Communications in Combinatorics and Optimization
Vol. xx, No. x (xxxx), pp. 1-17
https://doi.org/10.22049/cco.2025.30340.2425

CCO
Commun. Comb. Optim.

Research Article

General Randić index of unicyclic graphs with given maximum degree

Elize Swartz[†], **Tomáš Vetrík**[*]

Department of Mathematics and Applied Mathematics, University of the Free State,
Bloemfontein, South Africa
[†]swartze1@ufs.ac.za
[*]vetrikt@ufs.ac.za

Received: 7 February 2025; Accepted: 11 May 2025
Published Online: 17 May 2025

Abstract: The general Randić index of a graph G is defined as $R_a(G) = \sum_{uv \in E(G)} [d_G(u) d_G(v)]^a$, where $a \in \mathbb{R}$, $E(G)$ is the set of edges of G, and $d_G(u)$ and $d_G(v)$ are the degrees of vertices u and v, respectively. Among unicyclic graphs with given number of vertices and maximum degree, we present the graph with the largest value of R_a for $a < 0$, and graphs having the smallest values of R_a for $a > 0$.

Keywords: extremal graph, topological index, cycle.

AMS Subject classification: 05C09, 05C07, 05C35

1. Introduction

Let us denote by $V(G)$ and $E(G)$ the set of vertices and edges of a graph G. The degree $d_G(u)$ of a vertex u is the number of edges incident with u in G. The maximum degree Δ of G is the degree of a vertex whose degree is the largest in G. A pendant path of G is a subgraph of G containing two end vertices, one of them has degree at least 3 in G, the other end vertex has degree 1 in G, and all the internal vertices (if any) of that path have degree 2 in G. A unicyclic graph is a connected graph containing exactly one cycle. Let $C_k = u_1 u_2 \dots u_k u_1$ be the cycle with k vertices $u_1, u_2, \dots, u_k$ and k edges $u_1u_2, u_2u_3, \dots, u_{k-1}u_k, u_ku_1$. We denote the set of vertices adjacent to u in G by $N_G(u)$.

[*] *Corresponding Author*

Indices of graphs are investigated because of their wide applications. The general Randić index

$$R_a(G) = \sum_{uv \in E(G)} [d_G(u)\, d_G(v)]^a$$

defined for $a \in \mathbb{R}$ and a graph G was first investigated by Bollobás and Erdős [4]. Several special cases of R_a are well-known indices. From R_a, we get the Randić index if $a = -\frac{1}{2}$, reciprocal Randić index if $a = \frac{1}{2}$, second modified Zagreb index if $a = -1$, second Zagreb index if $a = 1$ and second hyper-Zagreb index if $a = 2$.

Unicyclic graphs belong to important classes of graphs. For unicyclic graphs with given number of vertices, Chen [5] proved that the cycle has the largest R_a if $-0.58 < a < 0$. For $a > 0$, this problem was investigated by Li, Shi and Xu [7]. The unicyclic graph having the minimum R_a for $a \geq -1$ was found by Wu and Zhang [12]. Li, Wang and Zhang [8] solved this problem for $a < -1$. The unicyclic graph with given number of vertices and diameter having the smallest R_a for $-0.64 \leq a < 0$ was obtained in [1]. Related topics were considered for example in [2], [6] and [10].

We study unicyclic graphs with prescribed maximum degree Δ and number of vertices n. For any unicyclic graph, we have $2 \leq \Delta \leq n-1$. The cycle C_n is the unique unicyclic graph for $\Delta = 2$ (and $n \geq 3$), and we obtain the unique unicyclic graph for $\Delta = n-1$ (where $n \geq 4$) by adding one edge to the star S_n. Thus, we consider Δ such that $3 \leq \Delta \leq n-2$.

Altassan and Imran [3] presented unicyclic graphs with given n and Δ having the largest R_a for $a_0 \leq a < 0$, where a_0 is about -0.21. In Theorem 2, we considerably extend their results by obtaining the unicyclic graph with given n and Δ having the largest R_a for every $a < 0$, where $\left\lceil \frac{n+1}{2} \right\rceil \leq \Delta \leq n-2$. Moreover, we obtain unicyclic graphs with given n and Δ having the smallest R_a for $a > 0$ in Theorem 1.

Lemmas 1 and 2 are used in both Sections 2 and 3, therefore we include them in this section. Lemma 1 was proved in [11].

Lemma 1. *Let $1 \leq x_1 < x_2$ and $c > 0$. Then for $a > 1$ and $a < 0$,*

$$(x_1 + c)^a - x_1^a < (x_2 + c)^a - x_2^a.$$

For $0 < a < 1$,

$$(x_1 + c)^a - x_1^a > (x_2 + c)^a - x_2^a.$$

Lemma 2. *Let $x > 0$, $c > s > 0$ and $a \neq 0$. Then the function*

$$f(x) = (cx)^a - (sx)^a$$

is strictly increasing.

Proof. We get $f'(x) = (c^a - s^a)ax^{a-1}$. Clearly $x^{a-1} > 0$. We have $c^a > s^a$ for $a > 0$, and $c^a < s^a$ for $a < 0$. Thus $f'(x) > 0$ if $a \neq 0$, so $f(x)$ is strictly increasing. □

2. Smallest value of R_a for $a > 0$

Let us give a few lemmas. Lemma 3 was proved in [9].

Lemma 3. *Let $c, q, r, a \in \mathbb{R}$, where $c, q, r > 0$ and $\{q, r\} \neq \{1\}$. Then the function*

$$f_{c,q,r}(a) = c\,q^a + r^a$$

is strictly convex.

We use Lemma 3 in the proof of Lemma 4.

Lemma 4. *We have*

(i) $2(3^a) + 1 - 3(2^a) > 0$ *for* $a > 0$,

(ii) $6^a + 3^a - 2(4^a) > 0$ *for* $a > 0$,

(iii) $6^a + 3(2^a) - 4(3^a) > 0$ *for* $a > 1$.

Proof. By Lemma 3, the functions

$$f_{2,\frac{3}{2},\frac{1}{2}}(a) = 2\left(\frac{3}{2}\right)^a + \left(\frac{1}{2}\right)^a \quad \text{and} \quad f_{3,\frac{2}{3},2}(a) = 3\left(\frac{2}{3}\right)^a + 2^a$$

are strictly convex for $a \in \mathbb{R}$.

(i) We have $f_{2,\frac{3}{2},\frac{1}{2}}(-\frac{1}{10}) < 3$ and $f_{2,\frac{3}{2},\frac{1}{2}}(0) = 3$. Since $f_{2,\frac{3}{2},\frac{1}{2}}(a)$ is strictly convex, we get $f_{2,\frac{3}{2},\frac{1}{2}}(a) > 3$ for $a > 0$. So $2\left(\frac{3}{2}\right)^a + \left(\frac{1}{2}\right)^a > 3$, thus $2(3^a) + 1^a > 3(2^a)$ for $a > 0$.

(ii) This part was proved in [9].

(iii) We have $f_{3,\frac{2}{3},2}(0) = f_{3,\frac{2}{3},2}(1) = 4$. Since $f_{3,\frac{2}{3},2}(a)$ is strictly convex, we get $f_{3,\frac{2}{3},2}(a) > 4$ for $a > 1$. So $3\left(\frac{2}{3}\right)^a + 2^a > 4$, thus $3(2^a) + 6^a > 4(3^a)$ for $a > 1$.

□

Let us show that a graph U_1 does not have the smallest R_a for $a > 0$.

Lemma 5. *Let U_1 be a unicyclic graph with a pendant path having one end vertex u_0 such that $3 \leq d_{U_1}(u_0) \leq 4$. Let U_1 contain a vertex different from u_0 which has maximum degree. Then there exists a unicyclic graph with the same number of vertices and same maximum degree having smaller R_a for $a > 0$.*

Proof. Let u_0 and u_p be the end vertices of a pendant path of length $p \geq 1$ in U_1, where $3 \leq d_{U_1}(u_0) \leq 4$ and $d_{U_1}(u_p) = 1$. Let us denote the vertices adjacent to u_0 in U_1 which are not on that pendant path by u', u'' if $d_{U_1}(u_0) = 3$, and u', u'', u''' if $d_{U_1}(u_0) = 4$. Since U_1 is not a tree, we can assume that $d_{U_1}(u') \geq 2$. We remove the edge u_0u' from U_1 and add the edge u_pu' to obtain U_2 from U_1. Then U_2 is unicyclic, and U_1 and U_2 have the same maximum degree and number of vertices. We have

$$d_{U_2}(u_0) = d_{U_1}(u_0) - 1, \;\; d_{U_2}(u_p) = 2 \;\text{ and }\; d_{U_2}(w) = d_{U_1}(w) \;\text{ for }\; w \in V(U_1) \setminus \{u_0, u_p\}.$$

Let $p = 1$. If $d_{U_1}(u_0) = 3$, then

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u')]^a - [d_{U_2}(u_1)d_{U_2}(u')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u'')]^a - [d_{U_2}(u_0)d_{U_2}(u'')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u_1)]^a - [d_{U_2}(u_0)d_{U_2}(u_1)]^a \\
&= [3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + [3d_{U_1}(u'')]^a - [2d_{U_1}(u'')]^a \\
&\quad + (3 \cdot 1)^a - (2 \cdot 2)^a \\
&> [3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + 3^a - 4^a \\
&\geq 6^a - 4^a + 3^a - 4^a \\
&> 0,
\end{aligned}$$

since $[3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a \geq 6^a - 4^a$ for $d_{U_1}(u') \geq 2$ by Lemma 2, and $6^a - 4^a + 3^a - 4^a > 0$ by Lemma 4 (ii).

If $d_{U_1}(u_0) = 4$, then

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u')]^a - [d_{U_2}(u_1)d_{U_2}(u')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u'')]^a - [d_{U_2}(u_0)d_{U_2}(u'')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u''')]^a - [d_{U_2}(u_0)d_{U_2}(u''')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u_1)]^a - [d_{U_2}(u_0)d_{U_2}(u_1)]^a \\
&= [4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + [4d_{U_1}(u'')]^a - [3d_{U_1}(u'')]^a \\
&\quad + [4d_{U_1}(u''')]^a - [3d_{U_1}(u''')]^a + (4 \cdot 1)^a - (3 \cdot 2)^a \\
&> [4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + 4^a - 6^a \\
&\geq 8^a - 4^a + 4^a - 6^a \\
&> 0,
\end{aligned}$$

since from Lemma 2, we get $[4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a \geq 8^a - 4^a$ for $d_{U_1}(u') \geq 2$. So $R_a(U_1) > R_a(U_2)$.

Let $p \geq 2$. If $d_{U_1}(u_0) = 3$, then

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u')]^a - [d_{U_2}(u_p)d_{U_2}(u')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u'')]^a - [d_{U_2}(u_0)d_{U_2}(u'')]^a \\
&\quad + [2d_{U_1}(u_0)]^a - [2d_{U_2}(u_0)]^a + [2d_{U_1}(u_p)]^a - [2d_{U_2}(u_p)]^a \\
&= [3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + [3d_{U_1}(u'')]^a - [2d_{U_1}(u'')]^a \\
&\quad + (2 \cdot 3)^a - (2 \cdot 2)^a + (2 \cdot 1)^a - (2 \cdot 2)^a \\
&> [3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + 6^a + 2^a - 2(4^a) \\
&\geq 6^a - 4^a + 6^a + 2^a - 2(4^a) \\
&= 2^a[2(3^a) + 1 - 3(2^a)] \\
&> 0,
\end{aligned}$$

since $[3d_{U_1}(u')]^a - [2d_{U_1}(u')]^a \geq 6^a - 4^a$ for $d_{U_1}(u') \geq 2$ by Lemma 2, and $2(3^a) + 1 - 3(2^a) > 0$ by Lemma 4 (i).
If $d_{U_1}(u_0) = 4$, then

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u')]^a - [d_{U_2}(u_p)d_{U_2}(u')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u'')]^a - [d_{U_2}(u_0)d_{U_2}(u'')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u''')]^a - [d_{U_2}(u_0)d_{U_2}(u''')]^a \\
&\quad + [2d_{U_1}(u_0)]^a - [2d_{U_2}(u_0)]^a + [2d_{U_1}(u_p)]^a - [2d_{U_2}(u_p)]^a \\
&= [4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + [4d_{U_1}(u'')]^a - [3d_{U_1}(u'')]^a \\
&\quad + [4d_{U_1}(u''')]^a - [3d_{U_1}(u''')]^a + (2 \cdot 4)^a - (2 \cdot 3)^a + (2 \cdot 1)^a - (2 \cdot 2)^a \\
&> [4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a + 8^a - 6^a + 2^a - 4^a \\
&> 8^a - 6^a \\
&> 0,
\end{aligned}$$

since from Lemma 2, we get $[4d_{U_1}(u')]^a - [2d_{U_1}(u')]^a > 4^a - 2^a$ for $d_{U_1}(u') > 1$. So $R_a(U_1) > R_a(U_2)$. □

We prove that there is a unicyclic graph having R_a smaller than $R_a(U_1)$ for $a > 0$.

Lemma 6. *Let U_1 be a unicyclic graph having a vertex u_0 which is an end vertex of $p \geq 2$ pendant paths, where $d_{U_1}(u_0) = p + i$, $1 \leq i \leq 3$, and let U_1 contain a vertex of maximum degree other than u_0. Then there exists a unicyclic graph with the same number of vertices and same maximum degree having smaller R_a for $a > 0$.*

Proof. Let $d_{U_1}(u_0) = x$. We have $x \geq 3$. Let $u_0u_1 \dots u_s$ and $u_0u'_1 \dots u'_t$ be two longest pendant paths containing u_0. So $s, t \geq 1$ and $d_{U_1}(u_s) = d_{U_1}(u'_t) = 1$. Let U_2 be obtained from U_1 be removing the edge u_0u_1 and adding the edge u'_tu_1. We have

$$d_{U_2}(u_0) = x - 1, \quad d_{U_2}(u'_t) = 2 \quad \text{and} \quad d_{U_1}(u) = d_{U_2}(u)$$

for $u \in V(U_1)\backslash\{u_0, u_t'\}$. Then U_2 is unicyclic, and U_1 and U_2 have the same maximum degree and number of vertices. We consider several cases.

Case 1. $s, t \geq 2$.

We obtain

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u_1')]^a - [d_{U_2}(u_0)d_{U_2}(u_1')]^a \\
&\quad + [d_{U_1}(u_{t-1}')d_{U_1}(u_t')]^a - [d_{U_2}(u_{t-1}')d_{U_2}(u_t')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u_1)]^a - [d_{U_2}(u_t')d_{U_2}(u_1)]^a \\
&\quad + \sum_{u\in N_{U_1}(u_0)\backslash\{u_1,u_1'\}} ([d_{U_1}(u_0)d_{U_1}(u)]^a - [d_{U_2}(u_0)d_{U_2}(u)]^a) \\
&= (x\cdot 2)^a - [(x-1)2]^a + (2\cdot 1)^a - (2\cdot 2)^a + (x\cdot 2)^a - (2\cdot 2)^a \\
&\quad + \sum_{u\in N_{U_1}(u_0)\backslash\{u_1,u_1'\}} ([x\, d_{U_1}(u)]^a - [(x-1)d_{U_1}(u)]^a) \\
&> 2(2x)^a - (2x-2)^a - 2(4^a) + 2^a = f(x).
\end{aligned}$$

Then $f'(x) = a2^a[2x^{a-1} - (x-1)^{a-1}]$. For $a \geq 1$, we have $2x^{a-1} > (x-1)^{a-1}$, thus $f'(x) > 0$. For $0 < a < 1$, we have

$$2 > \left(1 + \frac{1}{x-1}\right)^{1-a} = \left(\frac{x}{x-1}\right)^{1-a} = \frac{(x-1)^{a-1}}{x^{a-1}},$$

thus again $2x^{a-1} > (x-1)^{a-1}$ and consequently $f'(x) > 0$. So $f(x)$ is increasing for $x \geq 3$, where $a > 0$. Thus $f(x) \geq f(3)$ for $x \geq 3$. We have

$$f(3) = 2(6^a) - 3(4^a) + 2^a = 2^a[2(3^a) + 1 - 3(2^a)] > 0$$

by Lemma 4 (i). Hence $R_a(U_1) - R_a(U_2) > f(x) \geq f(3) > 0$. So U_2 has smaller R_a.

Case 2. Either $s = 1$ or $t = 1$.

We can assume that $s \geq 2$ and $t = 1$. Then

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u_1')]^a - [d_{U_2}(u_0)d_{U_2}(u_1')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u_1)]^a - [d_{U_2}(u_1')d_{U_2}(u_1)]^a \\
&\quad + \sum_{u\in N_{U_1}(u_0)\backslash\{u_1,u_1'\}} ([d_{U_1}(u_0)d_{U_1}(u)]^a - [d_{U_2}(u_0)d_{U_2}(u)]^a) \\
&= (x\cdot 1)^a - [(x-1)2]^a + (x\cdot 2)^a - (2\cdot 2)^a \\
&\quad + \sum_{u\in N_{U_1}(u_0)\backslash\{u_1,u_1'\}} ([x\, d_{U_1}(u)]^a - [(x-1)d_{U_1}(u)]^a) \\
&> (2x)^a + x^a - (2x-2)^a - 4^a = f(x).
\end{aligned}$$

We obtain $f'(x) = a[(2^a+1)x^{a-1} - 2^a(x-1)^{a-1}]$. For $a \geq 1$, we have $(2^a+1)x^{a-1} > 2^a(x-1)^{a-1}$, thus $f'(x) > 0$. For $0 < a < 1$, we have

$$\frac{2^a+1}{2^a} = 1 + \frac{1}{2^a} > \frac{3}{2} > \left(1 + \frac{1}{x-1}\right)^{1-a} = \left(\frac{x}{x-1}\right)^{1-a} = \frac{(x-1)^{a-1}}{x^{a-1}},$$

thus again $(2^a+1)x^{a-1} > 2^a(x-1)^{a-1}$ and consequently $f'(x) > 0$. So $f(x)$ is increasing for $x \geq 3$, where $a > 0$. Thus $f(x) \geq f(3)$ for $x \geq 3$. By Lemma 4 (ii),

$$f(3) = 6^a + 3^a - 2(4^a) > 0,$$

hence $R_a(U_1) - R_a(U_2) > f(x) \geq f(3) > 0$. So R_a is smaller for U_2.

Case 3. $s = t = 1$ and $0 < a \leq 1$.

We obtain

$$\begin{aligned}
R_a(U_1) - R_a(U_2) &= [d_{U_1}(u_0)d_{U_1}(u_1')]^a - [d_{U_2}(u_0)d_{U_2}(u_1')]^a \\
&\quad + [d_{U_1}(u_0)d_{U_1}(u_1)]^a - [d_{U_2}(u_1')d_{U_2}(u_1)]^a \\
&\quad + \sum_{u \in N_{U_1}(u_0)\setminus\{u_1,u_1'\}} ([d_{U_1}(u_0)d_{U_1}(u)]^a - [d_{U_2}(u_0)d_{U_2}(u)]^a) \\
&= (x \cdot 1)^a - [(x-1)2]^a + (x \cdot 1)^a - (2 \cdot 1)^a \\
&\quad + \sum_{u \in N_{U_1}(u_0)\setminus\{u_1,u_1'\}} ([x\, d_{U_1}(u)]^a - [(x-1)d_{U_1}(u)]^a) \\
&> x^a - (2x-2)^a + x^a - 2^a \\
&\geq 0
\end{aligned}$$

for $0 < a \leq 1$, since $x^a - (2x-2)^a + x^a - 2^a = 0$ if $a = 1$, and by Lemma 1, we have $x^a - 2^a > (2x-2)^a - x^a$ if $0 < a < 1$. Hence $R_a(U_1) > R_a(U_2)$.

Case 4. $s = t = 1$ and $a > 1$.

We have $s = t = 1$, so all $p \geq 2$ pendant paths containing u_0 are of length 1. We replace those p pendant paths by one path of length p with an end vertex u_0 to obtain U_2' from U_1. Then U_2' is unicyclic, and U_1 and U_2' have the same maximum degree and number of vertices. We denote the vertices adjacent to u_0 in U_1 which have degree at least 2 by w_i, where $1 \leq i \leq 3$. The proof of this case is more complicated than the previous cases, therefore we use $d_{U_1}(u_0) = p + i$ instead of $d_{U_1}(u_0) = x$. Then $d_{U_2'}(u_0) = i + 1$, where $1 \leq i \leq 3$. We have $d_{U_1}(w_i) = d_{U_2'}(w_i) \geq 2$. Thus

$$[d_{U_1}(u_0)d_{U_1}(w_i)]^a - [d_{U_2'}(u_0)d_{U_2'}(w_i)]^a = [(p+i)d_{U_1}(w_i)]^a - [(i+1)d_{U_1}(w_i)]^a \geq [(p+i)2]^a - [(i+1)2]^a$$

by Lemma 2, since $d_{U_1}(w_i) \geq 2$. Therefore

$$\begin{aligned}R_a(U_1) - R_a(U_2') &= p[(p+i)1]^a - [2(i+1)]^a - (p-2)4^a - 2^a \\ &\quad + \sum_{j=1}^{i}([d_{U_1}(u_0)d_{U_1}(w_j)]^a - [d_{U_2'}(u_0)d_{U_2'}(w_j)]^a) \\ &\geq p(p+i)^a - (p-2)4^a - (2i+2)^a - 2^a + i([2(p+i)]^a - [2(i+1)]^a) \\ &= f(p).\end{aligned}$$

Let $i = 1$. Then

$$f(p) = p[(p+1)^a - 4^a] + [2(p+1)]^a - 2^a.$$

If $p \geq 3$, clearly $f(p) > 0$. If $p = 2$, then

$$f(2) = [6^a + 3^a - 2(4^a)] + (3^a - 2^a) > 0,$$

since by Lemma 4 (ii), we have $6^a + 3^a - 2(4^a) > 0$.
Let $2 \leq i \leq 3$. Then

$$f'(p) = (p+i)^a + ap(p+i)^{a-1} - 4^a + i2^a a(p+i)^{a-1} > 0,$$

since $(p+i)^a \geq 4^a$. So $f(p)$ is increasing for $p \geq 2$. Thus $f(p) \geq f(2)$ for $p \geq 2$.
If $i = 2$ and $p = 2$, then

$$f(2) = [(8^a - 6^a) - (6^a - 4^a)] + (8^a - 6^a) + (4^a - 2^a) > 0,$$

since by Lemma 1, we have $8^a - 6^a > 6^a - 4^a$ for $a > 1$. Hence $R_a(U_1) - R_a(U_2') \geq f(p) \geq f(2) > 0$.
If $i = 3$ and $p = 2$, then

$$f(2) = 3(10^a) - 4(8^a) + 2(5^a) - 2^a = 2[(10^a - 8^a) - (8^a - 6^a)] + [(10^a - 6^a) - (6^a - 2^a)] + 2(5^a - 2^a) > 0,$$

since by Lemma 1, we have $10^a - 8^a > 8^a - 6^a$ and $10^a - 6^a > 6^a - 2^a$ for $a > 1$. Hence $R_a(U_1) - R_a(U_2') \geq f(p) \geq f(2) > 0$. So $R_a(U_1) > R_a(U_2')$. $\square$

For $\Delta \geq 3$ and $2 \leq t \leq n - \Delta - 1$, we obtain the graph $CPS_{n-\Delta-t+2,t,\Delta-1}$ from the path of length $t-1$ by connecting one of its end vertices to $\Delta - 1$ new vertices, and by identifying the other end vertex of that path with one vertex of the cycle $C_{n-\Delta-t+2}$; see Figure 1.

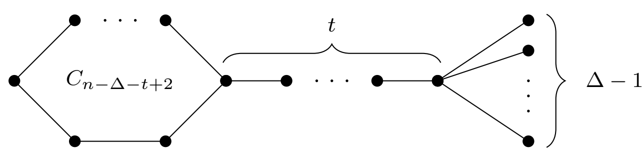

Figure 1. **Graph** $CPS_{n-\Delta-t+2,t,\Delta-1}$

For $3 \leq \Delta \leq n-1$, we obtain the graph $CS_{n-\Delta+2,\Delta-2}$ by joining one vertex of the cycle $C_{n-\Delta+2}$ to $\Delta - 2$ new vertices; see Figure 2.

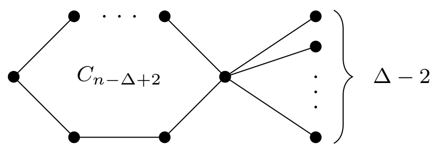

Figure 2. **Graph** $CS_{n-\Delta+2,\Delta-2}$

We show that graphs presented in Figures 1 and 2 are extremal graphs for Theorem 1.

Theorem 1. *Among unicyclic graphs containing n vertices and maximum degree $\Delta \geq 3$, the following graphs have the smallest values of R_a:*

(i) $CS_{4,\Delta-2}$ *for* $\Delta = n-2$ *and* $a > 0$,

(ii) $CS_{5,\Delta-2}$ *for* $\Delta = n-3$ *and* $a \geq 1$,

(iii) *For* $\Delta = n-3$ *and* $0 < a < 1$:
- $CS_{5,\Delta-2}$ *if* $(3\Delta)^a - 2(2\Delta)^a + \Delta^a + 2(6^a - 4^a) > 0$,
- $CPS_{3,2,\Delta-1}$ *if* $(3\Delta)^a - 2(2\Delta)^a + \Delta^a + 2(6^a - 4^a) < 0$,
- *both* $CS_{5,\Delta-2}$ *and* $CPS_{3,2,\Delta-1}$ *if* $(3\Delta)^a - 2(2\Delta)^a + \Delta^a + 2(6^a - 4^a) = 0$.

(iv) *For* $3 \leq \Delta \leq n-4$ *and* $a > 0$:
- $CPS_{n-\Delta-t+2,t,\Delta-1}$ *for any* $3 \leq t \leq n-\Delta-1$ *if* $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) > 0$
- $CS_{n-\Delta+2,\Delta-2}$ *if* $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) < 0$
- $CS_{n-\Delta+2,\Delta-2}$ *and* $CPS_{n-\Delta-t+2,t,\Delta-1}$ *for any* $3 \leq t \leq n-\Delta-1$ *if* $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) = 0$.

Proof. For $3 \leq \Delta \leq n-2$, let us denote by U' a unicyclic graph with n vertices and maximum degree Δ having the smallest R_a. We denote the cycle in U' by $C_k = v_1 v_2 \dots v_k v_1$ and a vertex of degree Δ by w. We can suppose that among vertices in C_k, v_1 is closest to w (possibly $w = v_1$). We denote a path between w and v_1 by P (its length is 0 if $w = v_1$). Let $S = V(P) \cup V(C_k)$.

Claim 1. The degree of every vertex not in S is at most 2.

To the contrary, suppose that there is a vertex not in S having degree greater than 2. Let v be a vertex of degree at least 3 furthest from S. It follows that v belongs to (at least) 2 pendant paths, hence from Lemma 6, U' is not a graph having the smallest R_a, a contradiction.

Claim 2. Every neighbour of a vertex from $S \setminus \{w\}$ is in S.

To the contrary, suppose that there exists $v \in S \setminus \{w\}$, having r neighbours not from S such that $r \geq 1$. By Claim 1, v belongs to r pendant paths. However, v cannot belong to two or more pendant paths, since from Lemma 6, U' would not have the minimum R_a. Thus $r = 1$. We have $3 \leq d_{U'}(v) \leq 4$ and from Lemma 5, U' is not a graph having the smallest R_a, a contradiction.

Claim 3. Every pendant path containing w has length 1.

To the contrary, suppose that U' contains a pendant path ending with w having length $p \geq 2$. We replace it with a path having length 1, and C_k is replaced with the cycle having length $p + k - 1$ to get U_1 from U'. We have

$$R_a(U') - R_a(U_1) = (2\Delta)^a - \Delta^a + 2^a - 4^a > 0$$

since by Lemma 2, we have $(2\Delta)^a - \Delta^a > (2 \cdot 2)^a - (1 \cdot 2)^a$. So $R_a(U') > R_a(U_1)$, a contradiction.

By Claims 1, 2 and 3, U' is $CS_{n-\Delta+2,\Delta-2}$ or $CPS_{n-\Delta-t+2,t,\Delta-1}$, where $2 \leq t \leq n - \Delta - 1$. Then $2 \leq n - \Delta - 1$ gives $\Delta \leq n - 3$, so $CPS_{n-\Delta-t+2,t,\Delta-1}$ does not exist for $\Delta = n - 2$.
(i) Let $\Delta = n - 2$. From the previous paragraph, clearly U' is $CS_{4,\Delta-2}$.
(ii) Let $\Delta = n - 3$. Then U' is $CS_{5,\Delta-2}$ or $CPS_{3,2,\Delta-1}$. Let us compare their R_a. We get

$$R_a(CPS_{3,2,\Delta-1}) = (\Delta - 1)\Delta^a + (3\Delta)^a + 4^a + 2(6^a)$$

and

$$R_a(CS_{5,\Delta-2}) = (\Delta - 2)\Delta^a + 2(2\Delta)^a + 3(4^a).$$

Thus

$$R_a(CPS_{3,2,\Delta-1}) - R_a(CS_{5,\Delta-2}) = (3\Delta)^a - 2(2\Delta)^a + \Delta^a + 2(6^a - 4^a). \tag{2.1}$$

For $a > 1$, we have $(3\Delta)^a - (2\Delta)^a > (2\Delta)^a - \Delta^a$ by Lemma 1, so $CS_{5,\Delta-2}$ has the smallest R_a.
For $a = 1$, we have $R_1(CPS_{3,2,\Delta-1}) - R_1(CS_{5,\Delta-2}) = 3\Delta - 2(2\Delta) + \Delta + 2(6-4) > 0$, so again $CS_{5,\Delta-2}$ has the smallest R_a.
(iii) For $0 < a < 1$ and $\Delta = n - 3$, by (2.1), $CS_{5,\Delta-2}$ has the smallest R_a if $(3\Delta)^a - 2(2\Delta)^a + \Delta^a + 2(6^a - 4^a) > 0$, $CPS_{3,2,\Delta-1}$ has the smallest R_a if $(3\Delta)^a - 2(2\Delta)^a + (\Delta)^a + 2(6^a - 4^a) < 0$, and both $CS_{5,\Delta-2}$ and $CPS_{3,2,\Delta-1}$ have the smallest R_a if $(3\Delta)^a - 2(2\Delta)^a + (\Delta)^a + 2(6^a - 4^a) = 0$.
(iv) Let $3 \leq \Delta \leq n - 4$.

Claim 4. P does not have length 1.

To the contrary, suppose that P is of length 1. So U' consists of C_k whose one vertex v_1 is adjacent to w, and w is a neighbour of $\Delta - 1$ vertices of degree 1 in U' (by Claim 3). So $n = \Delta + k$. Since $n \geq \Delta + 4$, we have $k \geq 4$. We replace C_k by the cycle having length $k-1$ and we replace P by the path having length 2 to obtain U_2 from U'. Then

$$R_a(U') - R_a(U_2) = (3\Delta)^a - (2\Delta)^a + 4^a - 6^a > 0,$$

since by Lemma 2, we have $(3\Delta)^a - (2\Delta)^a > (3 \cdot 2)^a - (2 \cdot 2)^a$. So $R_a(U') > R_a(U_2)$ which is a contradiction.

By Claims 1, 2, 3 and 4, P has length at least 2 or 0, so U' is $CS_{n-\Delta+2,\Delta-2}$ or any of the graphs $CPS_{n-\Delta-t+2,t,\Delta-1}$, where $3 \le t \le n-\Delta-1$. Let us compare their R_a. We get

$$R_a(CPS_{n-\Delta-t+2,t,\Delta-1}) = (2\Delta)^a + (\Delta-1)\Delta^a + 3(6^a) + (n-\Delta-3)4^a$$

and

$$R_a(CS_{n-\Delta+2,\Delta-2}) = 2(2\Delta)^a + (\Delta-2)\Delta^a + (n-\Delta)4^a.$$

Thus

$$R_a(CS_{n-\Delta+2,\Delta-2}) - R_a(CPS_{n-\Delta-t+2,t,\Delta-1}) = (2\Delta)^a - \Delta^a + 3(4^a - 6^a).$$

Hence, $CPS_{n-\Delta-t+2,t,\Delta-1}$ for $3 \le t \le n-\Delta-1$ has the smallest R_a if $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) > 0$, $CS_{n-\Delta+2,\Delta-2}$ has the smallest R_a if $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) < 0$, and $CS_{n-\Delta+2,\Delta-2}$ and $CPS_{n-\Delta-t+2,t,\Delta-1}$ for $3 \le t \le n-\Delta-1$ have the smallest R_a if $(2\Delta)^a - \Delta^a + 3(4^a - 6^a) = 0$. □

In Remark 1, we consider some special cases of Theorem 1 (iv).

Remark 1. Among unicyclic graphs containing n vertices and maximum degree Δ,

(i) $CS_{n-\Delta+2,\Delta-2}$ has the smallest R_a if $a > 0$, $\Delta = 3$ and $n \ge 7$,

(ii) $CPS_{n-\Delta-t+2,t,\Delta-1}$ for $3 \le t \le n-\Delta-1$ are the only graphs with the smallest R_a for $a \ge 1$ and $6 \le \Delta \le n-4$, except for the case when $a = 1$ and $\Delta = 6$. In that case, $CS_{n-\Delta+2,\Delta-2}$ also has the smallest R_a.

Proof. From the proof of Theorem 1, we know that for $a > 0$ and $3 \le \Delta \le n-4$, a graph with the smallest R_a is $CS_{n-\Delta+2,\Delta-2}$ or any of the graphs $CPS_{n-\Delta-t+2,t,\Delta-1}$, where $3 \le t \le n-\Delta-1$.
(i) Let $a > 0$ and $3 = \Delta \le n-4$. Then

$$R_a(CS_{n-\Delta+2,\Delta-2}) - R_a(CPS_{n-\Delta-t+2,t,\Delta-1}) = 6^a - 3^a + 3(4^a - 6^a) = (4^a - 6^a) - [6^a + 3^a - 2(4^a)] < 0,$$

since $4^a - 6^a < 0$ and $6^a - 2(4^a) + 3^a > 0$ by Lemma 4 (ii). Hence $CS_{n-\Delta+2,\Delta-2}$ has the smallest R_a if $\Delta = 3$,

(ii) Let $a \geq 1$ and $6 \leq \Delta \leq n-4$. For

$$R_a(CS_{n-\Delta+2,\Delta-2}) - R_a(CPS_{n-\Delta-t+2,t,\Delta-1}) = (2\Delta)^a - \Delta^a + 3(4^a - 6^a) = f(\Delta),$$

the derivative $f'(\Delta) = (2^a - 1)a\Delta^{a-1} > 0$, so the function $f(\Delta)$ is strictly increasing. Thus for $\Delta \geq 6$,

$$f(\Delta) \geq f(6) = 12^a - 6^a + 3(4^a - 6^a) = 2^a[6^a + 3(2^a) - 4(3^a)] > 0$$

if $a > 1$ by Lemma 4 (iii). If $a = 1$, then for $\Delta \geq 7$, we have and $f(\Delta) > f(6) = 0$. Remark 1 (ii) follows. □

3. Largest value of R_a for $a < 0$

For $\lceil \frac{n+1}{2} \rceil \leq \Delta \leq n-1$, we attach $n-\Delta-1$ pendant paths of length 2 and $2\Delta-n-1$ pendant paths of length 1 to one vertex of C_3 to obtain $CSI_{3,2\Delta-n-1,n-\Delta-1}$; see Figure 3.

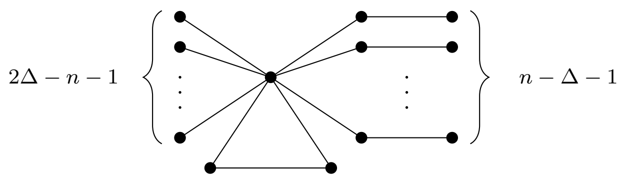

Figure 3. **Graph** $CSI_{3,2\Delta-n-1,n-\Delta-1}$

Let us show that $CSI_{3,2\Delta-n-1,n-\Delta-1}$ is the extremal graph for Theorem 2.

Theorem 2. *Among unicyclic graphs with n vertices and maximum degree Δ such that $\lceil \frac{n+1}{2} \rceil \leq \Delta \leq n-2$, the graph $CSI_{3,2\Delta-n-1,n-\Delta-1}$ has the largest value of R_a for $a < 0$.*

Proof. From $\lceil \frac{n+1}{2} \rceil \leq \Delta \leq n-2$ we get $n \geq 5$, so $\Delta \geq 3$. Note that $n \leq 2\Delta - 1$. Among unicyclic graphs with n vertices and maximum degree Δ, we denote a unicyclic graph with the largest R_a by U'. A vertex having degree Δ is denoted by w.
If w is not a neighbour of a vertex of degree 1, then every component of $U'-w$ has two or more vertices. There are $\Delta-1$ or more components, thus $n \geq 1+2(\Delta-1) = 2\Delta-1$. So $n = 2\Delta-1$, therefore $U'-w$ has exactly $\Delta-1$ components, where every component contains 2 vertices. Thus U' is $CSI_{3,0,\Delta-2}$ which is $CSI_{3,2\Delta-n-1,n-\Delta-1}$ if $n = 2\Delta-1$. In the rest of this proof, we can assume that w has a neighbour of degree 1, say w_0.

Claim 1. The vertex w belongs to the cycle of U'.

We denote the cycle of U' by $C_k = v_1v_2\dots v_kv_1$, where $k \geq 3$. To the contrary, suppose that $w \notin V(C_k)$. Thus, we can suppose that $d_{U'}(v_i) < \Delta$ for every $i = 1, 2, \dots, k$.

We can also suppose that a vertex of C_k closest to w is v_1. Let $u_1, u_2, \dots, u_s$, where $s \geq 0$, be the neighbours of v_2 in U' not in $V(C_k)$. Let U_1 have the same vertices as U' and $E(U_1) = \{w_0v_3, w_0u_1, \dots, w_0u_s\} \cup E(U') \setminus \{v_2v_3, v_2u_1, \dots, v_2u_s\}$. So U_1 is unicyclic and

$$R_a(U') - R_a(U_1) = (1 \cdot \Delta)^a - [d_{U'}(v_2) \cdot \Delta]^a + [d_{U'}(v_2)d_{U'}(v_1)]^a - [1 \cdot d_{U'}(v_1)]^a < 0,$$

since by Lemma 2, for $a < 0$,

$$[d_{U'}(v_2)d_{U'}(v_1)]^a - [1 \cdot d_{U'}(v_1)]^a < [d_{U'}(v_2) \cdot \Delta]^a - (1 \cdot \Delta)^a.$$

Thus $R_a(U') < R_a(U_1)$, a contradiction.

Claim 2. Every vertex of U' not on the cycle has degree at most 2.

We prove Claim 2 by contradiction. Among vertices not on the cycle having degree at least 3, let u be a vertex furthest from w. We have $d_{U'}(u) = s$, where $3 \leq s \leq \Delta$. So, there is a pendant path $uu_1 \dots u_p$, where $p \geq 1$ in U'. Let U_2 have the same vertices as U' and $E(U_2) = \{w_0u_1\} \cup E(U') \setminus \{uu_1\}$. We consider the cases $s \geq 4$ and $s = 3$ separately.

Case 1. $s \geq 4$.

Note that $\Delta \geq s \geq 4$. We have

$$\begin{aligned}
R_a(U') - R_a(U_2) &= \sum_{v \in N_{U'}(u) \setminus \{u_1\}} \left([d_{U'}(u)d_{U'}(v)]^a - [d_{U_2}(u)d_{U_2}(v)]^a\right) \\
&\quad + [d_{U'}(u)d_{U'}(u_1)]^a - [d_{U_2}(w_0)d_{U_2}(u_1)]^a \\
&\quad + [d_{U'}(w)d_{U'}(w_0)]^a - [d_{U_2}(w)d_{U_2}(w_0)]^a \\
&= \sum_{v \in N_{U'}(u) \setminus \{u_1\}} \left([s\, d_{U'}(v)]^a - [(s-1)d_{U'}(v)]^a\right) \\
&\quad + [s\, d_{U'}(u_1)]^a - [2\, d_{U'}(u_1)]^a + (\Delta \cdot 1)^a - (\Delta \cdot 2)^a \\
&< [s\, d_{U'}(u_1)]^a - [2\, d_{U'}(u_1)]^a + \Delta^a - (2\Delta)^a,
\end{aligned}$$

since $[s\, d_{U'}(v)]^a < [(s-1)d_{U'}(v)]^a$.
If $p \geq 2$, then $d_{U'}(u_1) = 2$. We obtain

$$\begin{aligned}
R_a(U') - R_a(U_2) &< (2s)^a - 4^a + \Delta^a - (2\Delta)^a \\
&\leq 8^a - 4^a + \Delta^a - (2\Delta)^a \\
&\leq 0,
\end{aligned}$$

since $(2s)^a \leq 8^a$, and by Lemma 2, we get $(2 \cdot 4)^a - 4^a \leq (2\Delta)^a - \Delta^a$ for $a < 0$ and $\Delta \geq 4$.

If $p = 1$, then $d_{U'}(u_1) = 1$. We get

$$\begin{aligned} R_a(U') - R_a(U_2) &< s^a - 2^a + \Delta^a - (2\Delta)^a \\ &\leq 4^a - 2^a + \Delta^a - (2\Delta)^a \\ &< 0, \end{aligned}$$

since $s^a \leq 4^a$, and by Lemma 2, we get $(2 \cdot 2)^a - 2^a < (2\Delta)^a - \Delta^a$ for $a < 0$ and $\Delta \geq 4$. Thus $R_a(U') < R_a(U_2)$ which is a contradiction.

Case 2. $s = 3$.

Let us denote the vertex adjacent to u in U' which is on a shortest path between u and w by u' (possibly $u' = w$). We denote the vertex adjacent to u in U' other than u' and u_1 by v. Since v is on a pendant path, we have $d_{U'}(v) \leq 2$, but we only use $d_{U'}(v) \leq 3$.
Clearly, in this case $n > 5$, thus $\Delta \geq 4$, since $\Delta \geq \left\lceil \frac{n+1}{2} \right\rceil$. We obtain

$$\begin{aligned} R_a(U') - R_a(U_2) &= [d_{U'}(u)d_{U'}(u')]^a - [d_{U_2}(u)d_{U_2}(u')]^a \\ &\quad + [d_{U'}(u)d_{U'}(v)]^a - [d_{U_2}(u)d_{U_2}(v)]^a \\ &\quad + [d_{U'}(u)d_{U'}(u_1)]^a - [d_{U_2}(w_0)d_{U_2}(u_1)]^a \\ &\quad + [d_{U'}(w)d_{U'}(w_0)]^a - [d_{U_2}(w)d_{U_2}(w_0)]^a \\ &= [3d_{U'}(u')]^a - [2d_{U'}(u')]^a + [3d_{U'}(v)]^a - [2d_{U'}(v)]^a \\ &\quad + [3\, d_{U'}(u_1)]^a - [2\, d_{U'}(u_1)]^a + (\Delta \cdot 1)^a - (\Delta \cdot 2)^a \\ &< 9^a - 6^a + [3\, d_{U'}(u_1)]^a - [2\, d_{U'}(u_1)]^a + \Delta^a - (2\Delta)^a, \end{aligned}$$

since $[3\, d_{U'}(u')]^a < [2\, d_{U'}(u')]^a$, and by Lemma 2, for $d_{U'}(v) \leq 3$, we have $[3\, d_{U'}(v)]^a - [2\, d_{U'}(v)]^a \leq (3 \cdot 3)^a - (2 \cdot 3)^a$.
If $p = 1$, then $d_{U'}(u_1) = 1$. We obtain

$$\begin{aligned} R_a(U') - R_a(U_2) &< 9^a - 6^a + 3^a - 2^a + 4^a - 8^a \\ &= 9^a - 8^a + 3^a - 2^a - (6^a - 4^a) \\ &< 0, \end{aligned}$$

since $9^a < 8^a$ for $a < 0$, and by Lemma 2, we get $3^a - 2^a < (2 \cdot 3)^a - (2 \cdot 2)^a = 6^a - 4^a$.
If $p \geq 2$, then $d_{U'}(u_1) = 2$. We get

$$\begin{aligned} R_a(U') - R_a(U_2) &< 9^a - 6^a + 6^a - 4^a + 4^a - 8^a \\ &= 9^a - 8^a \\ &< 0, \end{aligned}$$

since $9^a < 8^a$ for $a < 0$. So $R_a(U') < R_a(U_2)$ which is a contradiction. We have Claim 2.

Claim 3. The only vertex on the cycle having degree at least 3 in U' is w.

Assume to the contrary that C_k contain a vertex of degree at least 3 different from w. Let u have the largest degree among vertices in $V(C_k) \setminus \{w\}$. We have $d_{U'}(u) = s$, where $3 \leq s \leq \Delta$. From Claim 2 we also know that u is the end vertex of $s-2$ pendant paths. We denote a neighbour of u on one of those pendant paths by u_1.
If $s \geq 4$, then calculations given in Case 1 of Claim 2 can be used to show that U' does not have the largest R_a.
So $s = 3$. We denote the neighbours of u on C_k by u' and v (where possibly $u' = w$). We have $d_{U'}(v) \leq d_{U'}(u) = 3$.
If $n > 5$, then calculations given in Case 2 of Claim 2 can be used to show that U' does not have the largest R_a.
If $n = 5$, then $u' = w$, $C_k = C_3$ contains u, v and w. We have $d_{U'}(v) = 2$, u is adjacent to one vertex of degree 1 (which is u_1), and w is adjacent to one vertex of degree 1 (which is w_0). Then

$$R_a(U') - R_a(U_2) = 9^a - 6^a + 3^a - 2^a - (4^a - 3^a) < 0,$$

since $9^a < 6^a$ for $a < 0$, and by Lemma 1, we get $3^a - 2^a < 4^a - 3^a$. Thus $R_a(U') < R_a(U_2)$ which is a contradiction. So, we have Claim 3.

Thus U' contains a cycle with the vertex w which is the end vertex of $\Delta - 2$ pendant paths.
If U' would contain a pendant path of length greater than 2 or if the length of the cycle is greater than 3, then we can get a unicyclic graph U_3 from U' by replacing that path/cycle by a path/cycle having one less edge, and by joining a new vertex to w_0. We get

$$R_a(U') - R_a(U_3) = 4^a - 2^a + \Delta^a - (2\Delta)^a < 0,$$

since by Lemma 2, we have $4^a - 2^a < (2\Delta)^a - \Delta^a$ for $a < 0$. So we would have $R_a(U') < R_a(U_3)$.
Therefore the length of the cycle in U' is 3 and the length of each pendant path is 1 or 2. This implies that U' contains $n - \Delta - 1$ vertices at distance 2 from w, so w is contained in $n - \Delta - 1$ pendant paths of length 2 and $2\Delta - n - 1$ pendant paths of length 1. Thus U' is $CSI_{3,2\Delta-n-1,n-\Delta-1}$. □

4. Open problems

In this paper, unicyclic graphs having the smallest R_a for $a > 0$ and largest R_a for $a < 0$ are investigated. So, we state the following open problem.

Problem 1. Among unicyclic graphs with given number of vertices and maximum degree, find graphs with the smallest values of R_a for $a < 0$, and graphs having the largest R_a for $a > 0$.

Altassan and Imran [3] presented unicyclic graphs containing n vertices and maximum degree $\Delta \geq 3$ with the largest R_a for $a_0 \leq a < 0$, where a_0 is the negative solution of the equation $9^a + 2^a - 2(4^a) = 0$ which is about -0.21. Their result is extended in our Theorem 2 for $\lceil \frac{n+1}{2} \rceil \leq \Delta \leq n-2$ and every $a < 0$. Thus we state Problem 2.

Problem 2. Among unicyclic graphs containing n vertices and maximum degree Δ, find graphs with the largest values of R_a for $a < a_0$, where $3 \leq \Delta < \lceil \frac{n+1}{2} \rceil$.

Acknowledgements: The work of T. Vetrík is based on the research supported by the National Research Foundation of South Africa (Grant Number CPRR230530111607).

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

References

[1] M.R. Alfuraidan, K.C. Das, T. Vetrík, and S. Balachandran, *General Randić index of unicyclic graphs with given diameter*, Discrete Appl. Math. **306** (2022), 7–16.
https://doi.org/10.1016/j.dam.2021.09.016.

[2] A. Ali and T. Idrees, *A note on polyomino chains with extremum general sum-connectivity index*, Commun. Comb. Optim. **6** (2021), no. 1, 81–91.
https://doi.org/10.22049/cco.2020.26866.1153.

[3] A. Altassan and M. Imran, *General Randić index of unicyclic graphs and its applications to drugs*, Symmetry **16** (2024), no. 1, Article ID: 113.
https://doi.org/10.3390/sym16010113.

[4] B. Bollobás and P. Erdös, *Graphs of extremal weights*, Ars Combin. **50** (1998), 225–233.

[5] D. Chen, *Study of unicyclic graph with maximal general Randić index R_α for $\alpha <$* 0, Intelligent Computing and Information Science (Berlin, Heidelberg) (R. Chen, ed.), Springer Berlin Heidelberg, 2011, pp. 136–141.

[6] R. Hasni, N.H. Md Husin, and Z. Du, *Unicyclic graphs with maximum Randić indices*, Commun. Comb. Optim. **8** (2023), no. 1, 161–172.
https://doi.org/10.22049/cco.2021.27230.1216.

[7] X. Li, Y. Shi, and T. Xu, *Unicyclic graphs with maximum general Randić index for α¿ 0*, MATCH Commun. Math. Comput. Chem. **56** (2006), no. 3, 557–570.

[8] X. Li, L. Wang, and Y. Zhang, *Complete solution for unicyclic graphs with minimum general Randić index*, MATCH Commun. Math. Comput. Chem. **55** (2006), no. 2, 391–408.

[9] E. Swartz and T. Vetrík, *General sum-connectivity index and general Randić index of trees with given maximum degree*, Discret. Math. Lett. **12** (2023), 181–188.
https://doi.org/10.47443/dml.2023.140.

[10] ______, *General sum-connectivity index of unicyclic graphs with given maximum degree*, Discrete Appl. Math. **366** (2025), 238–249.
https://doi.org/10.1016/j.dam.2025.01.033.

[11] T. Vetrík and M. Masre, *General eccentric connectivity index of trees and unicyclic graphs*, Discrete Appl. Math. **284** (2020), 301–315.
https://doi.org/10.1016/j.dam.2020.03.051.

[12] B. Wu and L. Zhang, *Unicyclic graphs with minimum general Randić index*, MATCH Commun. Math. Comput. Chem. **54** (2005), no. 2, 455–464.