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,

\[
\text{irr}(G) = \sum_{xy \in E(G)} |d_G(x) - d_G(y)|,
\]

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

\[
I(G) = \sum_{xy \in E(G)} I_G(xy).
\]

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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Throughout the paper, we may suppose that the order of 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

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

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 pendant vertex. The (unique) $n$-vertex trees with 2 and $n-1$ pendant vertices are called path $P_n$ and star $S_n$, respectively. A unicyclic graph $G$ with circuit $C_m = v_1v_2\cdots v_mv_1$ of length $m$ is denoted by $C_m^{u_1,u_2,\ldots,u_k}(T_1,T_2,\ldots,T_k)$, where trees $T_1,T_2,\ldots,T_k$, $0 \leq k \leq m$, are all the nontrivial components of $G - E(C_m)$, and $u_i$ is the common vertex of $T_i$ and $C_m$, $1 \leq i \leq k$. 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 $k \geq 1$. 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 $C_3(S_2,S_3,T_3)$ 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 $N^1_G(x)$ and $N^2_G(x)$ of vertices of $G$ as $N^1_G(x) = \{u \in N_G(x); d_G(x) \geq d_G(u)\}$, and $N^2_G(x) = \{u \in N_G(x); d_G(x) < d_G(u)\}$; and suppose that $n^1_G(x) = |N^1_G(x)|$ and $n^2_G(x) = |N^2_G(x)|$.

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 $1 \leq r \leq n-2$, 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 \(P_3\), by attaching \(n - 5\) pendent
vertices to its central vertex. Also, we denote by \(H_n\) the tree of order \(n\) obtained from
\(P_3\) by joining \(n - 4\) pendent edges to only one of its endpoints, say \(a\) (see Figure 1).

\[
\begin{array}{c}
\text{Figure 1. Trees rooted at } a \text{ with large irregularity.}
\end{array}
\]

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 2.1.

### 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,

\[
\begin{align*}
&n^2 - 3n > n^2 - 5n + 6 > n^2 - 5n + 4 \\
&> n^2 - 7n + 16 > n^2 - 7n + 14 > n^2 - 7n + 12 > n^2 - 7n + 10 \\
&> n^2 - 9n + 30 > n^2 - 9n + 28 > n^2 - 9n + 24
\end{align*}
\]
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 $T \not\cong S_n, R_n, R_n, F_n, H_n$ 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

$$I(G) = \sum_{i=1}^{k} I(T_i) + 2 \sum_{i=1}^{k} \left( n_{T_i}^4(u_i) - n_{T_i}^2(u_i) + t_{u_i} \right) + \sum_{xy \in E(C_m)} I_G(xy),$$

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,

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

<table>
<thead>
<tr>
<th></th>
<th>$n = 3$</th>
<th></th>
<th>$n = 5$</th>
<th></th>
<th>$n = 6$</th>
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</thead>
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<td>$\text{irr}$</td>
<td>$\text{Graph}$</td>
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<td>$\text{Graph}$</td>
<td>$\text{irr}$</td>
<td>$\text{Graph}$</td>
</tr>
<tr>
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<td>$C_3$</td>
<td>10</td>
<td>$C_3(2)$</td>
<td>18</td>
<td>$C_3(3)$</td>
</tr>
<tr>
<td>4</td>
<td>$C_3(1)$</td>
<td>4</td>
<td>$C_3(R_{3,1})$</td>
<td>10</td>
<td>$C_3(R_{4,1})$</td>
</tr>
<tr>
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<td>$C_4$</td>
<td>8</td>
<td>$C_4(1, 1)_{n=2}$</td>
<td>4</td>
<td>$C_5(1)$</td>
</tr>
</tbody>
</table>

For the sake of completeness, we have computed the irregularity of all unicyclic graphs on $n = 3, 4, 5, 6$ vertices (see Table 2).
Since $d_G(u_i) = d_{T_i}(u_i) + 2$, then

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

\[
+ \sum_{d_{T_i}(u_i) = d_{T_i}(x) - 1} \left( \frac{2 - I_{T_i}(xu_i)}{2} \right) + \sum_{d_{T_i}(u_i) < d_{T_i}(x) - 1} \left( I_{T_i}(xu_i) - 2 \right) \right) + \sum_{xy \in E(C_m)} I_G(xy).
\]
On the other hand,
\[
\sum_{d_{T_i}(u_i) < d_{T_i}(x) - 1} (I_{T_i}(xu_i) - 2) = \sum_{d_{T_i}(u_i) < d_{T_i}(x)} (I_{T_i}(xu_i) - 2) - \sum_{d_{T_i}(u_i) = d_{T_i}(x) - 1} (I_{T_i}(xu_i) - 2) = \sum_{d_{T_i}(u_i) < d_{T_i}(x)} I_{T_i}(xu_i) - 2n_{u_i}^2 + \sum_{d_{T_i}(u_i) = d_{T_i}(x)} 1.
\]

Therefore, the lemma is proved.

We know that \( t_{u_i} \leq n_{T_i}^2(u_i) \) and \( d_{T_i}(u_i) = n_{T_i}^1(u_i) + n_{T_i}^2(u_i) \). 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
\[
I(G) \leq \sum_{i=1}^{k} I(T_i) + 2 \sum_{i=1}^{k} d_{T_i}(u_i) + \sum_{xy \in E(C_m)} I_G(xy)
\]
\[
= \sum_{i=1}^{k} I(T_i) + 2 \sum_{i=1}^{k} d_G(u_i) + \sum_{xy \in E(C_m)} I_G(xy) - 4k,
\]
with equality if and only if \( n_{T_i}^2(u_i) = 0 \) 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
\[
I(G) = \sum_{i=1}^{k} I(S_{l_{i}+1}) + 2 \sum_{i=1}^{k} d_{S_{l_{i}+1}}(u_i) + \sum_{xy \in E(C_m)} I_G(xy)
\]
\[
= \sum_{i=1}^{k} l_i^2 + (n - m) + \sum_{xy \in E(C_m)} I_G(xy).
\]

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, \( I(G_2) > I(G_1) \). \( \square \)

**Lemma 4.2.** Let \( G_2 = C_{m_1}^{u_1}(l_1, l_2, \ldots, l_k) \) and \( G_1 = C_{m_2}^{u_1}(T_1, \ldots, T_k) \), 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 \( T_i \not\cong S_{l_i+1} \), otherwise we have \( G_1 \cong G_2 \), and therefore \( I(G_1) = I(G_2) \). Without loss of generality, suppose that \( T_1 \not\cong S_{l_1+1} \) 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 \( l_1 \) pendant 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,

\[
I(G_1^0) - I(G_1) = I(S_{l_1+1}) + 2l_1 - I(T_1) - 2 \left( n_{T_1}^1(v_1) - n_{T_1}^2(v_1) + t_{v_1} \right) \\
+ \sum_{i=2}^{k} I(T_i) + 2 \sum_{i=2}^{k} \left( n_{T_i}^1(u_i) - n_{T_i}^2(u_i) + t_{u_i} \right) \\
- \sum_{i=2}^{k} I(T_i) - 2 \sum_{i=2}^{k} \left( n_{T_i}^1(u_i) - n_{T_i}^2(u_i) + t_{u_i} \right) - \sum_{xy \in E(C_m)} I_{G_1}(xy)
\]

\[
\geq 2l_1 - 2 \left( n_{T_1}^1(v_1) - n_{T_1}^2(v_1) + t_{v_1} \right) \\
+ I_{G_1^0}(v_1v_n) + I_{G_1^0}(v_1v_2) - I_{G_1}(v_1v_n) - I_{G_1}(v_1v_2)
\]

\[
\geq 2l_1 - 2d_{T_1}(v_1) + |d_{G_1}(v_1) - d_{G_1}(v_2) - d| - |d_{G_1}(v_1) - d_{G_1}(v_2)| \\
+ |d_{G_1}(v_1) - d_{G_1}(v_m) - d| - |d_{G_1}(v_1) - d_{G_1}(v_m)|
\]

\[
\geq 2l_1 - 2(l_1 - d) + 2d = 0.
\]

Therefore, \( I(G_1^0) > I(G_1) \), as desired. \( \square \)

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

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,

\[
n^2 - 9n + 24 = I(C_3(R_{n-2,3})) = I(C_4(2, n - 6)_{a=1}) = I(C_3(1, 2, n - 6))
\]
Without loss of generality, we can assume that \( I \geq l \) on other hand, one can see easily that the maximum value of \( I, I \) and \( I \).

\[
\begin{align*}
&= I (C_3(R_{4,1}, n - 6)) = I (C_3(R_{n-2, n-5})) = I (C_3(2, R_{n-4,1})) \\
&< I (C_4(2, n - 6))_\alpha \leq 2 \\
&< I (C_3(3, n - 6)) \\
&< I (C_4(R_{n-3,1})) = I (C_3(H_{n-2})) = I (C_3(F_{n-2})) = I (C_5(n - 5)) \\
&< I (C_3(R_{n-2,n-4})) = (C_3(R_{n-2,2})) = I (C_3(1, R_{n-3,1})) \\
&= I (C_4(1, n - 5))_\alpha = I (C_3(R_{3,1}, n - 5)) = I (C_3(1, 1, n - 5)) \\
&< I (C_4(1, n - 5))_\alpha \leq 2 \\
&< I (C_3(2, n - 5)) \\
&< I (C_3(R_{n-2,1})) = I (C_4(n - 4)) \\
&< I (C_3(1, n - 4)) \\
&< I (C_3(n - 3)) .
\end{align*}
\]

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 \( G \geq C_5(4, 5) \), then \( I(G) < n^2 - 9n + 24 = I(G_1) \), where \( G_1 = C_3^v (R_{n-2, 3}) \). 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, \( I(G) \leq I \left(C_m(l_1, l_2, \ldots, l_k) \right) \leq I \left(C_6(n - 6) \right) = n^2 - 9n + 18 < n^2 - 9n + 24 = I(G_1) \).

**Case 2:** \( m = 5 \). In this case, we will consider five separate subcases as follows.

(1) \( k = 1 \). Then \( G = C_5^v (T_1) \). By Lemma 3.2,

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

and \( I(G_1) = I(R_{n-2,3}) + 4d_{R_{n-2,3}}(v_1) \). It is clear that \( [n_{u_1}^2 - n_{u_1} + t_{u_1}] \leq d_{T_1}(u_1) \leq d_{R_{n-2,3}}(v_1) \). 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, \( I(G) \leq I \left(C_5(l_1, l_2) \right) \). On the other hand, one can see easily that the maximum value of \( I(C_5(l_1, l_2)) \) occurs when \( \alpha = d_{C_5}(u_1, u_2) = 2 \). By Corollary 3.2,

\[
I \left(C_5(l_1, l_2) \right) = l_1^2 + l_2^2 + 3(l_1 + l_2) = (n - 5)^2 - 2l_1l_2 + 3(n - 5) = n^2 - 7n - 2l_1l_2 + 10.
\]

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

(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
\[I(C_5(l_1, l_2, l_3)) = l_1^2 + l_2^2 + l_3 + 3(l_2 + l_3) + l_1.\]
Since \(l_1 + l_2 + l_3 = n - 5\), then
\[I(C_5(l_1, l_2, l_3)) = n^2 - 7n + 10 - 2l_1 - 2l_1 l_2 + l_1 l_3 + l_2 l_3.\]
Thus
\[I(G_1) - I(C_5(l_1, l_2, l_3)) = -2n + 14 + 2l_1 + 2(l_1 l_2 + l_1 l_3 + l_2 l_3) \geq 4 + 2l_1 > 0.\]

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 \(G = C_{4u}^1 (T_1)\). By assumption, \(G \not\cong C_4(n - 4)\) or \(C_4(R_{n-3,1})\). So, \(T_1 \not\cong S_{n-3}\) 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,
\[I(C_4(R_{n-3,2})) = I(C_4(R_{n-3,n-5})) = n^2 - 9n + 20 < I(G_1).\]
This means that \(I(G) < I(G_1)\).

(2) \(k = 2\). By Lemma 4.2, \(I(G) = I(C_4(T_1, T_2)) \leq I(C_4(l_1, l_2))\). Obviously, the maximal value of \(I(C_4(l_1, l_2))\) occurs when \(\alpha = d_{C_4}(u_1, u_2) = 2\). Hence, by Corollary 3.2 we have
\[I(C_4(l_1, l_2)) = n^2 - 5n - 2l_1 l_2 + 4.\]
Therefore,
\[I(G_1) - I(C_4(l_1, l_2)) = -4n + 2l_1 l_2 + 20.\]
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 \(G \cong C_4(l_1, R_{n-3-l_1,l_1})\). 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, \(I(G) \leq I(C_4(l_1, l_2, l_3))\).
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 \(I(C_4(l_1, l_2, l_3))\) occurs when \(\alpha = d_{C_4}(u_2, u_3) = 2\). Thus by Corollary 3.2, \(I(C_4(l_1, l_2, l_3)) = n^2 - 5n + 4 - 2l_1 l_2 - 2l_1 l_3 - 2l_2 l_3 - 4l_1\). Therefore,
\[I(G_1) - I(C_4(l_1, l_2, l_3)) = 2(-2n + 10 + l_1 l_2 + l_1 l_3 + l_2 l_3 + 2l_1).\]
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 \(l_1 l_3 + l_2 l_3 = nl_3 - 4l_3 - l_3^2\). 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:
\[I(G) \leq I(C_4(l_1, l_2, l_3, l_4)) < I(G_1).\]
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 ($n = 7, \ldots, 11$) with irregularity $\geq n^2 - 9n + 24$.  

<table>
<thead>
<tr>
<th>$n = 7$</th>
<th>$n = 8$</th>
<th>$n = 9$</th>
<th>$n = 10$</th>
<th>$n = 11$</th>
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<tr>
<td>$\text{irr}$</td>
<td>Graph</td>
<td>$\text{irr}$</td>
<td>Graph</td>
<td>$\text{irr}$</td>
</tr>
<tr>
<td>28</td>
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<td>40</td>
<td>$C_3(5)$</td>
<td>54</td>
</tr>
<tr>
<td>20</td>
<td>$C_3(1,3)$</td>
<td>30</td>
<td>$C_3(1,4)$</td>
<td>42</td>
</tr>
<tr>
<td>18</td>
<td>$C_3(3)$</td>
<td>28</td>
<td>$C_3(4)$</td>
<td>40</td>
</tr>
<tr>
<td>18</td>
<td>$C_3(R_{5,1})$</td>
<td>28</td>
<td>$C_3(R_{6,1})$</td>
<td>40</td>
</tr>
<tr>
<td>16</td>
<td>$C_3(2,2)$</td>
<td>24</td>
<td>$C_3(2,3)$</td>
<td>34</td>
</tr>
<tr>
<td>14</td>
<td>$C_4(1,2)_{\alpha=2}$</td>
<td>22</td>
<td>$C_4(1,3)_{\alpha=2}$</td>
<td>32</td>
</tr>
<tr>
<td>12</td>
<td>$C_4(1,2)_{\alpha=1}$</td>
<td>20</td>
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</tr>
<tr>
<td>12</td>
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</tr>
<tr>
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<td>$C_3(R_{6,4})$</td>
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</tr>
<tr>
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<td>20</td>
<td>$C_3(R_{6,2})$</td>
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<tr>
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<td>$C_3(2, R_{7,1})$</td>
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</tbody>
</table>

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References


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