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EXTREMELY IRREGULAR UNICYCLIC GRAPHS

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Abstract. The irregularity of a graph is defined to be the sum of absolute values of the differences of the degrees of endpoints of each edge. In this paper, we present some new results on the irregularity of unicyclic graphs, and then characterize all unicyclic graphs on n vertices with irregularity values greater than or equal to $n^2-9n+24$.

1. Introduction

A *unicyclic graph* is a connected graph with the same number of vertices and edges. Let $G=(V,E)$ be a simple, finite and undirected graph of order n. The *irregularity* of G is defined as,

$$\operatorname{irr}(G)=\sum_{xy\in E(G)}|d_G(x)-d_G(y)|, \tag{1.1}$$

where $d_G(x)$ is the degree of vertex x in G (see [4]). In this paper, we denote the irregularity of a graph G by $I(G)$. Moreover, for any edge xy of G, we denote $I_G(xy)=|d_G(x)-d_G(y)|$ and call it the *irregularity of the edge xy*. So, we have

$$I(G)=\sum_{xy\in E(G)} I_G(xy). \tag{1.2}$$

Obviously, a graph G has irregularity zero if and only if every component of G is a regular graph. Albertson [4] proved that the irregularity of any graph is an even number. Also, he presented upper bounds on the irregularity of bipartite and triangle-free graphs, and a sharp upper bound for trees. The irregularity of bipartite graphs are studied also in [11]. The relations between this quantity and the matching number of trees and unicyclic graphs were investigated in [12]. Hansen et al. [10] characterized

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the graphs with n vertices and m edges with maximal irregularity. Abdo and Dimitrov [3] considered the irregularity of graphs under several graph operations. Inspired by the structure of the equation (1.1), Abdo et al. [1] introduced a new measure of irregularity of a graph, so-called the *total irregularity*, as

$$\operatorname{irr}_t(G) = \frac{1}{2} \sum_{x,y \in V(G)} |d_G(x) - d_G(y)|.$$

Dimitrov and Škrekovski [7] compared the irregularity and total irregularity of graphs and gave some new appealing relations between them. Furthermore, the smallest graphs with equal irregularity measures are investigated in [6]. FathTabar [8] established some new bounds on the first and the second Zagrab indices that depend on the irregularity of graphs. Tavakoli et al. [18] characterized the graphs with minimum and maximum values of irregularity. Also, all graphs with the second minimum of the irregularity and total irregularity values are determined [13, 14], and the trees with the five smallest and five greatest irregularity values are characterized [9]. More references about this graph invariant can be found in [2, 5, 16, 17, 19].

Let u and v be two vertices of a (connected) graph G. Then the *distance* between u and v is the number of edges in a shortest path whose endpoints are u and v. This quantity is denoted by $d_G(u, v)$ and it is the main part of an old topological index (*Wiener index*) which has found interesting applications in chemistry. In [15], the extremal unicyclic graphs with respect to Wiener index is studied.

Recall that a vertex of degree one is called a *pendent vertex*. The (unique) n-vertex trees with 2 and $n-1$ pendent vertices are called *path* P_n, and *star* S_n, respectively. A unicyclic graph G with circuit $C_m = v_1 v_2 \cdots v_m v_1$ of length m is denoted by $C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$, where trees $T_1, T_2, \ldots, T_k$, $0 \le k \le m$, are all the nontrivial components of $G - E(C_m)$, and u_i is the common vertex of T_i and C_m, $1 \le i \le k$. Throughout the paper, we may suppose that the order of T_i is not greater than the order of T_{i+1}, for each $i = 1, 2, \ldots, k-1$. It is obvious that if $k = 0$, then $G \cong C_n$. For convenience, we denote $C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ by $C_m(T_1, T_2, \ldots, T_k)$, for $k \ge 1$. Let $n(T_i) = l_i + 1$ be the order of T_i, for $i = 1, 2, \ldots, k$, then we have $\sum_{i=1}^{k} l_i = n - m$. Also, if a tree T_i is the star S_{l_i+1} then we replace it by l_i, for example we denote $C_3(S_2, S_5, T_3)$ by $C_3(1, 4, T_3)$.

Let x be a vertex of the graph G. We denote by $N_G(x)$ the set of all vertices of G that are adjacent to x. Also, we define the subsets $N_G^1(x)$ and $N_G^2(x)$ of vertices of G as $N_G^1(x) = \{u \in N_G(x); d_G(x) \ge d_G(u)\}$, and $N_G^2(x) = \{u \in N_G(x); d_G(x) < d_G(u)\}$; and suppose that $n_G^1(x) = |N_G^1(x)|$ and $n_G^2(x) = |N_G^2(x)|$.

2. Main Result

In this section, we first introduce some notations and definitions of trees that are involved in the main result of this work.

Let $V(P_2) = \{a, b\}$ and r be a natural number such that $1 \le r \le n-2$, then we use $R_{n,r}$ to denote the n-vertex tree that is obtained from P_2, by joining r pendent edges to b and $n-2-r$ pendent edges to a. Throughout this paper, the notation F_n represents the tree of order n that is obtained from P_5, by attaching $n-5$ pendent vertices to its central vertex. Also, we denote by H_n the tree of order n obtained from P_4 by joining $n-4$ pendent edges to only one of its endpoints, say a (see Figure 1).

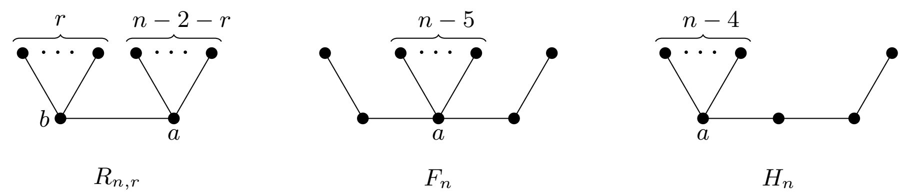

Figure 1. Trees rooted at a with large irregularity.

The following theorem is the main result of this paper that characterizes twenty four unicyclic graphs with the greatest irregularity.

Theorem 2.1. *Let G be a unicyclic graph on $n \geq 12$ vertices. If G is not isomorphic to any of graphs appeared in Table* 1*, then either $I(G) < n^2 - 9\,n + 24$ or $G \cong C_3(4,5)$.*

Table 1. The unicyclic graphs with the first twenty four greatest irregularity.

Graph	$C_3(n-3)$	$C_3(1, n-4)$	$C_4(n-4)$	$C_3(R_{n-2,1})$	$C_3(2, n-5)$	$C_4(1, n-5)_{\alpha=2}$
irr	$n^2-3\,n$	$n^2-5\,n+6$	$n^2-5\,n+4$	$n^2-5\,n+4$	$n^2-7\,n+16$	$n^2-7\,n+14$
Graph	$C_3(1, 1, n-5)$	$C_3(R_{3,1}, n-5)$	$C_4(1, n-5)_{\alpha=1}$	$C_3(1, R_{n-3,1})$	$C_3(R_{n-2,2})$	$C_3(R_{n-2,n-4})$
irr	$n^2-7\,n+12$	$n^2-7\,n+12$	$n^2-7\,n+12$	$n^2-7\,n+12$	$n^2-7\,n+12$	$n^2-7\,n+12$
Graph	$C_5(n-5)$	$C_3(F_{n-2})$	$C_3(H_{n-2})$	$C_4(R_{n-3,1})$	$C_3(3, n-6)$	$C_4(2, n-6)_{\alpha=2}$
irr	$n^2-7\,n+10$	$n^2-7\,n+10$	$n^2-7\,n+10$	$n^2-7\,n+10$	$n^2-9\,n+30$	$n^2-9\,n+28$
Graph	$C_3(R_{n-2,n-5})$	$C_3(2, R_{n-4,1})$	$C_3(R_{4,1}, n-6)$	$C_3(1, 2, n-6)$	$C_4(2, n-6)_{\alpha=1}$	$C_3(R_{n-2,3})$
irr	$n^2-9\,n+24$	$n^2-9\,n+24$	$n^2-9\,n+24$	$n^2-9\,n+24$	$n^2-9\,n+24$	$n^2-9\,n+24$

Remark 2.1. Note that Theorem 2.1 indicates that for $n \geq 13$, there exist exactly 24 unicyclic graphs on n vertices with irregularity greater than or equal to $n^2 - 9n + 24$, and in the special case $n = 12$ the number of such graphs is 25. Bear in mind that for $n \geq 12$ we have,

$$\begin{aligned} n^2 - 3\,n &> n^2 - 5\,n + 6 > n^2 - 5\,n + 4 \\ &> n^2 - 7\,n + 16 > n^2 - 7\,n + 14 > n^2 - 7\,n + 12 > n^2 - 7\,n + 10 \\ &> n^2 - 9\,n + 30 > n^2 - 9\,n + 28 > n^2 - 9\,n + 24. \end{aligned}$$

Table 2. Irregularity of all unicyclic graphs on n vertices for $n = 3, 4, 5, 6$.

$n=3$		$n=5$		$n=6$					
irr	**Graph**	**irr**	**Graph**	**irr**	**Graph**	**irr**	**Graph**	**irr**	**Graph**
0	C_3	10	$C_3(2)$	18	$C_3(3)$	6	$C_4(1,1)_{\alpha=1}$	4	$C_4(R_{3,1})$
$n=4$		6	$C_3(1,1)$	12	$C_3(1,2)$	6	$C_3(R_{4,2})$	4	$C_3(H_4)$
irr	**Graph**	4	$C_4(1)$	10	$C_4(2)$	6	$C_3(1, R_{3,1})$	0	C_6
4	$C_3(1)$	4	$C_3(R_{3,1})$	10	$C_3(R_{4,1})$	6	$C_3(1,1,1)$	–	–
0	C_4	0	C_5	8	$C_4(1,1)_{\alpha=2}$	4	$C_5(1)$	–	–

For the sake of completeness, we have computed the irregularity of all unicyclic graphs on $n = 3, 4, 5, 6$ vertices (see Table 2).

Also, we have collected all unicyclic graphs on $n = 7, 8, \ldots, 11$ vertices, each of which has the irregularity greater than or equal to $n^2 - 9n + 24$, as presented in Table 3, at the end of the paper.

To demonstrate the forms of the maximal unicyclic graphs with respect to irregularity value, some types of maximal graphs are displayed in Figure 2.

3. Lemmas

This section restates its first and foremost lemma, which has been proved in [9]. Then it proves relevant propositions that are required in the proof of the results that will be reported in the next section.

The following lemma characterizes all trees with the first five greatest irregularity values.

Lemma 3.1. [9] *Let T be a tree on n vertices. If $T \ncong S_n, R_{n,1}, R_{n,2}, F_n, H_n$ or $R_{n,3}$, then $I(T) < I(R_{n,3}) < I(H_n) = I(F_n) < I(R_{n,2}) < I(R_{n,1}) < I(S_n)$.*

Lemma 3.2. *Let $G = C_m^{u_1,\ldots,u_k}(T_1, \ldots, T_k)$ be a unicyclic graph of order n, then*

$$I(G) = \sum_{i=1}^{k} I(T_i) + 2\sum_{i=1}^{k} \left(n_{T_i}^1(u_i) - n_{T_i}^2(u_i) + t_{u_i} \right) + \sum_{xy \in E(C_m)} I_G(xy),$$

where $t_{u_i} = |\{v \in N_{T_i}(u_i); d_{T_i}(u_i) = d_{T_i}(v) - 1\}|$.

Proof. Applying formula (1.2), we can rewrite the irregularity of unicyclic graphs as:

$$I(G) = \sum_{i=1}^{k} \sum_{xy \in E(T_i)} I_G(xy) + \sum_{xy \in E(C_m)} I_G(xy).$$

So,

$$I(G) = \sum_{i=1}^{k} \left[\sum_{\substack{\{x,y\} \subseteq V(T_i) \setminus \{u_i\} \\ xy \in E(T_i)}} I_G(xy) + \sum_{xu_i \in E(T_i)} I_G(xu_i) \right] + \sum_{xy \in E(C_m)} I_G(xy).$$

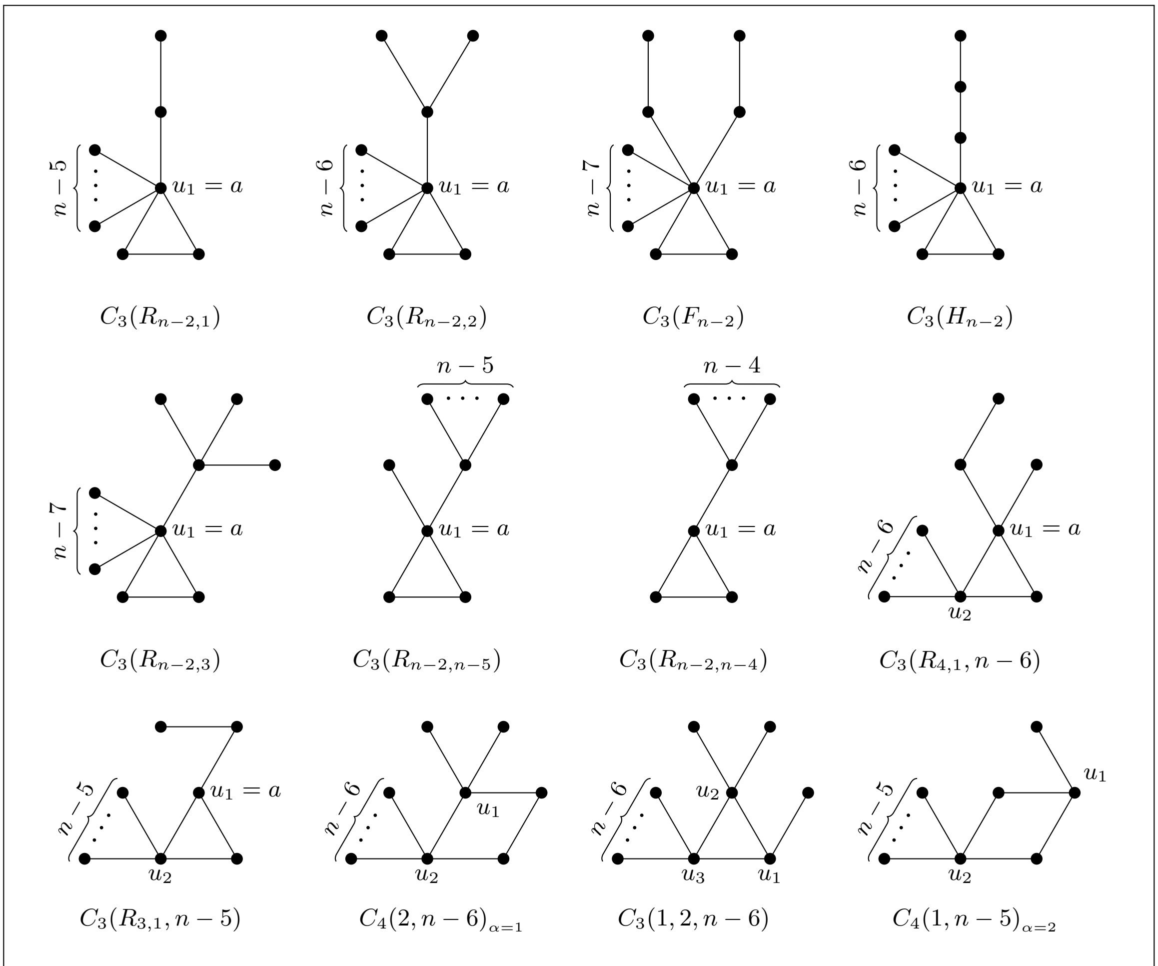

FIGURE 2. Some types of maximal unicyclic graphs with respect to irregularity value.

Since $d_G(u_i) = d_{T_i}(u_i) + 2$, then

$$I(G) = \sum_{i=1}^{k} \left(\sum_{\substack{\{x,y\} \subseteq V(T_i) \setminus \{u_i\} \\ xy \in E(T_i)}} I_{T_i}(xy) + \sum_{\substack{d_{T_i}(u_i) \geq d_{T_i}(x) \\ xu_i \in E(T_i)}} \Big(I_{T_i}(xu_i) + 2 \Big) \right.$$

$$\left. + \sum_{\substack{d_{T_i}(u_i) = d_{T_i}(x) - 1 \\ xu_i \in E(T_i)}} \Big(\underbrace{2 - I_{T_i}(xu_i)}_{1} \Big) + \sum_{\substack{d_{T_i}(u_i) < d_{T_i}(x) - 1 \\ xu_i \in E(T_i)}} \Big(I_{T_i}(xu_i) - 2 \Big) \right)$$

$$+ \sum_{xy \in E(C_m)} I_G(xy).$$

On the other hand,

$$\begin{aligned}\sum_{\substack{d_{T_i}(u_i)<d_{T_i}(x)-1\\ xu_i\in E(T_i)}}\Big(I_{T_i}(xu_i)-2\Big) &= \sum_{\substack{d_{T_i}(u_i)<d_{T_i}(x)\\ xu_i\in E(T_i)}}\Big(I_{T_i}(xu_i)-2\Big)\\ &\quad-\sum_{\substack{d_{T_i}(u_i)=d_{T_i}(x)-1\\ xu_i\in E(T_i)}}\Big(I_{T_i}(xu_i)-2\Big)\\ &= \sum_{\substack{d_{T_i}(u_i)<d_{T_i}(x)\\ xu_i\in E(T_i)}} I_{T_i}(xu_i)-2n^2_{u_i}+\sum_{\substack{d_{T_i}(u_i)=d_{T_i}(x)\\ xu_i\in E(T_i)}}1.\end{aligned}$$

Therefore, the lemma is proved. □

We know that $t_{u_i} \leq n^2_{T_i}(u_i)$ and $d_{T_i}(u_i) = n^1_{T_i}(u_i) + n^2_{T_i}(u_i)$. So, we have the following results.

Corollary 3.1. *Let $G = C_m(T_1, T_2, \ldots, T_k)$ be a unicyclic graph of order n, then*

$$\begin{aligned}I(G) &\leq \sum_{i=1}^{k} I(T_i) + 2\sum_{i=1}^{k} d_{T_i}(u_i) + \sum_{xy\in E(C_m)} I_G(xy)\\ &= \sum_{i=1}^{k} I(T_i) + 2\sum_{i=1}^{k} d_G(u_i) + \sum_{xy\in E(C_m)} I_G(xy) - 4k,\end{aligned}$$

with equality if and only if $n^2_{T_i}(u_i) = 0$ for $i = 1, \ldots, k$.

Corollary 3.2. *Let $G = C_m(l_1, l_2, \ldots, l_k)$ be a unicyclic graph of order n, then*

$$\begin{aligned}I(G) &= \sum_{i=1}^{k} I(S_{l_i+1}) + 2\sum_{i=1}^{k} d_{S_{l_i+1}}(u_i) + \sum_{xy\in E(C_m)} I_G(xy)\\ &= \sum_{i=1}^{k} {l_i}^2 + (n-m) + \sum_{xy\in E(C_m)} I_G(xy).\end{aligned}$$

4. Proof of Theorem 2.1

In this section, we shall first present some preliminary lemmas which are necessary in the proof of Theorem 2.1. Afterwards, we use all gathered propositions to prove our main result. Eventually, we give two tables to report the special cases $3 \leq n \leq 11$.

Lemma 4.1. *Let $G_1 = C_m(n-m)$ and $G_2 = C_{m-1}(n-m+1)$ be unicyclic graphs of order n. Then $I(G_2) > I(G_1)$.*

Proof. By a simple calculation, one can easily see that $I(G_1) = (n-m+3)(n-m)$ and $I(G_2) = (n-m+3)(n-m+1)$. Therefore, $I(G_2) > I(G_1)$. □

Lemma 4.2. *Let $G_2 = C_m^{u_1,\ldots,u_k}(l_1, \ldots, l_k)$ and $G_1 = C_m^{u_1,\ldots,u_k}(T_1, \ldots, T_k)$, where $n(T_i) = l_i + 1$, for each $i = 1, \ldots, k$. Then $I(G_2) \geq I(G_1)$, with the equality if and only if $G_2 \cong G_1$.*

Proof. Let $C_m = v_1v_2\cdots v_mv_1$. Suppose that there exists at least one index i such that $T_i \ncong S_{l_i+1}$, otherwise we have $G_1 \cong G_2$, and therefore $I(G_1) = I(G_2)$. Without loss of generality, suppose that $T_1 \ncong S_{l_1+1}$ and v_1 is the common vertex of T_1 and C_m. Also, let G_1^0 be the graph obtained from G_1, by removing vertices $V(T_1)\setminus\{v_1\}$, and attaching l_1 pendent vertices to v_1. To prove the lemma, it is sufficient to show that $I(G_1^0) > I(G_1)$. Set $d = d_{G_1^0}(v_1) - d_{G_1}(v_1) = l_1 - d_{T_1}(v_1)$. Then by Lemmas 3.1 and 3.2, we have,

$$\begin{aligned}
I(G_1^0) - I(G_1) =& I(S_{l_i+1}) + 2l_1 - I(T_1) - 2\left(n^1_{T_1}(v_1) - n^2_{T_1}(v_1) + t_{v_1}\right)\\
&+ \sum_{i=2}^{k} I(T_i) + 2\sum_{i=2}^{k}\left(n^1_{T_i}(u_i) - n^2_{T_i}(u_i) + t_{u_i}\right) + \sum_{xy\in E(C_m)} I_{G_1^0}(xy)\\
&- \sum_{i=2}^{k} I(T_i) - 2\sum_{i=2}^{k}\left(n^1_{T_i}(u_i) - n^2_{T_i}(u_i) + t_{u_i}\right) - \sum_{xy\in E(C_m)} I_{G_1}(xy)\\
>& 2l_1 - 2\left(n^1_{T_1}(v_1) - n^2_{T_1}(v_1) + t_{v_1}\right)\\
&+ I_{G_1^0}(v_1v_n) + I_{G_1^0}(v_1v_2) - I_{G_1}(v_1v_n) - I_{G_1}(v_1v_2)\\
\geq& 2\,l_1 - 2\,d_{T_1}(v_1) + |d_{G_1}(v_1) - d_{G_1}(v_2) - d| - |d_{G_1}(v_1) - d_{G_1}(v_2)|\\
&+ |d_{G_1}(v_1) - d_{G_1}(v_m) - d| - |d_{G_1}(v_1) - d_{G_1}(v_m)|\\
\geq& 2l_1 - 2\,(l_1 - d) + 2\,d\\
=& 0.
\end{aligned}$$

Therefore, $I(G_1^0) > I(G_1)$, as desired. □

Lemma 4.3. *Let $G \cong C_m(l_1, l_2, \ldots, l_k)$ be a unicyclic graph of order n, such that $l = l_1 + l_2 + \cdots + l_k = n - m$, then $I(G) \leq I\,(C_m(l))$, with the equality if and only if $G \cong C_m(l)$.*

Proof. By applying corollary 3.2, we have $I\,(C_m(l)) = (n-m)^2 + (n-m)$ and $I(G) \leq (n-m)^2 + (n-m) + \sum_{xy\in E(C_m)} I_G(xy)$. Also, for any vertex x of C_m, $d_G(x) \geq 2$. So,

$$\sum_{xy\in E(C_m)} I_G(xy) \leq 2\sum_{i=1}^{k}(l_i + 2 - 2) = 2(n-m).$$

Therefore, $I(G) \leq (n-m)^3 + 3(n-m) = I\,(C_m(l))$. □

Now we are ready to prove the main result of this paper.

Proof of Theorem 2.1**.** By Remark 2.1 and Table 1, we have,

$$n^2 - 9n + 24 = I\,(C_3(R_{n-2,3})) = I\,(C_4(2, n-6)_{\alpha=1}) = I\,(C_3(1, 2, n-6))$$

$$
\begin{aligned}
&= I\left(C_3(R_{4,1}, n-6)\right) = I\left(C_3(R_{n-2,n-5})\right) = I\left(C_3(2, R_{n-4,1})\right)\\
&< I\left(C_4(2, n-6)_{\alpha=2}\right)\\
&< I\left(C_3(3, n-6)\right)\\
&< I\left(C_4(R_{n-3,1})\right) = I\left(C_3(H_{n-2})\right) = I\left(C_3(F_{n-2})\right) = I\left(C_5(n-5)\right)\\
&< I\left(C_3(R_{n-2,n-4})\right) = \left(C_3(R_{n-2,2})\right) = I\left(C_3(1, R_{n-3,1})\right)\\
&= I\left(C_4(1, n-5)_{\alpha=1}\right) = I\left(C_3(R_{3,1}, n-5)\right) = I\left(C_3(1, 1, n-5)\right)\\
&< I\left(C_4(1, n-5)_{\alpha=2}\right)\\
&< I\left(C_3(2, n-5)\right)\\
&< I\left(C_3(R_{n-2,1})\right) = I\left(C_4(n-4)\right)\\
&< I\left(C_3(1, n-4)\right)\\
&< I\left(C_3(n-3)\right).
\end{aligned}
$$

So, it is enough to prove that if G is a unicyclic graph on $n \geq 12$ vertices, such that it is not isomorphic to any of graphs in Table 1 and $G \ncong C_3(4,5)$, then $I(G) < n^2 - 9n + 24 = I(G_1)$, where $G_1 = C_3^{v_1}(R_{n-2,3})$. We will consider four separate cases ($m = 3$, $m = 4$, $m = 5$ and $m > 5$). We have the following.

Case 1: $m > 5$. We first assume that $k = 0$. Then $0 = I(G) < n^2 - 9n + 24 = I(G_1)$. We now assume that $k \geq 1$. Then by Corollary 3.2 and Lemmas 4.1, 4.2 and 4.3, $I(G) \leq I\Big(C_m(l_1, l_2, \ldots, l_k)\Big) \leq I\Big(C_6(n-6)\Big) = n^2 - 9n + 18 < n^2 - 9n + 24 = I(G_1)$.

Case 2: $m = 5$. In this case, we will consider five separate subcases as follows.

(1) $k = 1$. Then $G = C_5^{u_1}(T_1)$. By Lemma 3.2,

$$I(G) = I(T_1) + 2[n_{u_1}^1 - n_{u_1}^2 + t_{u_1}] + 2d_{T_1}(u_1)$$

and $I(G_1) = I(R_{n-2,3}) + 4d_{R_{n-2,3}}(v_1)$. It is clear that $[n_{u_1}^1 - n_{u_1}^2 + t_{u_1}] \leq d_{T_1}(u_1) \leq d_{R_{n-2,3}}(v_1)$. Also, by Lemma 3.1, $I(T_1) < I(R_{n-2,3})$. Therefore, $I(G) < I(G_1)$, as desired.

(2) $k = 2$. In this case $G = C_5(T_1, T_2)$. Assume that T_1 and T_2 are trees of orders $l_1 + 1$ and $l_2 + 1$, respectively. By Lemma 4.2, $I(G) \leq I\Big(C_5(l_1, l_2)\Big)$. On the other hand, one can see easily that the maximum value of $I\left(C_5(l_1, l_2)\right)$ occurs when $\alpha = d_{C_5}(u_1, u_2) = 2$. By Corollary 3.2,

$$I\Big(C_5(l_1, l_2)_{\alpha=2}\Big) = {l_1}^2 + {l_2}^2 + 3(l_1 + l_2) = (n-5)^2 - 2l_1l_2 + 3(n-5) = n^2 - 7n - 2l_1l_2 + 10.$$

Therefore, $I(G_1) - I\Big(C_5(l_1, l_2)_{\alpha=2}\Big) = -2n + 2l_1l_2 + 14$. This will be minimum if ($l_1 = 1$, $l_2 = n-6$) or ($l_1 = n-6$, $l_2 = 1$). Thus in this case $I(G_1) - I\left(C_5(l_1, l_2)_{\alpha=2}\right) = 2 > 0$. Hence we have $I(G) \leq I\left(C_5(l_1, l_2)_{\alpha=2}\right) < I(G_1)$.

(3) $k = 3$. In this case $G = C_5(T_1, T_2, T_3)$. Assume that T_1, T_2 and T_3 are trees of orders $l_1 + 1, l_2 + 1$ and $l_3 + 1$, respectively. By Lemma 4.2, $I(G) \leq I\left(C_5(l_1, l_2, l_3)\right)$. Without loss of generality, we can assume that $l_3 \geq l_2 \geq l_1$. It is clear that the maximal value of $I\left(C_5(l_1, l_2, l_3)\right)$ occurs when $d_{C_5}(u_1, u_2) = d_{C_5}(u_2, u_3) = 2$ or $d_{C_5}(u_1, u_3) =$

$d_{C_5}(u_2, u_3) = 2$. By Corollary 3.2, in the last situation we have

$$I\left(C_5(l_1, l_2, l_3)\right) = {l_1}^2 + {l_2}^2 + {l_3}^2 + 3(l_2 + l_3) + l_1.$$

Since $l_1 + l_2 + l_3 = n - 5$, then $I\left(C_5(l_1, l_2, l_3)\right) = n^2 - 7n + 10 - 2l_1 - 2(l_1 l_2 + l_1 l_3 + l_2 l_3)$. Thus

$$I(G_1) - I\left(C_5(l_1, l_2, l_3)\right) = -2n + 14 + 2l_1 + 2\underbrace{(l_1 l_2 + l_1 l_3 + l_2 l_3)}_{\geq l_1 + l_2 + l_3 = n-5} \geq 4 + 2l_1 > 0.$$

Therefore, $I(G) < I(G_1)$, as desired.

If $k = 4$ or 5, then a similar argument as in subcases when $k = 1, 2, 3$ shows that $I(G) < I(G_1)$.

Case 3: $m = 4$. In this case, we will consider three separate cases ($k = 1$, $k = 2$, $k = 3$ and $k = 4$).

(1) $k = 1$. Then $G = C_4^{u_1}(T_1)$. By assumption, $G \ncong C_4(n-4)$ or $C_4(R_{n-3,1})$. So, $T_1 \ncong S_{n-3}$ or $R_{n-3,1}$, thus by Lemmas 3.1 and 3.2, G has a maximum irregularity if $T_1 \cong R_{n-3,2}$ or $R_{n-3,n-5}$. On the other hand,

$$I\left(C_4(R_{n-3,2})\right) = I\left(C_4(R_{n-3,n-5})\right) = n^2 - 9n + 20 < I(G_1).$$

This means that $I(G) < I(G_1)$.

(2) $k = 2$. By Lemma 4.2, $I(G) = I\left(C_4(T_1, T_2)\right) \leq I\left(C_4(l_1, l_2)\right)$. Obviously, the maximal value of $I\left(C_4(l_1, l_2)\right)$ occurs when $\alpha = d_{C_4}(u_1, u_2) = 2$. Hence, by Corollary 3.2 we have $I\Big(C_4(l_1, l_2)\Big) = n^2 - 5n - 2l_1 l_2 + 4$. Therefore,

$$I(G_1) - I\Big(C_4(l_1, l_2)\Big) = -4n + 2l_1 l_2 + 20.$$

Since neither $C_4(1, n-5)$ nor $C_4(2, n-6)$ is isomorphic to G, we know that if $G \cong C_4(l_1, l_2)$ and $l_1 \in \{1, 2\}$, then T_2 is not a star. Assume that $l_2 \geq l_1$. If $l_1 \leq 2$, then G has a maximum irregularity when $G \cong C_4(l_1, R_{n-3-l_1, l_1})_{\alpha=2}$. Therefore $I(G) < I(G_1)$. So, let $l_1 \geq 3$. Then $-4n + 2l_1 l_2 + 20$ will be minimum if $l_1 = 3$ and $l_2 = n - 7$. Therefore, $-4n + 2l_1 l_2 + 20 = 2n - 22 > 0$, for $n \geq 12$. Hence $I(G) < I(G_1)$, for $n \geq 12$.

(3) $k = 3$. In this case $G = C_4(T_1, T_2, T_3)$. Assume that T_1, T_2 and T_3 are trees of orders $l_1 + 1, l_2 + 1$ and $l_3 + 1$, respectively. By Lemma 4.2, $I(G) \leq I\left(C_4(l_1, l_2, l_3)\right)$. Without loss of generality, we can assume that $l_3 \geq l_2 \geq l_1$. It is easy to check that the maximum value of $I\left(C_4(l_1, l_2, l_3)\right)$ occurs when $\alpha = d_{C_4}(u_2, u_3) = 2$. Thus by Corollary 3.2, $I\left(C_4(l_1, l_2, l_3)\right) = n^2 - 5n + 4 - 2l_1 l_2 - 2l_1 l_3 - 2l_2 l_3 - 4l_1$. Therefore, $I(G_1) - I\left(C_4(l_1, l_2, l_3)\right) = 2(-2n + 10 + l_1 l_2 + l_1 l_3 + l_2 l_3 + 2l_1)$. If $l_1 = l_2 = 1$, $l_3 = n - 6$, then $2(-2n + 10 + l_1 l_2 + l_1 l_3 + l_2 l_3 + 2l_1) = 2 > 0$. Now if $l_1 \geq 1$, $l_2, l_3 \geq 2$, then $l_1 + l_2 = n - 4 - l_3 \geq 3$, consequently $n \geq l_3 + 7$ and $l_1 l_3 + l_2 l_3 = n l_3 - 4l_3 - {l_3}^2$. Therefore, $2(-2n + 10 + l_1 l_2 + l_1 l_3 + l_2 l_3 + 2l_1) = 2l_3 > 0$. This means that $I(G) < I(G_1)$ which completes this case.

(4) $k = 4$. A similar argument as in subcases when $k = 2, 3$ shows that:

$$I(G) \leq I\Big(C_4(l_1, l_2, l_3, l_4)\Big) < I(G_1).$$

Case 4: $m = 3$. In this case, we will consider three separate cases as follows.

(1) $k = 1$. We have $G = C_3^{u_1}(T_1)$. By assumption, for $r = 1, 2, 3, n-4$ and $n-5$, $G \ncong C_3(n-3), C_3(R_{n-2,r}), C_3(F_{n-2})$ or $C_3(H_{n-2})$. Therefore, $T_1 \ncong S_{n-2}, R_{n-2,r}, F_{n-2}$ or H_{n-2}. Also, by Lemma 3.2, $I(G) = I(T_1) + 2[n^1_{u_1} - n^2_{u_1} + t_{u_1}] + 2d_{T_1}(u_1) \leq I(T_1)+4d_{T_1}(u_1)$ and $I(G_1) = I(R_{n-2,3})+4d_{R_{n-2,3}}(v_1)$. Obviously, $d_{T_1}(u_1) \leq d_{R_{n-2,3}}(v_1)$. Also, by Lemma 3.1, $I(T_1) < I(R_{n-2,3})$. Therefore, $I(G) < I(G_1)$, as desired.

(2) $k = 2$. In this case, assume that T_1 and T_2 are trees of orders $l_1 + 1$ and $l_2 + 1$, respectively. By Lemma 4.2, $I(G) = I\Big(C_3(T_1, T_2)\Big) \leq I\Big(C_3(l_1, l_2)\Big)$. By assumption, $n \geq 12$ and $G \ncong C_3(3, n-6)$ so, we have $l_2 \geq l_1 \geq 4$ and $l_2 \neq 4$. On the other hand, $I\Big(C_3(l_1, l_2)\Big) = n^2 - 3n - 2l_1l_2 - 2l_1$. So, $I(G_1) - I\Big(C_3(l_1, l_2)\Big) = -6n + 24 + 2l_1l_2 + 2l_1$. Since $l_1+l_2 = n-3$, then $n \geq l_2+7$. Thus $-6n+24+2l_1l_2+2l_1 \geq 2(l_2-5) \geq 0$. Hence for $n \geq 13$, $I(G) < I(G_1)$ and $I\Big(C_3(l_1, l_2)\Big) = I(G_1)$ if and only if $(n = 12, l_1 = 4, l_2 = 5)$. Therefore, for $n \geq 13$, $I(G) < I(G_1)$. For $n = 12$, $I(G_1) = I\Big(C_3(4, 5)\Big)$, as desired.

(3) $k = 3$. In this case, assume that T_1, T_2 and T_3 are trees of orders $l_1 + 1$, $l_2 + 1$ and $l_3 + 1$, respectively and $l_3 \geq l_2 \geq l_1$. By Lemmas 3.2 and 4.2, $I(G) = I\Big(C_3(T_1, T_2, T_3)\Big) \leq I\Big(C_3(l_1, l_2, l_3)\Big) = n^2 - 5n + 6 - 2(l_1l_2 + l_1l_3 + l_2l_3) + 2(l_3 - l_1)$. By assumption, $G \ncong C_3(1, 1, n-5), C_3(1, 2, n-6)$ and so, the cases ($l_1 = l_2 = 1$, $l_3 = n-5$) and ($l_1 = 1$, $l_2 = 2$, $l_3 = n-6$) cannot occur. If $l_1 = 1$ and $l_2, l_3 \geq 3$, then $I(G_1) - I\Big(C_3(l_1, l_2, l_3)\Big) = -4n + 20 + 2l_2 + 2l_2l_3$. $-4n + 20 + 2l_2 + 2l_2l_3$ will be minimum if ($l_2 = 3$, $l_3 = n-7$) and in this case $-4n + 20 + 2l_2 + 2l_2l_3 = 2n - 16 > 0$, for $n \geq 12$. Hence $I(G) < I(G_1)$.

If $l_1, l_2, l_3 \geq 2$, then $l_2 = n - l_1 - l_3 - 3 \geq 2$. So, $n \geq l_1 + l_3 + 5$ and

$$\begin{aligned}
I(G_1) - I\left(C_3(l_1, l_2, l_3)\right) =& 2\left(l_1(n - l_1 - l_3 - 3) + l_1l_3 + (n - l_1 - l_3 - 3)l_3 - l_3 + l_1\right) \\
& - 4n + 18 \\
=& 2\left(n(l_1 + l_3 - 2) + 9 - {l_1}^2 - {l_3}^2 - 4l_3 - 2l_1 - l_1l_3\right) \\
\geq& 2\Big((l_1 + l_3 + 5)(l_1 + l_3 - 2) \\
& + 9 - {l_1}^2 - {l_3}^2 - 4l_3 - 2l_1 - l_1l_3\Big) \\
=& 2(l_1 - 1)(l_3 + 1) > 0.
\end{aligned}$$

Therefore, $I(G) < I(G_1)$. This completes our argument. □

Remark 4.1. Recall that in Theorem 2.1 we have characterized 24 types of n-vertex unicyclic graphs with the greatest irregularity values, for $n \geq 12$. Additionally, using computer calculations, we have also determined the irregularity of unicyclic graphs on less than 12 vertices, which are reported in Tables 2 and 3. More precisely, we have specified the irregularity of all unicyclic graphs up to 6 vertices in Table 2, and all possible unicyclic graphs on $n = 7, \ldots, 11$ vertices with irregularity greater than or equal to $n^2 - 9n + 24$, in Table 3.

Table 3. All possible unicyclic graphs on n vertices ($n = 7, \dots, 11$) with irregularity$\geq n^2 - 9\,n + 24$.

$n=7$		$n=8$		$n=9$		$n=10$		$n=11$	
irr	**Graph**	**irr**	**Graph**	**irr**	**Graph**	**irr**	**Graph**	**irr**	**Graph**
28	$C_3(4)$	40	$C_3(5)$	54	$C_3(6)$	70	$C_3(7)$	88	$C_3(8)$
20	$C_3(1,3)$	30	$C_3(1,4)$	42	$C_3(1,5)$	56	$C_3(1,6)$	72	$C_3(1,7)$
18	$C_4(3)$	28	$C_4(4)$	40	$C_4(5)$	54	$C_4(6)$	70	$C_4(7)$
18	$C_3(R_{5,1})$	28	$C_3(R_{6,1})$	40	$C_3(R_{7,1})$	54	$C_3(R_{8,1})$	70	$C_3(R_{9,1})$
16	$C_3(2,2)$	24	$C_3(2,3)$	34	$C_3(2,4)$	46	$C_3(2,5)$	60	$C_3(2,6)$
14	$C_4(1,2)_{\alpha=2}$	22	$C_4(1,3)_{\alpha=2}$	32	$C_4(1,4)_{\alpha=2}$	44	$C_4(1,5)_{\alpha=2}$	58	$C_4(1,6)_{\alpha=2}$
12	$C_4(1,2)_{\alpha=1}$	20	$C_4(2,2)_{\alpha=2}$	30	$C_4(1,4)_{\alpha=1}$	42	$C_4(1,5)_{\alpha=1}$	56	$C_4(1,6)_{\alpha=1}$
12	$C_3(R_{5,3})$	20	$C_4(1,3)_{\alpha=1}$	30	$C_3(R_{7,5})$	42	$C_3(R_{8,6})$	56	$C_3(R_{9,7})$
12	$C_3(R_{5,2})$	20	$C_3(R_{6,4})$	30	$C_3(R_{7,2})$	42	$C_3(R_{8,2})$	56	$C_3(R_{9,2})$
12	$C_3(2,R_{3,1})$	20	$C_3(R_{6,2})$	30	$C_3(R_{3,1},4)$	42	$C_3(R_{3,1},5)$	56	$C_3(R_{3,1},6)$
12	$C_3(1,R_{4,1})$	20	$C_3(3,R_{3,1})$	30	$C_3(1,R_{6,1})$	42	$C_3(1,R_{7,1})$	56	$C_3(1,R_{8,1})$
12	$C_3(1,1,2)$	20	$C_3(1,R_{5,1})$	30	$C_3(3,3)$	42	$C_3(1,1,5)$	56	$C_3(1,1,6)$
10	$C_5(2)$	20	$C_3(1,1,3)$	30	$C_3(1,1,4)$	40	$C_5(5)$	54	$C_5(6)$
10	$C_4(R_{4,1})$	18	$C_5(3)$	28	$C_5(4)$	40	$C_4(R_{7,1})$	54	$C_4(R_{8,1})$
10	$C_3(H_5)$	18	$C_4(R_{5,1})$	28	$C_4(2,3)_{\alpha=2}$	40	$C_3(H_8)$	54	$C_3(H_9)$
10	$C_3(F_5)$	18	$C_3(H_6)$	28	$C_4(R_{6,1})$	40	$C_3(F_8)$	54	$C_3(F_9)$
–	–	18	$C_3(F_6)$	28	$C_3(H_7)$	40	$C_3(3,4)$	52	$C_3(3,5)$
–	–	16	$C_4(2,2)_{\alpha=1}$	28	$C_3(F_7)$	38	$C_4(2,4)_{\alpha=2}$	50	$C_4(2,5)_{\alpha=2}$
–	–	16	$C_3(R_{6,3})$	24	$C_4(2,3)_{\alpha=1}$	36	$C_4(3,3)_{\alpha=2}$	48	$C_3(4,4)$
–	–	16	$C_3(2,R_{4,1})$	24	$C_3(R_{7,4})$	34	$C_4(2,4)_{\alpha=1}$	46	$C_4(3,4)_{\alpha=2}$
–	–	16	$C_3(1,2,2)$	24	$C_3(R_{7,3})$	34	$C_3(R_{8,5})$	46	$C_4(2,5)_{\alpha=1}$
–	–	–	–	24	$C_3(3,R_{4,1})$	34	$C_3(R_{8,3})$	46	$C_3(R_{9,6})$
–	–	–	–	24	$C_3(2,R_{5,1})$	34	$C_3(R_{4,1},4)$	46	$C_3(R_{9,3})$
–	–	–	–	24	$C_3(1,2,3)$	34	$C_3(2,R_{6,1})$	46	$C_3(R_{4,1},5)$
–	–	–	–	–	–	34	$C_3(1,2,4)$	46	$C_3(2,R_{7,1})$
–	–	–	–	–	–	–	–	46	$C_3(1,2,5)$

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References

[1] H. Abdo, S. Brandt and D. Dimitrov, *The total irregularity of a graph*, Discrete Math. Theor. Comput. Sci. **16** (2014), 201–206.

[2] H. Abdo, N. Cohen and D. Dimitrov, *Graphs with maximal irregularity*, Filomat **28** (2014), 1315–1322.

[3] H. Abdo and D. Dimitrov, *The irregularity of graphs under graph operations*, Discuss. Math. Graph Theory **34** (2014), 263–278.

[4] M. O. Albertson, *The irregularity of a graph*, Ars Combin. **46** (1997), 219–225.

[5] F. K. Bell, *A note on the irregularity of graphs*, Linear Algebra Appl. **161** (1992), 45–54.
[6] D. Dimitrov and T. Réti, *Graphs with equal irregularity indices*, Acta Polytechnica Hungarica **11** (2014), 41–57.
[7] D. Dimitrov and R. Škrekovski, *Comparing the irregularity and the total irregularity of graphs*, Ars Math. Contemp. **9** (2015), 45–50.
[8] G. H. Fath-Tabar, *Old and new zagreb indices of graphs*, MATCH Commun. Math. Comput. Chem. **65** (2011), 79–84.
[9] G. H. Fath-Tabar, I. Gutman and R. Nasiri, *Extremely irregular trees*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) **38** (2013), 1–8.
[10] P. Hansen and H. Mélot, *Variable neighborhood search for extremal graphs. 9. bounding the irregularity of a graph*, Discrete Math. Theor. Comput. Sci. **69** (2005), 253–264.
[11] M. A. Henning and D. Rautenbach, *On the irregularity of bipartite graphs*, Discrete Math. **307** (2007), 1467–1472.
[12] W. Luo and B. Zhou, *On the irregularity of trees and unicyclic graphs with given matching number*, Util. Math. **83** (2010), 141–147.
[13] R. Nasiri, H. R. Ellahi, A. Gholami and G. H. Fath-Tabar, *The irregularity and total irregularity of eulerian graphs*, Iranian J. Math. Chem. **9**(2) (2018), 101–111.
[14] R. Nasiri and G. H. Fath-Tabar, *The second minimum of the irregularity of graphs*, Electron. Notes Discrete Math. **45** (2014), 133–140.
[15] R. Nasiri, H. Yousefi-Azari, M. R. Darafsheh and A. R. Ashrafi, *Remarks on the wiener index of unicyclic graphs*, J. Appl. Math. Comput. **41** (2013), 49–59.
[16] T. Réti and D. Dimitrov, *On irregularities of bidegreed graphs*, Acta Polytechnica Hungarica **10** (2013), 117–134.
[17] M. Tavakoli, F. Rahbarnia and A. R. Ashrafi, *Some new results on irregularity of graphs*, J. Appl. Math. Inform. **32** (2014), 675–685.
[18] M. Tavakoli, F. Rahbarnia, M. Mirzavaziri, A. R. Ashrafi and I. Gutman, *Extremely irregular graphs*, Kragujevac J. Math. **37** (2013), 135–139.
[19] B. Zhou and W. Luo, *On irregularity of graphs*, Ars Combin. **88** (2008), 55–64.

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