2 \\
&\geq && \Delta^2 - \Delta - 2 \qquad (4)
\end{aligned}
$$

since $d_G(x) \geq 2$, $d_G(y) \geq 2$, and $d_G(w) = \Delta$.

From the above two cases, we get the required inequality. Suppose now that the equality holds in (3). Then w lies on the cycle and $d_G(x) = d_G(y) = 2$, it follows that each vertex on the cycle of G, different from w, has degree two. We also must have

$$\sum_{i=1}^{\Delta-2} imb_G(w, w_i) = \sum_{i=1}^{\Delta-2} |d_G(w) - d_G(w_i)|.$$

Then, similarly as in the proof of Theorem 1, we can show that all paths (w, w_i), $1 \leq i \leq \Delta - 2$ are pendent. Hence $G \in \mathcal{A}_n(g, \Delta)$. On the other hand, if $G \in \mathcal{A}_n(g, \Delta)$, then by Lemma 2, $irr(G) = \Delta^2 - \Delta - 2$. This completes the proof. ■

Theorem 3. *Let G be a unicyclic graph of order n with maximum degree Δ. Then*

$$irr(G) \geq \Delta^2 - \Delta - 2 \qquad (5)$$

with equality holding if and only if $G \in \bigcup_{g=3}^{n-\Delta+2} \mathcal{A}_n(g, \Delta)$.

Proof. Let g be the girth of G. Then $3 \leq g \leq n - \Delta + 2$. By Theorem 2, $irr(G) \geq \Delta^2 - \Delta - 2$ with equality holding if and only if $G \in \mathcal{A}_n(g, \Delta)$. Hence, the equality holds in (5) if and only if $G \in \bigcup_{g=3}^{n-\Delta+2} \mathcal{A}_n(g, \Delta)$. ■

Corollary 3. *Let G be a unicyclic graph of order n with girth g which is* *different from C_n. Then $irr(G) \geq 4$ with equality holding if and only if G is isomorphic to the graph obtained by attaching one pendent vertex of a path P_{n-g+1} to one vertex of C_g.*

Proof. Let Δ be the maximum degree in G. Since G is different from C_n, we have $\Delta \geq 3$. By Theorem 2, $irr(G) \geq \Delta^2 - \Delta - 2 \geq 4$ with equality holding if and only if $G \in \mathcal{A}_n(g,3)$. Clearly, $\mathcal{A}_n(g,3)$ consists of only one graph that is isomorphic to the graph obtained by attaching one pendent vertex of P_{n-g+1} to one vertex of C_g. ■

We now establish a lower bound on the irregularity of graphs in terms of the number of pendent vertices and the maximum degree.

Theorem 4. *Let G be a graph of order n with k pendent vertices and maximum degree Δ, different from P_n. Then $irr(G) \geq 2k + \Delta - 3$.*

Proof. Let $v_1, v_2, \ldots, v_k$ be the pendent vertices of G. Denote by u_i, $1 \leq i \leq k$ the nearest vertex from v_i that has degree greater than two. Clearly, we can always find the vertices u_i, because G is different from P_n. Let w be the maximum degree vertex. Then one can easily see that the paths $(w,u_1),(u_1,v_1),(u_2,v_2),\ldots,(u_k,v_k)$ are edge-disjoint. Then by the definition and Lemma 1, we have

$$\begin{aligned} irr(G) &\geq \sum_{i=1}^{k} imb_G(u_i,v_i) + imb_G(w,u_1) \\ &\geq |d_G(u_1)-1| + \sum_{i=2}^{k} |d_G(u_i)-1| + |\Delta - d_G(u_1)| \\ &\geq d_G(u_1) - 1 + (k-1)(3-1) + \Delta - d_G(u_1) \\ &= 2k + \Delta - 3 \end{aligned}$$

since $d_G(u_i) \geq 3$ for $1 \leq i \leq k$ and Δ is the maximum degree of G. ■

Denote by $\mathcal{G}_{n,k}$ the class of graphs of order n with k pendent vertices and maximum degree three in which every vertex of degree two lies on a pendent path. If $1 \leq k \leq (n+2)/2$, then $\mathcal{G}_{n,k} \neq \emptyset$. For example, the graph obtained by attaching $k-2$ pendent edges to the consecutive $k-2$ non-pendent vertices of P_{n-k+2} belongs to $\mathcal{G}_{n,k}$.

Tavakoli et al. [33] proved that if G is a graph of order n with k pendent vertices, then $irr(G) \geq k$ with equality if and only if G is isomorphic to P_n. We now improve this result and give a sharp lower bound on the irregularity of graphs.

Theorem 5. *Let G be a graph of order n with k pendent vertices, different from P_n. Then*

$$irr(G) \geq 2k \tag{6}$$

with equality holding if and only if $G \in \mathcal{G}_{n,k}$, $1 \leq k \leq (n+2)/2$.

Proof. Let $v_1, v_2, \ldots, v_k$ be the pendent vertices of G. Denote by u_i, $1 \leq i \leq k$ the nearest vertex from v_i that has degree greater than two. Then similarly as in the proof of Theorem 4, we get

$$irr(G) \geq \sum_{i=1}^{k} imb_G(u_i, v_i) \geq \sum_{i=1}^{k} |d_G(u_i) - 1| \geq k(3-1) = 2k \tag{7}$$

since $d_G(u_i) \geq 3$ for $1 \leq i \leq k$.

Suppose that the equality holds in (7). Then $\Delta = 3$ by Theorem 4. Also for all $1 \leq i \leq k$, we have $d_G(u_i) = 3$ and it follows that $imb_G(e) = 0$ for all $e \notin (u_i, v_i)$, $1 \leq i \leq k$. If $G \notin \mathcal{G}_{n,k}$, then there exists a vertex x of degree two that has two neighbors y and z of degree three. Then $xy \notin (u_i, v_i)$, $imb_G(xy) = 1$ and we get a contradiction. Therefore, $G \in \mathcal{G}_{n,k}$. If $k > (n+2)/2$, then we have $2(n-1) \leq 2|E(G)| \leq k + \Delta(n-k)$ and it follows that

$$\Delta \geq 1 + \frac{n-2}{n-k} > 1 + \frac{n-2}{n-(n+2)/2} = 3\,.$$

Thus, $\mathcal{G}_{n,k} = \emptyset$.

Conversely, if $G \in \mathcal{G}_{n,k}$ then imb of all pendent paths are two and imb of all other edges are zero. Hence, it is easy to see that the equality holds in (6). ∎

3 Irregularity of maximally irregular graphs

In this section, we study the irregularity of maximally irregular graphs. Albertson [5] proved that the irregularity of a graph is an even number.

Theorem 6. *Let G be a maximally irregular graph with maximum degree Δ. Then $irr(G) \geq 2\lfloor \Delta/2 \rfloor$ and the bound is tight.*

Proof. Since G is a maximally irregular graph, there exists a path (u, v) with $d_G(u) = \Delta$ and $d_G(v) = 1$. We thus get

$$irr(G) \geq imb_G(u, v) \geq |d_G(u) - d_G(v)| = \Delta - 1 \tag{8}$$

by Lemma 1. Therefore, since the irregularity of G is even, we obtain the required bound.

We now show that the above bound is tight. If $\Delta = 1$ or $\Delta = 2$, then $irr(P_2) = 0$ and $irr(P_3) = 2$. Therefore, we assume that $\Delta \geq 3$. Let t be an odd positive integer. Let M be a maximum matching in K_{t+2} and e an edge of K_{t+2} such that one end vertex of e is M-unsaturated. Denote by H_t the graph obtained from K_{t+2} by deleting the edges in M and e. Note that H_t is the graph with one vertex of degree $t - 1$ and all other vertices of degree t. Also, K'_i denotes the graph obtained from K_i by deleting an edge. We denote by x_i and y_i the vertices of degree $i - 2$ in K'_i.

Case (i). Δ is odd. Then, we construct a new graph G from the graphs P_2, $K'_4, \ldots, K'_\Delta$ and H_Δ as shown in Figure 1.

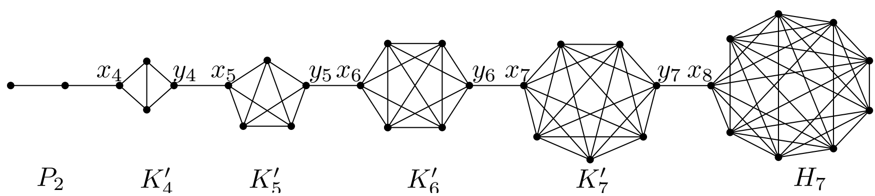

Figure 1. A maximally irregular graph G with maximum degree 7 and $irr(G) = 6$

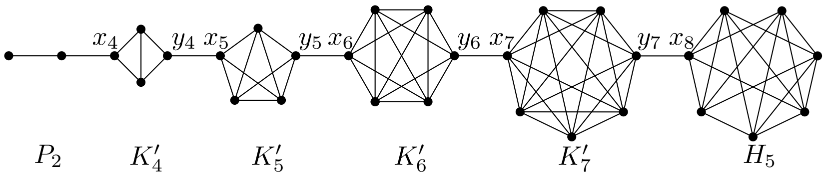

Figure 2. A maximally irregular graph G with maximum degree 6 and $irr(G) = 6$

Case (ii). Δ is even. Then we construct a new graph G from the graphs P_2, $K_4', \ldots, K_{\Delta+1}'$ and $H_{\Delta-1}$ as shown in Figure 2.

In the above two cases, one can easily see that G is the maximally irregular graph with maximum degree Δ such that $irr(G) = 2\lfloor \Delta/2 \rfloor$. ■

From the proof of Theorem 6, we obtain the following result which is the inverse problem for the irregularity of maximally irregular graphs.

Theorem 7. *For any even positive integer t, there exists a maximally irregular graph G such that $irr(G) = t$.*

A graph is *quasiperfect* if it has exactly two vertices of same degree. In [8], it was shown that for any positive integer n, there exists a unique quasiperfect graph of order n. We denote it by QP_n. One can easily check that $irr(QP_n) = \lfloor n^2/4 \rfloor$.

Lemma 3. [20, 23] Let G be a maximally irregular graph of order n. Then $|E(G)| \leq \lfloor n^2/4 \rfloor$.

We now give an upper bound on the irregularity of maximally irregular graphs.

Theorem 8. *Let G be a maximally irregular graph of order n with maximum degree Δ. Then*

$$irr(G) \leq \frac{1}{48}\left(6n^2\,\Delta + 3\Delta^2\,n - 2\Delta^3 - 4\Delta\right).$$

Proof. Let n_i be the number of vertices of degree i in G, $1 \leq i \leq \Delta$. Then $n_1 + n_2 + \cdots + n_\Delta = n$ and $n_i \geq 1$ for $1 \leq i \leq \Delta$ since G is maximally irregular. This implies

$$\sum_{i=1}^{\lfloor \Delta/2 \rfloor} n_i \leq n - \lceil \Delta/2 \rceil \,. \tag{9}$$

If $1 \leq i \leq \lfloor \Delta/2 \rfloor$, then $imb_G(e) \leq \Delta - i$ for all edges e incident with vertices of degree i. In addition, the imbalance of the remaining edges is at most $\lfloor \Delta/2 \rfloor$. Therefore,

$$\begin{aligned} irr(G) &\leq \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i\, n_i(\Delta - i) + \lfloor \Delta/2 \rfloor \left(|E(G)| - \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i n_i \right) \\ &= \lceil \Delta/2 \rceil \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i - \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i^2 + \lfloor \Delta/2 \rfloor |E(G)| \\ &+ \sum_{i=1}^{\lfloor \Delta/2 \rfloor} (n_i - 1) i (\lceil \Delta/2 \rceil - i) \,. \end{aligned} \tag{10}$$

On the other hand, one can easily see that

$$\lceil \Delta/2 \rceil \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i - \sum_{i=1}^{\lfloor \Delta/2 \rfloor} i^2 = \begin{cases} \dfrac{(\Delta+3)(\Delta^2-1)}{48}, & \Delta \text{ is odd} \\[2ex] \dfrac{\Delta(\Delta^2-4)}{48}, & \Delta \text{ is even} \end{cases} \tag{11}$$

and

$$\begin{aligned} \sum_{i=1}^{\lfloor \Delta/2 \rfloor} (n_i - 1) i (\lceil \Delta/2 \rceil - i) &\leq \frac{1}{4} \lceil \Delta/2 \rceil^2 \sum_{i=1}^{\lfloor \Delta/2 \rfloor} (n_i - 1) \\ &\leq \begin{cases} \dfrac{(n-\Delta)(\Delta+1)^2}{16}, & \Delta \text{ is odd} \\[2ex] \dfrac{(n-\Delta)\Delta^2}{16}, & \Delta \text{ is even} \end{cases} \end{aligned} \tag{12}$$

because of inequality (9). Then, substituting (11) and (12) back into (10), we obtain

$$irr(G) \leq \lfloor \Delta/2 \rfloor |E(G)| + \begin{cases} \dfrac{3n(\Delta+1)^2 - 2\Delta^3 - 3\Delta^2 - 4\Delta - 3}{48}, & \Delta \text{ is odd} \\ \dfrac{3\Delta^2 n - 2\Delta^3 - 4\Delta}{48}, & \Delta \text{ is even} \end{cases} \tag{13}$$

and it follows that

$$irr(G) \leq \begin{cases} \dfrac{n^2(\Delta-1)}{8} + \dfrac{3n(\Delta+1)^2 - 2\Delta^3 - 3\Delta^2 - 4\Delta - 3}{48}, & \Delta \text{ is odd} \\ \dfrac{n^2\Delta}{8} + \dfrac{3\Delta^2 n - 2\Delta^3 - 4\Delta}{48}, & \Delta \text{ is even} \end{cases}$$

by Lemma 3. Hence, we get the required inequality. ■

4 Conclusion

A natural issue is to characterize the graphs with maximum irregularity in the class of graphs with given order. We pose the following conjecture.

Conjecture 1. *Among maximally irregular graphs of order n, the quasi-perfect graph QP_n is the unique graph with maximal irregularity.*

By using the SageMath software, the validity of Conjecture 1 could be confirmed for the first few values of n, that is $n \leq 10$. We conclude this paper by giving an additional support on this conjecture.

Lemma 4. [20] Let G be a maximally irregular graph of order n with maximum degree Δ. If

$$\Delta \leq n - \frac{1}{2}\left(\sqrt{4n + 3 - 2(-1)^n} - 1\right),$$

then $|E(G)| \leq \lfloor \Delta(2n - \Delta + 1)/4 \rfloor$.

Theorem 9. *Let G be a maximally irregular graph of order n. If $\Delta \leq 3n/5$, then Conjecture 1 holds.*

Proof. If $n \leq 10$ then Conjecture 1 is found to be true by using the Sage-Math software. Let therefore $n > 10$. Then, since $\Delta \leq 3n/5$, we have $\Delta \leq n - \frac{1}{2}\left(\sqrt{4n+3-2(-1)^n} - 1\right)$. From (13), we get

$$irr(G) \leq \lfloor \Delta/2 \rfloor |E(G)| + \begin{cases} \dfrac{3n(\Delta+1)^2 - 2\Delta^3 - 3\Delta^2 - 4\Delta - 3}{48}, & \Delta \text{ is odd} \\ \dfrac{3\Delta^2 n - 2\Delta^3 - 4\Delta}{48}, & \Delta \text{ is even} \end{cases}$$

$$\leq \frac{\Delta}{2} \cdot \frac{\Delta(2n - \Delta + 1)}{4} + \frac{3\Delta^2 n - 2\Delta^3 - 4\Delta}{48}$$

$$= \frac{\Delta}{48}(15n\Delta - 8\Delta^2 + 6\Delta - 4)$$

by Lemma 4. Therefore from the above inequality, we obtain

$$irr(G) \leq \frac{n(153n^2 + 90n - 100)}{2000} \tag{14}$$

because $\Delta \leq 3n/5$ and the function $f(x) = x(15n\,x - 8x^2 + 6x - 4)$ is increasing for all $1 \leq x < n$. On the other hand, we easily see that

$$irr(QP_n) = \begin{cases} \dfrac{1}{12}(n^3 - n), & n \text{ is odd} \\ \dfrac{1}{12}(n^3 - 4n), & n \text{ is even} \end{cases}. \tag{15}$$

By (14) and (15), we get $irr(G) < irr(QP_n)$ for $n > 10$ which is our required result. ■

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