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THE EXTREMAL IRREGULARITY OF CONNECTED GRAPHS WITH GIVEN NUMBER OF PENDANT VERTICES

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Abstract. The irregularity of a graph $G = (V, E)$ is defined as the sum of imbalances $|d_u - d_v|$ over all edges $uv \in E$, where d_u denotes the degree of the vertex u in G. This graph invariant, introduced by Albertson in 1997, is a measure of the defect of regularity of a graph. In this paper, we completely determine the extremal values of the irregularity of connected graphs with n vertices and p pendant vertices ($1 \leqslant p \leqslant n-1$), and characterize the corresponding extremal graphs.

Keywords: graph irregularity; connected graph; pendant vertex; extremal graph

MSC 2020: 05C07, 05C35

1. Introduction

We consider finite, undirected, and simple graphs throughout this paper. Let G be a graph with the vertex set $V(G)$ and edge set $E(G)$. For a nonempty set $U \subseteq V(G)$, denote by $G[U]$ the graph induced by the vertices in U. Let $G - uv$ denote the graph obtained from G by deleting an edge $uv \in E(G)$, and if $vw \notin E(G)$, let $G + vw$ denote the graph obtained from G by adding an edge between the vertices v and w. For a vertex v in G, denote by $N_G(v)$ the set of vertices that are adjacent to v and by $d_G(v)$ the degree of v, which is equal to $|N_G(v)|$. We call v a *pendant vertex* if $d_G(v) = 1$. We also write $\Delta(G)$ for the maximum degree of the vertices in G and let $\Delta_2(G) := \max(\{d_G(v)\colon\ v \in V(G)\} \setminus \{\Delta(G)\})$.

A clique (or an independent set) of G is a set of mutually adjacent (or nonadjacent, respectively) vertices in G. As usual, let S_n and P_n be the star and the path on n vertices, respectively. For $1 \leqslant k \leqslant \frac{1}{2}n - 1$, we denote by $D_{n,k}$ the graph obtained by

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joining the centers of S_{k+1} and S_{n-k-1} with an edge, which is usually named a *double tree*, see Figure 1. For $1 \leqslant \omega \leqslant n-1$, let $CS_{n,\omega}$ be the graph obtained by joining each vertex of a clique of order ω with each vertex of an independent set of order $n-\omega$, which is usually called a *complete split graph*. We also use $H_{n,s,t}$ to denote the graph obtained by joining the center of S_{s+1} with each vertex of $CS_{n-s-1,t}$, where $1 \leqslant s \leqslant n-3$ and $1 \leqslant t \leqslant n-s-2$, see Figure 1.

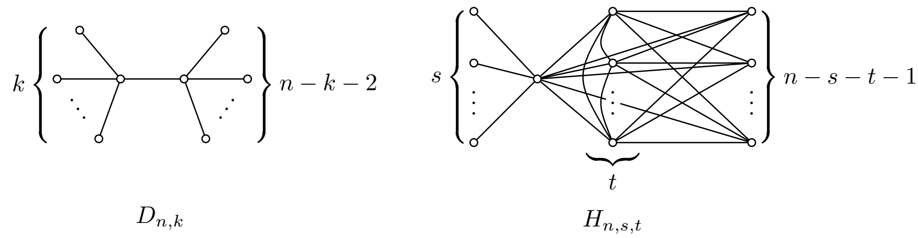

Figure 1. The graphs $D_{n,k}$ and $H_{n,s,t}$.

In 1997, Albertson in [3] defined the imbalance of an edge $e = uv \in E(G)$ as $\mathrm{imb}_G(e) = |d_G(u) - d_G(v)|$ and the irregularity of a graph G as

$$\mathrm{irr}(G) = \sum_{e \in E(G)} \mathrm{imb}_G(e) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

The idea of imbalance of an edge appeared implicitly in [4] where it was related to Ramsey problems with repeated degrees. For a connected graph G, $\mathrm{irr}(G) = 0$ if and only if G is regular, and for an irregular graph G, $\mathrm{irr}(G)$ is a measure of the defect of regularity of G. It should be also mentioned that the irregularity of a graph has found many applications in chemical graph theory, where it was met under the names the Albertson index (see [11], [19]), the misbalance deg index (see [21]), and the third Zagreb index, see [8].

For a general graph G on n vertices, Albertson in [3] first gave an asymptotically tight upper bound: $\mathrm{irr}(G) \leqslant \frac{1}{27}4n^3$. This upper bound was later improved by Abdo et al. (see [1]) as $\mathrm{irr}(G) \leqslant \lfloor \frac{1}{3}n \rfloor \lceil \frac{1}{3}2n \rceil (\lceil \frac{1}{3}2n \rceil - 1)$, with the equality holding if and only if $G \cong CS_{n,\lfloor \frac{1}{3}n \rfloor}$, see also [20]. Hansen and Mélot in [12] also characterized the graphs with n vertices and m edges and having the maximal irregularity. Nasiri and Fath-Tabar in [16] determined all the connected graphs with the second-minimal irregularity. Henning and Rautenbach in [13] characterized the structure of bipartite graphs having the maximal irregularity with given sizes of the partite sets and a given number of edges, they also derived a corresponding result for bipartite graphs with given sizes of the partite sets and gave an upper bound on the irregularity of these graphs. Luo and Zhou in [15], [22] determined the maximal values and corresponding extremal graphs of the irregularity of several classes of graphs, including the trees and unicyclic graphs with a fixed matching number or fixed number of pendant vertices. For some other results about graph irregularity, one can refer to [2], [5], [6], [7], [9], [10], [14], [17], [18] and the references cited therein.

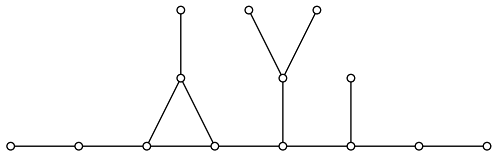

Figure 2. A graph in $\widehat{\Gamma}^{(3)}_{14,6}$.

In this paper, we focus on the extremal values and the corresponding extremal graphs of the irregularity of connected graphs with given order and given number of pendant vertices. For two positive integers n and p with $1 \leqslant p \leqslant n-1$, let

$$\Gamma_{n,p} = \{G\colon\ G \text{ is a connected graph of order } n \text{ with } p \text{ pendant vertices}\}.$$

Note that $\Gamma_{n,n-1} = \{S_n\}$ and $\Gamma_{n,n-2} = \{D_{n,k}\colon\ 1 \leqslant k \leqslant \frac{1}{2}n - 1\}$. Moreover, let

$$\widehat{\Gamma}^{(3)}_{n,p} = \{G \in \Gamma_{n,p}\colon\ \Delta(G) = 3 \text{ and } G[V_G^{(3)}] \text{ is connected}\},$$

where $V_G^{(i)} = \{v \in V(G)\colon\ d_G(v) = i\}$, see Figure 2 for illustration. Note that the graphs in $\widehat{\Gamma}^{(3)}_{n,p}$ all have the same irregularity regardless of the distribution of the vertices of degree 2 and the internal structure, as every path from a pendant vertex to a degree 3 vertex whose internal vertices are all of degree 2 contributes 2 to the irregularity. The main results of this paper are as follows:

Theorem 1. *Let $G \in \Gamma_{n,p}$, where n and p are positive integers such that $1 \leqslant p \leqslant n-1$.*

(i) *If $p = n-1$, then*

$$\operatorname{irr}(G) \leqslant n^2 - 3n + 2$$

with equality if and only if $G \cong S_n$.

(ii) *If $p = n-2$, then*

$$\operatorname{irr}(G) \leqslant n^2 - 5n + 6$$

with equality if and only if $G \cong D_{n,1}$.

(iii) *If $1 \leqslant p \leqslant n-3$, then*

$$\operatorname{irr}(G) \leqslant k^3 - 2(n-p-2)k^2 + [(n-p-1)(n-p-4)+1]k + (n-2)(n-1)$$

with equality if and only if $G \cong H_{n,p,k}$*, where* $k = \max\{1, \lfloor \frac{1}{3}(n-p-1) \rfloor - 1 + \varepsilon\}$*, and*

▷ *if* $n-p-1 \equiv 0 \pmod 3$*, then* $\varepsilon = 0$*;*
▷ *if* $n-p-1 \equiv 1 \pmod 3$*, then* $\varepsilon \in \{0,1\}$*;*
▷ *if* $n-p-1 \equiv 2 \pmod 3$*, then* $\varepsilon = 1$*.*

Theorem 2. *Let* $G \in \Gamma_{n,p}$*, where* n *and* p *are positive integers such that* $1 \leqslant p \leqslant n-1$*. If* $G \ncong P_n$*, then* $\mathrm{irr}(G) \geqslant 2p$*, with equality if and only if* $G \in \widehat{\Gamma}^{(3)}_{n,p}$*.*

The proofs of Theorems 1 and 2 are given in the following section.

2. Proofs

We first present the proof of Theorem 1. To this end, we need to establish two auxiliary results in advance.

Lemma 3. *Let* $f(x) := x^3 - 2(\theta-1)x^2 + (\theta^2 - 3\theta + 1)x + (n-2)(n-1)$ *be a continuous function on the closed interval* $[1,\theta]$*, where* n *and* θ *are positive integers such that* $3 \leqslant \theta \leqslant n-2$*. Then the function* $f(x)$ *attains its maximum uniquely at* $x = \max\bigl\{1, \frac{1}{3}\bigl(2\theta - 2 - \sqrt{\theta^2+\theta+1}\bigr)\bigr\}$*.*

P r o o f. Consider the derivative of the function $f(x)$ on $[1,\theta]$,

$$f'(x) = 3x^2 - 4(\theta-1)x + \theta^2 - 3\theta + 1,$$

whose two zero points are

$$x_1 = \frac{2\theta - 2 - \sqrt{\theta^2+\theta+1}}{3} \quad \text{and} \quad x_2 = \frac{2\theta - 2 + \sqrt{\theta^2+\theta+1}}{3}.$$

Note that $x_1 < 1$ if $3 \leqslant \theta \leqslant 5$ and $x_1 > 1$ if $6 \leqslant \theta \leqslant n-2$. Clearly, $f(x)$ must attain its maximum at 1, θ, $x_1 (\geqslant 1)$, or x_2. Moreover, for $3 \leqslant \theta \leqslant n-2$, we have

$$\begin{aligned}
f(1) - f(\theta) &= 2(\theta^2 - 3\theta + 2) > 0,\\
f(1) - f(x_2) &= \frac{1}{27}\bigl[2\bigl(\sqrt{\theta^2+\theta+1} - \theta\bigr)\theta^2 + \bigl(51\theta + 2\sqrt{\theta^2+\theta+1} - 159\bigr)\theta\\
&\quad + 2\bigl(\sqrt{\theta^2+\theta+1} + 55\bigr)\bigr] > 0,\\
f(x_1) - f(1) &= \frac{1}{27}\bigl[\bigl(2\sqrt{\theta^2+\theta+1} + 2\theta - 51\bigr)\theta^2 + \bigl(2\sqrt{\theta^2+\theta+1} + 159\bigr)\theta\\
&\quad + 2\bigl(\sqrt{\theta^2+\theta+1} - 55\bigr)\bigr] > 0;
\end{aligned}$$

one might check that the third inequality holds for $3 \leqslant \theta \leqslant 12$ by direct calculation and for $\theta \geqslant 13$ by the fact that

$$f(x_1) - f(1) > \frac{\theta^2}{27}\big(2\sqrt{\theta^2+\theta+1} + 2\theta - 51\big) > \frac{\theta^2}{27}\big(4\theta - 51\big) > 0.$$

This proves that $f(x)$ attains its maximum uniquely at $x = \max\{1, x_1\}$, as desired, completing the proof of Lemma 3. $\square$

Lemma 4. *Let $G \in \Gamma_{n,p}$, where n and p are positive integers such that $1 \leqslant p \leqslant n-3$. If G has the maximal irregularity, then $\Delta(G) = n-1$ and $\Delta_2(G) = n-p-1$.*

Proof. For convenience, let $d_v = d_G(v)$ for any vertex $v \in V(G)$, and let u_1 and u_2 be two vertices of G such that $d_{u_1} = \Delta(G)$ and $d_{u_2} = \Delta_2(G)$, respectively. We first show that $\Delta(G) = n-1$. By contradiction, we suppose that $\Delta(G) \leqslant n-2$. Clearly, there is a vertex v_1 nonadjacent to the vertex u_1 (that is, $u_1v_1 \notin E(G)$). We consider the following two cases:

Case 1: $N_G(v_1) \nsubseteq N_G(u_1)$. In this case, there exists a vertex $u \notin N_G(u_1)$ such that $v_1u \in E(G)$. Let $G_1 = G - v_1u + u_1v_1 + u_1u$. Obviously, G_1 has p pendant vertices. However,

$$\begin{aligned}\operatorname{irr}(G_1) - \operatorname{irr}(G) &= (d_{u_1} + 2 - d_{v_1}) + (d_{u_1} + 2 - d_u) - |d_{v_1} - d_u| \\ &\quad + \sum_{x \in N_G(u_1)} [(d_{u_1} + 2 - d_x) - (d_{u_1} - d_x)] \\ &= 4d_{u_1} + 4 - d_{v_1} - d_u - |d_{v_1} - d_u| \\ &\geqslant 4d_{u_1} + 4 - 2\max\{d_{v_1}, d_u\} > 0,\end{aligned}$$

which contradicts the assumption that G has the maximal irregularity.

Case 2: $N_G(v_1) \subseteq N_G(u_1)$. In this case, for any vertex $z \in N_G(v_1)$, we have $d_z \geqslant 2$. We further consider the following subcases.

Subcase 2.1: $d_z \leqslant d_{v_1}$ for any vertex $z \in N_G(v_1)$. Let $G_2 = G + u_1v_1$. One can see that G_2 still has p pendant vertices. However, we have

$$\begin{aligned}\operatorname{irr}(G_2) - \operatorname{irr}(G) &= [(d_{u_1} + 1) - (d_{v_1} + 1)] \\ &\quad + \sum_{x \in N_G(u_1)} [(d_{u_1} + 1 - d_x) - (d_{u_1} - d_x)] \\ &\quad + \sum_{y \in N_G(v_1)} [(d_{v_1} + 1 - d_y) - (d_{v_1} - d_y)] \\ &= 2d_{u_1} > 0,\end{aligned}$$

which again contradicts the maximality of G.

Subcase 2.2: There is (at least) one vertex $w \in N_G(v_1)$ so that $d_w > d_{v_1}$. If $d_w \geqslant 3$, then let $G_3 = G - v_1w + v_1u_1$. Clearly, G_3 has p pendant vertices. However, we obtain

$$\begin{aligned}\operatorname{irr}(G_3) - \operatorname{irr}(G) &= (d_{u_1} + 1 - d_{v_1}) + [(d_{u_1} + 1) - (d_w - 1)] - (d_{u_1} - d_w) \\ &\quad - (d_w - d_{v_1}) + \sum_{x \in N_G(u_1) - \{w\}} [(d_{u_1} + 1 - d_x) - (d_{u_1} - d_x)] \\ &\quad + \sum_{y \in N_G(w) - \{u_1, v_1\}} (|d_w - 1 - d_y| - |d_w - d_y|) \\ &\geqslant 2d_{u_1} - 2d_w + 4 > 0,\end{aligned}$$

a contradiction.

If $d_w = 2$, then $d_{v_1} = 1$. Suppose that w' is a vertex in $N_G(u_1) - \{w\}$ such that $d_{w'} \geqslant d_z$ for any vertex $z \in N_G(u_1) - \{w\}$. Then, we have $d_{w'} \geqslant 2$ (since $1 \leqslant p \leqslant n - 3$). Let $G_4 = G - v_1w + v_1u_1 + ww'$. Clearly, G_4 still has p pendant vertices. However, we get

$$\begin{aligned}\operatorname{irr}(G_4) - \operatorname{irr}(G) &= (d_{u_1} + 1 - 1) + (d_{u_1} + 1 - 2) + [(d_{u_1} + 1) - (d_{w'} + 1)] \\ &\quad + (d_{w'} + 1 - 2) - (d_{u_1} - d_{w'}) - (d_{u_1} - 2) - (2 - 1) \\ &\quad + \sum_{x \in N_G(u_1) - \{w, w'\}} [(d_{u_1} + 1 - d_x) - (d_{u_1} - d_x)] \\ &\quad + \sum_{y \in N_G(w') - \{u_1\}} (|d_{w'} + 1 - d_y| - |d_{w'} - d_y|) \\ &\geqslant 2d_{u_1} - 2 > 0,\end{aligned}$$

a contradiction as well. This proves that $\Delta(G) = n - 1$.

Since G has p pendant vertices, there is exactly one vertex of degree $n - 1$ in G. We further prove that $\Delta_2(G) = n - p - 1$. Again by contradiction, we suppose that $\Delta_2(G) \leqslant n - p - 2$. Let $U = \{v \in V(G)\colon\ d_v \neq 1,\ d_v \neq n - 1\}$. Clearly, $|U| = n - p - 1$ and there is a vertex v_2 in U nonadjacent to the vertex u_2 (that is, $u_2v_2 \notin E(G)$). We consider the following two cases:

Case 3: $N_G(v_2) \nsubseteq N_G(u_2)$. In this case, there exists a vertex $u \notin N_G(u_2)$ such that $v_2u \in E(G)$. Let $G_5 = G - v_2u + u_2v_2 + u_2u$. Obviously, G_5 has p pendant vertices. However,

$$\begin{aligned}\operatorname{irr}(G_5) - \operatorname{irr}(G) &= (d_{u_2} + 2 - d_u) + (d_{u_2} + 2 - d_{v_2}) - |d_{v_2} - d_u| \\ &\quad + [n - 1 - (d_{u_2} + 2)] - (n - 1 - d_{u_2}) \\ &\quad + \sum_{x \in N_G(u_2) - \{u_1\}} [(d_{u_2} + 2 - d_x) - (d_{u_2} - d_x)] \\ &\geqslant 4d_{u_2} - 2\max\{d_{v_2}, d_u\} > 0,\end{aligned}$$

which contradicts the assumption that G has the maximal irregularity.

Case 4: $N_G(v_2) \subseteq N_G(u_2)$. In this case, let $G_6 = G - v_2w + v_2u_2$, where $w \in N_G(v_2) - \{u_1\}$. Note that $d_w \geqslant 3$ and hence G_6 still has p pendant vertices. However, we obtain

$$\begin{aligned}
\operatorname{irr}(G_6) - \operatorname{irr}(G) &= [d_{u_2} + 1 - (d_w - 1)] + (d_{u_2} + 1 - d_{v_2}) - (d_{u_2} - d_w) \\
&\quad - |d_w - d_{v_2}| + [n - 1 - (d_{u_2} + 1)] - (n - 1 - d_{u_2}) \\
&\quad + [n - 1 - (d_w - 1)] - (n - 1 - d_w) \\
&\quad + \sum_{x \in N_G(u_2) - \{u_1, w\}} [(d_{u_2} + 1 - d_x) - (d_{u_2} - d_x)] \\
&\quad + \sum_{y \in N_G(w) - \{u_1, u_2, v_2\}} (|d_w - 1 - d_y| - |d_w - d_y|) \\
&\geqslant 2d_{u_2} + 4 - 2\max\{d_{v_2}, d_w\} > 0,
\end{aligned}$$

a contradiction, as desired. This proves that $\Delta_2(G) = n - p - 1$.

The proof of Lemma 4 is thus completed. $\square$

We are now ready to give the proof of Theorem 1.

Proof of Theorem 1. Clearly, (i) follows from the fact that $\Gamma_{n,n-1} = \{S_n\}$.

For (ii), noting that $\Gamma_{n,n-2} = \{D_{n,k}\colon\ 1 \leqslant k \leqslant \frac{1}{2}n - 1\}$, we have

$$\operatorname{irr}(G) = 2k^2 - 2k(n-1) + n^2 - 3n + 2 \leqslant n^2 - 5n + 6,$$

with equality if and only if $k = 1$, i.e., $G \cong D_{n,1}$.

For (iii), we can suppose that $G (\in \Gamma_{n,p})$ has the maximal irregularity. Then we have the following claim.

Claim 5. $G \cong H_{n,p,k}$, $1 \leqslant k \leqslant n - p - 2$.

Proof of Claim 5. By Lemma 4, we know that $\Delta(G) = n - 1$ and $\Delta_2(G) = n - p - 1$. For $1 \leqslant i \leqslant n - 1$, let $V_G^{(i)} = \{z \in V(G)\colon\ d_z = i\}$. It is easy to see that $|V_G^{(1)}| = p$ and $|V_G^{(n-1)}| = 1$. Moreover, let $q = |V_G^{(n-p-1)}|$ and let

$$W = V(G) - (V_G^{(1)} \cup V_G^{(n-p-1)} \cup V_G^{(n-1)}).$$

Note that $1 \leqslant q \leqslant n - p - 3$ or $q = n - p - 1$.

If $q = n - p - 1$, then $|W| = n - p - q - 1 = 0$ and hence $W = \emptyset$; in this case, we have $G \cong H_{n,p,n-p-2}$.

If $q = n-p-3$, then $|W| = 2$. Moreover, since $n-p-1 > d_z \geqslant q+1 = n-p-2$ for any vertex $z \in W$, W must be an independent set, implying that $G \cong H_{n,p,n-p-3}$.

If $1 \leqslant q \leqslant n - p - 4$, then $|W| \geqslant 3$. We can also prove that W must be an independent set, which implies that $G \cong H_{n,p,q}$. Indeed, by letting u be a vertex in W such that $d_u = \max\{d_z\colon\ z \in W\}$, we just need to show that $d_u = q+1$. By contradiction, we can now suppose that $d_u > q+1$. Let $W' = W - (N_G(u) \cup \{u\})$. Since $q+1 < d_u < n-p-1$, we have $1 \leqslant |W'| \leqslant |W|-2$. We consider the following two cases.

Case 1: W' is not an independent set. In this case, there is an edge vw such that $v, w \in W'$. Let $G_1 = G - vw + uv$. Clearly, G_1 still has p pendant vertices. However, we obtain

$$\begin{aligned}
\operatorname{irr}(G_1) - \operatorname{irr}(G) = {} & (d_u + 1 - d_v) - |d_v - d_w| \\
& + [(n-1-d_w+1) - (n-1-d_w)] \\
& + [(n-1-d_u-1) - (n-1-d_u)] \\
& + q[(n-p-1-d_w+1) - (n-p-1-d_w)] \\
& + q[(n-p-1-d_u-1) - (n-p-1-d_u)] \\
& + \sum_{x \in N_G(u) \cap W} [(d_u + 1 - d_x) - (d_u - d_x)] \\
& + \sum_{y \in N_G(w) \cap W - \{v\}} (|d_w - 1 - d_y| - |d_w - d_x|) \\
\geqslant {} & 2d_u + 2 - 2\max\{d_v, d_w\} \\
> {} & 0,
\end{aligned}$$

which contradicts the assumption that G has the maximal irregularity.

Case 2: W' is an independent set.

Subcase 2.1: There is an edge vw such that $v \in W'$ and $w \in N_G(u) \cap W$. Let $G_2 = G - vw + vu$. Clearly, G_2 has p pendant vertices. However,

$$\begin{aligned}
\operatorname{irr}(G_2) - \operatorname{irr}(G) = {} & (d_u + 1 - d_v) + [(d_u+1) - (d_w - 1)] - (d_u - d_w) \\
& - |d_v - d_w| + (n-1-d_u-1) - (n-1-d_u) \\
& + (n-1-d_w+1) - (n-1-d_w) \\
& + q[(n-p-1-d_u-1) - (n-p-1-d_u)] \\
& + q[(n-p-1-d_w+1) - (n-p-1-d_w)] \\
& + \sum_{x \in N_G(u) \cap W - \{w\}} [(d_u + 1 - d_x) - (d_u - d_x)] \\
& + \sum_{y \in N_G(w) \cap W - \{u,v\}} (|d_w - 1 - d_y| - |d_w - d_y|) \\
\geqslant {} & 2d_u + 4 - 2\max\{d_v, d_w\} \\
> {} & 0,
\end{aligned}$$

which again contradicts the maximality of G.

Subcase 2.2: There is no edge vw such that $v \in W'$ and $w \in N_G(u) \cap W$. If $q < \frac{1}{3}(n-p-1)-1$, let $\lambda = |W'|$ and let G_3 be the graph obtained from G by joining the vertex u with each vertex in W'. Clearly, G_3 has p pendant vertices and $d_u + p + \lambda + 1 = n$. However, we get

$$\begin{aligned}
\operatorname{irr}(G_3) - \operatorname{irr}(G) = &\ [(n-1-d_u-\lambda)-(n-1-d_u)] \\
&+ \lambda[(n-1-q-2)-(n-1-q-1)] \\
&+ q[(n-p-1-d_u-\lambda)-(n-p-1-d_u)] \\
&+ q\lambda[(n-p-1-q-2)-(n-p-1-q-1)] \\
&+ \lambda(d_u+\lambda-q-2) \\
&+ \sum_{x \in N_G(u) \cap W} [(d_u+\lambda-d_x)-(d_u-d_x)] \\
= &\ \lambda(2d_u - 4q + \lambda - 5) \\
= &\ \lambda(n-p-1+d_u-4q-5) \\
\geqslant &\ \lambda[(n-p-1)-3q-3] \\
> &\ 0,
\end{aligned}$$

a contradiction.

If $q \geqslant \frac{1}{3}(n-p-1)-1$, let G_4 be the graph obtained from G by deleting all the edges of $G[W-W']$. Clearly, G_4 still has p pendant vertices. However,

$$\begin{aligned}
\operatorname{irr}(G_4) - \operatorname{irr}(G) = &\ \sum_{w \in W-W'} q[n-p-1-(q+1)-(n-p-1-d_w)] \\
&+ \sum_{w \in W-W'} [n-1-(q+1)-(n-1-d_w)] \\
&- \frac{1}{2} \sum_{w \in W-W'} \sum_{x \in N_G(w) \cap W} |d_w - d_x| \\
\geqslant &\ \sum_{w \in W-W'} (q+1)(d_w-q-1) \\
&- \frac{1}{2} \sum_{w \in W-W'} (d_w-q-1)[(n-p-2)-(q+2)] \\
= &\ \frac{1}{2}[3q-(n-p-1)+5] \sum_{w \in W-W'} (d_w-q-1) \\
> &\ 0,
\end{aligned}$$

a contradiction as well. This proves that $d_u = q+1$ and hence W is an independent set, which implies that $G \cong H_{n,p,q}$. Claim 5 thus follows. □

We next determine the exact value of k such that $\operatorname{irr}(H_{n,p,k})$ attains its maximum.

If $p = n-3$, then by the definition of $H_{n,p,k}$, we have $1 \leqslant k \leqslant n-p-2 = 1$, that is, $k = 1 = \max\{1, \lfloor\frac{1}{3}(n-p-1)\rfloor - 1 + \varepsilon\}$, where $\varepsilon \in \{0,1\}$.

If $1 \leqslant p \leqslant n-4$, by setting $\theta = n-p-1$, we have $3 \leqslant \theta \leqslant n-2$. Moreover, by some calculations, we have

$$\begin{aligned}\operatorname{irr}(H_{n,p,k}) &= [n-1-(n-p-1)]k + [n-1-(k+1)](n-p-1-k)\\ &\quad + (n-1-1)p + [(n-p-1)-(k+1)](n-p-1-k)k\\ &= k^3 - 2(\theta-1)k^2 + (\theta^2 - 3\theta + 1)k + (n-2)(n-1)\\ &= f(k),\end{aligned}$$

where $f(x) = x^3 - 2(\theta-1)x^2 + (\theta^2 - 3\theta+1)x + (n-2)(n-1)$. By Lemma 3, we know that $f(x)$ attains its maximum uniquely at $x = \max\{1, \frac{1}{3}(2\theta - 2 - \sqrt{\theta^2+\theta+1})\}$.

When $3 \leqslant \theta \leqslant 5$, we have $\frac{1}{3}(2\theta-2-\sqrt{\theta^2+\theta+1}) < 1$ and hence, $f(k)$ attains its maximum at $k = 1 = \max\{1, \lfloor\frac{1}{3}(n-p-1)\rfloor - 1 + \varepsilon\}$, where $\varepsilon \in \{0,1\}$.

When $6 \leqslant \theta \leqslant n-2$, we have $\frac{1}{3}(2\theta-2-\sqrt{\theta^2+\theta+1}) > 1$ and hence $f(k)$ attains its maximum at

$$q_1 = \Big\lfloor \frac{2\theta - 2 - \sqrt{\theta^2+\theta+1}}{3} \Big\rfloor \quad \text{or} \quad q_2 = \Big\lceil \frac{2\theta - 2 - \sqrt{\theta^2+\theta+1}}{3} \Big\rceil.$$

Observing that $\frac{1}{3}(\theta-3) < \frac{1}{3}(2\theta-2-\sqrt{\theta^2+\theta+1}) < \frac{1}{3}(\theta-\frac{5}{2})$, we can check that $q_1 = \lfloor\frac{1}{3}\theta\rfloor - 1$ and $q_2 = \lfloor\frac{1}{3}\theta\rfloor$. Furthermore, we have

- ▷ if $\theta = 3t$, then $q_1 = t-1$, $q_2 = t$, and $f(q_1) - f(q_2) = 2t > 0$;
- ▷ if $\theta = 3t+1$, then $q_1 = t-1$, $q_2 = t$, and $f(q_1) - f(q_2) = 0$;
- ▷ if $\theta = 3t+2$, then $q_1 = t-1$, $q_2 = t$, and $f(q_1) - f(q_2) = -2(t+1) < 0$.

Now, by combining the above arguments, we may conclude that

$$k = \Big\lfloor\frac{n-p-1}{3}\Big\rfloor - 1 + \varepsilon = \max\Big\{1, \Big\lfloor\frac{n-p-1}{3}\Big\rfloor - 1 + \varepsilon\Big\},$$

where $\varepsilon = 0$ if $n-p-1 \equiv 0 \pmod 3$, $\varepsilon \in \{0,1\}$ if $n-p-1 \equiv 1 \pmod 3$, and $\varepsilon = 1$ if $n-p-1 \equiv 2 \pmod 3$, as desired.

This completes the proof of Theorem 1. □

Proof of Theorem 2. Suppose that $G \in \Gamma_{n,p}$ $(1 \leqslant p \leqslant n-1)$. For an integer $l \geqslant 1$, let $Q := u_0u_1\ldots u_l$ be a path of length l in G. We call Q a pendant path of length l if $d_{u_0} \geqslant 3$, $d_{u_l} = 1$, and $d_{u_i} = 2$ for all i with $1 \leqslant i \leqslant l-1$. It is easy to check that the contribution of a pendant path Q in G to $\operatorname{irr}(G)$ is always $d_{u_0} - 1$.

On the other hand, since $G \not\cong P_n$, every pendant vertex of G uniquely determines a pendant path of G and vice versa, which yields that there are exactly p pendant paths in G. Thus, we have

$$\operatorname{irr}(G) \geqslant p \cdot (d_{u_0} - 1) \geqslant 2p. \tag{2.1}$$

Moreover, noting that all pendant paths (of arbitrary length) have the same minimal irr-value 2 if and only if their initial vertices have degree 3, we can conclude that the equality holds in (2.1) if and only if G has p pendant paths whose initial vertices have degree 3 and all other vertices not in these p pendant paths (if exist) have degree 3, that is, $G \in \widehat{\Gamma}^{(3)}_{n,p}$.

The proof of Theorem 2 is completed. □

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