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Sum of Powers of the Degrees of Graphs: Extremal Results and Bounds

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Abstract

For any real number α, the sum of the α-th powers of the degrees of a (molecular) graph G, denoted by ${}^0R_\alpha(G)$, is known as the general zeroth–order Randić index as well as the general first Zagreb index and variable first Zagreb index. Research on the graph invariant ${}^0R_\alpha$ (for specific values of α) began in the 1970s, when the first Zagreb index ${}^0R_2$ and the zeroth–order connectivity/Randić index ${}^0R_{-1/2}$ were introduced within the study of molecular modeling. After that, several other specific versions of the invariant ${}^0R_\alpha$ were also studied. These versions include inverse degree (or modified total adjacency index) ${}^0R_{-1}$, modified first Zagreb index ${}^0R_{-2}$, and forgotten topological index ${}^0R_3$. The main purpose of the present survey is to present bounds and extremal results related to the invariant ${}^0R_\alpha$, including all the aforementioned specific versions of ${}^0R_\alpha$.

1 Introduction

All the graphs considered in the present study are assumed to be finite and simple. Undefined notations and terminologies from (chemical) graph theory can be found in [16, 67, 72, 143].

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For the graph $G = (V, E)$ with vertex set $V = \{1, 2, \ldots, n\}$ and edge set $E = \{e_1, e_2, \ldots, e_m\}$, we will take $d_1 \geq d_2 \geq \cdots \geq d_n$ and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$, where $d_i = d(i)$ is the vertex degree and $d(e_i)$ is edge degree. In addition, we will use standard notation; $\Delta = d_1$, $\Delta_2 = d_2$, $\delta = d_m$, $\delta_2 = d_{m-1}$, $\Delta_{e_1} = d(e_1) + 2$, $\Delta_{e_2} = d(e_2) + 2$, $\delta_{e_1} = d(e_m) + 2$, $\delta_{e_2} = d(e_{m-1}) + 2$. If the vertices i and j are adjacent (respectively, non-adjacent), then we denote it by $i \sim j$ (respectively $i \nsim j$). As usual, $L(G)$ denotes a line graph of the graph G.

In graph theory, an invariant is a property of graphs that depends only on its abstract structure, not on graph representations such as particular labeling or drawing of the graph. Such quantities are also called topological indices. Topological indices represent an important type of molecular descriptors. Hundreds of different such invariants have been employed to date, with varying success, in QSAR (quantitative structure–activity relationship) and QSPR (quantitative structure–property relationship) studies. Topological indices have gained considerable popularity and many new topological indices have been proposed and studied in the mathematical chemistry literature in recent years.

The first and second Zagreb indices are vertex–degree–based graph invariants defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{i \sim j} d_i\, d_j\,. \tag{1}$$

The quantity M_1 was first time considered in 1972 [69], whereas M_2 in 1975 [68]. These are the oldest and most thoroughly examined vertex–degree–based topological indices. Details of their theory and applications can be found in surveys [17, 18, 57, 59, 123] and in the references quoted therein. Thereby, in the present survey, we do not include those results which are concerned only with Zagreb indices.

As shown in [39, 123], the first Zagreb index can be also represented as

$$M_1 = \sum_{i \sim j} (d_i + d_j)\,. \tag{2}$$

Bearing in mind that for the edge e connecting the vertices i and j,

$$d(e) = d_i + d_j - 2$$

the index M_1 can also be considered as an edge-degree based topological index, since according to (2) holds [114]

$$M_1 = \sum_{i=1}^{m} \big[d(e_i) + 2 \big]\,. \tag{3}$$

A so-called forgotten topological index, F, is defined as [50]

$$F = F(G) = \sum_{i=1}^{n} d_i^3 \,.$$

It is worth noting that the graph invariant F was considered already in the paper [69], but in the next more than 40 years it did not attract any attention and was completely ignored. For this reason, the name "forgotten" has been proposed for this topological index [50].

Various generalizations of the Zagreb indices have been proposed. In [77] a so called general zeroth–order Randić index was introduced. It is defined as

$$^0R_\alpha = {}^0R_\alpha(G) = \sum_{i=1}^{n} d_i^\alpha$$

where α is an arbitrary real number. It is also met under the names first general Zagreb index [95] and variable first Zagreb index [116].

For specific values of α, specific notations (and hence specific names) are being used. For example, ${}^mM_1 = {}^0R_{-2}$ (the modified first Zagreb index [123]), ${}^0R = {}^0R_{-\frac{1}{2}}$ (the zeroth–order connectivity/Randić index [86]), $ID = {}^0R_{-1}$ (inverse degree or modified total adjacency index [45] and [123]), $M_1 = {}^0R_2$ (the first Zagreb index [8]), $F = {}^0R_3$ (the forgotten topological index [50]), and so on.

A relation between ${}^0R_\alpha$ and ${}^0R_{1/\alpha}$ for $\alpha = p$, a positive integer, was studied in [139]. The graph invariant ${}^0R_\alpha$ was studied for any real number $\alpha \geq 1$ in [130]. The invariant $\sum_{v \in V(G)} f(d_v)$ (a generalization of ${}^0R_\alpha$) was considered in [83]. Mathematical properties of ${}^0R_\alpha$ for $0 < \alpha < 1$ were explored in [99]. An extremal problem concerning ${}^0R_\alpha$, for $\alpha = -k, -\frac{1}{k}, \frac{1}{k}, k$, where $k \geq 2$ is a positive integer, was studied in [94]. The invariant ${}^0R_\alpha$, for $\alpha = 2\lambda$, where λ is real number, was considered in [116] under the name variable first Zagreb index.

Based on (2), the general sum–connectivity index, X_α was defined as [166]

$$X_\alpha = X_\alpha(G) = \sum_{i \sim j} (d_i + d_j)^\alpha \,.$$

Particulary interesting for us is the case $\alpha = -\frac{1}{2}$, namely

$$X_{-1/2} = SCI = SCI(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}}$$

defined in [165], and referred to as the (ordinary) sum–connectivity index.

Generalization of the second Zagreb index, reported in the [12], known as general Randić index, R_α is defined as

$$R_\alpha = R_\alpha(G) = \sum_{i\sim j} (d_i\, d_j)^\alpha$$

where α is a real number. It is also referred to as variable second Zagreb index, denoted as ${}^\lambda M_2$ (see [116]). Some well known special cases are R_{-1} (general Randić index R_{-1}, [133], also referred to as modified second Zagreb index, denoted as M_2^* [123]), $R = R_{-\frac{1}{2}}$ (ordinary Randić index [133]), $RR = R_{1/2}$ (reciprocal Randić index, [62]), and so on.

Multiplicative versions of topological indices were proposed in 2010 [141], whereas the first and second multiplicative Zagreb indices, denoted by Π_1 and Π_2, respectively, were first considered in a paper [56] published in 2011, and were promptly followed by numerous additional studies. These indices are defined as:

$$\Pi_1 = \Pi_1(G) = \prod_{i=1}^{n} d_i^2 \qquad \text{and} \qquad \Pi_2 = \Pi_2(G) = \prod_{i\sim j} d_i\, d_j\,.$$

One year later, the multiplicative sum Zagreb index, Π_1^* , was introduced [41], defined as

$$\Pi_1^* = \Pi_1^*(G) = \prod_{i\sim j} (d_i + d_j)\,.$$

It can be easily observed that Π_1^* can be also expressed as

$$\Pi_1^* = \prod_{i=1}^{m} \left[d(e_i) + 2 \right]$$

meaning that Π_1^* can be considered as an edge-degree based topological index as well.

Another vertex–degree–based topological index, $NK = NK(G)$, known as the Narumi–Katayama index, is defined as [120]

$$NK = NK(G) = \det D = \prod_{i=1}^{n} d_i\,.$$

It can be easily seen that $\Pi_1 = NK^2$.

The atom-bond connectivity index, ABC, is defined as [44]

$$ABC = ABC(G) = \sum_{i\sim j} \sqrt{\frac{d_i - d_j - 2}{d_i\, d_j}}\,.$$

The (first) geometric–arithmetic index of a graph is defined as [148]

$$GA = GA_1 = GA_1(G) = \sum_{i\sim j} \frac{2\sqrt{d_i\, d_j}}{d_i + d_j}\,.$$

As an irregularity measure of a graph, the Albetson index was introduced in [2]

$$A = A(G) = \sum_{i\sim j} |d_i - d_j| \,. \tag{4}$$

The inverse indeg index is defined as [149]

$$ISI = ISI(G) = \sum_{i\sim j} \frac{d_i\, d_j}{d_i + d_j} \,. \tag{5}$$

The harmonic index is defined [45] as

$$H = H(G) = \sum_{i\sim j} \frac{2}{d_i + d_j} \,. \tag{6}$$

Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ be the Laplacian eigenvalues values of the graph G. Then the Kirchhoff index, Kf, is defined as [66,168]

$$Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} \,.$$

By $\alpha(n)$ we will denote the expression

$$\alpha(n) = \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor\right) = \frac{1}{4} \left(1 - \frac{(-1)^{n+1} + 1}{2n^2}\right).$$

Before we proceed, let us define one special class of d-regular graphs Γ_d (see [124]). Let $N(i)$ be a set of all neighbors of the vertex i, i.e., $N(i) = \{k \mid k \in V,\, k \sim i\}$, and $d(i,j)$ the distance between vertices i and j. Denote by Γ_d a set of d-regular graphs, $1 \leq d \leq n-1$, with diameter 2, and $|N(i) \cap N(j)| = d$ for $i \nsim j$

For the sake of notation uniformity, throughout this survey, we use ${}^0R_\alpha$ for any specific value of α.

Needless to say, there exist many papers in the literature, dealing with the

- chemical applicability of ${}^0R_\alpha$ (for some particular values of α),
- mathematical properties of ${}^0R_\alpha$, other than bounds and extremal results.

However, here, we focus only on the bounds and extremal results, for the sake of brevity.

The survey is organized as follows. The next section is devoted to results pertaining to general inequalities for ${}^0R_\alpha$, where α is an arbitrary real number (or integer). In this section, we also outline relations between ${}^0R_\alpha$ and other topological indices as well as bounds and extremal values for ${}^0R_\alpha$. Sections 3 to 6 are devoted to the results obtained for some specific values of α. Section 3 gives a survey of the results for the modified Zagreb index, ${}^0R_{-2}$, Section 4 for the inverse–degree index, ${}^0R_{-1}$, Section 5 for the zeroth–order Randić index, ${}^0R_{-\frac{1}{2}}$, and, finally, Section 6 results for the forgotten topological index, ${}^0R_3$. From Section 3 to Section 6, each section contains two subsections, namely "Bounds" and "Extremal results".

Throughout this survey, whenever the condition on α is not mentioned, it is assumed that α is any real number.

2 Some general results for the invariant ${}^0R_\alpha$

2.1 General inequalities for ${}^0R_\alpha$

In 1992, Székely [139] established an upper bound on ${}^0R_\alpha$ in terms of ${}^0R_{1/\alpha}$, when α is a positive integer.

Theorem 1. [139] *If α is a positive integer and G is any graph, then*

$$ {}^0R_\alpha(G) \leq \frac{1}{c}\left({}^0R_{1/\alpha}(G)\right)^\alpha $$

holds for $c = 1$ whereas the inequality is not always true for $c > 1$. The equality sign in the above inequality holds if and only if $\alpha = 1$ or G has size zero.

Caro and Yuster [20] derived an upper bound on ${}^0R_\alpha$ under certain conditions, as stated in the following theorem.

Theorem 2. [20] *Let $\alpha \geq 2$ be an integer, let $\frac{1}{2} < s \leq 1$ and let $t > s$ be a real number. If G is an n-vertex graph with maximal degree $\leq sn$ and size $\leq tn$, then*

$$ {}^0R_\alpha(G) \leq \frac{t}{s}(sn)^\alpha + o(n^\alpha)\,. $$

Denote by $B_{n,t}$ the n-vertex graph with exactly t vertices of degree $n-1$ and the remaining of $n-t$ vertices forming an independent set.

Theorem 3. [28] *If G is a connected n-vertex graph with size m, minimal degree δ, maximal degree Δ, and α is a positive real number, then*

$$ {}^0R_{\alpha+1}(G) \leq \frac{2m}{n}\left[{}^0R_\alpha(G) + (n-1)(\Delta^\alpha - \delta^\alpha)\right] - \frac{\Delta^\alpha - \delta^\alpha}{n}\,{}^0R_2(G) \tag{7} $$

with equality if and only if $G \cong B_{n,t}$ for some $1 \leq t \leq n$ or G is regular.

Inequality (7) can be improved when G is a certain type of triangle–free graph and α is an integer greater than 1 (see Theorem 5).

Theorem 4. [28] *If G is a connected n-vertex graph with size m and α is a positive real number, then*

$$ {}^0R_{\alpha+1}(G) \geq \frac{2m}{n}\, {}^0R_\alpha(G) \tag{8} $$

with equality if and only if G is regular.

Let $p = (p_i)$ be a sequence of real numbers, and $a = (a_i)$ and $b = (b_i)$ sequences of non-negative real numbers of similar monotonicity. Then by the Chebyshev inequality (see for example [117]),

$$ \sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i\, a_i\, b_i \geq \sum_{i=1}^{n} p_i\, a_i \sum_{i=1}^{n} p_i\, b_i\,. $$

For $p_i = \frac{1}{d_i}$, $a_i = d_i^{\alpha+1}$, $b_i = d_i$, $\alpha \geq -1$, we get

$$ {}^0R_{\alpha+1}(G) \geq \frac{n\, {}^0R_\alpha(G)}{{}^0R_{-1}(G)}\,. \tag{9} $$

For $p_i = 1$, $a_i = d_i^\alpha$, $b_i = d_i$, $\alpha \geq 0$, the inequality (8) is obtained.

For $p_i = d_i$, $a_i = d_i^{\alpha-1}$, $b_i = d_i$, $\alpha \geq 1$, we obtain

$$ {}^0R_{\alpha+1}(G) \geq \frac{{}^0R_2(G)\, {}^0R_\alpha(G)}{2m}\,. \tag{10} $$

This inequality is stronger than (8) for $\alpha \geq 1$.

For $p_i = d_i^2$, $a_i = d_i^{\alpha-2}$, $b_i = d_i$, $\alpha \geq 2$, we get

$$ {}^0R_{\alpha+1}(G) \geq \frac{{}^0R_3(G)\, {}^0R_\alpha(G)}{{}^0R_2(G)} \tag{11} $$

which is stronger than (8) for $\alpha \geq 2$.

Let $\mathfrak{F}$ be the class of triangle–free graphs G with the property that G contains a vertex u such that $d_v = \Delta$ for all $v \in N(u)$ and $d_v = \delta$ for $v \in V(G) \setminus N[u]$, where $N[u] = N(u) \cup \{u\}$ and $N(u)$ is the neighborhood of u. The bounds, given in the following theorem, are improved versions of inequality (7) under some certain conditions.

Theorem 5. [19] *Let $\alpha \geq 2$ be an integer. Let G be a connected non-regular triangle–free n-vertex graph with minimal degree δ, maximal degree Δ, size m and $n \geq 2\Delta + 1$. Then*

$$ {}^0R_{\alpha+1}(G) \leq \frac{2m}{n}\left[{}^0R_\alpha(G) + (n-1)(\Delta^\alpha - \delta^\alpha) - \frac{1}{2}\left[(\delta+1)^\alpha - \delta^\alpha\right]\right] - \frac{\Delta^\alpha - \delta^\alpha}{n}\, {}^0R_2(G)\,. $$

In addition to the above assumptions, if $G \notin \mathfrak{F}$ then the bound can be strengthened to

$$ {}^0R_{\alpha+1}(G) \le \frac{2m}{n} \left[{}^0R_\alpha(G) + (n-1)(\Delta^\alpha - \delta^\alpha) - [(\delta+1)^\alpha - \delta^\alpha] \right] - \frac{\Delta^\alpha - \delta^\alpha}{n} \, {}^0R_2(G) \, . $$

Theorem 6. [101] *If G is any (n,m)-graph without isolated vertices, then*

$$ {}^0R_{-\alpha}(G) \cdot {}^0R_\alpha(G) \ge n^2 $$

for any real α.

The lower bound given in Theorem 134 is a special case of the inequality, stated in Theorem 6. In Theorem 7, we will see that the inequality given in Theorem 6 can be strengthened.

Recently, making the use of the generalization of the Szőkefalvi Nagy's inequality, some inequalities involving ${}^0R_\alpha$ were obtained in [60].

Theorem 7. [60] *If G is an n-vertex graph with minimal degree δ, maximal degree Δ and no isolated vertices, then the following inequalities hold for any real number α:*

$$ \begin{aligned} {}^0R_\alpha(G) \cdot {}^0R_{\alpha-2}(G) &\ge \left[{}^0R_{\alpha-1}(G) \right]^2 + \frac{(\Delta\delta)^{\alpha-2} \, (\Delta - \delta)^2}{\Delta^{\alpha-2} + \delta^{\alpha-2}} \cdot {}^0R_{\alpha-2}(G) \\ {}^0R_\alpha(G) \cdot {}^0R_{\alpha-2}(G) &\ge \left[{}^0R_{\alpha-1}(G) \right]^2 + \frac{(\Delta\delta)^{\alpha-2} \, (\Delta - \delta)^2}{\Delta^\alpha + \delta^\alpha} \cdot {}^0R_\alpha(G) \\ {}^0R_\alpha(G) \cdot {}^0R_{-\alpha}(G) &\ge n^2 + \frac{(\Delta^\alpha - \delta^\alpha)^2}{(\Delta\,\delta)^\alpha \, (\Delta^\alpha + \delta^\alpha)} \cdot {}^0R_\alpha(G) \, . \end{aligned} $$

The equality sign in any of the above equality holds if and only if G is regular.

The third inequality of Theorem 7 is stronger than the one, given in Theorem 6. Recently, two of the present authors *et al.* [112] derived several inequalities involving ${}^0R_\alpha$.

Theorem 8. [112] *If G is an n-vertex graph, $n \ge 3$, with minimal degree δ, maximal degree Δ and no isolated vertices, then the following inequalities hold for any real number α:*

$$ {}^0R_{\alpha+1}(G) \le (\Delta + \delta) \cdot {}^0R_\alpha(G) - \Delta\delta \cdot {}^0R_{\alpha-1}(G) \tag{12} $$

$$ {}^0R_{\alpha+1}(G) \le \frac{1}{4} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2 \frac{\left[{}^0R_\alpha(G) \right]^2}{{}^0R_{\alpha-1}(G)} \, . \tag{13} $$

The equality sign in (12) holds if and only if G is regular or biregular, while the equality sign in (13) holds if and only if G is regular.

The inequality (13) is stronger than (7) if $G \cong P_n$, $G \cong K_{\frac{n}{2},\frac{n}{2}}$ (n is even), or G is a bidegreed graph.

In 2004, Miličević and Nikolić [116] considered the invariant ${}^0R_\alpha$ for all real values of α (in their definition, they used the real exponent 2λ which also, obviously, covers all real numbers) and named it as variable first Zagreb index. The variable first Zagreb index (${}^\lambda M_1$) and variable second Zagreb index (${}^\lambda M_2$) of a graph G are defined [116] as

$$ {}^\lambda M_1(G) = \sum_{v \in V(G)} (d_v)^{2\lambda} \qquad \text{and} \qquad {}^\lambda M_2(G) = \sum_{u \sim v} (d_u\, d_v)^\lambda $$

where λ is any real number. Clearly, ${}^0R_{2\lambda} = {}^\lambda M_1$ and ${}^\lambda M_2 = R_\lambda$, where R_λ is the general Randić index introduced by Bollobás and Erdős [12].

For an (n,m)-graph G, the following inequality (known as the generalized Zagreb indices inequality) was firstly analyzed in [145]:

$$ \frac{{}^\lambda M_1(G)}{n} \le \frac{{}^\lambda M_2(G)}{m} \tag{14} $$

which is equivalent to say that the invariant ${}^0R_\alpha$ is bounded above by $\frac{n}{m}\left(R_{\alpha/2}\right)$, i.e.,

$$ {}^0R_\alpha(G) \le \frac{n}{m}\, R_{\alpha/2}(G)\,. \tag{15} $$

Background of inequality (14) can be found in the survey [102] and related references listed therein. Inequality (15) (and hence (14)) does not hold in the general case. Several authors have reported conditions under which the inequality (15) is valid. In what follows, we summarize these conditions.

Theorem 9. [145] *If $0 \le \alpha \le 2$ and G is an (n,m)-molecular graph, then inequality (15) holds.*

Theorem 10. [7,145] *If $0 \le \alpha \le 1$ and G is an (n,m)-graph, then inequality (15) holds.*

Theorem 11. [11] *If $1 < \alpha \le \sqrt{2}$ and G is an (n,m)-graph, then inequality (15) holds.*

Theorem 12. [103] *Let G be an (n,m)-graph with minimal degree δ and maximal degree Δ. Let G satisfy at least one of the following conditions:*

1. $\Delta - \delta \le 2$.

2. $\Delta - \delta \le 3$ and $\delta \ne 2$.

If $0 \le \alpha \le 2$, then inequality (15) holds.

Theorem 13. [146] *If G is an n-vertex tree, then inequality (15) holds if and only if $0 \leq \alpha \leq 2$.*

Theorem 14. [73] *If $0 \leq \alpha \leq 2$ and G is a connected unicyclic n-vertex graph, then inequality (15) holds. For $0 < \alpha \leq 2$ the equality sign in (15) holds if and only if $G \cong C_n$.*

The following opposite inequality of (14) was also studied in several papers:

$$\frac{{}^{\lambda}M_1(G)}{n} \geq \frac{{}^{\lambda}M_2(G)}{m}$$

which is equivalent to

$$ {}^{0}R_\alpha(G) \geq \frac{n}{m} \cdot R_{\alpha/2}(G)\,. \tag{16}$$

Now, we collect the results concerning inequality (16).

Theorem 15. [145] *Let G be an unbalanced complete bipartite n-vertex graph with size m. If $\alpha < 0$ or $\alpha > 1$, then inequality (16) holds.*

Theorem 16. [160] *If G is a connected unicyclic n-vertex graph, then inequality (16) holds for $\alpha \leq 0$. Moreover, if $\alpha < 0$, then the equality sign in (16) holds if and only if $G \cong C_n$.*

Theorem 17. [80] *If $\alpha < 0$ and G is an (n,m)-graph, then inequality (16) holds, with equality if and only if G is regular.*

Theorem 18. [103] *Let G be an (n,m)-graph with minimal degree δ and maximal degree Δ. Let G satisfy at least one of the following conditions:*

1. $\Delta - \delta \leq 2$.

2. $\Delta - \delta \leq 3$ and $\delta \neq 2$.

If $\alpha < 0$, then inequality (16) holds, with equality if and only if G is regular.

Clearly, every (n,m)-molecular graph satisfies at least one of the conditions, stated in Theorem 18, which implies the next result.

Corollary 19. [103] *Let G be an (n,m)-molecular graph. If $\alpha < 0$, then inequality (16) holds, with equality if and only if G is regular.*

Recently, Rodríguez *et al.* [134] established several general inequalities involving the invariant ${}^{0}R_\alpha$.

Theorem 20. [134] *If G is a non-trivial n-vertex graph with maximal degree Δ and minimal degree δ, and α, β are real numbers, then*

$$\begin{aligned} {}^0R_\alpha(G) &\leq \delta^{\alpha-\beta} \cdot {}^0R_\beta(G) \quad \text{if } \alpha \leq \beta \\ {}^0R_\alpha(G) &\leq \Delta^{\alpha-\beta} \cdot {}^0R_\beta(G) \quad \text{if } \alpha \geq \beta \\ {}^0R_\alpha(G) &\geq \frac{\Delta^{\alpha+\beta}\, n^2}{{}^0R_\beta(G)} \quad \text{if } \alpha \leq -\beta \\ {}^0R_\alpha(G) &\geq \frac{\delta^{\alpha+\beta}\, n^2}{{}^0R_\beta(G)} \quad \text{if } \alpha \geq -\beta\,. \end{aligned}$$

The equality is attained in the lower bound with $(\alpha, \beta) \neq (0,0)$ if and only if G is regular. If $\alpha = \beta = 0$, then the lower bound is attained for every graph. The equality holds in the upper bound for some $\alpha \neq \beta$ if and only if G is regular. If $\alpha = \beta$, then the upper bound is attained for every graph.

Theorem 21. [134] *If G is a non-trivial n-vertex graph, α is a real number, and $s > 0$, then*

$$s^2 \cdot {}^0R_\alpha(G) + {}^0R_{-\alpha}(G) \geq 2ns\,.$$

Theorem 22. [134] *If G is a non-trivial n-vertex graph, α is a real number, and $\beta > 0$, then*

$${}^0R_{\alpha\beta}(G) \cdot {}^0R_{-\alpha\beta}(G) \geq n^{\beta+1}$$

with equality for $\alpha \neq 0$, if and only if G is regular.

Theorem 23. [134] *If G is a non-trivial graph with maximal degree Δ and $\alpha \geq 1 \geq \beta > 0$, then*

$$\left[{}^0R_\alpha(G)\right]^{1/\alpha} \leq \Delta^{1-\beta} \cdot {}^0R_\beta(G)\,.$$

Theorem 24. [134] *If G is a non-trivial n-vertex graph with maximal degree Δ and minimal degree δ, and α is a real number, then*

$$\frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha + \delta^\alpha} \sqrt{n\ {}^0R_{2\alpha}(G)} \leq {}^0R_\alpha(G) \leq \sqrt{n\ {}^0R_{2\alpha}(G)}\,.$$

The lower bound is attained if G is regular. The upper bound is attained, for $\alpha \neq 0$, if and only if G is regular.

Theorem 25. [134] *If G is a non-trivial n-vertex graph with maximal degree Δ and minimal degree δ, and α is a real number, then*

$$^{0}R_{\alpha}(G) + (\Delta\,\delta)^{\alpha} \cdot {}^{0}R_{-\alpha}(G) \leq n(\Delta^{\alpha} + \delta^{\alpha})$$

with equality, for $\alpha \neq 0$, if and only if $d_u \in \{\delta, \Delta\}$ for every $u \in V(G)$.

Theorem 26. [134] *If G is a non-trivial n-vertex graph and α, β are real numbers with $\alpha > 0$, then*

$$n + \alpha \cdot {}^{0}R_{\beta}(G) \begin{cases} \leq \left(\left({}^{0}R_{\alpha\beta}(G)\right)^{1/\alpha} + n^{1/\alpha} \right)^{\alpha} & \text{if } \alpha \geq 1 \\ \geq \left(\left({}^{0}R_{\alpha\beta}(G)\right)^{1/\alpha} + n^{1/\alpha} \right)^{\alpha} & \text{if } 0 < \alpha < 1\,. \end{cases}$$

Theorem 27. [134] *If G is a non-trivial n-vertex graph and α, β are real numbers with $\beta > 0$, then*

$$^{0}R_{\alpha+\beta}(G) \begin{cases} \geq \frac{1}{n}\ {}^{0}R_{\alpha}(G) \cdot {}^{0}R_{\beta}(G) & \text{if } \alpha \geq 0 \\ \leq \frac{1}{n}\ {}^{0}R_{\alpha}(G) \cdot {}^{0}R_{\beta}(G) & \text{if } \alpha \leq 0\,. \end{cases}$$

The equality sign in any of the above inequalities holds, for $\alpha \neq 0$, if and only if G is regular.

2.2 Relations between $^{0}R_{\alpha}$ and other topological indices

For a positive integer χ, let $f(\chi)$ be the minimal order of a triangle–free graph having chromatic number χ and put $f(0) = 0$.

Theorem 28. [19] *If $\alpha \geq 2$ is an integer, then for every triangle–free n-vertex graph G with m edges and chromatic number χ, the following inequality holds*

$$^{0}R_{\alpha}(G) \leq m\,[n - f\,(\chi - 2)]\,[n - f\,(\chi - 2) - \delta]^{\alpha-2}\,.$$

In 2004, Lu *et al.* [107] derived some inequalities, stated in the next four theorems, related to the invariant $^{0}R_{\alpha}$.

Theorem 29. [107] *If G is a connected n-vertex graph without isolated vertices, then*

$$2R_{\alpha}(G) + \left({}^{0}R_{2\alpha}(G) - \frac{\left[{}^{0}R_{\alpha}(G)\right]^2}{n} \right) \mu_{n-1} \leq {}^{0}R_{2\alpha+1}(G)$$

$$\leq 2R_{\alpha}(G) + \left({}^{0}R_{2\alpha}(G) - \frac{\left[{}^{0}R_{\alpha}(G)\right]^2}{n} \right) \mu_1$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ *are the eigenvalues of the Laplacian matrix of* G. *Also,* $2R_\alpha(G) = {}^0R_{2\alpha+1}(G)$ *and* $n \cdot {}^0R_{2\alpha}(G) - [{}^0R_\alpha(G)]^2 = 0$ *if and only if* G *is regular.*

Theorem 30. [107] *If* $\alpha \neq 0$ *and* G *is a connected* n*-vertex graph without isolated vertices, then*

$$^0R_{2\alpha+1}(G) \geq 2R_\alpha(G)$$

with equality if and only if G *is regular.*

Theorem 31. [107] *If* $\alpha \neq 0$ *and* G *is a non-regular* n*-vertex graph without isolated vertices, then*

$$^0R_{2\alpha+1}(G) \leq 2R_\alpha(G) - \left[{}^0R_\alpha(G)\right]^2 + n \cdot {}^0R_{2\alpha}(G)$$

with equality if $G \cong S_n$.

Theorem 32. [107] *Let* G *be an* n*-vertex graph without isolated vertices and* $\rho(G)$ *be the largest eigenvalue of the adjacency matrix of* G. *Then*

$$\frac{1}{2}\, {}^0R_{2\alpha}(G) \cdot \rho(G) \geq R_\alpha(G)$$

with equality if and only if G *is regular.*

Liu and one of the present authors [100] established several bounds on the invariant $^0R_\alpha$.

Theorem 33. [100] *Let* G *be an* (n, m)*-graph with minimal degree* δ, *maximal degree* Δ *and no isolated vertices.*
i) *If* α *is any real number, then*

$$^0R_\alpha(G) \geq 2R_{(\alpha-1)/2}(G)$$

with equality if and only if every component of G *is regular or* $\alpha = 1$.
ii) *If* α *is any positive integer, then*

$$^0R_\alpha(G) \leq m(m+1)^{\alpha-1}\,.$$

If G *is connected, then the equality sign in the above inequality holds if and only if* $\alpha = 2$ *and* $G \cong S_n$.
iii) *If* G *is connected, then*

$$^0R_3(G) \leq m(m+1)^2 - 2M_2(G)$$

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

iv) *If* $\alpha \geq 2$ *is any real number, then*

$$^0R_\alpha(G) \leq 2m\delta^{\alpha-1} + (2m - n\delta)\sum_{j=0}^{\alpha-2} \Delta^{\alpha-j-1}\delta^j$$

with equality if G *is regular or biregular.*

v) *If* α *is any positive real number, then*

$$\begin{aligned} & \left[{}^0R_\alpha(G)\right]^2 - (n-1)\Delta^\alpha \cdot {}^0R_\alpha(G) + \Delta^\alpha \cdot {}^0R_{\alpha+1}(G) - 2R_\alpha(G) \leq {}^0R_{2\alpha}(G) \\ \leq \; & \left[{}^0R_\alpha(G)\right]^2 - (n-1)\delta^\alpha \cdot {}^0R_\alpha(G) + \delta^\alpha \cdot {}^0R_{\alpha+1}(G) - 2R_\alpha(G)\,. \end{aligned}$$

The inequality stated in Theorem 33(i) was also derived in [107, 167]. The equality case mentioned in Theorem 33(i) is due to Zhou and Vukičević [167].

Theorem 34. [167] *Let* G *be an* n*-vertex graph without isolated vertices and with clique number* ω. *If* G *has at least one edge, then*

$$\frac{2\omega}{\omega-1} \cdot R_\alpha(G) \leq \left[{}^0R_\alpha(G)\right]^2 \leq 2R_\alpha(G) + n \cdot {}^0R_{2\alpha}(G) - {}^0R_{2\alpha+1}(G)$$

with right equality if and only if $\alpha = 0$ *or every pair of non-adjacent vertices of* G *has the same degree. The left equality holds if and only if one of the following conditions holds:*

i) $\alpha = 1$ *and* G *is either a complete bipartite graph for* $\omega = 2$ *or a regular complete* ω*-partite graph for* $\omega \geq 3$.

ii) $\alpha < 1$ *and* G *is regular complete* ω*-partite graph.*

iii) $\alpha > 1$ *and* G *is either a regular complete* ω*-partite graph or*

$$G \cong K_{\underbrace{n_1,\ldots,n_1}_{a-times},\underbrace{n_2,\ldots,n_2}_{b-times}}$$

where $n_1 \neq n_2$, $a + b = \omega$, $n_1\left[(a-1)n_1 + bn_2\right]^\alpha = n_2\left[an_1 + (b-1)n_2\right]^\alpha$.

The right inequality, given in Theorem 34, was also derived in [107]. However, most of the graphs that attain equality were not mentioned there. Also, the left inequality, stated in Theorem 34, was independently established in [42].

Theorem 35. [105] *If* G *is a connected non-trivial* n*-vertex graph, then*

$$^0R_\alpha(G) \begin{cases} > \displaystyle\sum_{i=1}^{n-1}(\mu_i)^\alpha & \text{for } 0 < \alpha < 1 \\ < \displaystyle\sum_{i=1}^{n-1}(\mu_i)^\alpha & \text{for } \alpha < 0 \text{ or } \alpha > 1 \end{cases}$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ *are the eigenvalues of the Laplacian matrix of* G.

Das and Dehmer [34] proved that ${}^0R_\alpha$ is bounded above by X_α, when α is a real number greater than 1.

Theorem 36. [34] *If* G *is an* n*-vertex graph and* $\alpha \geq 1$, *then*

$$ {}^0R_\alpha(G) \leq X_\alpha(G) $$

with equality if and only if $G \cong nK_1$ *or* $G \cong tK_2 \cup (n-2t)K_1$ $(t \leq \frac{n}{2})$ *with* $\alpha = 1$.

Theorem 37. [112] *If* α *is a non-negative integer and* G *is an* (n, m)*-graph,* $n \geq 3$, *with minimal degree* δ, *maximal degree* Δ, *and no isolated vertices, then*

$$ {}^0R_{\alpha+1}(G) \leq (\Delta-\delta)^{-1}\left[2m(\Delta^{\alpha+1}-\delta^{\alpha+1}) - n\Delta\delta(\Delta^\alpha - \delta^\alpha)\right] \tag{17} $$

$$ {}^0R_{\alpha+1}(G) \leq (\Delta-\delta)^{-1}\left[{}^0R_2(G)(\Delta^\alpha-\delta^\alpha) - 2m\Delta\delta(\Delta^{\alpha-1} - \delta^{\alpha-1})\right]. \tag{18} $$

The equality sign in any of the inequalities (17), (18) holds if and only if G *is regular or biregular. Moreover, equality sign in (17) holds if* $\alpha = 0$, *and in (18) if* $\alpha = 1$.

The inequalities given in the next theorem are due Elphick and Réti [42], who independently obtained these inequalities within the study of variable first Zagreb index. The first inequality of this result (Theorem 38) had already been proved in [167], within the study of general zeroth–order Randić index.

Theorem 38. [42] *If* G *is any graph with clique number* ω, *then*

$$ \frac{1}{2\omega}\left[{}^0R_\alpha(G)\right]^2(\omega-1) \geq R_\alpha(G). $$

Also, if G *is a triangle–free graph, then*

$$ \frac{1}{4}\left[{}^0R_\alpha(G)\right]^2 \geq R_\alpha(G). $$

It is assumed that G *does not contain isolated vertices when* $\alpha < 0$.

Let

$$ \alpha(n) = \frac{1}{4}\left(1 - \frac{(-1)^{n+1}+1}{2n^2}\right). $$

In [65] the following relationships between ${}^0R_\alpha$ and Π_1 were reported.

Theorem 39. *Let G be a simple connected graph with $n \geq 2$ vertices. Then, for any real $\alpha \geq 0$*

$$\left(\Delta^{\alpha/2} - \delta^{\alpha/2}\right)^2 \leq {}^0R_\alpha(G) - n\,(\Pi_1(G))^{\alpha/2n} \leq n^2\,\alpha(n)\left(\Delta^{\alpha/2} - \delta^{\alpha/2}\right)^2 .$$

If $\alpha < 0$, then

$$\left(\delta^{\alpha/2} - \Delta^{\alpha/2}\right)^2 \leq {}^0R_\alpha(G) - n\,(\Pi_1(G))^{\alpha/2n} \leq n^2\,\alpha(n)\left(\delta^{\alpha/2} - \Delta^{\alpha/2}\right)^2 .$$

Equalities on the right–hand sides hold if and only if G is regular. Equalities on the left–hand sides hold if and only if $d_2 = \cdots = d_{n-1} = \sqrt{\Delta\,\delta}$.

Theorem 40. *Let G be a simple connected graph with n vertices. If $n \geq 3$ and $\alpha \geq 0$, then*

$$\begin{aligned}\Delta^\alpha + \left(\Delta_2^{\alpha/2} - \delta^{\alpha/2}\right)^2 &\leq {}^0R_\alpha(G) - (n-1)\left(\frac{\Pi_1(G)}{\Delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \Delta^\alpha + (n-1)^2\,\alpha(n-1)\left(\Delta_2^{\alpha/2} - \delta^{\alpha/2}\right)^2 .\end{aligned}$$

If $n \geq 3$ and $\alpha \leq 0$, then

$$\begin{aligned}\Delta^\alpha + \left(\delta^{\alpha/2} - \Delta_2^{\alpha/2}\right)^2 &\leq {}^0R_\alpha(G) - (n-1)\left(\frac{\Pi_1(G)}{\Delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \Delta^\alpha + (n-1)^2\,\alpha(n-1)\left(\delta^{\alpha/2} - \Delta_2^{\alpha/2}\right)^2 .\end{aligned}$$

Equalities on the right–hand sides hold if and only if $\Delta_2 = d_2 = \cdots = d_n = \delta$. Equalities on the left–hand sides hold if and only if $d_3 = \cdots = d_{n-1} = \sqrt{\Delta_2 \delta}$

Theorem 41. *Let G be a simple connected graph with n vertices. If $n \geq 3$ and $\alpha \geq 0$, then*

$$\begin{aligned}\delta^\alpha + \left(\Delta^{\alpha/2} - \delta_2^{\alpha/2}\right)^2 &\leq {}^0R_\alpha(G) - \left(\frac{\Pi_1(G)}{\delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \delta^\alpha + (n-1)^2\,\alpha(n-1)\left(\Delta^{\alpha/2} - \delta_2^{\alpha/2}\right)^2 .\end{aligned}$$

If $n \geq 3$ and $\alpha \leq 0$, then

$$\begin{aligned}\delta^\alpha + \left(\delta_2^{\alpha/2} - \Delta^{\alpha/2}\right)^2 &\leq {}^0R_\alpha - \left(\frac{\Pi_1}{\delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \delta^\alpha + (n-1)^2\,\alpha(n-1)\left(\delta_2^{\alpha/2} - \Delta^{\alpha/2}\right)^2 .\end{aligned}$$

Equalities on the right–hand side of the above inequalities hold if and only if $\Delta = d_1 = \cdots = d_{n-1} = \delta_1$, and on the left–hand side if and only if $\Delta_2 = d_2 = \cdots = d_{n-2} = \sqrt{\Delta\,\delta_2}$.

Theorem 42. *Let G be a simple connected graph with n vertices. If $n \geq 4$ and $\alpha \geq 0$, then*

$$\begin{aligned}\Delta^\alpha + \delta^\alpha + \left(\Delta_2^{\alpha/2} - \delta_2^{\alpha/2}\right)^2 &\leq {}^0R_\alpha - \left(\frac{\Pi_1}{\Delta^2\,\delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \Delta^\alpha + \delta^\alpha + (n-2)^2\,\alpha(n-2)\left(\Delta_2^{\alpha/2} - \delta_2^{\alpha/2}\right)^2 .\end{aligned}$$

If $n \geq 4$ and $\alpha \leq 0$, then

$$\begin{aligned}\Delta^\alpha + \delta^\alpha + \left(\delta_2^{\alpha/2} - \Delta_2^{\alpha/2}\right)^2 &\leq {}^0R_\alpha - \left(\frac{\Pi_1}{\Delta^2\,\delta^2}\right)^{\frac{\alpha}{2(n-1)}} \\ &\leq \Delta^\alpha + \delta^\alpha + (n-2)^2\,\alpha(n-2)\left(\delta_2^{\alpha/2} - \Delta_2^{\alpha/2}\right)^2 .\end{aligned}$$

Equalities on the left–hand sides of the above inequalities hold if and only if $\Delta_2 = d_2 = \cdots = d_{n-1} = \delta_2$, and on the right–hand sides if and only if $d_3 = \cdots = d_{n-2} = \sqrt{\Delta_2\,\delta_2}$.

In [111] the following auxiliary result was proved.

Theorem 43. [111] *Let G be a simple connected graph with $m \geq 1$ edges. Then, for any $\alpha \geq 1$ or $\alpha \leq 0$*

$$ {}^0R_{\alpha+1}(G) \geq \frac{({}^0R_2(G))^\alpha}{(2m)^{\alpha-1}} $$

with equality if G is regular, or $\alpha = 0$, or $\alpha = 1$.

Recently, Rodríguez *et al.* [134] found inequalities between general Randić index, multiplicative second Zagreb index, and the invariant ${}^0R_\alpha$.

Theorem 44. [134] *If G is a non-trivial graph with maximal degree Δ and minimal degree δ, then*

$$2\Delta^{1-\alpha}\cdot R_{\alpha-1}(G) \leq {}^0R_\alpha(G) \leq 2\delta^{1-\alpha}\; R_{\alpha-1}(G) \quad \text{if} \quad \alpha \geq 1$$

$$2\delta^{1-\alpha}\cdot R_{\alpha-1}(G) \leq {}^0R_\alpha(G) \leq 2\Delta^{1-\alpha}\; R_{\alpha-1}(G) \quad \text{if} \quad \alpha \leq 1\,.$$

The equality sign in any of the above inequalities holds, for $\alpha \neq 1$, if and only if G is regular.

Theorem 45. [134] *If G is a non-trivial (n,m)-graph and α is a real number, then*

$$ {}^0R_\alpha(G) \geq 2m\,[\Pi_2(G)]^{\frac{\alpha-1}{2m}} $$

with equality, for $\alpha \neq 1$, if and only if G is regular.

2.3 Bounds

Theorem 46. [28] *If G is a connected n-vertex graph with m edges, then*

$$^0R_{1/2}(G) \geq \frac{1}{2}\left[\sqrt{8mn + \left(\sqrt{\Delta}-\sqrt{\delta}\right)^2\left(n-1-\frac{2m}{n}\right)^2} - \left(\sqrt{\Delta}-\sqrt{\delta}\right)\left(n-1-\frac{2m}{n}\right)\right]$$

with equality if and only if G is regular.

A family of graphs is said to be monotone if it is closed under taking subgraphs [49]. Füredi and Kündgen [49] established some asymptotically sharp bounds for $\frac{1}{n}\,{}^0R_\alpha(G)$ (which is known as the α-th moment of degree sequence of the n-vertex graph G), when G is in a monotone family and α is a non-negative integer.

Theorem 47. [71] *If α is a positive integer and G is a connected planar graph with $n \geq 4$ vertices, size m, and minimal degree δ, then*

$$^0R_\alpha(G) \leq 2(n-1)^\alpha + 4^\alpha(n-4) + 2\cdot 3^\alpha - 2[(\delta+1)^\alpha - \delta^\alpha](3n-m-6)\,.$$

Theorem 48. [71] *If α is a positive integer and G is a connected planar graph with minimal degree δ and maximal degree $\Delta \geq 6$, then*

$$^0R_\alpha(G) \leq \frac{(6-\delta)\Delta^\alpha + (\Delta-6)\delta^\alpha}{\Delta-\delta}\left(n-\frac{12}{6-\delta}\right) + \frac{12}{6-\delta}\,\delta^\alpha\,.$$

Theorem 49. [71] *If $\alpha \geq 2$ is an integer and G is a planar graph without isolated vertices and with maximal degree $\Delta \geq 7$, then*

$$\begin{aligned} {}^0R_\alpha(G) \;\; &\leq \;\; \left(\frac{2(\Delta^\alpha-1)}{\Delta-6} + 6^\alpha - \frac{2(6^\alpha-1)(\Delta-1)}{5(\Delta-6)}\right) n \\ &- \;\; \frac{16}{\Delta-6}\left(\Delta^\alpha - 1 - \frac{(6^\alpha-1)(\Delta-1)}{5}\right) - \frac{12(6^\alpha-1)}{5}\,. \end{aligned}$$

Bollobás and Nikiforov [15] strengthened the Erdős–Stone theorem by using ${}^0R_\alpha$ (letting α as a positive integer) instead of the number of edges, and obtained the upper bound on ${}^0R_\alpha$, stated in the following theorem.

Theorem 50. [15] *Let t, α be integers such that $t \geq 2$ and $1 \leq \alpha \leq t+1$. If G is a K_{t+1}–free n-vertex graph, then*

$$^0R_\alpha(G) \leq \left(1-\frac{1}{t}\right)^\alpha n^{\alpha+1}\,.$$

Xu *et al.* [154] proved the following theorem, which recovers Theorem 48 if one takes $p = 3$ and $q = 6$.

Theorem 51. [154] *Let α, p and q be positive integers. If G is an n-vertex graph with size $m \leq np - q$, minimal degree δ, and maximal degree $\Delta \geq 2p$, then*

$$ {}^0R_\alpha(G) \leq \frac{(2p-\delta)\Delta^\alpha + (\Delta - 2p)\delta^\alpha}{\Delta - \delta} \left(n - \frac{2q}{2p-\delta} \right) + \frac{2q}{2p-\delta}\,\delta^\alpha \,. $$

A graph is 1-planar if it can be drawn in the plane so that each edge is crossed by at most one other edge. In what follows, we state some consequences of Theorem 51.

Corollary 52. [154] *If α is a positive integer and G is any 1-planar graph with maximal degree $\Delta \geq 8$, then*

$$ {}^0R_\alpha(G) \leq \frac{(8-\delta)\Delta^\alpha + (\Delta - 8)\delta^\alpha}{\Delta - \delta} \left(n - \frac{16}{8-\delta} \right) + \frac{16}{8-\delta}\,\delta^\alpha \,. $$

A graph G is said to be t-degenerate if for every subgraph H of G, the minimal degree of H is at most t.

Corollary 53. [154] *If α is a positive integer, then for every t-degenerate graph G with maximal degree $\Delta \geq 2t$, the following inequality holds*

$$ {}^0R_\alpha(G) \leq \frac{(2t-\delta)\Delta^\alpha + (\Delta - 2t)\delta^\alpha}{\Delta - \delta} \left(n - \frac{t^2+t}{2t-\delta} \right) + \frac{t^2+t}{2t-\delta}\,\delta^\alpha \,. $$

A (simple) graph is series–parallel if it may be turned into K_2 by a sequence of the following operation: replacement of a pair of edges incident to a vertex of degree 2 with a single edge.

Corollary 54. [154] *If α is a positive integer and G is any series–parallel graph with minimal degree δ and maximal degree $\Delta \geq 3$, then*

$$ {}^0R_\alpha(G) \leq \frac{(4-\delta)\Delta^\alpha + (\Delta - 4)\delta^\alpha}{\Delta - \delta} \left(n - \frac{6}{4-\delta} \right) + \frac{6}{4-\delta}\,\delta^\alpha \,. $$

The next result is due to Czap *et al.* [29]. It gives a simple but elegant upper bound on ${}^0R_\alpha$(G), when G is a 1-planar graph and α is an integer greater than 1.

Theorem 55. [29] *If $\alpha \geq 2$ is an integer, then for every 1-planar n-vertex graph G,*

$$ {}^0R_\alpha(G) \leq 2(n-1)^\alpha + o(n) \,. $$

The bound is asymptotically tight.

Su *et al.* [138] generalized the results of Dankelmann *et al.* [30].

Theorem 56. [138] *Let G be a connected non-trivial n-vertex graph with minimal degree δ. If G is not a maximally edge-connected graph, then*

$$^0R_\alpha(G) \geq 2\delta^\alpha - \delta^{\alpha+1} + (\delta-1)(\delta+1)^\alpha + (\delta-1)(n-\delta-1)^\alpha + (2n-3\delta-2)(n-\delta-2)^\alpha$$

for all $\alpha \leq -1$.

Theorem 56 is a generalized version of Theorem 148.

Theorem 57. [138] *Let G be a connected triangle–free n-vertex graph, $n \geq 2$, with minimal degree δ. If G is not a maximally edge-connected graph, then*

$$^0R_\alpha(G) \geq \delta^\alpha - \delta^{\alpha+1} + (\delta-1)(\delta+1)^\alpha + \frac{(\delta-1)(n-2\delta+2)^\alpha}{2^\alpha} + \frac{(2n-5\delta+1)(n-2\delta)^\alpha}{2^\alpha}$$

for all $\alpha \leq -1$.

Theorem 57 is a generalized version of Theorem 150. Su *et al.* [137] extended the results of [138] to $0 < \alpha < 1$. The lower bounds mentioned in Theorem 56 and Theorem 57 become upper bounds when $0 < \alpha < 1$.

Theorem 58. [137] *Let G be a connected non-trivial n-vertex graph with minimal degree δ. If G is not a maximally edge-connected graph, then*

$$^0R_\alpha(G) \leq 2\delta^\alpha - \delta^{\alpha+1} + (\delta-1)(\delta+1)^\alpha + (\delta-1)(n-\delta-1)^\alpha + (2n-3\delta-2)(n-\delta-2)^\alpha$$

for $0 < \alpha < 1$.

Theorem 59. [137] *Let G be a connected triangle–free n-vertex graph, $n \geq 2$, with minimal degree δ. If G is not a maximally edge-connected graph, then*

$$^0R_\alpha(G) \leq \delta^\alpha - \delta^{\alpha+1} + (\delta-1)(\delta+1)^\alpha + \frac{(\delta-1)(n-2\delta+2)^\alpha}{2^\alpha} + \frac{(2n-5\delta+1)(n-2\delta)^\alpha}{2^\alpha}$$

for $0 < \alpha < 1$.

Volkmann [144] found several bounds on the invariant $^0R_\alpha$ for certain types of digraphs.

Theorem 60. [144] *Let D be a strongly connected diagraph with minimal degree δ and order $n \geq 3$. If D is not a maximally edge-connected diagraph, then*

$$
{}^0R_\alpha(D)\begin{cases}\geq 2\delta^\alpha - \delta^{\alpha+1} + 2(n-\delta-2)^{\alpha+1} - (\delta-2)(n-\delta-2)^\alpha + \Lambda & \text{for } \alpha \leq -1\\ \geq 2\delta^\alpha + \delta^{\alpha+1} - (\delta-2)(n-\delta-2)^\alpha + \Lambda & \text{for } -1 \leq \alpha < 0\\ \leq 2\delta^\alpha - (n-2\delta)(n-\delta-2)^\alpha + \Lambda & \text{for } 0 < \alpha < 1\\ \geq 3\delta^\alpha + \delta^{\alpha+1} - (\delta-1)(n-\delta-2)^\alpha + \Lambda & \text{for } 1 < \alpha \leq 2\end{cases}
$$

where $\Lambda = (\delta-1)(\delta+1)^\alpha + (\delta-1)(n-\delta-1)^\alpha$.

Corollary 61. [144] *Let G be a connected graph with minimal degree δ and order $n \geq 3$. If G is not a maximally edge-connected graph, then the bounds given in Theorem 60 for ${}^0R_\alpha(D)$ also hold for ${}^0R_\alpha(G)$.*

With regard to the third bound of Theorem 60, the bound concerning ${}^0R_\alpha(G)$ is an improvement of the bound given in Theorem 58. Corresponding to the first bound of Theorem 60, the bound concerning ${}^0R_\alpha(G)$ was also reported in [27].

Theorem 62. [144] *Let D be a strongly connected diagraph with minimal degree δ and order $n \geq 3$. If D is not a maximally edge-connected diagraph and either $-\frac{1}{3} \leq \alpha < 0$ or $-\frac{\delta-1}{\delta+1} \leq \alpha < 0$, then*

$$
{}^0R_\alpha(D) \geq 2\delta^\alpha - (n-2\delta)(n-\delta-2)^\alpha + \Lambda
$$

where $\Lambda = (\delta-1)(\delta+1)^\alpha + (\delta-1)(n-\delta-1)^\alpha$.

Chen *et al.* [27] extended the results of [137, 138] to $-1 \leq \alpha < 0$ and $1 < \alpha \leq 2$.

Theorem 63. [27] *Let G be a connected graph with minimal degree δ and order $n \geq 2$. If G is not a maximally edge-connected graph, then*

$$
{}^0R_\alpha(G) < 2^{2-\alpha}[n^2 - (2\delta+4)n + \delta^2 + 5\delta + 3]^\alpha
$$

for $1 < \alpha \leq 2$.

Theorem 64. [27] *Let G be a connected triangle–free graph with minimal degree δ and order $n \geq 2$. If G is not a maximally edge-connected graph, then the following inequality holds for $-1 \leq \alpha < 0$:*

$$
{}^0R_\alpha(G) \geq min\,\{\phi_1(\alpha,\delta), \phi_2(\alpha,\delta)\}
$$

where

$$\phi_1(\alpha,\delta) = \delta^\alpha + 3\delta^{\alpha+1} + (\delta-1)(\delta+1)^\alpha + \frac{(\delta-1)(n-2\delta+2)^\alpha}{2^\alpha} - \frac{(\delta-1)(n-2\delta)^\alpha}{2^\alpha}$$

and

$$\phi_2(\alpha,\delta) = \delta^\alpha + 2\delta^{\alpha+1} + 2\delta(\delta+1)^\alpha + \frac{(\delta-2)(n-2\delta)^\alpha}{2^\alpha} - \frac{(\delta-2)(n-2\delta-2)^\alpha}{2^\alpha}\,.$$

In [54], a lower bound on ${}^0R_\alpha(T)$ in terms of p was obtained, where T is a tree with p pendent vertices.

Su *et al.* [136] derived several lower bounds on the invariant ${}^0R_\alpha$, when α is a positive integer. In order to state the first result of [136], we need to recall the cyclomatic number of a graph: the minimal number of edges of a graph G whose removal makes G acyclic.

Theorem 65. [136] *Let α be a positive integer. If G is a connected graph with n_1 pendent vertices, cyclomatic number ν, and no vertex of degree 3, then*

$${}^0R_\alpha(G) \geq 4^\alpha(\nu-1) + (1 + 2^{-1}\cdot 4^\alpha)n_1$$

with equality if and only if every non-pendent vertex of G has degree 4, provided that such graphs exist.

Theorem 66. [136] *Let α be a positive integer and T be an n-vertex tree with n_1 pendent vertices. Then*

$$\begin{aligned} {}^0R_\alpha(T) \ &\geq\ n_1 + \left((n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 2 - n_1\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 1\right)^\alpha \\ &+\ \left(n-2-(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 2\right)^\alpha \end{aligned}$$

with equality if and only if T consists of n_1 pendent vertices, $(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 2 - n_1$ vertices of degree $\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 1$ and $n-2-(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor$ vertices of degree $\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 2$.

Theorem 67. [136] *Let α be a positive integer and U be a connected unicyclic n-vertex graph with n_1 pendent vertices. Then*

$$\begin{aligned} {}^0R_\alpha(U) \ &\geq\ n_1 + \left((n-n_1)\left\lfloor\frac{n}{n-n_1}\right\rfloor - n_1\right)\left(\left\lfloor\frac{n}{n-n_1}\right\rfloor + 1\right)^\alpha \\ &+\ \left(n-(n-n_1)\left\lfloor\frac{n}{n-n_1}\right\rfloor\right)\left(\left\lfloor\frac{n}{n-n_1}\right\rfloor + 2\right)^\alpha \end{aligned}$$

with equality if and only if U consists of n_1 pendent vertices, $(n-n_1)\left\lfloor\frac{n}{n-n_1}\right\rfloor - n_1$ vertices of degree $\left\lfloor\frac{n}{n-n_1}\right\rfloor + 1$ and $n-(n-n_1)\left\lfloor\frac{n}{n-n_1}\right\rfloor$ vertices of degree $\left\lfloor\frac{n}{n-n_1}\right\rfloor + 2$.

Theorem 68. [136] *Let α be a positive integer and B be a connected bicyclic n-vertex graph with n_1 pendent vertices. Then*

$$\begin{aligned} {}^0R_\alpha(B) \;\geq\; & n_1 + \left((n-n_1)\left\lfloor\frac{n+2}{n-n_1}\right\rfloor - 2 - n_1\right)\left(\left\lfloor\frac{n+2}{n-n_1}\right\rfloor + 1\right)^\alpha \\ + \; & \left(n+2-(n-n_1)\left\lfloor\frac{n+2}{n-n_1}\right\rfloor\right)\left(\left\lfloor\frac{n+2}{n-n_1}\right\rfloor + 2\right)^\alpha \end{aligned}$$

with equality if and only if B consists of n_1 pendent vertices, $(n-n_1)\left\lfloor\frac{n+2}{n-n_1}\right\rfloor - 2 - n_1$ vertices of degree $\left\lfloor\frac{n+2}{n-n_1}\right\rfloor + 1$ and $n+2-(n-n_1)\left\lfloor\frac{n+2}{n-n_1}\right\rfloor$ vertices of degree $\left\lfloor\frac{n+2}{n-n_1}\right\rfloor + 2$.

For a connected c-cyclic n-vertex graph G, $0 \leq c \leq 6$, upper and lower bounds on ${}^0R_\alpha(G)$ in terms of n were established in [10] (see Table 2 of [10] - the bounds given in this table corresponds to $\alpha < 0$ and $\alpha > 1$, and the lower (respectively, upper) bounds are interchanged with upper (respectively, lower) bounds for the case $0 < \alpha < 1$).

Ilić and Stevanović [81] derived a lower bound on the invariant ${}^0R_\alpha$, within the study of variable first Zagreb index.

Theorem 69. [81] *If G is an (n,m)-graph and $\alpha \geq 1$, then*

$${}^0R_\alpha(G) \geq n\left(\frac{2m}{n}\right)^\alpha .$$

Having in mind (10) and (11), and Jensen's inequality (see for example [117]) it can be easily verified that the following inequalities are valid:

$${}^0R_\alpha(G) \geq {}^0R_2(G)\left(\frac{2m}{n}\right)^{\alpha-2}, \qquad \alpha \geq 2$$

and

$${}^0R_\alpha(G) \geq \frac{{}^0R_3(G)n}{{}^0R_2(G)}\left(\frac{2m}{n}\right)^{\alpha-1}, \qquad \alpha \geq 3 .$$

For $\alpha \geq 2$ and $\alpha \geq 3$, the above inequalities are stronger than the one given in Theorem 69.

Some bounds on the expected value and distribution function of ${}^0R_\alpha$, for certain trees and certain values of α, can be found in the paper [118]. Recently, Rodriguez *et al.* [134] derived several bounds for the invariant ${}^0R_\alpha$.

Theorem 70. [134] *If G is a non-trivial graph with m edges, maximal degree Δ and minimal degree δ, then*

$$2\Delta^{\alpha-1}m \leq {}^0R_\alpha(G) \leq 2\delta^{\alpha-1}m \quad if \quad \alpha < 1$$

$$2\delta^{\alpha-1}\, m \le {}^0R_\alpha(G) \le 2\Delta^{\alpha-1}\, m \quad if \quad \alpha \ge 1\,.$$

The equality sign in any of the above inequalities holds, for $\alpha \neq 1$, if and only if G is regular.

Theorem 71. [134] *If G is a non-trivial (n,m)-graph, then*

$$^0R_\alpha(G) \begin{cases} \ge 2m\alpha + n(1-\alpha) & if \;\; \alpha \le 0 \;\; or \; \alpha \ge 1 \\ \le 2m\alpha + n(1-\alpha) & if \;\; 0 < \alpha < 1\,. \end{cases}$$

The equality sign in any of the above inequalities holds, for $\alpha \neq 0, 1$, if and only if G is a union of pairwise disjoint edges.

2.4 Extremal results

In this section, we collect some extremal results concerning $^0R_\alpha$. Let $t_\alpha(n,H)$ denote the maximal value of $^0R_\alpha$ taken over all H–free n-vertex graphs.

The Turán graph $T_k(n)$ is a complete k-partite n-vertex graph, whose classes are as equal as possible.

Theorem 72. [20,21] *If $\alpha = 1, 2, 3$ and $k \ge 3$ is a positive integer, then*

$$t_\alpha(n, K_k) = {}^0R_\alpha(T_{k-1}(n))\,.$$

Motivated by Theorem 72, Bollobás and Nikiforov [14] established some related results:

Theorem 73. [14] *If $0 < \alpha \le 3$, then $t_\alpha(n, K_3) = {}^0R_\alpha(T_2(n))$. For every $\epsilon > 0$, there exists δ such that if $\alpha > 3 + \delta$, then for sufficiently large n,*

$$t_\alpha(n, K_3) > (1+\epsilon)\,{}^0R_\alpha(T_2(n))\,.$$

Theorem 74. [14] *For every $k \ge 3$, $0 < \alpha < k-1$, and sufficiently large n, it holds that*

$$t_\alpha(n, K_k) = {}^0R_\alpha(T_{k-1}(n))\,.$$

Later in this section, we will see a result (Theorem 90) related to Theorems 72, 73, and 74.

Theorem 75. [14] *For $k \geq 3$ and $\alpha > 0$, there exists $c = c(\alpha, k)$ such that the following assertion holds. If $t_\alpha(n, K_k) = {}^0R_\alpha(G)$ for some K_k–free graph G of order n, then G is a complete $(k-1)$-partite graph having $k-2$ vertex classes of size $cn + o(n)$.*

Theorem 76. [14] *For every $k \geq 3$, and $\alpha > 0$,*

$$t_\alpha(n, H) = t_\alpha(n, K_k) + o(n^{\alpha+1}).$$

The next theorem determines $t_\alpha(n, P_k)$ for n sufficiently large (for small values of n there are exceptions). In order to state this result, we need to define the graph $H(n, k)$ for $n \geq k \geq 4$ as follows. The vertex set of H is composed of two parts A and B where $|B| = \lfloor \frac{k}{2} \rfloor - 1$ and $|A| = n - |B|$. B induces a complete graph, and A induces an independent set when k is even, or a single edge plus $|A| - 2$ isolated vertices when k is odd. All possible edges between A and B exist.

Theorem 77. [20] *Let $\alpha \geq 2$ be an integer, $k \geq 4$ and $n > n_0(k)$. Then,*

$$t_\alpha(n, P_k) = {}^0R_\alpha(H(n, k)).$$

Furthermore, $H(n, k)$ is the unique extremal graph.

A linear forest is a forest whose components are paths. An even linear forest is a forest whose components are paths with an even number of vertices (distinct components may have different lengths).

Theorem 78. [20] *Let α and k be integers greater than 1. If F is an even linear forest with $2k$ vertices then, for n sufficiently large, $t_\alpha(n, F) = {}^0R_\alpha(H(n, 2k))$.*

Theorem 79. [20] *If α and k are integers greater than 1, then*

$$t_\alpha(n, S_k) = \begin{cases} n(n-1)^\alpha & \text{if } n \leq k-2 \\ n(k-2)^\alpha & \text{if } n > k-2 \text{ and } nk \text{ is even} \\ (n-1)(k-2)^\alpha + (k-3)^\alpha & \text{if } n > k-2 \text{ and } nk \text{ is odd.} \end{cases}$$

Let S_k^* be the tree obtained from S_{k-1} by attaching one new pendent vertex to one of the pendent vertices.

Theorem 80. [20] *If α and k are integers greater than 1 such that $n > 2k$, then $t_\alpha(n, S_k^*) = {}^0R_\alpha(S_n) = (n-1)^\alpha + (n-1)$.*

A connected bipartite graph is equipartite if the two vertex classes forming the bipartition have equal sizes. For a given graph H and positive integer n, the Turán number $t(n, H)$ is the maximal number of edges in an H-free n-vertex graph.

Theorem 81. [20] *Let α and k be integers greater than 1. If H is an equipartite tree with $2k$ vertices, and $t(n,H) \leq (k-1)n$ then*

$$t_\alpha(n, H) = (k-1)n^\alpha + o(n^\alpha)\,.$$

Let $C^{(e)}$ be the family of even cycles. A matching in a graph is a set of pairwise non-adjacent edges. A maximal matching is one which covers as many vertices as possible. The friendship graph F_n is the one, obtained from S_n by adding a maximal matching on the set of pendent vertices. Thus, F_n has exactly $\lfloor 3(n-1)/2 \rfloor$ edges, and no even cycle.

Theorem 82. [20] *If n is sufficiently large and $\alpha \geq 2$ is an integer, then*

$$t_\alpha\left(n, C^{(e)}\right) = {}^0R_\alpha(F_n)$$

and F_n is the unique extremal graph.

Theorem 83. [20] *Let α, a and k be integers such that $2 \leq a \leq k$. Then $t_\alpha[n, K_{a,k}] = (a-1)n^k[1+o(1)]$ for all $\alpha \geq 2$. Furthermore, if $\alpha \geq k$ then*

$$t_\alpha(n, K_{2,k}) = n^\alpha\big[1+o(1)\big]\,.$$

Conjecture 84. [20] *Let H be a graph with chromatic number $\chi \geq 3$. If $\alpha \geq 1$ is an integer, then*

$$t_\alpha(n, H) = \left(\frac{\chi-2}{\chi-1}\right)^\alpha n^{\alpha+1}\big[1+o(1)\big]\,.$$

Bollobás and Nikiforov [14] proved a result that completely settles, with appropriate changes, Conjecture 84.

Conjecture 85. [20] *Let $\alpha > 2$ be an integer and H be a fixed graph. There exists $n_0 = n_0(\alpha, H)$ such that for all $n > n_0$ and for all H–free n-vertex graphs G, it holds that $t_\alpha(n,H) = {}^0R_\alpha(G)$ if and only if $t_2(n,H) = {}^0R_2(G)$.*

Conjecture 85 was disproved in [14].

Conjecture 86. [20] *If $\alpha > 1$ is an integer, then* $t_\alpha(n, C_{2k}) = (k-1)n^\alpha\big[1+o(1)\big]$.

Nikiforov [122] proved Conjecture 86. Here, it should be mentioned that some new results on the generalization of the Turán problem, introduced by Caro and Yuster [20], were reported by Pikhurko [131]. The next result is due to Gu *et al.* [55], which is an extension of Theorem 82.

Theorem 87. [55] *For any positive integer α and sufficiently large n, there exists a constant $c = c(\alpha)$ such that the following holds: If $t_\alpha(n, C_5) = {}^0R_\alpha(G)$ for some C_5–free graph G of order n, then G is a complete bipartite graph having one vertex class of size $cn + o(n)$ and the other of size $(1 - c)n + o(n)$.*

Theorem 88. [99] *Let $m = \binom{k}{2}$. Among (n, m)-graphs, the graph having $n - k$ isolated vertices and a complete subgraph K_k, is the unique graph with the minimal ${}^0R_{1/2}$ value.*

Linial and Rozenman [99] studied the graph invariant $\sum_{v\in V(G)} f(d_v)$ (a generalization of ${}^0R_\alpha$) and proved that Theorem 88 cannot be extended to every concave increasing function f. The authors of [99] asked the following questions: what is the family of functions f for which Theorem 88 remains valid? Is Theorem 88 valid for ${}^0R_\alpha$, $\alpha < 1$? Also, in [99], it was conjectured that among (n, m)-graphs, $\binom{k-1}{2} < m < \binom{k}{2}$, the graph whose only non-trivial component is the graph obtained from K_{k-1} by adding one new vertex of degree $m - \binom{k-1}{2}$, is the unique graph with minimal ${}^0R_{1/2}$ value. Soon after the proposal of this conjecture, it was confirmed by Ismailescu and Stefanica [83] by proving a more general result:

Theorem 89. [83] *Let k be the unique positive integer satisfying $\binom{k-1}{2} < m \leq \binom{k}{2}$. Among (n, m)-graphs, the graph with $n - k$ isolated vertices, a complete subgraph K_{k-1}, and one vertex of degree $m - \binom{k-1}{2}$ connected to vertices of the complete subgraph, is the unique graph with minimal ${}^0R_\alpha$ value for $0 < \alpha \leq \frac{1}{2}$.*

The authors of [83] conjectured that Theorem 89 remains valid for $\frac{1}{2} < \alpha < 1$. Hota and Sundaram [74] generalized Theorem 89 to functions that satisfy a more general set of conditions.

Vukičević [147] obtained the following extremal result, which is related to Theorems 72, 73, and 74.

Theorem 90. [147] *If $k \geq 2$ is an integer and $n = kx$, then*

$$t_\alpha(n, K_{k+1}) = {}^0R_\alpha(T_k(n))$$

for $0 \le \alpha \le 3$. Moreover, this statement cannot be extended to any $\alpha < 0$ or $\alpha > 3$ (for $\alpha < 0$, it is assumed that G does not contain any isolated vertex).

The double star S_{n_1,n_2}, where $n_1, n_2 \ge 1$, is the graph consisting of the union of two disjoint stars S_{n_1} and S_{n_2} together with an edge connecting their centers. Denote by $\mathcal{C}_{n,\nu}$ the set of all connected n-vertex graphs with cyclomatic number ν. Let

$$\begin{aligned} \mathcal{T}^{(1)} &= \{P_n\} \\ \mathcal{T}^{(2)} &= \{T \in \mathcal{C}_{n,0} : n_1 = 3, n_2 = n-4, n_3 = 1, n_i = 0 \text{ for } \ i \ge 4\} \\ \mathcal{T}^{(3)} &= \{T \in \mathcal{C}_{n,0} : n_1 = 4, n_2 = n-6, n_3 = 2, n_i = 0 \text{ for } \ i \ge 4\}. \end{aligned}$$

In 2004, Li and Zhao [94] determined the trees (respectively, chemical trees) with first three (respectively, first two) extremal ${}^0R_\alpha$ values for certain, but infinitely many, values of α.

Theorem 91. [94] *Let $\alpha = -k, k, -\frac{1}{k}$ or $\frac{1}{k}$ where $k \ge 2$ is an integer. Among the n-vertex trees, the trees with maximal, second maximal, third maximal, minimal, second minimal, third minimal ${}^0R_\alpha$ values are those given in Table 1.*

	$\alpha = k$	$\alpha = -k$	$\alpha = \frac{1}{k}$	$\alpha = -\frac{1}{k}$
maximal	S_n	S_n	P_n	S_n
minimal	P_n	P_n	S_n	P_n
second maximal	$S_{n-2,2}$	$S_{n-2,2}$	members of $\mathcal{T}^{(2)}$	$S_{n-2,2}$
second minimal	members of $\mathcal{T}^{(2)}$	members of $\mathcal{T}^{(2)}$	$S_{n-2,2}$	members of $\mathcal{T}^{(2)}$
third maximal	$S_{n-3,3}$	$S_{n-3,3}$	members of $\mathcal{T}^{(3)}$	$S_{n-3,3}$
third minimal	members of $\mathcal{T}^{(3)}$	members of $\mathcal{T}^{(3)}$	$S_{n-3,3}$	members of $\mathcal{T}^{(3)}$

Table 1: Trees, referred in Theorem 91, with the first three extremal ${}^0R_\alpha$ values.

Denote by $\mathbb{CG}^*_{n,m}$ the set of connected molecular (n,m)-graphs containing at most one vertex of degree 2 or 3.

Theorem 92. [94] *Let $\mathbb{CT}_n$ be the class of n-vertex chemical trees. Let $n-2 = 3a+i$, $i = 0,1,2$ and take*

$$\begin{aligned} \mathcal{T}_a^{(1)} &= \{T \in \mathbb{CT}_n : n_1 = n-a-1, n_2 = n_3 = 1, n_4 = a-1\} \\ \mathcal{T}_a^{(2)} &= \{T \in \mathbb{CT}_n : n_1 = n-a-1, n_2 = 0, n_3 = 2, n_4 = a-1\} \\ \mathcal{T}_a^{(3)} &= \{T \in \mathbb{CT}_n : n_1 = n-a-2, n_2 = 2, n_3 = 0, n_4 = a\}\,. \end{aligned}$$

1) *If* $\alpha = -k$, k, *or* $-\frac{1}{k}$, *where* $k \geq 2$ *is an integer, and* $T \in \mathbb{CT}_n$, *then*

1a) ${}^0R_\alpha(T)$ *attains the maximal value if and only if* $T \in \mathbb{CG}^*_{n,n-1}$.

1b) ${}^0R_\alpha(T)$ *attains the second maximal value if and only if* $T \in \mathcal{T}_a^{(i+1)}$ *for* $i = 0, 1, 2$.

2) *If* $\alpha = \frac{1}{k}$, *where* $k \geq 2$ *is an integer, and* $T \in \mathbb{CT}_n$ *then*

2a) ${}^0R_\alpha(T)$ *attains the minimal value if and only if* $T \in \mathbb{CG}^*_{n,n-1}$.

2b) ${}^0R_\alpha(T)$ *attains the second minimal value if and only if* $T \in \mathcal{T}_a^{(i+1)}$ *for* $i = 0, 1, 2$.

Li and Zheng [95] found the extremal trees with respect to the invariant ${}^0R_\alpha$.

Theorem 93. [95] *Among n-vertex trees, the unique trees with maximal and minimal* ${}^0R_\alpha$ *values are listed in Table 2.*

	$0 < \alpha < 1$	$\alpha < 0$ or $\alpha > 1$
maximal	P_n	S_n
minimal	S_n	P_n

Table 2: Trees, referred in Theorem 93, with extremal ${}^0R_\alpha$ values.

Following the technique adopted in [94], Theorems 91 and 92 can be easily extended for all values of α. More precisely, those statements of Theorems 91 and 92 that hold for $\alpha = -k, k, -\frac{1}{k}$ (respectively, for $\alpha = \frac{1}{k}$), also hold for $\alpha < 0$ and $\alpha > 1$ (respectively, for $0 < \alpha < 1$), see [90]. Trees with the first four maximal ${}^0R_\alpha$ values for $\alpha < 0$ and $\alpha > 1$, and trees with the first four minimal ${}^0R_\alpha$ values for $0 < \alpha < 1$, were determined in [104], using majorization technique. Furthermore, recently, Eliasi and Ghalavand [40] found trees with the first three minimal ${}^0R_\alpha$ values (for $\alpha < 0$ and $\alpha > 1$) and first three maximal ${}^0R_\alpha$ values (for $0 < \alpha < 1$), using majorization technique.

The set $\mathbb{CG}^*$ has been defined in connection with Theorem 92. Let $\mathbb{CG}^\circ_{n,m}$ be the set of connected molecular (n, m)-graphs satisfying $\Delta - \delta \leq 1$. Hu *et al.* [77] characterized the connected molecular (n, m)-graphs with the maximal and minimal ${}^0R_\alpha$ values.

Theorem 94. [77] *Among (connected) molecular* (n, m)*-graphs which satisfy at least one of the following conditions:*

1. $m = n - 1$,

2. $m \geq n \geq 6$, *for* $n = 6$,$m \geq 10$, *and for* $n = 7$, $m \neq 8$,

the graphs with maximal and minimal ${}^0R_\alpha$ *values are specified in Table 3.*

	$0<\alpha<1$	$\alpha<0$ or $\alpha>1$
maximal	members of $\mathbb{CG}^{\circ}_{n,m}$	members of $\mathbb{CG}^{*}_{n,m}$
minimal	members of $\mathbb{CG}^{*}_{n,m}$	members of $\mathbb{CG}^{\circ}_{n,m}$

Table 3: Molecular (n,m)-graphs, specified in Theorem 94, with extremal ${}^0R_\alpha$ values.

Denote by S_n^+ the graph obtained from S_n, where $n \geq 4$, by adding an edge between any two pendent vertices. Zhang and Zhang [162] identified the connected unicyclic graphs with the first three extremal ${}^0R_\alpha$ values. In order to state their result, we need the following graph classes:

$$\mathcal{U}^{(1)} = \{C_n\}$$

$$\mathcal{U}^{(2)} = \{U \in \mathcal{C}_{n,1} : n_1 = 1, n_2 = n-2, n_3 = 1, n_i = 0 \text{ for } i \geq 4\}$$

$$\mathcal{U}^{(3)} = \{U \in \mathcal{C}_{n,1} : n_1 = 2, n_2 = n-4, n_3 = 2, n_i = 0 \text{ for } i \geq 4\}$$

where $\mathcal{C}_{n,1}$ is the set of connected unicyclic n-vertex graphs.

Theorem 95. [162] *Among connected unicyclic n-vertex graphs, where $n \geq 5$, the graphs with the maximal, second maximal, third maximal, minimal, second minimal, third minimal ${}^0R_\alpha$ values are those specified in Table 4 and Fig. 1.*

	$0<\alpha<1$	$\alpha<0$ or $\alpha>1$
maximal	C_n	S_n^+
minimal	S_n^+	C_n
second maximal	members of $\mathcal{U}^{(2)}$	U_1'
second minimal	U_1'	members of $\mathcal{U}^{(2)}$
third maximal	members of $\mathcal{U}^{(3)}$	U_2', U_3' or U_4'
third minimal	U_2', U_3' or U_4'	members of $\mathcal{U}^{(3)}$

Table 4: Connected unicyclic graphs with first three extremal ${}^0R_\alpha$ values. The graphs U_1', U_2', U_3' and U_4' are depicted in Fig. 1.

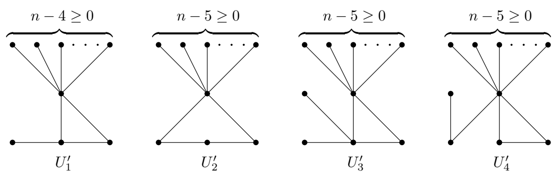

Figure 1: The graphs U_1', U_2', U_3' and U_4', specified in Table 4.

A part of Theorem 95 was also proved in [104] by another simple method. Wang and Deng [150] determined the unique graph with maximal ${}^0R_\alpha$ value among connected unicyclic n-vertex graphs with fixed cycle length, for certain, but infinitely many, values of α.

Let G_1 and G_2 be disjoint graphs and $v_i \in V(G_i)$ for $i = 1, 2$. The chain graph of G_1 and G_2 is denoted by $C(G_1, G_2; v_1, v_2)$ and is defined [108] as the graph obtained from G_1 and G_2 by identifying v_1 with v_2.

Theorem 96. [150] *Let $n \geq k+1$ and $\alpha = -r, r$ or $-\frac{1}{r}$, where $r \geq 2$ is an integer. Among connected unicyclic n-vertex graphs in which the length of the cycle is k, the chain graph $C(C_k, S_{n-k+1}; u, w)$ is the unique graph with maximal ${}^0R_\alpha$ value, where u is any vertex of the cycle C_k and w is the center of the star S_{n-k+1}.*

Hua and Deng [78] completely solved the extremal problem, attacked in [150]. More precisely, they extended Theorem 96 to all real values of α and found extremal graphs for all possible values of α.

Theorem 97. [78] *Among connected unicyclic n-vertex graphs in which the length of the cycle is k, where $n \geq k+1$, the only graphs with maximal and minimal ${}^0R_\alpha$ values are those listed in Table 5.*

	$0 < \alpha < 1$	$\alpha < 0$ or $\alpha > 1$
maximal	$C(C_k, P_{n-k+1}; u, v)$	$C(C_k, S_{n-k+1}; u, w)$
minimal	$C(C_k, S_{n-k+1}; u, w)$	$C(C_k, P_{n-k+1}; u, v)$

Table 5: Extremal graphs referred in Theorem 97. The vertex u is any vertex of the cycle C_k, v is a pendent vertex of the path P_{n-k+1} and w is the center of the star S_{n-k+1}.

Theorem 97 was also proved in [96] independently.

For $3 \leq p \leq n-2$, let $\mathcal{T}(n,p)$ and $\mathcal{U}(n,p)$ be the sets of n-vertex trees and connected unicyclic n-vertex graphs, respectively, with p pendent vertices. Let $\mathcal{T}^*(n,\Delta)$ and $\mathcal{U}^*(n,\Delta)$ be the sets of n-vertex trees and connected unicyclic n-vertex graphs, respectively, with maximal degree Δ, where $n-2 = a(\Delta-1)+k-1$, a is an integer, $k = 1, 2, 3, \ldots, \Delta-1$, and $3 \leq \Delta \leq n-2$.

For the set $\mathcal{T}(n,p)$, Zhang and Zhou [157] characterized the trees with first three maximal ${}^0R_\alpha$ values for $\alpha < 0$ and $\alpha > 1$, and trees with first three minimal ${}^0R_\alpha$ values for $0 < \alpha < 1$.

Theorem 98. [157] *Among members of $\mathcal{T}(n,p)$, the unique trees with first three maximal (respectively, minimal) ${}^0R_\alpha$ values, for $\alpha < 0$ and $\alpha > 1$ (respectively, $0 < \alpha < 1$), have the degree sequences, specified in Table 6.*

	$0 < \alpha < 1$	$\alpha < 0$ or $\alpha > 1$
maximal		$(p, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p})$
minimal	$(p, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p})$	
second maximal		$(p-1, 3, \underbrace{2, \ldots, 2}_{n-p-2}, \underbrace{1, \ldots, 1}_{p})$, $p \geq 4$
second minimal	$(p-1, 3, \underbrace{2, \ldots, 2}_{n-p-2}, \underbrace{1, \ldots, 1}_{p})$, $p \geq 4$	
third maximal		$(p-2, 4, \underbrace{2, \ldots, 2}_{n-p-2}, \underbrace{1, \ldots, 1}_{p})$, $p \geq 6$
third minimal	$(p-2, 4, \underbrace{2, \ldots, 2}_{n-p-2}, \underbrace{1, \ldots, 1}_{p})$, $p \geq 6$	

Table 6: Degree sequences of the trees referred in Theorem 98.

Theorem 99. [157] *Let $T \in \mathcal{T}^*(n,\Delta)$ such that $n-2 = a(\Delta-1)+k-1$, where a is an integer, $k = 1, 2, \ldots, \Delta-1$ and $3 \leq \Delta \leq n-2$. Then ${}^0R_\alpha(T)$ attains maximal (respectively, minimal) value for $\alpha < 0$ and $\alpha > 1$ (respectively, for $0 < \alpha < 1$) if and only if T has the degree sequence $(\underbrace{\Delta, \ldots, \Delta}_{a}, \underbrace{1, \ldots, 1}_{n-a})$ if $k = 1$ and $(\underbrace{\Delta, \ldots, \Delta}_{a}, k, \underbrace{1, \ldots, 1}_{n-a-1})$ if $k \geq 2$.*

For the set $\mathcal{T}^*(n,\Delta)$, elements with the second

- minimal ${}^0R_\alpha$ values for $0 < \alpha < 1$,
- maximal ${}^0R_\alpha$ values for $\alpha < 0$ and $\alpha > 1$,

were also obtained in [157]. Also, Zhang and Zhou [157] determined graphs from the classes $\mathcal{U}(n,p)$, $\mathcal{U}^*(n,\Delta)$ having the first three, first two, respectively,

- minimal ${}^0R_\alpha$ values for $0 < \alpha < 1$,
- maximal ${}^0R_\alpha$ values for $\alpha < 0$ and $\alpha > 1$.

Moreover, in the set $\mathcal{U}(n,p)$, the unique graphs with maximal (for $\alpha < 0$ and $\alpha > 1$) and minimal (for $0 < \alpha < 1$) ${}^0R_\alpha$ values were determined in [96] independently. Furthermore, Lin *et al.* [96] characterized the unique graphs with minimal (for $\alpha < 0$ and $\alpha > 1$) and maximal (for $0 < \alpha < 1$) ${}^0R_\alpha$ values, from the set $\mathcal{U}(n,p)$.

Theorem 100. [96] *In the class $\mathcal{U}(n,p)$, graphs with the degree sequence*

$$\Big(\underbrace{3+\mu_{n,p},\dots,3+\mu_{n,p}}_{p-\lambda_{n,p}},\underbrace{2+\mu_{n,p},\dots,2+\mu_{n,p}}_{n-2p+\lambda_{n,p}},\underbrace{1,\dots,1}_{p}\Big)\ ,$$

are the only graphs with

i) *minimal ${}^0R_\alpha$ value for $\alpha > 1$ and $\alpha < 0$,*

ii) *maximal ${}^0R_\alpha$ value for $0 < \alpha < 1$, where*

$$\mu_{n,p} = \left\lfloor \frac{p-1}{n-p} \right\rfloor \qquad \text{and} \qquad \lambda_{n,p} = (n-p)\mu_{n,p}\,.$$

The graphs with the minimal ${}^0R_\alpha$ value, $\alpha > 1$, were determined in [61], for the set of all n-vertex connected c-cyclic graphs with maximal degree $\geq 2c$ (respectively, maximal degree ≥ 3) with $c \geq 1$ (respectively, $c = 0$).

Theorem 101. [61]

i) *Among the members of $\mathcal{T}^*(n,\Delta)$, $\Delta \geq 3$, the starlike trees have the minimal ${}^0R_\alpha$ value for $\alpha > 1$.*

ii) *Let $\alpha > 1$ and $c \geq 1$. Among n-vertex connected c-cyclic graphs with maximal degree $\Delta \geq 2c$, the graph obtained by connecting c pairs of pendent vertices of a starlike tree having maximal degree Δ, has the minimal ${}^0R_\alpha$ value.*

For $\Delta < 2c$, the connected c-cyclic graphs with minimal ${}^0R_\alpha$ value, $\alpha > 1$, have no pendent vertices [61]. The next extremal result is due to Yamaguchi [155].

Theorem 102. [155] *If $n \geq 3$ and $n-1 \geq d \geq 2$, then among the n-vertex trees with diameter d, the unique trees with first three extremal ${}^0R_\alpha$ values have the degree sequences listed in Table 7. The degree sequences, corresponding to second and third extremal ${}^0R_\alpha$ values, must satisfy the conditions $n-3 \geq d \geq 3$ and $n-5 \geq d \geq 3$, respectively.*

An extremal result, similar to Theorem 102, for the set of n-vertex trees with fixed radius, was also proved in [155].

Let $P_d = v_0v_1\dots v_d$ be a path of length d and let $G_{n,d,i,j}$ be the graph obtained from P_d by attaching $n-d-1$ pendent vertices to v_i and joining one of the new pendent vertices to v_j. Let $\mathbb{G}_{n,d} = \{G_{n,d,i,j}\ :\ 2 \leq i \leq d-1 \ \text{ and } \ 1 \leq j = i-1 \ \text{ or } \ i-2\}$. Among connected unicyclic graphs with fixed order and diameter, Pan *et al.* [125] determined the unique graphs with minimal and maximal ${}^0R_\alpha$ values for all α.

	$0<\alpha<1$	$\alpha<0$ or $\alpha>1$
maximal		$(n-d+1,\underbrace{2,\ldots,2}_{d-2},\underbrace{1,\ldots,1}_{n-d+1})$
minimal	$(n-d+1,\underbrace{2,\ldots,2}_{d-2},\underbrace{1,\ldots,1}_{n-d+1})$	
second maximal		$(n-d,3,\underbrace{2,\ldots,2}_{d-3},\underbrace{1,\ldots,1}_{n-d+1})$
second minimal	$(n-d,3,\underbrace{2,\ldots,2}_{d-3},\underbrace{1,\ldots,1}_{n-d+1})$	
third maximal		$(n-d-1,4,\underbrace{2,\ldots,2}_{d-3},\underbrace{1,\ldots,1}_{n-d+1})$
third minimal	$(n-d-1,4,\underbrace{2,\ldots,2}_{d-3},\underbrace{1,\ldots,1}_{n-d+1})$	

Table 7: Degree sequences of the extremal trees, mentioned in Theorem 102.

Theorem 103. [125] *Let $3 \le d \le n-2$. In the set of connected unicyclic n-vertex graphs with diameter d, members of $\mathbb{G}_{n,d}$ are the only graphs with*
i) *maximal ${}^0R_\alpha$ value for $\alpha > 1$ and $\alpha < 0$;*
ii) *minimal ${}^0R_\alpha$ value for $0 < \alpha < 1$.*

Theorem 104. [125] *Let $3 \le \lfloor \frac{n}{2} \rfloor \le d \le n-2$. In the set of connected unicyclic n-vertex graphs with diameter d, the chain graphs $C(C_{2n-2d}, P_{2d-n+1}; u, v)$ and $C(C_{2n-2d-1}, P_{2d-n+2}; u, v)$ for $3 \le \lfloor \frac{n}{2} \rfloor \le d \le n-2$, and the cycle C_n for $d = \lfloor \frac{n}{2} \rfloor$, are the only graphs with*
i) *minimal ${}^0R_\alpha$ value for $\alpha > 1$ and $\alpha < 0$,*
ii) *maximal ${}^0R_\alpha$ value for $0 < \alpha < 1$,*
where u is any vertex of the cycle graph and v is a pendent vertex of the path graph.

The definition of a chain graphs is found earlier in connection with Theorem 96.

Zhang *et al.* [161] characterized the connected bicyclic graphs with first three extremal ${}^0R_\alpha$ values for all α. In order to state this result, we need the following graph classes:

$$\mathcal{B}^{(1)} = \{B \in \mathcal{C}_{n,2} : n_1 = 0, n_2 = n-2, n_3 = 2, n_i = 0 \text{ for } i \ge 4\}$$

$$\mathcal{B}^{(2)} = \{B \in \mathcal{C}_{n,2} : n_1 = 0, n_2 = n-1, n_3 = 0, n_4 = 1, n_i = 0 \text{ for } i \ge 5\}$$

$$\mathcal{B}^{(3)} = \{B \in \mathcal{C}_{n,2} : n_1 = 1, n_2 = n-4, n_3 = 3, n_i = 0 \text{ for } i \ge 4\}$$

where $\mathcal{C}_{n,2}$ is the set of connected bicyclic n-vertex graphs.

Theorem 105. [161] *Among the n-vertex connected bicyclic graphs, where $n \geq 6$, the graphs with maximal, second maximal, third maximal, minimal, second minimal, third minimal ${}^0R_\alpha$ values are those specified in Table 8 and Fig. 2.*

	$\alpha < 0$	$0 < \alpha < 1$	$1 < \alpha < 2$	$\alpha > 2$
maximal	B_1'	members of $\mathcal{B}^{(1)}$	B_1'	B_1'
minimal	members of $\mathcal{B}^{(1)}$	B_1'	members of $\mathcal{B}^{(1)}$	members of $\mathcal{B}^{(1)}$
second maximal	B_3'	members of $\mathcal{B}^{(2)}$	B_2', B_3' or B_4'	B_2'
second minimal	members of $\mathcal{B}^{(2)}$	B_2'	members of $\mathcal{B}^{(2)}$	members of $\mathcal{B}^{(3)}$
third maximal	B_2' or B_4'	members of $\mathcal{B}^{(3)}$	B_2', B_3' or B_4'	B_3' or B_4'
third minimal	members of $\mathcal{B}^{(3)}$	B_3'	members of $\mathcal{B}^{(3)}$	members of $\mathcal{B}^{(2)}$

Table 8: Connected bicyclic graphs, referred in Theorem 105, with the first three extremal ${}^0R_\alpha$ values. The graphs B_1', B_2', B_3' and B_4' are depicted in Fig. 2.

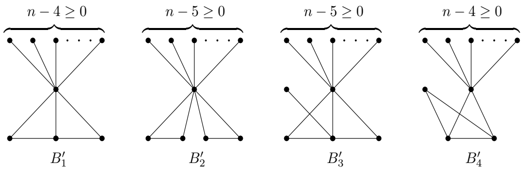

Figure 2: The graphs B_1', B_2', B_3' and B_4', mentioned in Table 8.

Chen and Deng [25], also, independently determined the connected bicyclic graphs with the extremal ${}^0R_\alpha$ values. The next extremal result is due to Liu and Liu [104].

Theorem 106. [104] *Let $c \geq 0$ and $1 \leq p \leq n-2c-1$. In the class of connected c-cyclic n-vertex graphs with p pendent vertices, the graphs with the degree sequence $(2c+p, \underbrace{2,\dots,2}_{n-p-1}, \underbrace{1,\dots,1}_{p})$ are the only graphs with*

i) *maximal ${}^0R_\alpha$ value for $\alpha > 1$ and $\alpha < 0$;*

ii) *minimal ${}^0R_\alpha$ value for $0 < \alpha < 1$.*

For $c = 2$ and $p \leq n-5$, Pan and Lv [127] independently proved Theorem 106. They, also, characterized the extremal graphs corresponding to the case $c = 2$, $p = n-4$. Moreover, the next theorem was also proved in [127].

Theorem 107. [127] *Among connected bicyclic n-vertex graphs with p pendent vertices, graphs with degree sequence* $(\underbrace{3+\mu_{n,p},\dots,3+\mu_{n,p}}_{p+2-\lambda_{n,p}},\underbrace{2+\mu_{n,p},\dots,2+\mu_{n,p}}_{n-2p-2+\lambda_{n,p}},\underbrace{1,\dots,1}_{p})$ *are the only graphs with*

i) *minimal $^0R_\alpha$ value for $\alpha > 1$ and $\alpha < 0$,*

ii) *maximal $^0R_\alpha$ value for $0 < \alpha < 1$, where*

$$\mu_{n,p} = \left\lfloor \frac{p+1}{n-p} \right\rfloor \quad \textit{and} \quad \lambda_{n,p} = (n-p)\mu_{n,p}\ .$$

In what follows, we denote the degree of the vertex $v_i \in V(G)$ as d_i instead of d_{v_i}, for the sake of simplicity. We recall a graph family, defined in [13]. Let $\widetilde{G} = G(d_1, d_2, \dots, d_N)$ be an n-vertex graph having vertex set $\bigcup_{j=0}^{N} I_j$ as disjoint union, where $I_0 = \{v_1, v_2, \dots, v_N\}$, $|I_j| = d_j - d_{j+1}$ for $j = 1, 2 \dots, N-1$, $|I_N| = d_N - (N-1)$ and $d_1 \geq d_2 \geq \cdots \geq d_N \geq N-1$. Also, for $1 \leq j \leq N$, we set $N_{\widetilde{G}}(v_j) = (I_0 \setminus \{v_j\}) \cup \left(\bigcup_{k=j}^{N} I_k \right)$ and suppose that all members of $\bigcup_{j=1}^{N} I_j$ are pairwise non-adjacent. The graph $\widetilde{G}$ is depicted in Fig. 3. Let $\mathcal{F}$ be the set of graphs of the form $\widetilde{G}$. Denote by $\mathbb{C}^*$ the set of connected (n,m)-graphs satisfying $\Delta - \delta \leq 1$. Hu *et al.* [76] identified connected (n,m)-graphs with maximal and minimal $^0R_\alpha$ values.

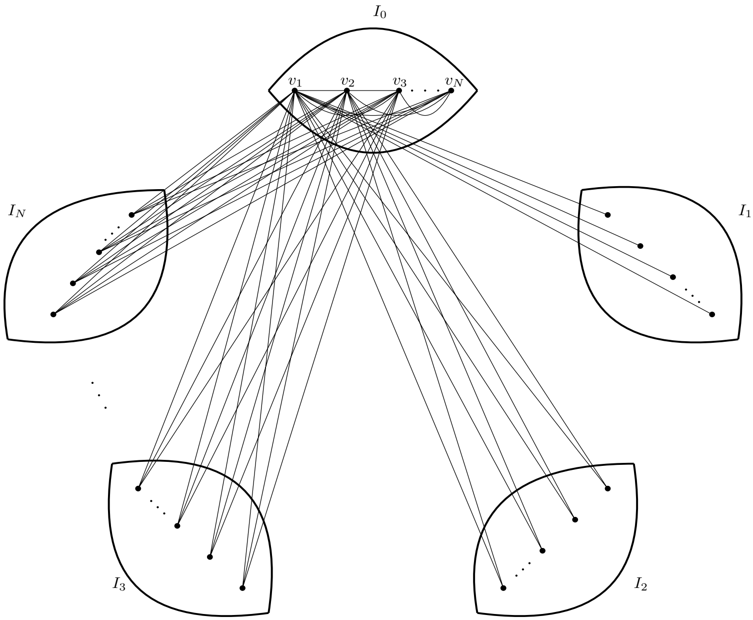

Figure 3: The graphical representation of $\widetilde{G}$.

Theorem 108. [76] *Among connected* (n, m)*-graphs, the graphs with maximal and minimal* ${}^0R_\alpha$ *values are mentioned in Table 9.*

	$0 < \alpha < 1$	$\alpha < 0$ or $\alpha > 1$
maximal	members of $\mathbb{C}^*$	some graph(s) in $\mathcal{F}$
minimal	some graph(s) in $\mathcal{F}$	members of $\mathbb{C}^*$

Table 9: Connected (n, m)-graphs, referred in Theorem 108, with extremal ${}^0R_\alpha$ values.

Theorem 108 indicates that the graph with maximal ${}^0R_\alpha$ value, for $\alpha \leq -1$, must belongs to the set $\mathcal{F}$. Hu *et al.* [76] determined the exact structure of this extremal graph. However, unfortunately, the proof of this fact contains some error, which was identified by Li and Shi [91], and Pavlović *et al.* [129] independently – in both of these papers not only the aforementioned proof was corrected but also the same result was extended for $\alpha < 0$, and thereby Theorem 188 was generalized for any negative value of α.

Theorem 109. [91, 129] *Among connected n-vertex graphs with $n+\frac{k(k-3)}{2}+p$ edges, where $2 \le k \le n-1$ and $0 \le p \le k-2$, the graph $K_k^{n-k}(p)$ has the maximal ${}^0R_\alpha$ value for all $\alpha < 0$.*

A matching containing $\widetilde{m}$ edges is known as an $\widetilde{m}$-matching. A graph with an $\widetilde{m}$-matching is a graph having at least one $\widetilde{m}$-matching [75]. A matching M of a graph G is said to be perfect if for every vertex $u \in V(G)$ there is another vertex $v \in V(G)$ such that $uv \in M$.

Let n and $\widetilde{m}$ be positive integers such that $n \ge 2\widetilde{m}$ and let $\mathbb{T}(n,\widetilde{m})$ be the class of n-vertex trees with an $\widetilde{m}$-matching. A tree $T^0(n,\widetilde{m})$ is defined as follows: $T^0(n,\widetilde{m})$ is obtained from the star $S_{n-\widetilde{m}+1}$ by attaching a pendent edge to each of $\widetilde{m}-1$ pendent vertices of $S_{n-\widetilde{m}+1}$. Then $T^0(n,\widetilde{m})$ is an n-vertex tree with an $\widetilde{m}$-matching. In particular, the tree $T^0(2\widetilde{m},\widetilde{m})$ has a perfect matching.

Theorem 110. [79] *Among the members of $\mathbb{T}(2\widetilde{m},\widetilde{m})$, $\widetilde{m} \ge 1$, the unique trees with maximal and minimal ${}^0R_\alpha$ values are those mentioned in Table 10.*

	$0<\alpha<1$	$\alpha<0$ or $\alpha>1$
maximal	$P_{2\widetilde{m}}$	$T^0(2\widetilde{m},\widetilde{m})$
minimal	$T^0(2\widetilde{m},\widetilde{m})$	$P_{2\widetilde{m}}$

Table 10: The unique trees with extremal ${}^0R_\alpha$ values from the set $\mathbb{T}(2\widetilde{m},\widetilde{m})$.

A conjugated graph is the graph having perfect matchings. Among connected conjugated unicyclic graphs with fixed order and girth, the graphs having extremal ${}^0R_\alpha$ values were determined in [79, 159]. Li and Zhang [89] characterized the graphs with extremal ${}^0R_\alpha$ values from the class of all connected conjugated bicyclic graphs having fixed order. For $\alpha > 2$, Pan and Liu [126] discovered the graphs with maximal ${}^0R_\alpha$ value from the set of connected conjugated tricyclic graphs having fixed order.

A graph G is said to be a quasi–tree if there exists some vertex $v \in V(G)$ such that $G-v$ is a tree. Obviously, every non-trivial tree is also a quasi–tree. Qiao [132] determined the unique quasi–trees with maximal and minimal ${}^0R_\alpha$ values.

Theorem 111. [132] *Among n-vertex ($n \ge 3$) quasi–trees containing cycles, the unique graphs with maximal and minimal ${}^0R_\alpha$ values are those listed in Table 11.*

	$\alpha < 0$	$0 < \alpha < 1$	$\alpha = 1$	$\alpha > 1$
maximal	S_n^+	$P_1 + P_{n-1}$	$P_1 + T_{n-1}$	$K_{1,1,n-2}$
minimal	$P_1 + P_{n-1}$	S_n^+	C_n	C_n

Table 11: Extremal quasi–trees mentioned in Theorem 111, where T_{n-1} is any $(n-1)$-vertex tree.

The unique graphs with extremal ${}^0R_\alpha$ values, from the set of n-vertex $(n \geq 3)$ quasi–tree graphs (including trees), were also determined in [132] (see Theorem 5 of [132]). The next result, which covers a part of Theorem 176, is due to Li and Yan [88].

Theorem 112. [88] *Among n-vertex connected graphs with k cut edges, the unique graphs with extremal ${}^0R_\alpha$ values are those listed in Table 12.*

	$0 < \alpha < 1$	$\alpha < 0$	$\alpha > 1$
maximal		$C(C_{n-k}, S_{k+1}; u, w)$	$C(K_{n-k}, S_{k+1}; t, w)$
minimal	$C(C_{n-k}, S_{k+1}; u, w)$		$C(C_{n-k}, P_{k+1}; u, v)$

Table 12: The extremal graphs, referred in Theorem 112. The vertices $u \in V(C_{n-k})$, $t \in V(K_{n-k})$ are arbitrary, $v \in V(P_{k+1})$ is a pendent vertex and $w \in V(S_{k+1})$ is the center.

Recently, Wu *et al.* [151] independently proved that the graph $C(K_{n-k}, S_{k+1}; t, w)$, mentioned in Theorem 112, is the unique graph with maximal ${}^0R_\alpha$ value, for $\alpha > 1$, among the n-vertex connected graphs with k cut edges.

A connected graph G is a cactus if and only if every edge of G lies on at most one cycle. Lin and Lu [98] determined the unique cacti having extremal ${}^0R_\alpha$ values, among cacti with fixed order and number of cycles.

Theorem 113. [98] *Let G be an n-vertex cactus with $c \geq 2$ cycles such that $n = 2c + j$ where $1 \leq j \leq c - 1$. Then*

$${}^0R_\alpha \begin{cases} \leq (c+2)2^{\alpha+1} + (c-j)4^\alpha + (j-1)2 \cdot 3^\alpha & \text{for } 0 < \alpha < 1 \\ \geq (c+2)2^{\alpha+1} + (c-j)4^\alpha + (j-1)2 \cdot 3^\alpha & \text{for } \alpha < 0 \text{ and } \alpha > 1. \end{cases}$$

The equality sign in any of the above inequalities holds if and only if $n_4 = c-j$, $n_3 = 2j-2$, $n_2 = c+2$, $n_1 = 0$, $n_i = 0$ for $i \geq 5$.

Theorem 114. [98] *Let G be an n-vertex cactus with $c \geq 2$ cycles such that $n = 2c + j$ where $j \geq c$. Then*

$${}^0R_\alpha \begin{cases} \leq (j+2)2^\alpha + (c-1)2 \cdot 3^{\alpha+1} & \text{for } 0 < \alpha < 1 \\ \geq (j+2)2^\alpha + (c-1)2 \cdot 3^{\alpha+1} & \text{for } \alpha < 0 \text{ and } \alpha > 1. \end{cases}$$

The equality sign in any of the above inequalities holds if and only if $n_3 = 2c+2$, $n_2 = j+2$, $n_1 = 0$, $n_i = 0$ *for* $i \geq 4$.

Theorem 115. [98] *Let* $n \geq 5$. *Among the* n*-vertex cacti with* c *cycles, the graph obtained from* S_n *by adding* c *mutually independent edges, uniquely*

- *maximize* ${}^0R_\alpha$ *for* $\alpha < 0$ *and* $\alpha > 1$,
- *minimize* ${}^0R_\alpha$ *for* $0 < \alpha < 1$.

Theorem 115 was also proved in [4], independently.

Next, we state some results concerning specific k-polygonal chain graphs. For this, we need some definitions. A k-polygonal system is a connected geometric figure obtained by concatenating congruent regular k-polygons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent regular k-polygons. For $k = 3, 4, 6$, the k-polygonal system corresponds to triangular animals [53], polyominoes [52], and benzenoid system [58] respectively. In a k-polygonal system, two polygons are said to be adjacent if they share a side. The characteristic graph (or dualist or inner dual) of a given k-polygonal system consists of vertices corresponding to k-polygons of the system; two vertices are adjacent if and only if the corresponding k-polygons are adjacent. A k-polygonal system whose characteristic graph is the path graph is called k-polygonal chain. In a k-polygonal chain, a k-polygon having one (respectively two) neighboring k-polygon(s) is called terminal (respectively non-terminal). A k-polygonal chain can be represented by a graph (called k-polygonal chain graph) in which the edges represent sides of a k-polygon while the vertices correspond to the points where two sides of a k-polygon meet.

In a 4-polygonal (polyomino) chain graph, a non-terminal square having a vertex of degree 2 is known as a kink. A linear polyomino chain graph is the one, without kinks. A zigzag polyomino chain graph is the one, consisting of only kinks and terminal squares.

Theorem 116. [4,5] *Among the polyomino chain graphs with* $n = 2h+2$ *vertices,* $h \geq 3$,

- *the linear polyomino chain graph uniquely minimizes (respectively, maximizes)* ${}^0R_\alpha$ *for* $\alpha < 0$ *and* $\alpha > 1$ *(respectively, for* $0 < \alpha < 1$*)*,
- *the zigzag polyomino chain graph uniquely maximizes (respectively, minimizes)* ${}^0R_\alpha$ *for* $\alpha < 0$ *and* $\alpha > 1$ *(respectively, for* $0 < \alpha < 1$*)*.

In a 5-polygonal (pentagonal) chain graph, a kink is a non-terminal pentagon which contains an edge connecting the vertices of degree 2. The linear pentagonal chain graph is the one, having no kink. A pentagonal chain graph consisting of only kinks and terminal pentagons is called zigzag pentagonal chain graph. A segment of a pentagonal chain graph, is the maximal linear chain subgraph, including kinks and/or terminal pentagons at its end. A segment containing terminal pentagon(s) is called a terminal segment and a segment that is not terminal is known as a non-terminal segment. The number of pentagons in a segment is called its length. Let Ω_n be the set of of pentagonal chain graphs with $n = 3h + 2$ vertices, $h \geq 3$, in which every non-terminal segment of length 3 (if such does exist) contains no edge connecting the both vertices of degree 3. The next result directly follows from Theorem 3.6 of [6].

Theorem 117. [6] *If $\alpha < 0$ or $\alpha > 1$, then among the members of the set Ω_n,*

- *the linear pentagonal chain graph uniquely minimizes ${}^0R_\alpha$,*
- *the zigzag pentagonal chain graph uniquely maximizes ${}^0R_\alpha$.*

A 3-polygonal (triangular) chain graph in which every vertex has degree at most four is said to be a linear triangular chain graph. An induced subgraph H of a triangular chain graph T_c is said to be segment if H forms a maximal linear triangular chain subgraph of T_c. Denote by $s(T_c)$ (or simply by s) the number of segments in a triangular chain graph T_c. Obviously, $s \geq 1$ and $s = 1$ if and only if T_c is linear. Denote by $\mathfrak{T}_n$ the set of triangular chain graphs with $n = h + 2$ vertices, $h \geq 4$, in which every vertex has degree at most 5. If $T_c \in \mathfrak{T}_n$, then by using a result from [3], we have

$$ {}^0R_\alpha(T_c) = 4^\alpha + 2^{\alpha+1} + 3^\alpha - 5^\alpha + (3^\alpha - 2 \cdot 4^\alpha + 5^\alpha)s \, . $$

But, by virtue of Lagrange's mean value theorem,

$$ 3^\alpha - 2 \cdot 4^\alpha + 5^\alpha \begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ < 0 & \text{if } 0 < \alpha < 1 \end{cases} $$

and hence (bearing in mind the fact $s \geq 1$), it follows:

Theorem 118. [3] *Among the elements of the set $\mathfrak{T}_n$, the linear triangular chain graph uniquely*

- *minimizes ${}^0R_\alpha$ for $\alpha < 0$ and $\alpha > 1$,*
- *maximizes ${}^0R_\alpha$ for $< 0 < \alpha < 1$.*

Tomescu *et al.* [142] determined the unique species having maximal ${}^0R_\alpha$ value, $\alpha \geq 1$, among graphs with fixed order and connectivity (and with fixed order and edge-connectivity).

Theorem 119. [142] *Among the n-vertex graphs, $n \geq 3$, with connectivity $\kappa \geq 1$, $K_\kappa + (K_1 \cup K_{n-\kappa-1})$ is the unique graph with maximal ${}^0R_\alpha$ value for $\alpha \geq 1$.*

Corollary 120. [142] *If the connectivity "κ" is replaced by the edge-connectivity "λ" throughout Theorem 119, then the resulting statement remains true.*

The next theorem and corollary, extended versions of Theorem 119 and Corollary 120, respectively, are due to Wu *et al.* [151].

Theorem 121. [151] *Let $n \geq 3$ and $1 \leq \kappa \leq n-2$. Among the n-vertex graphs with connectivity κ, $K_\kappa + (K_1 \cup K_{n-\kappa-1})$ is the unique graph with*

- *maximal ${}^0R_\alpha$ value for $\alpha > 0$,*
- *minimal ${}^0R_\alpha$ value for $\alpha < 0$.*

Corollary 122. [151] *If the connectivity "κ" is replaced by the edge-connectivity "λ" throughout Theorem 121, then the resulting statement remains true.*

Let $S(n,r)$ be the graph obtained by attaching exactly one pendent path (possibly of zero length) to each vertex of the complete graph K_{n-r} such that the lengths of the attached pendent paths differ by at most 1. For $\frac{n}{2} \leq r \leq n-2$, let $\mathbb{H}_{n,r}$ be the class of graphs obtained by attaching exactly one pendent path (with length ≥ 1) to each vertex of the complete graph K_{n-r}.

Theorem 123. [151] *For $\alpha > 1$, among the connected n-vertex graphs with r cut vertices,*

- *$S(n,r)$ is the unique graph with the maximal ${}^0R_\alpha$ value for $0 < r \leq \frac{n}{2}$,*
- *the graph with the maximal ${}^0R_\alpha$ value, for $\frac{n}{2} < r \leq n-2$, belongs to the set $\mathbb{H}_{n,r}$.*

The next result is also due to Tomescu *et al.* [142].

Theorem 124. [142] *Let G be a 2-connected or 2-edge-connected graph with $n \geq 3$ vertices. Then for $\alpha > 0$, ${}^0R_\alpha(G)$ is minimal if and only if $G \cong C_n$.*

Chen *et al.* [23] characterized the unique graph having maximal (respectively, minimal) ${}^0R_\alpha$ value for $\alpha > 0$ (respectively, $\alpha < 0$), among bipartite connected graphs with fixed order and matching number.

Theorem 125. [23] *Among the bipartite connected n-vertex graphs with matching number β, $K_{\beta,n-\beta}$ is the unique graph with*

- *maximal ${}^0R_\alpha$ value for $\alpha > 0$,*
- *minimal ${}^0R_\alpha$ value for $\alpha < 0$.*

Yu and Feng [156] determined the unique graph having maximal ${}^0R_\alpha$ value for $\alpha > 1$, among all connected graphs with fixed order and matching number.

Theorem 126. [156] *Among the connected n-vertex graphs with matching number β, $K_\beta + \overline{K}_{n-\beta}$ is the unique graph with maximal ${}^0R_\alpha$ value for $\alpha > 1$.*

The vertex bipartiteness of a graph G is denoted by $v_b(G)$ (or simply by v_b) and is defined as the minimal number of vertices of G whose removal makes G bipartite [47]. Let $\mathfrak{G}_{n,a}$ be the set of connected n-vertex graphs satisfying $v_b \le a \le n-2$. We end this section with the following extremal result, which was recently proved by Chen *et al.* [24].

Theorem 127. [24] *Let $a \ge 1$ and $n \ge 4$. In the set $\mathfrak{G}_{n,a}$, $K_a + K_{\lfloor \frac{n-a}{2} \rfloor, \lceil \frac{n-a}{2} \rceil}$ is the unique graph with the*

- *maximal ${}^0R_\alpha$ value for $0 < \alpha \le 1$,*
- *minimal ${}^0R_\alpha$ value for $\alpha < 0$.*

Recently, some extremal results for the invariant ${}^0R_\alpha$ were established in [85].

Theorem 128. [85] *If T is an n-vertex tree, $n \ge 6$, with p pendent vertices, $3 \le p \le n-2$, then*

$$
{}^0R_\alpha(T) \begin{cases} \le 2^\alpha n + p^\alpha - (2^\alpha - 1)p - 2^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ \ge 2^\alpha n + p^\alpha - (2^\alpha - 1)p - 2^\alpha & \text{if } 0 < \alpha < 1\,. \end{cases}
$$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(p, \underbrace{2,\ldots,2}_{n-p-1}, \underbrace{1,\ldots,1}_{p})$.

Theorem 129. [85] *If T is an n-vertex tree, $n \ge 6$, with p pendent vertices, $3 \le p \le n-2$, then*

$$
{}^0R_\alpha(T) \begin{cases} \ge [(n-p)t - n + 2]t^\alpha + [2n - p - (n-p)t - 2](t+1)^\alpha + p & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ \le [(n-p)t - n + 2]t^\alpha + [2n - p - (n-p)t - 2](t+1)^\alpha + p & \text{if } 0 < \alpha < 1\,. \end{cases}
$$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(\underbrace{t+1,\ldots,t+1}_{2n-p-(n-p)t-2}, \underbrace{t,\ldots,t}_{(n-p)t-n+2}, \underbrace{1,\ldots,1}_{p})$.

Theorem 130. [85] *If T is an n-vertex tree, $n \geq 6$, with b branching vertices, $1 \leq b \leq n/2-1$, then*

$$ {}^0R_\alpha(T) \begin{cases} \geq 2^\alpha n + (3^\alpha - 2^{\alpha+1}+1)b - 2^{\alpha+1}+2 & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ \leq 2^\alpha n + (3^\alpha - 2^{\alpha+1}+1)b - 2^{\alpha+1}+2 & \text{if } 0 < \alpha < 1 . \end{cases} $$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(\underbrace{3,\dots,3}_{b},\underbrace{2,\dots,2}_{n-2b-2},\underbrace{1,\dots,1}_{b+2})$.

Theorem 131. [85] *If T is an n-vertex tree, $n \geq 6$, with b branching vertices, $1 \leq b \leq n/2-1$, then*

$$ {}^0R_\alpha(T) \begin{cases} \leq (n-2b+1)^\alpha + n + (3^\alpha - 1)b - 3^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ \geq (n-2b+1)^\alpha + n + (3^\alpha - 1)b - 3^\alpha & \text{if } 0 < \alpha < 1 . \end{cases} $$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(n-2b+1,\underbrace{3,\dots,3}_{b-1},\underbrace{1,\dots,1}_{n-b})$.

A segment of a tree is a path P, whose terminal vertices are branching or/and pendent, and all non-terminal vertices (if such exist) have degree 2. A vertex with degree 2 is called an even-prime vertex [85]. The number of segments of a tree T can be determined from the number of even-prime vertices of T and vise versa [97]. Hence, the problem of finding trees with extremal ${}^0R_\alpha$ values among all n-vertex trees with fixed segments is equivalent to the problem of finding trees with extremal ${}^0R_\alpha$ values from the collection of n-vertex trees with fixed even-prime vertices.

Theorem 132. [85] *If T is an n-vertex tree, $n \geq 6$, with k segments, $3 \leq k \leq n-2$, then*

$$ {}^0R_\alpha(T) \begin{cases} \leq 2^\alpha n + k^\alpha - (2^\alpha - 1)k - 2^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1 \\ \geq 2^\alpha n + k^\alpha - (2^\alpha - 1)k - 2^\alpha & \text{if } 0 < \alpha < 1 . \end{cases} $$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(k,\underbrace{2,\dots,2}_{n-k-1},\underbrace{1,\dots,1}_{k})$.

Theorem 133. [85] *Let T be an n-vertex tree, $n \geq 6$, with k segments, $3 \leq k \leq n-2$. If $\alpha < 0$ or $\alpha > 1$, then the following inequality holds:*

$$ {}^0R_\alpha(T) \geq \begin{cases} f(n,k) + 4^\alpha - 2\cdot 3^\alpha - 2^\alpha + 2 & \text{if } k \text{ is even} \\ f(n,k) + \frac{1}{2}\left[3 - 3^\alpha - 2^{\alpha+1}\right] & \text{if } k \text{ is odd} \end{cases} $$

where $f(n,k) = 2^\alpha n + \frac{1}{2}\left[3^\alpha - 2^{\alpha+1} + 1\right]k$. If $0 < \alpha < 1$, then the inequality is reversed. In either case, the bound is best possible and is attained if and only if T has the degree sequence π:

$$ \pi = \begin{cases} (4, \underbrace{3,\dots,3}_{\frac{k-4}{2}}, \underbrace{2,\dots,2}_{n-k-1}, \underbrace{1,\dots,1}_{\frac{k+4}{2}}) & \text{if } k \text{ is even} \\ (\underbrace{3,\dots,3}_{\frac{k-1}{2}}, \underbrace{2,\dots,2}_{n-k-1}, \underbrace{1,\dots,1}_{\frac{k+3}{2}}) & \text{if } k \text{ is odd}. \end{cases} $$

3 Modified first Zagreb index

The graph invariant ${}^0R_{-2}$ was considered in [123] under the name modified first Zagreb index.

3.1 Bounds

Hao [70] obtained some bounds on the invariant ${}^0R_{-2}$.

Theorem 134. [70] *Let G be a connected non-trivial n-vertex graph with minimal degree δ and maximal degree Δ. If n is even, then*

$$ \frac{n^2}{{}^0R_2(G)} \leq {}^0R_{-2}(G) \leq \frac{1}{{}^0R_2(G)}\left[n^2 + \left(\frac{\Delta}{\delta} - \frac{\delta}{\Delta}\right)^2 \left\lfloor \frac{n}{2} \right\rfloor^2\right]. $$

If n is odd, then

$$ \frac{n^2}{{}^0R_2(G)} \leq {}^0R_{-2}(G) \leq \frac{1}{{}^0R_2(G)}\left[n^2 + \left(\frac{\Delta}{\delta} - \frac{\delta}{\Delta}\right)^2 \left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right)\right]. $$

The equality $n^2 = {}^0R_2(G) \cdot {}^0R_{-2}(G)$ holds if and only if G is a regular graph.

Theorem 135. [70] *If G is a connected non-trivial (n,m)-graph with minimal degree δ, maximal degree Δ, and*

$$ \Theta = m\left[\frac{2m}{n-1} + \frac{\Delta(n-2)}{n-1} + (\Delta - \delta)\left(1 - \frac{\Delta}{n-1}\right)\right] $$

then

$$\max\left\{\frac{n^3}{4m^2}, \frac{n^2}{\Theta}, \frac{n}{\left(\sqrt[n]{NK(G)}\right)^2}\right\} \le {}^0R_{-2}(G) \le n-1+\frac{1}{(n-1)^2}$$

with left equality if and only if G is regular, and with right equality if and only if $G \cong S_n$.

In addition to other results, some lower bounds on ${}^0R_{-2}$ were also derived in [60].

Theorem 136. [60] *If G is an n-vertex graph with minimal degree δ, maximal degree Δ, and no isolated vertices, then*

$$ {}^0R_{-2}(G) \ \ge\ \frac{n^2}{{}^0R_2(G)} + \frac{1}{\Delta^2+\delta^2}\left(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\right)^2$$

$$ {}^0R_{-2}(G) \ \ge\ \frac{\left({}^0R_{-1}(G)\right)^2}{n} + \frac{1}{2}\left(\frac{1}{\delta}-\frac{1}{\Delta}\right)^2 .$$

The equality sign in any of the above inequalities holds if and only if G is regular.

Clearly, the first lower bound, stated in Theorem 136 is better than the one, given in Theorem 134.

Theorem 137. [60] *If G is an n-vertex graph with minimal degree δ, maximal degree Δ, and no isolated vertices, then*

$$ {}^0R_{-2}(G) \ge {}^0R_{-1}(G)\left(\frac{1}{\delta}+\frac{1}{\Delta}\right) - \frac{n-2}{4}\left(\frac{1}{\delta}+\frac{1}{\Delta}\right)^2$$

with equality if and only if G has the degree sequence $(\Delta, \underbrace{c,\dots,c}_{n-2}, \delta)$, where $c = \frac{\Delta+\delta}{2}$.

3.2 Extremal results

We could not find any extremal result, concerning the invariant ${}^0R_{-2}$ only. Needless to say, most of the extremal results concerning general ${}^0R_\alpha$ (collected in Section 2.1) cover also those concerning ${}^0R_{-2}$.

4 Inverse degree or modified total adjacency index

It seems that the graph invariant ${}^0R_{-1}$ was first considered within pure graph theory under the name inverse degree – in some conjectures generated by the computer program

Graffiti [45]. The invariant ${}^0R_{-1}$ was also introduced independently within chemical graph theory, under the name modified total adjacency index [123]. In this section, we collect all bounds and extremal results concerning ${}^0R_{-1}$.

4.1 Bounds

The average distance of a graph G is defined as the average of the distances between all unordered pairs of vertices of G. Recall that it is closely related to the Wiener index, namely the sum of distances between all unordered pairs of vertices [37, 135, 153].

The diameter of a graph G is the greatest distance between two vertices of G. In 1988, Erdős *et al.* [43], refuted the following Graffiti conjecture, related to a lower bound on ${}^0R_{-1}$ and obtained an inequality involving ${}^0R_{-1}$, given in Theorem 139.

Conjecture 138. *If μ is the average distance of a connected non-trivial graph G, then*

$$ {}^0R_{-1}(G) \geq \mu \,. $$

Theorem 139. [43] *If G is a connected non-trivial n-vertex graph with diameter d, then*

$$ \left[6\,{}^0R_{-1}(G) + 2 + o(1)\right] \frac{\log n}{\log \log n} \geq d \,. $$

The eccentricity of a vertex v in a graph is the distance from v to a vertex farthest from v. The radius of a graph G is the minimal vertex eccentricity in G. Dankelmann *et al.* [31] disproved the following Graffiti conjecture, related to a lower bound on ${}^0R_{-1}$.

Conjecture 140. *If a connected non-trivial graph G has average distance μ and radius r, then*

$$ {}^0R_{-1}(G) \geq r - \mu \,. $$

The matching number of a graph is the number of edges in a maximal matching. In [106, 163], the following conjecture of Graffiti, concerning a lower bound on ${}^0R_{-1}$, was disproved and a related lower bound was derived (mentioned in Theorem 142).

Conjecture 141. *If T is a non-trivial n-vertex tree with matching number β, then*

$$ {}^0R_{-1}(T) \geq n - 2 - \beta \,. $$

Let $\mathbb{F}$ be the class of trees satisfying the following properties:

1. The star S_5 is a member of $\mathbb{F}$,

2. If $T \in \mathbb{F}$, then the tree $(T \cup S_4) + uv$ also belongs to $\mathbb{F}$, where $V(T) \cap V(S_4) = \emptyset$, $u \in V(T)$ is a pendent vertex and $v \in V(S_4)$ is the branching vertex. Also, let $\mathbb{F}' = \{T_k, k = 0, 1, 2, \ldots\}$, where $T_0 = P_4$, $V(T_k) = V(T_{k-1}) \cup \{u_1, u_2\}$, $E(T_k) = E(T_{k-1}) \cup \{v'u_1, u_1u_2\}$, $u_1, u_2 \notin V(T_{k-1})$ and the vertex $v' \in V(T_{k-1})$ has degree $k+1 = \frac{1}{2}|V(T_{k-1})|$ in T_{k-1}. The authors of [106, 163] obtained lower and upper bound on ${}^0R_{-1}$, stated in the next theorem.

Theorem 142. [106, 163] *If T is an n-vertex tree, $n \geq 5$, then*

$$\frac{15n+9}{16} - \beta \leq {}^0R_{-1}(T) \leq \frac{5}{4}n - \frac{1}{2} + \frac{2}{n} - \beta$$

with left equality if and only if $T \in \mathbb{F}$, and with right equality if and only $T \in \mathbb{F}'$.

Cioabă [28] proved the following result, whose lower bound can be obtained from a more general result – Theorem 6.

Theorem 143. [28] *If G is a connected n-vertex non-trivial graph with size m, minimal degree δ, and maximal degree Δ, then*

$$\frac{n^2}{2m} \leq {}^0R_{-1}(G) \leq \frac{n^2}{2m} + \left(\frac{1}{\delta} - \frac{1}{\Delta}\right)\left(n - 1 - \frac{2m}{n}\right)$$

with equality if and only if G is regular or $G \cong S_n$.

Liu and one of the present authors [100] established several bounds on the invariant ${}^0R_{-1}$.

Theorem 144. [100] *If G is an n-vertex graph without isolated vertices, then*

$$\frac{1}{n}\left[{}^0R_{-1/2}(G)\right]^2 \leq {}^0R_{-1}(G) \leq \sqrt{n \cdot {}^0R_{-2}(G)}$$

with equality if and only if G is regular.

Theorem 145. [100] *If G is an n-vertex graph without isolated vertices, then*

$$\sqrt{{}^0R_{-2}(G) \cdot 2M_2^*(G)} \leq {}^0R_{-1}(G) \leq \left[{}^0R_{-1/2}(G)\right]^2 - 2R(G),$$

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

Theorem 146. [100] *If G is a non-trivial (n,m)-graph without isolated vertices, then*

$$\sqrt{{}^0R_{-2}(G) + n(n-1)\,[NK(G)]^{-2/n}} \leq {}^0R_{-1}(G) \leq \left[{}^0R_{-\frac{1}{2}}(G)\right]^2 - n(n-1)\,[NK(G)]^{-1/n}$$

with equality if and only if G is regular. Also, it holds that

$$n\,[NK(G)]^{-1/n} < {}^0R_{-1}(G) < \frac{n^2}{n^2\sqrt{NK(G)} - 2m(n-1)}$$

and

$$n\left[\frac{n \cdot NK(G)}{2m}\right]^{-1/(n-1)} \leq {}^0R_{-1}(G) \leq \left(\frac{2m}{n}\right)^{n-1} \frac{n}{NK(G)}\,.$$

The next bound, which improves the bound given in Theorem 139, is due to Dankelmann *et al.* [32].

Theorem 147. [32] *If G is a connected non-trivial n-vertex graph with diameter d and large n, then*

$$\left[3\,{}^0R_{-1}(G) + 2 + o(1)\right] \frac{\log n}{\log\log n} \geq d\,.$$

Due to the fact $\mu(G) \leq d(G)$, both inequalities mentioned in Theorems 139 and 147 can be rewritten in terms of $\mu(G)$. Li and Shi [92] improved a bound on ${}^0R_{-1}$ given by Dankelmann et al. [32], for the case of trees and unicyclic graphs.

An edge-cut of a connected graph G is a set of edges whose removal disconnects G. The edge connectivity is denoted by $\lambda(G)$ (or simply by λ) and is defined as the minimal cardinality of an edge-cut over all edge-cuts of G. A graph is said to be maximally edge-connected if $\lambda = \delta$. Dankelmann *et al.* [30] established some lower bounds on ${}^0R_{-1}$ for particular graph types.

Theorem 148. [30] *Let G be a connected non-trivial n-vertex graph with minimal degree δ. If G is not a maximally edge-connected graph, then*

$${}^0R_{-1}(G) \geq 2 + \frac{2}{\delta(\delta+1)} + \frac{n-2\delta}{(n-\delta-2)(n-\delta-1)}\,.$$

Corollary 149. [30] *Let G be a connected non-trivial n-vertex graph. If G is not a maximally edge-connected graph, then ${}^0R_{-1}(G) \geq 2$.*

Theorem 150. [30] *Let G be a connected triangle–free n-vertex graph, $n \geq 2$, with minimal degree δ. If G is not a maximally edge-connected graph, then*

$${}^0R_{-1}(G) \geq 4 - 4(\delta-1)\left(\frac{1}{4\delta(\delta+1)} + \frac{1}{(n-2\delta)(n-2\delta+2)}\right).$$

Su *et al.* [138] generalized Theorems 148 and 150 (see Theorems 56 and 57, respectively).

An edge-cut S of a graph is a minimal edge-cut if $|S| = \lambda$. A graph G is called super edge-connected if every minimal edge-cut consists of edges incident with a vertex of minimal degree. Clearly, every super edge-connected graph is also a maximally edge-connected graph. Tian *et al.* [140] extended the results of Dankelmann *et al.* [30] to super edge-connected graphs.

Theorem 151. [140] *Let G be a connected non-trivial n-vertex graph with minimal degree δ. If G is not super edge-connected, then*

$$ {}^{0}R_{-1}(G) \geq 2 + \frac{n-2\delta}{(n-\delta-1)(n-\delta)} \,. $$

If G contains no K_δ with all its vertices of degree δ, then the bound given in Theorem 151 can be improved slightly:

Theorem 152. [140] *Let G be a connected non-trivial n-vertex graph with minimal degree δ, such that it contains no K_δ with all its vertices of degree δ. If G is not super edge-connected, then*

$$ {}^{0}R_{-1}(G) \geq 2 + \frac{1}{\delta(\delta+1)} + \frac{n-2\delta-1}{(n-\delta-1)(n-\delta-2)} \,. $$

Theorem 153. [140] *Let G be a connected triangle–free n-vertex graph with minimal degree $\delta \geq 3$. If G is not super edge-connected, then*

$$ {}^{0}R_{-1}(G) \geq 4 - \frac{1}{\delta} - \frac{4\delta}{(n-2\delta+1)(n-2\delta+3)} \,. $$

Mukwembi [119] established several bounds on ${}^{0}R_{-1}$ and posed two upper bounds as conjecture.

Theorem 154. [119] *If T is a tree with $n \geq 3$ vertices and diameter d, then*

$$ \frac{n}{2} + \sqrt{\frac{n}{2}} - d \leq {}^{0}R_{-1}(T) \leq \frac{3n}{2} - d \,. $$

The upper bound is tight. The lower bound is close to the best possible in the sense that there exist trees T_n satisfying the hypothesis of the theorem such that

$$ {}^{0}R_{-1}(T_n) + d(T_n) = \frac{n}{2} + 2\sqrt{n-1} + o(1) \,. $$

Theorem 155. [119] *Let T be a tree with n_1 pendent vertices and diameter d. If q and ε, $0 \le \varepsilon < d-1$, are unique integers for which $n_1 - 2 = q(d-1) + \varepsilon$, then*

$$^0R_{-1}(T) \ge n_1 + \frac{d-1}{q+2} - \frac{\varepsilon}{(q+2)(q+3)} .$$

Moreover the bound is sharp for all values of d and n_1.

Theorem 156. [119] *If G is a k-regular connected graph, $k \ge 3$, with diameter d, then*

$$^0R_{-1}(G) \ge \frac{k+1}{3k}\left(d + \frac{6}{k+1} - 1\right)$$

and this inequality is tight.

Theorem 157. [119] *If G is a connected non-trivial molecular graph with diameter d, then*

$$^0R_{-1}(G) \ge \frac{d-3}{3} .$$

Also, if G is a connected planar graph with $n \ge 3$ vertices and diameter d, then

$$^0R_{-1}(G) \ge \frac{1}{6}\left(d + \frac{4}{n-2} + 3\right) .$$

As the bounds given in Theorem 157 seem to be not the best possible, Mukwembi [119] conjectured that, for molecular and planar graphs, essentially the bound for 4-regular and 3-regular graphs apply respectively:

Conjecture 158. [119] *If G is a connected non-trivial molecular graph with diameter d, then*

$$d \le \frac{12}{5} \cdot {^0R_{-1}(G)} + o(1)$$

and this inequality is tight. Also, if G is a connected planar non-trivial graph with diameter d, then

$$d \le \frac{9}{4} \cdot {^0R_{-1}(G)} + o(1)$$

and this inequality is also tight.

Chen and Fujita [26] settled the first inequality of Conjecture 158. Das *et al.* [36] obtained several additional bound on $^0R_{-1}$.

Theorem 159. [36] *Let G be an n-vertex graph, $n \ge 3$, with size m, minimal degree δ, maximal degree Δ, and without isolated vertices. Then*

$$^0R_{-1}(G) \ge \frac{\Delta+\delta}{\Delta\delta} + \sqrt{\frac{4(n-2)^3\Delta\delta}{(\Delta+\delta)^2\left[2m(\Delta+\delta) - n\Delta\delta - \Delta^2 - \delta^2\right]}}$$

with equality if and only if G is regular.

Theorem 160. [36] *Let G be an n-vertex graph, $n \geq 3$, with size m, minimal degree δ, maximal degree Δ, and without isolated vertices. Then*

$$\frac{\Delta+\delta}{\Delta\delta}+\frac{(n-2)^2}{2m-\Delta-\delta} \leq {}^0R_{-1}(G) \leq \frac{\Delta+\delta}{\Delta\delta}+\frac{(n-2)[(n-3)(\Delta^2+\delta^2)+2\delta\Delta]}{2\delta\Delta(2m-\Delta-\delta)}$$

with left equality if and only if G has the degree sequence $(d_1, \underbrace{d_2, \ldots, d_2}_{n-2}, d_n)$, where $d_1 \geq d_2 \geq d_n$, and the right equality holds for regular graphs.

In the next two theorems relations between ${}^0R_{-1}(G)$ and the Kirchhoff index $Kf(G)$ are given.

Theorem 161. [36] *If G is a connected non-trivial n-vertex graph having m edges such that $2m\sqrt{n} \leq (n-1)^2\delta$, then*

$$ {}^0R_{-1}(G) \leq \frac{1}{\sqrt{n}}\, Kf(G)\,. $$

Theorem 162. [164] *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$ Kf(G) \geq -1 + (n-1)\, {}^0R_{-1}(G)\,, $$

with equality if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \leq r \leq \lceil \frac{n}{2} \rceil$.

Theorem 163. [36] *If G is a graph with minimal degree $\delta \geq 2$, then*

$$ {}^0R_{-1}(G) < ABC(G). $$

Theorem 164. [36] *If $\overline{G}$ is the complement graph of a graph G and minimal degrees of both G, $\overline{G}$ are greater than 1, then*

$$ {}^0R_{-1}(G) + {}^0R_{-1}\left(\overline{G}\right) < ABC(G) + ABC\left(\overline{G}\right). $$

Theorem 165. [36] *If G is a graph with average degree $\overline{d}$, minimal degree δ and maximal degree Δ such that*

$$ \overline{d} \geq \sqrt{\frac{\Delta}{\delta^3}} $$

then ${}^0R_{-1}(G) \leq GA(G)$.

The lower bound on ${}^0R_{-1}$, stated in Theorem 143, can be strengthened as:

Theorem 166. [60] *Let G be an n-vertex graph without isolated vertices, size m, minimal degree δ, and maximal degree Δ. If*

$$\Theta = \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2$$

then

$$\frac{n^2}{2m} + \frac{\Theta}{\Delta + \delta} \le {}^0R_{-1}(G) \le \frac{1}{\Delta} + \frac{1}{\delta} + \frac{(n-2)^2}{2m - \Delta - \delta} + \frac{(n-2)(n-3)\Theta}{2(2m - \Delta - \delta)}\,.$$

The left equality holds if and only if G has the degree sequence $(\Delta, \underbrace{c, \ldots, c}_{n-2}, \delta)$, where $c = \frac{\Delta+\delta}{2}$, and the right equality holds if and only if G is regular.

The next result is an immediate consequence of Theorem 166.

Corollary 167. [60] *Let G be an n-vertex graph without isolated vertices, size m, minimal degree δ, and maximal degree Δ. It holds that*

$${}^0R_{-1}(G) \le \frac{n^2}{2m} + \frac{n(n-1)}{4m} \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2$$

with equality if and only if G is regular.

An inequality establishing a relationship between ${}^0R_{-1}$ and Π_1 was proved in [65].

Theorem 168. [65] *Let G be a simple connected graph with $n \ge 2$ vertices. Then*

$$\frac{(\sqrt{\Delta} - \sqrt{\delta})^2}{\Delta\delta} \le {}^0R_{-1}(G) - n\big(\Pi_1(G)\big)^{-1/2n} \le n^2\alpha(n)\, \frac{(\sqrt{\Delta} - \sqrt{\delta})^2}{\Delta\delta}\,.$$

Recently Das *et al.* [33] derived several bounds on the invariant ${}^0R_{-1}$.

Theorem 169. [33] *If G is a connected non-trivial n-vertex graph with maximal degree Δ and minimal degree δ, then*

$${}^0R_{-1}(G) \ge \frac{2}{\Delta} \left[R(G) + \frac{\Delta - \delta}{4\Delta\delta^2\,(\delta+1)} + \frac{1}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{1+\delta}} \right)^2 \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right) \right]$$

with equality if and only if G is regular.

Theorem 170. [33] *If G is a connected non-trivial (n,m)-graph with maximal degree Δ and minimal degree δ, then*

$${}^0R_{-1}(G) \ge \frac{2}{\delta} \left[R(G) + \frac{m}{2} \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right)^2 + \frac{m}{4} \left(\frac{1}{\delta^2} - \frac{1}{\Delta^2} \right) (\Delta - \delta) \right]$$

with equality if and only if G is regular.

Theorem 171. [33] *If G is a connected non-trivial n-vertex graph with maximal degree Δ, then*

$$ {}^0R_{-1}(G) \geq \frac{2}{\Delta} H(G) $$

where $H(G)$ is the harmonic index, Eq. (6). Equality holds if and only if G is regular.

Theorem 172. [33] *If G is a connected non-trivial n-vertex graph with $d_i \geq d_j \geq \sqrt{d_i}+1$ for any edge $ij \in E(G)$, then ${}^0R_{-1}(G) < H(G)$.*

Theorem 173. [33] *If T is a non-trivial tree, then ${}^0R_{-1}(T) > \max\{R(T), H(T)\}$.*

4.2 Extremal results

Xu and Das [152] solved several extremal problems concerning the graph invariant ${}^0R_{-1}$. In order to state the first result of [152], we need the definition of the chain of two graphs given earlier in connection with Theorem 96.

Theorem 174. [152] *If G is a connected n-vertex graph with chromatic number χ, $2 \leq \chi \leq n-1$, then*

$$ {}^0R_{-1}\left(T_\chi(n)\right) \leq {}^0R_{-1}(G) \leq {}^0R_{-1}\left(C(K_\chi, S_{n-\chi+1}; t, w)\right). $$

The left equality holds if and only if $G \cong T_\chi(n)$. The right equality holds if and only if $G \cong C(K_\chi, S_{n-\chi+1}; t, w)$, where $T_\chi(n)$ is the Turán graph, t is any vertex of the complete graph K_χ, and w is the center of the star $S_{n-\chi+1}$.

A clique of a graph G is a maximal subset of mutually adjacent vertices of G. The clique number of G is denoted by $\omega(G)$ (or simply by ω) and is defined as the number of vertices of a largest clique in G.

Theorem 175. [152] *If the chromatic number χ is replaced by the clique number ω throughout Theorem 174, then the resulting statement remains true.*

A cut edge of a connected graph G is an edge whose removal disconnects G (in two components).

Theorem 176. [152] *If G is a connected n-vertex graph with k cut edges, $1 \leq k \leq n-3$, then*

$$ {}^0R_{-1}\left(C(K_k, P_{n-k+1}; t, v)\right) \leq {}^0R_{-1}(G) \leq {}^0R_{-1}\left(C(C_{n-k}, S_{k+1}; u, w)\right) $$

with left equality if and only if $G \cong C(K_k, P_{n-k+1}; t, v)$*, and with right equality if and only if* $G \cong C(C_{n-k}, S_{k+1}; u, w)$*, where the vertices* $u \in V(C_{n-k})$*,* $t \in V(K_k)$ *are arbitrary,* $v \in V(P_{n-k+1})$ *is a pendent vertex, and* $w \in V(S_{k+1})$ *is the center.*

Theorem 177. [152] *If the number of cut edges* k *is replaced by the clique number* ω *throughout Theorem 176, then the resulting statement remains true.*

The (vertex) connectivity of a non-trivial graph G is denoted by $\kappa(G)$ (or simply by κ) and is defined as the minimal number of vertices whose removal either increases the number of components of G or makes G a trivial graph. Let $\mathcal{V}(n,\ell)$ and $\mathcal{E}(n,\ell)$ be the sets of all non-trivial n-vertex graphs with connectivity κ and edge-connectivity λ, respectively, such that: $\kappa, \lambda \leq \ell \leq n-1$. Denote by $\mathcal{V}(n,\kappa)$ and $\mathcal{E}(n,\lambda)$ the sets of connected non-trivial n-vertex graphs with connectivity κ and edge-connectivity λ, respectively.

Theorem 178. [152] *If* $1 \leq \ell \leq n-1$ *and* $G \in \mathcal{V}(n,\ell)$ *or* $G \in \mathcal{E}(n,\ell)$ *then*

$$^{0}R_{-1}(G) \leq {}^{0}R_{-1}\left(S_n\right)$$

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

Theorem 179. [152] *If* $1 \leq \ell \leq n-1$ *and* $G \in \mathcal{E}(n,\ell)$*, then*

$$^{0}R_{-1}(G) \geq {}^{0}R_{-1}\left(K_\ell + (K_1 \cup K_{n-\ell-1})\right)$$

with equality if and only if $G \cong K_\ell + (K_1 \cup K_{n-\ell-1})$*.*

Theorem 180. [142,152] *If the number* ℓ *is replaced by the edge-connectivity* λ *throughout Theorem 179, then the resulting statement remains true.*

Theorem 181. [152] *If* $1 \leq \ell \leq n-1$ *and* $G \in \mathcal{V}(n,\ell)$*, then*

$$^{0}R_{-1}(G) \geq {}^{0}R_{-1}\left(K_\ell + (K_1 \cup K_{n-\ell-1})\right)$$

with equality if and only if $G \cong K_\ell + (K_{n_1} \cup K_{n_2})$*,* $n_1 + n_2 = n-1$ *for* $\ell = 1$*, and* $G \cong K_\ell + (K_1 \cup K_{n-\ell-1})$ *for* $\ell \geq 2$*.*

Theorem 182. [142, 152] *If the number* ℓ *is replaced with the connectivity* κ *throughout Theorem 181, then the resulting statement remains true.*

A set of mutually non-adjacent vertices of a graph is said to be an independent (or stable) set. The independence (or stability) number of a graph G is defined as the cardinality of a maximal independent set in G. Let $\mathcal{B}(n,\beta)$ and $\mathcal{A}(n,\alpha')$ be the set of connected non-trivial n-vertex graphs with matching number β and independence number α', respectively. Denote by $S^*_{n,a}$ the tree obtained from the star S_{a+1} by attaching a pendent vertex to each of its $n-a-1$ pendent vertices.

Theorem 183. [152] *If $\alpha' < n-1$ and $G \in \mathcal{A}(n,\alpha')$, then*

$$^0R_{-1}\left(K_{n-\alpha'} + \overline{K}_{\alpha'}\right) \le {}^0R_{-1}(G) \le {}^0R_{-1}\left(S^*_{n,\alpha'}\right)$$

with left equality if and only if $G \cong K_{n-\alpha'} + \overline{K}_{\alpha'}$, and with right equality if and only if $G \cong S^*_{n,\alpha'}$.

Theorem 184. [152] *If $\beta = \lfloor \frac{n}{2} \rfloor$ and $G \in \mathcal{B}(n,\beta)$, then $^0R_{-1}(G) \ge {}^0R_{-1}(K_n)$ with equality if and only if $G \cong K_n$. If $2 \le \beta < \lfloor \frac{n}{2} \rfloor$ and $G \in \mathcal{B}(n,\beta)$, then*

$$^0R_{-1}(G) \ge {}^0R_{-1}\left(K_\beta + \overline{K}_{n-\beta}\right)$$

with equality if and only if $G \cong K_\beta + \overline{K}_{n-\beta}$.

Theorem 185. [152] *If $2 \le \beta \le \lfloor \frac{n}{2} \rfloor$ and $G \in \mathcal{B}(n,\beta)$, then*

$$^0R_{-1}(G) \le {}^0R_{-1}\left(S^*_{n,n-\beta}\right)$$

with equality if and only if $G \cong S^*_{n,n-\beta}$.

5 Zeroth–order Randić index

The graph invariant $^0R_{-1/2}$ (nowadays, known as the zeroth–order Randić index) was initially consider by Kier and Hall [86] in 1976. In this section, we outline the existing results concerning this invariant.

5.1 Bounds

Liu and one of the present authors [100] derived the lower bounds on $^0R_{-1/2}$, stated in the following theorem.

Theorem 186. [100] *Let G be an n-vertex graph without isolated vertices.*

$$^0R_{-1/2}(G) \geq \sqrt{^0R_{-1}(G) + 2R(G)}$$

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

$$^0R_{-1/2}(G) \geq \sqrt{^0R_{-1}(G) + n(n-1)\left[NK(G)\right]^{-1/n}}$$

with equality if and only if G is regular.

Das and Dehmer [34] established some inequalities between the sum–connectivity index and $^0R_{-1/2}$.

Theorem 187. [34] *If G is a connected n-vertex non-trivial graph with maximal degree Δ, then*

$$^0R_{-1/2}(G) \geq \frac{2\sqrt{2}}{\Delta} \cdot SCI(G)$$

with equality if and only if G is regular.

If T is an n-vertex non-trivial tree, then

$$^0R_{-1/2}(T) > SCI(T)\,.$$

If G is an n-vertex graph such that $d_v \geq 2n^{1/3}$ for all $v \in V(G)$, then

$$^0R_{-1/2}(G) < SCI(G)\,.$$

5.2 Extremal results

Let K_k^{n-k} be the graph obtained by attaching $n-k$ pendent vertices to one vertex of the k-vertex complete graph K_k. For any positive integer $p < k$, let $K_k^{n-k}(p)$ be the graph obtained by adding p new edges between one pendent vertex of K_k^{n-k} and p vertices with degree $k-1$. Pavlović [128] solved an extremal problem concerning $^0R_{-1/2}$, related to Theorem 89, for the case of connected (n,m)-graphs.

Theorem 188. [128] *Among the connected n-vertex graphs with $n + \frac{k(k-3)}{2} + p$ edges, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$, the graph $K_k^{n-k}(p)$ has the maximal $^0R_{-1/2}$ value.*

Recently, Eliasi and Ghalavand [40] determined the trees with the first eight maximal ${}^0R_{-1/2}$ values, using majorization technique. Li and Zhang [93] obtained extremal results for some graph families.

Let $\mathcal{W}_{n,\widetilde{m}}$ be the set of all connected n-vertex non-trivial graphs with maximum matching of cardinality $\widetilde{m}$.

For $n \leq 4m$, let

$$\mathcal{M} = \left\{ s : h(s) = \min_{1 \leq x \leq \widetilde{m}} \left(\frac{x}{\sqrt{n-1}} + \frac{n - 2\widetilde{m} + x - 1}{\sqrt{x}} + \frac{2\widetilde{m} - 2x + 1}{\sqrt{2\widetilde{m} - x}} \right) \right\}.$$

Theorem 189. [93] *Let $G \in \mathcal{W}_{n,\widetilde{m}}$. If $n \geq 4\widetilde{m} + 1$, then*

$${}^0R_{-1/2}(G) \geq \frac{\widetilde{m}}{\sqrt{n-1}} + \frac{n - \widetilde{m}}{\sqrt{\widetilde{m}}}$$

with equality if and only if $G \cong K_{\widetilde{m}} + \overline{K}_{n-\widetilde{m}}$.

If $s \in \mathcal{M}$ and $2\widetilde{m} \leq n \leq 4\widetilde{m}$, then

$${}^0R_{-1/2}(G) \geq \frac{s}{\sqrt{n-1}} + \frac{n - 2\widetilde{m} + s - 1}{\sqrt{s}} + \frac{2\widetilde{m} - 2s + 1}{2\widetilde{m} - s}$$

with equality if and only if there exists $k \in \mathcal{M}$ such that $G \cong K_{2\widetilde{m}-2k+1} + \overline{K}_{n-2\widetilde{m}+k-1}$.

Theorem 190. [93] *If $n \geq 6$ and $G \in \mathcal{W}_{n,\widetilde{m}}$, then*

$${}^0R_{-1/2}(G) \leq \frac{1}{\sqrt{n - \widetilde{m}}} + \frac{\widetilde{m} - 1}{\sqrt{2}} + n - \widetilde{m}$$

with equality if and only if $G \cong T^0(n, \widetilde{m})$.

Let $P_{n,p}$ be the graph obtained from K_{n-p} by adding p pendent vertices to it such that the vertices of K_{n-p} have almost equal number of pendent vertices. Let $ST(n,p)$ be the graph with degree sequence $(p, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p})$.

Theorem 191. [93] *If G is a connected n-vertex non-trivial graph with p pendent vertices, then*

$${}^0R_{-1/2}(P_{n,p}) \leq {}^0R_{-1/2}(G) \leq {}^0R_{-1/2}(ST(n,p))$$

with left equality if and only if $G \cong P_{n,p}$ and right equality if and only if $G \cong ST(n,p)$.

A ϕ–vertex coloring of a graph G is an assignment of ϕ colors $1, 2, \cdots, \phi$ to the vertices of G. The coloring is proper if no two distinct adjacent vertices have the same color. A graph is ϕ–colorable if it has a proper ϕ–vertex coloring. Denote by $CP(n, \phi)$ those complete ϕ-partite graph in which the number of vertices in any two-partite sets are almost equal.

Theorem 192. [93] *If G is a connected proper ϕ–colorable graph with n vertices, $n \geq 2$, then*

$$^0R_{-1/2}(CP(n,\phi)) \leq {}^0R_{-1/2}(G) \leq {}^0R_{-1/2}(S_n)\,.$$

The unique graphs attaining the lower and upper bounds are $CP(n,\phi)$ and S_n, respectively.

A Hamiltonian cycle of a graph G is a cycle containing every vertex of G. A graph is Hamiltonian if it contains a Hamiltonian cycle.

Theorem 193. [93] *If G is a Hamiltonian graph, then*

$$^0R_{-1/2}(K_n) \leq {}^0R_{-1/2}(G) \leq {}^0R_{-1/2}(C_n)\,.$$

The unique graphs attaining the lower and upper bounds are K_n and C_n, respectively.

6 Forgotten topological index

Recently, Furtula and one of the present authors [50] named the invariant $^0R_3$ the forgotten topological index and showed that it has interesting chemical applications. In this section, we present the main results, obtained so far, for the forgotten topological index.

6.1 Bounds

In the very first paper on the forgotten topological index [50], three bounds were established. From these three bounds, two are in terms of the renowned graph invariant R_1, known as the second Zagreb index, which was considered within the study of molecular branching [68].

Theorem 194. [50] *If G is a connected (n,m)-vertex graph, then*

$$^0R_3(G) \leq 2R_1(G) + m(n-2)^2$$

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

Theorem 195. [50] *If a graph G has m edges, then*

$$^0R_3(G) \geq \frac{\left[{}^0R_2(G)\right]^2}{2m}$$

$$^0R_3(G) \geq \frac{\left[{}^0R_2(G)\right]^2}{m} - 2R_1(G)\,.$$

The equality sign in any of the above inequality holds if and only if G is regular.

Furtula *et al.* [51] derived several bounds on the invariant ${}^0R_3$.

Theorem 196. [51] *If G is an (n,m)-vertex graph, then*

$$ {}^0R_3(G) \geq \frac{2m}{n} \cdot {}^0R_2(G) \tag{19} $$

with equality if G is regular;

$$ {}^0R_3(G) \leq m(n^2 - 6n + 4m + 6) \tag{20} $$

with equality if $G \cong S_n$;

$$ {}^0R_3(G) \leq m[(n-2)^2 + 4m - 2(\delta - 1)(n - 1 - \Delta)] \tag{21} $$

with equality if $G \cong S_n$, where δ is minimal degree and Δ is maximal degree of G;

$$ {}^0R_3(G) \leq \frac{\omega - 1}{\omega} \left[{}^0R_2(G)\right]^2 \tag{22} $$

where ω is the clique number of G.

Inequality (19) also follows from inequality (8).

Che and Chen [22] obtained various bounds for the invariant ${}^0R_3$. By $A(G)$ is denoted the Albertson index, Eq. (4).

Theorem 197. [22] *If G is a connected graph with m edges, then*

$$ {}^0R_3(G) \geq \frac{[A(G)]^2}{m} + 2R_1(G) \tag{23} $$

with equality if and only if $|d_u - d_v|$ is constant for all edges $uv \in E(G)$;

$$ {}^0R_3(G) \geq \frac{[A(G)]^2 + \left[{}^0R_2(G)\right]^2}{2m} \tag{24} $$

with equality if and only if G is regular or biregular.

Theorem 198. [22] *If G is a connected (n,m)-graph with minimal degree δ and maximal degree Δ, then*

$$ \begin{aligned} {}^0R_3(G) &\leq (\Delta+\delta)[2m(\Delta+\delta) - n\Delta\delta] \\ &+ \frac{1}{2}(\Delta-\delta)\sqrt{mn[2m(\Delta+\delta) - n\Delta\delta] - 4m^3} - 2m\delta\Delta \\ {}^0R_3(G) &\leq (\Delta+\delta) \cdot {}^0R_2(G) + \frac{1}{2}(\Delta-\delta) \cdot A(G) - 2m\delta\Delta\,. \end{aligned} $$

The equality sign in any of the above inequalities holds if and only if G is regular.

Theorem 199. [22] *Let G be a connected K_{k+1}–free (n,m)-graph with minimal degree δ and maximal degree Δ, where $n \geq 2$ and $k \geq 2$. Then*

$$^0R_3(G) \leq \frac{2mn(k-1)(\Delta+\delta)}{k} + \frac{m(\Delta-\delta)}{2} \cdot \sqrt{\frac{2n^2(k-1)}{k} - 4m - 2m\delta\Delta}$$

with equality if and only if G is a regular complete k-partite graph;

$$^0R_3(G) \leq \frac{m(k-1)}{k}\left[\frac{(k^2+2k-4)n^2}{k} - 4m\right]$$

with equality if and only if G is a complete bipartite graph for $k=2$ and a regular complete k-partite graph for $k \geq 3$.

The next result, obtained with the study of spectral moments of the signless Laplacian matrix, is due to Lekishvili [87].

Theorem 200. [87] *If G is a graph with m edges, then*

$$^0R_3(G) \geq 3\,^0R_2(G) - 4m\,.$$

In addition to the other results, proved in [60], the next three lower bounds for $^0R_3$ were also established there.

Theorem 201. [60] *If G is a non-trivial (n,m)-graph with minimal degree $\delta \geq 1$ and maximal degree Δ graph, then*

$$^0R_3(G) \geq \frac{\left[^0R_2(G)\right]^2}{2m} + \frac{\Delta\delta(\Delta-\delta)^2}{\Delta+\delta}$$

with equality if G is regular.

Theorem 202. [60] *If G is a non-trivial (n,m)-graph with minimal degree δ and maximal degree Δ, then*

$$^0R_3(G) \geq (\Delta+\delta)\,^0R_2(G) - \frac{m(\Delta+\delta)^2}{2} + \frac{(\Delta+\delta)(\Delta-\delta)^2}{4}$$

with equality if and only if G has the degree sequence $(\Delta, \underbrace{c,\ldots,c}_{n-2}, \delta)$, where $c = \frac{\Delta+\delta}{2}$.

Corollary 203. [60] *If G is a non-trivial (n,m)-graph with minimal degree δ and maximal degree Δ, then*

$$^0R_3(G) \geq (\Delta+\delta)\left[\frac{4m^2}{n} - \frac{m(\Delta+\delta)}{2} + \frac{3(\Delta-\delta)}{4}\right]$$

with equality if and only if G has the degree sequence $(\Delta, \underbrace{c,\ldots,c}_{n-2}, \delta)$, where $c = \frac{\Delta+\delta}{2}$.

The F-coindex [51] and second Zagreb coindex [35, 38] of a graph G are denoted by $\overline{F}(G)$ and $\overline{M}_2(G)$, respectively, and are defined as

$$\overline{F}(G) = \sum_{u \nsim v, u \neq v} \left(d_u^2 + d_v^2\right), \quad \overline{M}_2(G) = \sum_{u \nsim v, u \neq v} (d_u\, d_v).$$

The next theorem is due to Khaksari and Ghorbani [84].

Theorem 204. [84] *If G is an (n,m)-graph with minimal degree δ and maximal degree Δ, then*

$$max\left\{6m - 2n, \frac{8m^3}{n^2}\right\} \leq {}^0R_3(G) \leq \left[{}^0R_2(G)\right]^2 - 2R_1(G) \leq \left[{}^0R_2(G)\right]^3$$

$$2[R_1(G) + \overline{M}_2(G)] - \overline{F}(G) \leq {}^0R_3(G) \leq (n-1)\, {}^0R_2(G) + \Delta^2\, m(n-3) - \overline{F}(G)$$

$${}^0R_3(G) \geq 6\, {}^0R_2(G) + 3n - 12m - \frac{2n}{\delta+1}\left[\frac{4}{(\delta+1)^2} + 3(\Delta-1)^2 + \frac{6(\Delta-1)}{\delta+1}\right].$$

Two of the present authors and Matejić [110] derived several lower bounds on the invariant ${}^0R_3$.

Theorem 205. [110] *Let G be a connected (n,m)-graph, $n \geq 3$, with minimal degree δ, maximal degree Δ, and degree sequence $(d_1, d_2, \ldots, d_n)$ where $d_1 \geq d_2 \geq \cdots \geq d_n$. If $\Delta_2 = d_2$, then*

$$\begin{aligned}
{}^0R_3(G) &\geq \frac{\left[{}^0R_2(G)\right]^2}{2m} + \frac{\Delta_2\Delta(\Delta-\Delta_2)^2}{2m} \\
{}^0R_3(G) &\geq \frac{8m^3}{n^2} + \frac{\Delta_2\Delta(\Delta-\Delta_2)^2}{2m} \\
{}^0R_3(G) &\geq \delta^3 + \frac{\left({}^0R_2(G) - \delta^2\right)^2}{2m-\delta} + \frac{\Delta_2\Delta(\Delta-\Delta_2)^2}{2m-\delta} \\
{}^0R_3(G) &\geq 2m\delta^2 + \frac{\Delta_2\Delta(\Delta-\Delta_2)^2}{2m-\delta}.
\end{aligned}$$

The equality sign in any of the above inequalities holds if and only if G is regular.

The inverse indeg index ISI is defined in Eq. (5). The inequalities, given in the next theorem, between the invariants ${}^0R_3$ and ISI are due to Nezhad *et al.* [121].

Theorem 206. [121] *If G is any graph with minimal degree δ and maximal degree Δ, then*

$$4\delta\left(\frac{{}^0R_2(G)}{2} - ISI(G)\right) \leq {}^0R_3(G) \leq 4\Delta\left(\frac{{}^0R_2(G)}{2} - ISI(G)\right)$$

and

$$^{0}R_3(G) \geq 4\delta \cdot ISI(G)\,.$$

The equality sign in any of the above inequalities holds if and only if G is regular.

Relationships between $^{0}R_3(G)$ and Π, Π_1^*, and Π_2 are established by the following theorems [65].

Theorem 207. [65] *Let G be a simple connected graph with $n \geq 2$ vertices. Then*

$$\left(\Delta^{3/2} - \delta^{3/2}\right)^2 \leq \; ^{0}R_3(G) - n\left(\Pi_1(G)\right)^{3/2n} \leq n^2\alpha(n)\left(\Delta^{3/2} - \delta^{3/2}\right)^2 \,.$$

Theorem 208. [65] *Let G be a simple connected graph with n vertices and $m \geq 1$ edges. Then*

$$\begin{aligned}(\Delta_{e_1} - \delta_{e_1})^2 - 2R_1(G) \leq \; & ^{0}R_3(G) - m\left(\Pi_1^*(G)\right)^{2/m} \\ & \leq m^2\alpha(m)\left(\Delta_{e_1} - \delta_{e_1}\right)^2 - 2R_1(G) \qquad (25) \\ & \leq 4m^2\alpha(m)\left(\Delta - \delta\right)^2 - 2R_1(G)\,.\end{aligned}$$

Theorem 209. [65] *Let G be a simple connected graph with n vertices and $m \geq 1$ edges. Then*

$$\begin{aligned} ^{0}R_3(G) - m\left(\Pi_2(G)\right)^{2/m} & \leq m^2\alpha(m)\left(\Delta_{e_1} - \delta_{e_1}\right)^2 - 2R_1(G) \\ & \leq 4m^2\alpha(m)\left(\Delta - \delta\right)^2 - 2R_1(G)\,.\end{aligned}$$

Theorem 210. [46] *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$^{0}R_3(G) \geq m\left(\Pi_1^*(G)\right)^{2/m} - 2R_1(G)\,.$$

Note that the left–hand part of (25) is stronger than the inequality given in Theorem 210.

Relationships between $^{0}R(G)$ and the general sum–connectivity index $X_\alpha(G)$ and $R_1(G)$ are given by the next two theorems [115].

Theorem 211. [115] *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then for $\alpha \geq 2$*

$$X_\alpha(G)\Delta_{e_1}^{2-\alpha} - 2R_1(G) \leq \, ^{0}R_3(G) \leq X_\alpha(G)\delta_{e_1}^{2-\alpha} - 2R_1(G)\,.$$

It $\alpha \leq 2$, the the opposite inequalities are valid. Equalities are attained when $\alpha = 2$, or if the line graph $L(G)$ is regular.

Theorem 212. [115] *Let G be a simple connected graph with n vertices and m edges. Then, for any real $\alpha, \alpha \leq 1$ or $\alpha \geq 2$,*

$$^0R_3(G) \leq \left[X_\alpha(G)\, {}^0R_2^{\alpha-2}(G)\right]^{\frac{1}{\alpha-1}} - 2R_1(G)\,.$$

If $1 \leq \alpha \leq 2$, the opposite inequality is valid. Equality is attained if and only if $\alpha = 1$, or $\alpha = 2$, or if $L(G)$ is regular.

The next result gives relationship between $^0R_3(G)$ and the Kirchhoff index Kf.

Theorem 213. [113] *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$^0R_3(G) \geq \frac{4(n-1)m^2}{1+Kf(G)}$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

In the next theorems relationships between $^0R(G)$ and/or the first and second Zagreb indices are given.

Theorem 214. [82] *Let G be a simple (n,m)-graph. Then*

$$^0R_3(G) \geq \frac{n\, {}^0R_2(G)}{m}\,.$$

Equality holds if and only if G is regular.

Theorem 215. [82] *Let G be a simple (n,m)-graph. Then*

$$^0R_3(G) \leq (\Delta+\delta)\, {}^0R_2(G) - 2m\Delta\,\delta\,.$$

Equality holds if and only if G is regular or biregular.

Theorem 216. [46] *Let G be a simple (n,m)-graph without pendent vertices. Then*

$$\delta {}^0R_2(G) \leq {}^0R_3(G) \leq \Delta\, {}^0R_2(G)$$

$$^0R_3(G) \leq 2(\Delta+\delta)\, {}^0R_2(G) - 2R_1(G) - 4m\delta\,\Delta$$

$$^0R_3(G) \leq \frac{(\Delta+\delta)^2}{4m\Delta\,\delta}\left({}^0R_2(G)\right)^2 - 2R_1(G)\,.$$

Equalities hold if and only if G is regular.

Theorem 217. [114] *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ {}^0R_3(G) \geq \frac{\left({}^0R_2(G)\right)^2}{m} + \frac{1}{2}(\Delta_{e_1} - \delta_{e_1})^2 - 2R_1(G) $$

with equality if and only if $L(G)$ is regular, or $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$ and $\Delta_{e_1} + \delta_{e_1} = 2\Delta_{e_2}$.

Corollary 218. [114] *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ {}^0R_3(G) \geq \delta_{e_1}\,{}^0R_2(G) + \frac{1}{2}(\Delta_{e_1} - \delta_{e_1})^2 - 2R_1(G) $$

with equality if and only if $L(G)$ is regular.

Theorem 219. [114] *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ {}^0R_3(G) \leq (\Delta_{e_1} + \delta_{e_1})\,{}^0R_2(G) - m\Delta_{e_1}\delta_{e_1} - 2R_1(G) $$

with equality if and only if there exists an integer k, $1 \leq k \leq m$, such that $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$.

Corollary 220. [114] *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ {}^0R_3(G) \leq \frac{\left({}^0R_2(G)\right)^2}{4m} \left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} + \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}} \right) - 2R_1(G) $$

with equality if and only if $L(G)$ is regular.

Theorem 221. [114] *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ {}^0R_3(G) \leq \frac{\left({}^0R_2(G)\right)^2}{m} + m\alpha(m)(\Delta_{e_1} - \delta_{e_1})^2 - 2R_1(G)\,. $$

Equality holds if and only if $L(G)$ is regular.

In [109] the following results were proved.

Theorem 222. [109] *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$ {}^0R_3(G) \geq \frac{\left({}^0R_2(G)\right)^2}{m} + \frac{(\Delta_{e_1} - \Delta_{e_2})^2}{m} - 2R_1(G) $$

and

$$ {}^0R_3(G) \geq \frac{\left({}^0R_2(G)\right)^2}{2m} + \frac{(\Delta_{e_1} - \Delta_{e_2})^2}{2m}\,. $$

Equality in the first inequality holds if and only if $L(G)$ is regular, whereas in the second if and only if G is regular.

Theorem 223. [109] *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$^{0}R_3(G) \geq \delta_{e_1}^2 + \frac{\left({}^{0}R_2(G) - \delta_{e_1}\right)^2}{m-1} + \frac{\left(\Delta_{e_1} - \Delta_{e_2}\right)^2}{m-1} - 2R_1(G)$$

and

$$^{0}R_3(G) \geq \frac{1}{2}\delta_{e_1}^2 + \frac{\left({}^{0}R_2(G) - \delta_{e_1}\right)^2}{2(m-1)} + \frac{\left(\Delta_{e_1} - \Delta_{e_2}\right)^2}{2(m-1)}$$

with equalities if and only if $L(G)$ is regular.

The next, recently established, bound is due to Rodríguez et *al.* [134].

Theorem 224. [134] *If G is a non-trivial graph with maximal degree Δ and minimal degree δ, then*

$$\frac{4R_2(G)}{\Delta^2} - 2R_2(G) \leq {}^{0}R_3(G) \leq \frac{4R_2(G)}{\delta^2} - 2R_2(G)$$

with equality if and only if G is regular.

6.2 Extremal results

We recall that $\mathcal{C}_{n,\nu}$ is the set of connected n-vertex graphs with cyclomatic number ν. Recently, graphs from the set $\mathcal{C}_{n,\nu}$ for $\nu = 0, 1, \ldots, 5$, with the first few minimal $^{0}R_3$ values, were determined in [63]. In order to state the first result of [63], we need the following tree classes:

$$\mathcal{T}^{(4)} = \{T \in \mathcal{C}_{n,0} : n_1 = 5, n_2 = n-8, n_3 = 3, n_i = 0 \text{ for } i \geq 4\}$$

$$\mathcal{T}^{(5)} = \{T \in \mathcal{C}_{n,0} : n_1 = 4, n_2 = n-5, n_3 = 0, n_4 = 1, n_i = 0 \text{ for } i \geq 5\}$$

$$\mathcal{T}^{(6)} = \{T \in \mathcal{C}_{n,0} : n_1 = 6, n_2 = n-10, n_3 = 4, n_i = 0 \text{ for } i \geq 4\}.$$

Theorem 225. [63] *Let $n \geq 10$, $T_j \in \mathcal{T}^{(j)}$, $j = 1, 2, \ldots, 6$, and $T \in \mathcal{C}_{n,0} \setminus \bigcup_{j=1}^{6} \mathcal{T}^{(j)}$. Then*

$$^{0}R_3(T_1) < {}^{0}R_3(T_2) < {}^{0}R_3(T_3) < {}^{0}R_3(T_4) < {}^{0}R_3(T_5) < {}^{0}R_3(T_6) < {}^{0}R_3(T)$$

where the tree classes $\mathcal{T}^{(1)}, \mathcal{T}^{(2)}$, and $\mathcal{T}^{(3)}$ are defined before Theorem 91.

Trees with the first three minimal ${}^0R_3$ values were also determined in [40, 94], within the study of the invariant ${}^0R_\alpha$. For example, see Theorem 91.

Theorem 226. [63] *Let* $n \geq 5$, $U_j \in \mathcal{U}^{(j)}$, $j = 1,2,3$, *and* $U \in \mathcal{C}_{n,1} \setminus \bigcup_{j=1}^{3} \mathcal{U}^{(j)}$. *Then*

$$ {}^0R_3(U_1) < {}^0R_3(U_2) < {}^0R_3(U_3) < {}^0R_3(U) $$

where the graph classes $\mathcal{U}^{(1)}, \mathcal{U}^{(2)}$, *and* $\mathcal{U}^{(3)}$ *are defined before Theorem 95.*

Theorem 226, also, follows from Theorem 95.

Theorem 227. [63] *Let* $n \geq 7$, $B_j \in \mathcal{B}^{(j)}$, $j = 1,2,3$, *and* $B \in \mathcal{C}_{n,2} \setminus \bigcup_{j=1}^{3} \mathcal{B}^{(j)}$. *Then*

$$ {}^0R_3(B_1) < {}^0R_3(B_3) < {}^0R_3(B_2) < {}^0R_3(B) $$

where the graph classes $\mathcal{B}^{(1)}, \mathcal{B}^{(2)}$, *and* $\mathcal{B}^{(3)}$ *are defined before Theorem 105.*

There is a typo in Theorem 2.11 of [63]: the inequality ${}^0R_3(G_2) < {}^0R_3(G_3)$, mentioned there, should be written as ${}^0R_3(G_3) < {}^0R_3(G_2)$. Theorem 227, also, follows from Theorem 105.

We need the following graph classes for stating the next three extremal results:

$$
\begin{aligned}
\mathcal{G}^{(1)} &= \{G \in \mathcal{C}_{n,3} : n_1 = 0, n_2 = n-4, n_3 = 4, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{G}^{(2)} &= \{G \in \mathcal{C}_{n,3} : n_1 = 1, n_2 = n-6, n_3 = 5, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{G}^{(3)} &= \{G \in \mathcal{C}_{n,3} : n_1 = 0, n_2 = n-3, n_3 = 2, n_4 = 1, n_i = 0 \text{ for } \ i \geq 5\} \\
\mathcal{G}^{(4)} &= \{G \in \mathcal{C}_{n,3} : n_1 = 2, n_2 = n-8, n_3 = 6, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{H}^{(1)} &= \{H \in \mathcal{C}_{n,4} : n_1 = 0, n_2 = n-6, n_3 = 6, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{H}^{(2)} &= \{H \in \mathcal{C}_{n,4} : n_1 = 1, n_2 = n-8, n_3 = 7, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{J}^{(1)} &= \{J \in \mathcal{C}_{n,5} : n_1 = 0, n_2 = n-8, n_3 = 8, n_i = 0 \text{ for } \ i \geq 4\} \\
\mathcal{J}^{(2)} &= \{J \in \mathcal{C}_{n,5} : n_1 = 1, n_2 = n-10, n_3 = 9, n_i = 0 \text{ for } \ i \geq 4\}\,.
\end{aligned}
$$

Theorem 228. [63] *Let* $n \geq 11$, $G_j \in \mathcal{G}^{(j)}$, $j = 1,2,3,4$, *and* $G \in \mathcal{C}_{n,3} \setminus \bigcup_{j=1}^{4} \mathcal{G}^{(j)}$. *Then*

$$ {}^0R_3(G_1) < {}^0R_3(G_2) < {}^0R_3(G_3) < {}^0R_3(G_4) < {}^0R_3(G)\,. $$

Theorem 229. [63] *Let* $n \geq 12$, $H_j \in \mathcal{H}^{(j)}$, $j = 1, 2$, *and* $H \in \mathcal{C}_{n,4} \setminus \bigcup_{j=1}^{2} \mathcal{H}^{(j)}$. *Then*

$$^0R_3(H_1) < {}^0R_3(H_2) < {}^0R_3(H)\,.$$

Theorem 230. [63] *Let* $n \geq 16$, $J_j \in \mathcal{J}^{(j)}$, $j = 1, 2$, *and* $J \in \mathcal{C}_{n,5} \setminus \bigcup_{j=1}^{2} \mathcal{J}^{(j)}$. *Then*

$$^0R_3(J_1) < {}^0R_3(J_2) < {}^0R_3(J)\,.$$

Recently, Abdo *et al.* [1] obtained the following two extremal results for the invariant $^0R_3$.

Theorem 231. [1] *Let* T^* *be a tree with maximal* $^0R_3$ *value among the* n*-vertex trees with maximal degree* Δ. *Then the following holds:*
1. If $n-2 \equiv 0$ *mod* $(\Delta - 1)$, *then* T^* *contains* $\frac{n-2}{\Delta-1}$ *vertices of degree* Δ *and* $\frac{n(\Delta-2)+2}{\Delta-1}$ *pendent vertices. In this case,*

$$^0R_3(T^*) = \Delta(\Delta+1)(n-2) + 2(n-1)\,.$$

2. If $n-2 \not\equiv 0$ *mod* $(\Delta-1)$, *then* T^* *contains* $\frac{n-x-1}{\Delta-1}$ *vertices of degree* Δ, $\frac{(n-1)(\Delta-2)+x}{\Delta-1}$ *pendent vertices, and one vertex of degree* x, *where* x *is uniquely determined by* $2 \leq x \leq \Delta - 1$ *and* $n - x - 1 \equiv 0$ *mod* $(\Delta - 1)$. *In this case,*

$$^0R_3(T^*) = (\Delta^2 + \Delta + 2)(n-1) - (\Delta^2 + \Delta + 1)x + x^3\,.$$

Theorem 231 follows, also, from Theorem 99.

Theorem 232. [1] *Let* $T^\star$ *has the maximal* $^0R_3$ *value among the* n*-vertex chemical trees. Then the following holds:*
1. If $n-2 \equiv 0$ *mod* 3, *then* $T^\star$ *contains* $\frac{n-2}{3}$ *vertices of degree 4 and* $\frac{2n+2}{3}$ *pendent vertices, and* $^0R_3(T^\star) = 22n - 42$.
2. If $n-2 \not\equiv 0$ *mod* 3, *then* $T^\star$ *contains* $\frac{n-x-1}{3}$ *vertices of degree 4,* $\frac{2(n-1)+x}{3}$ *pendent vertices, and one vertex of degree* x, *where* x *is uniquely determined by* $2 \leq x \leq 3$ *and* $n - x - 1 \equiv 0$ *mod* 3. *Then,* $^0R_3(T^\star) = 22(n-1) - 21x + x^3$.

Theorem 232 follows, also, from Theorem 94.

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