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Preface

In the recent years, the mathematical–chemistry literature is flooded by countless graph–based topological indices, proposed to serve as molecular structure descriptors.

Topological indices have attracted much attention of chemical and mathematical researchers, especially those focussing on graph theory, from all over the world. Nowadays many interesting results and lot of open problems on it have been reported in literature. In most cases, the mathematical investigation of these indices consist of finding lower and upper bounds for them, and characterizing the graphs for which these inequalities become equalities. Again, the number of results obtained along these lines, and the number of respective publications, is so large that no human can satisfactorily follow them and recognize what is significant and what is not.

In order to help colleagues to find their way through the data jungle, we decided to devote one book in our "*Mathematical Chemistry Monographs*" series to bounds on topological indices and the related extremal graphs. To this end, in the Summer of 2016 we invited a number of colleagues to contribute chapters to our book. The scholars invited were among those who are currently active and who publish in this field of chemical graph theory. Their response was beyond anything what we could have expected.

Thus, instead of a single "*Mathematical Chemistry Monograph*", we had to produce three volumes, that is:

- Mathematical Chemistry Monograph No. 19:
  Bounds in Chemical Graph Theory – Basics
  Faculty of Science & University, Kragujevac, 2017
- Mathematical Chemistry Monograph No. 20:
  Bounds in Chemical Graph Theory – Mainstreams
  Faculty of Science & University, Kragujevac, 2017
- Mathematical Chemistry Monograph No. 21:
  Bounds in Chemical Graph Theory – Advances
  Faculty of Science & University, Kragujevac, 2017

The present book is the "*Mathematical Chemistry Monograph*" No. 20, completed in January 2017.

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On Energy, Laplacian Energy and Signless Laplacian Energy of Graphs

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1. Introduction

In this paper we are concerned with simple, undirected, and unweighted graphs. Let $G = (V, E)$ be a graph on vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$, where $|E(G)| = m$. Also let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by $\delta = \delta(G)$ and the maximum by $\Delta = \Delta(G)$. Let N_i be the neighbor set of the vertex $v_i \in V(G)$, $i = 1, 2, \ldots, n$. The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices v_i and v_j are adjacent if and only if they are not adjacent in G. If vertices v_i and v_j are adjacent in G, we denote that by $v_iv_j \in E(G)$.

The adjacency matrix $A(G)$ of G is defined by its entries $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n$ denote the eigenvalues of $A(G)$. When more than one graph is under consideration, then we write $\lambda_i(G)$ instead of λ_i. The energy of the graph G is defined as

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i| \,, \tag{1}$$

where λ_i, $i = 1, 2, \ldots, n$ are the eigenvalues of graph G. For its basic properties, applications including various lower and upper bounds, see [10, 13, 15–17, 26, 28], book [30] and the references cited therein.

The $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ be, respectively, the Laplacian matrix and the signless Laplacian matrix of the graph G, where $D(G)$ is the diagonal matrix of vertex degrees. The eigenvalues of $L(G)$ and $Q(G)$ will be denoted by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ and $q_1 \geq q_2 \geq \cdots \geq q_{n-1} \geq q_n$, respectively. Then the Laplacian energy and the signless Laplacian energy of G are defined as

$$LE = LE(G) = \sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right| \text{ and } LE^+ = LE^+(G) = \sum_{i=1}^{n} \left|q_i - \frac{2m}{n}\right|,$$

respectively. Details on the properties of Laplacian energy, including various lower and upper bounds, see [9,11,13,16,18,38,42]. The Laplacian energy LE found applications not only in theoretical organic chemistry (see, [21, 36]), but also in image processing [40] and information theory [29]. The signless Laplacian energy was until now studied only to a limited extent [1, 12, 15]. We denote by K_n, $K_{p,\,q}$ $(p + q = n)$ and S_n $(\cong K_{1,\,n-1})$, the complete graph, the complete bipartite graph and the star on n vertices, respectively, throughout this paper.

The paper is organized as follows. In Section 2, we give several lower and upper bounds on energy of graphs. In Section 3, we discuss lower and upper bounds on the Laplacian energy of graphs. In Section 4, we present several relations between different graph energies of graphs.

2. On energy of graphs

Recall that ν^+ and ν^- are the number of positive and negative eigenvalues of the adjacency matrix $A(G)$ of graph G, respectively. Then from the definition of the energy of a graph and the trace of the matrix $A(G)$, one can get the following result [14]:

Lemma 2.1. [14] *Let G be a graph of order n. Then*

$$\mathcal{E}(G) = 2\sum_{i=1}^{\nu^+} \lambda_i = -2\sum_{i=1}^{\nu^-} \lambda_{n-i+1} = 2 \max_{1\leq k\leq n} \left(\sum_{i=1}^{k} \lambda_i\right) = 2 \max_{1\leq k\leq n} \left(\sum_{i=1}^{k} -\lambda_{n-i+1}\right),$$

where ν^+ and ν^- are the number of positive and negative eigenvalues of $A(G)$, respectively.

Li et. al [30] gave the following lower bound in terms of m:

Theorem 2.2. [30] *For a graph G with m edges,*

$$\mathcal{E}(G) \geq 2\sqrt{m} \tag{2}$$

with equality holding if and only if G consists of a complete bipartite graph $K_{a,\,b}$ such that $a \cdot b = m$ and arbitrarily many isolated vertices.

It is well known that

$$\prod_{i=1}^{n} \lambda_i = \det\, \mathbf{A},$$

where $\det\, \mathbf{A}$ is the determinant of the adjacency matrix of graph G. McClelland [34] obtained the following lower bound in terms of n, m and the determinant of the adjacency matrix of graph G:

Theorem 2.3. [34] *Let G be a graph of order n with m edges. Then*

$$\mathcal{E}(G) \geq \sqrt{2m + n(n-1)|\det\, \mathbf{A}|^{2/n}}\,, \tag{3}$$

where $\det\, \mathbf{A}$ *is the determinant of the adjacency matrix of graph G.*

A graph G is said to be singular if at least one of its adjacency eigenvalues is equal to zero. For singular graphs, evidently, $\det\, \mathbf{A} = 0$. A graph is nonsingular if all its eigenvalues are different from zero. Then, $|\det\, \mathbf{A}| > 0$. In [17], the authors presented the following lower bound on $\mathcal{E}(G)$:

Theorem 2.4. [17] *Let G be a connected nonsingular graph of order n with m edges. Then*

$$\mathcal{E}(G) \geq \frac{2m}{n} + n - 1 + \ln|det(A)| - \ln\frac{2m}{n}. \tag{4}$$

Equality holds in (4) *if and only if G is isomorphic to the complete graph K_n.*

Remark 2.5. *In* [17]*, the authors mentioned that the lower bound in* (4) *is better than the lower bounds in* (2) *and* (3) *for different class of graphs.*

The following three lower bounds on $\mathcal{E}(G)$ of graph G is obtained in [13].

Theorem 2.6. [13] *Let G be a connected graph of order n and m edges. Then*

$$\mathcal{E}(G) \geq \min\left\{\frac{2m}{n} + \sqrt{2m - \frac{4m^2}{n^2} + Z}\,,\ \sqrt{2m-n+1} + \sqrt{n-1+Z}\right\}, \tag{5}$$

where

$$Z = (n-1)(n-2)\left(\frac{(\det\, \mathbf{A})^2}{2m-n+1}\right)^{\frac{1}{n-1}}$$

and $\det\, \mathbf{A}$ *is the determinant of the adjacency matrix of graph G. Moreover, the equality holds in* (5) *if and only if $G \cong K_n$.*

Corollary 2.1. [13] *Let G be a connected graph of order n and m edges. Then*

$$\mathcal{E}(G) \geq \frac{2m}{n} + \sqrt{(n-1)\left[1 + (n-2)\left(\frac{(\det \mathbf{A})^2}{2m-n+1}\right)^{\frac{1}{n-1}}\right]}, \tag{6}$$

where $\det\, \mathbf{A}$ *is the determinant of the adjacency matrix of graph G. Moreover, the equality holds in* (6) *if and only if $G \cong K_n$.*

Corollary 2.2. [13] *Let G be a connected graph of order n with m edges and maximum degree Δ. Then*

$$\mathcal{E}(G) \geq \frac{2m}{n} + \sqrt{(n-1)\left[1 + (n-2)\left(\frac{\det \mathbf{A}}{\Delta}\right)^{\frac{2}{n-1}}\right]}, \tag{7}$$

where $\det\, \mathbf{A}$ *is the determinant of the adjacency matrix of graph G. Moreover, the equality holds in* (7) *if and only if $G \cong K_n$.*

A d-regular graph G on n vertices is strongly d-regular (denote by srg($n,\ d,\ \lambda,\ \mu$)) if there exist positive integers d, λ and μ such that every vertex has d neighbors, every adjacent pair of vertices has λ common neighbors, and every nonadjacent pair has μ common neighbors. For example, the complete graph and Petersen graph are strongly regular graphs. Strongly regular graphs were introduced by Bose in 1963 [5]. The complement of an srg($n,\ d,\ \lambda,\ \mu$)) is also strongly regular. It is an srg($n,\ n-d-1,\ n-2-2d+\mu,\ n-2d+\lambda$)). The adjacency matrix of srg($n,\ d,\ \lambda,\ \mu$) has exactly three distinct eigenvalues:
(i) d of multiplicity 1,

(ii) $\dfrac{\lambda-\mu+\sqrt{(\lambda-\mu)^2+4(d-\mu)}}{2}$ of multiplicity $\dfrac{1}{2}\left[n-1-\dfrac{2d+(n-1)(\lambda-\mu)}{\sqrt{(\lambda-\mu)^2+4(d-\mu)}}\right]$,

(iii) $\dfrac{\lambda-\mu-\sqrt{(\lambda-\mu)^2+4(d-\mu)}}{2}$ of multiplicity $\dfrac{1}{2}\left[n-1+\dfrac{2d+(n-1)(\lambda-\mu)}{\sqrt{(\lambda-\mu)^2+4(d-\mu)}}\right]$.

Koolen and Moulton [26] gave the following upper bound in terms on n and m:

Theorem 2.7. [26] *If $2m \geq n$ and G is a graph on n vertices with m edges, then the inequality*

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m-\left(\frac{2m}{n}\right)^2\right)} \tag{8}$$

holds. Moreover, equality holds in (8) *if and only if G is either $\frac{n}{2}K_2$, K_n, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value*

$$\sqrt{\left(2m-\left(\frac{2m}{n}\right)^2\right)/(n-1)}\,.$$

The first Zagreb index $M_1(G)$ is the oldest and popular degree based topological index, both from theoretical point of view and applications. The first Zagreb index has been introduced more than forty years ago by Gutman and Trinajstić [23] and is defined as

$$M_1(G) = \sum_{v_i\in V(G)} d_i^2\,.$$

Some recent results on the first Zagreb index were reported in [7] and review [4], where also references to the previous mathematical research in this area can be found. This index reflect the extent of branching of the molecular carbon–atom skeleton, and can thus be viewed as molecular structure-descriptors [2]. Zhou [44] obtained the following upper bound on n, m and the first Zagreb index $M_1(G)$:

Theorem 2.8. [44] *If G is a graph with n vertices, m edges and degree sequence $d_1,\ d_2,\ldots,\ d_n$, then*

$$\mathcal{E}(G) \leq \sqrt{\frac{M_1(G)}{n}} + \sqrt{(n-1)\left(2m-\left(\sqrt{\frac{M_1(G)}{n}}\right)^2\right)}\,. \tag{9}$$

Moreover, equality in (9) *holds if and only if* G *is either* $\frac{n}{2}\,K_2$ $(n = 2m)$*,* K_n $(m = n(n-1)/2)$*, a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value* $\sqrt{\left(2m - \left(\frac{2m}{n}\right)^2\right)/(n-1)}$*, or* $n\,K_1$ $(m = 0)$*.*

In [10], the authors found the upper bound on energy $\mathcal{E}(G)$ of graphs G in terms of n, m and δ.

Theorem 2.9. [10] *Let* G *be a connected graph of order* n $(n \geq 6)$*,* m *edges with minimum degree* δ*. Then*

$$\mathcal{E}(G) \leq \frac{2(m-\delta)}{n-1} + \sqrt{(n-1)\left[2m - \frac{4(m-\delta)^2}{(n-1)^2}\right]}\,. \tag{10}$$

Corollary 2.3. [10] *Let* G *be a connected graph of order* n $(n \geq 6)$*,* m *edges with at least a pendent vertex. Then*

$$\mathcal{E}(G) \leq \frac{2(m-1)}{n-1} + \sqrt{(n-1)\left[2m - \frac{4(m-1)^2}{(n-1)^2}\right]}\,. \tag{11}$$

Remark 2.10. *In* [10]*, the authors mentioned that* (10) *is better than* (8) *for* $m \geq n\delta$ *and* (9) *for* $4n\,(m-\delta)^2 \geq M_1(G)\,(n-1)^2$.

The rank of a matrix is defined as the maximum number of linearly independent row (or column) vectors in the matrix. The rank r of an undirected graph is defined as the rank of its adjacency matrix, that is, the number of non-zero eigenvalues are called the rank of graph. Analogously, the nullity of the graph of order n is the nullity of its adjacency matrix, which equals $n-r$. Let $G(n,\,m)$ be a set of graphs of order n and m edges. Now we define

$$\Gamma_1 = \left\{G \,:\, G \in G(n,\,m) \ \text{ and } \ \sum_{i=1}^{k} \mu_i(G) \leq m + \frac{k^2+k}{2}\,,\ 1 \leq k \leq n\right\}$$

$$\text{and} \qquad \Gamma_2 = \left\{G \,:\, G \in G(n,\,m) \ \text{ and } \ \sum_{i=1}^{k} q_i(G) \leq m + \frac{k^2+k}{2}\,,\ 1 \leq k \leq n\right\}.$$

One can easily see that tree, unicyclic, bicyclic and regular graphs are belong to $\Gamma_1 \cap \Gamma_2$. The following upper bound on energy $\mathcal{E}(G)$ was obtained in [12].

Theorem 2.11. [12] *Let* G *be a graph of order* n *with* $m > 0$ *edges. If* $G \in \Gamma_1 \cap \Gamma_2$*, then*

$$\mathcal{E}(G) \leq m + \frac{r^2+r}{4} - 1,$$

where $r = rank(A)$*.*

The following four upper bounds were obtained in [13]:

Theorem 2.12. [13] *Let G be a connected graph of order n, m edges, Δ maximum degree and the first Zagreb index $M_1(G)$. Then*

$$\mathcal{E}(G) \leq \Delta + \sqrt{\frac{2m(n^2-2m)}{n^2} + P}\,,$$

where

$$P = \sqrt{\binom{r-1}{2}\left[\frac{8m^2(n^2-2m)^2}{n^4} - 2M_1(G) - \frac{2\left(M_1(G)-2m\right)^2}{n(n-1)} + 2\Delta^4\right]}$$

and r is the rank of the adjacency matrix of graph G. Moreover, the equality holds if and only if $G \cong K_n$ or $G \cong K_{n/2,\,n/2}$ or $G \cong$ srg $\left(n,\, d,\, \frac{d(d-1)}{n-1},\, \frac{d(d-1)}{n-1}\right)$.

Corollary 2.4. [13] *Let G be a d-regular connected graph of order n. Then*

$$\mathcal{E}(G) \leq d + \sqrt{(n-1)\,d\,(n-d)}$$

with equality holding if and only if $G \cong K_n$ or $G \cong$ srg $\left(n,\, d,\, \frac{d(d-1)}{n-1},\, \frac{d(d-1)}{n-1}\right)$.

Corollary 2.5. [34] *Let G be a d-regular connected graph of order n. Then*

$$\mathcal{E}(G) \leq \frac{n(\sqrt{n}+1)}{2}$$

with equality holding if and only if $G \cong$ srg $\left(n,\, \frac{n+\sqrt{n}}{2},\, \frac{n+2\sqrt{n}}{4},\, \frac{n+2\sqrt{n}}{4}\right)$.

Corollary 2.6. [13] *Let G be a connected graph of order n, m edges, maximum degree Δ and the first Zagreb index $M_1(G)$. Then*

$$\mathcal{E}(G) \leq \Delta + \sqrt{\frac{2m(n^2-2m)}{n^2} + P}\,,$$

where

$$P = \sqrt{\binom{n-1}{2}\left[\frac{8m^2(n^2-2m)^2}{n^4} - 2M_1(G) - \frac{2\left(M_1(G)-2m\right)^2}{n(n-1)} + 2\Delta^4\right]}\,.$$

Moreover, the equality holds if and only if $G \cong K_n$ or $G \cong$ srg $\left(n,\, d,\, \frac{d(d-1)}{n-1},\, \frac{d(d-1)}{n-1}\right)$.

A bipartite graph is a graph whose vertices can be divided into two disjoint sets U and V (that is, U and V are each independent sets) such that every edge connects a vertex in U to one in V. Vertex sets U and V are usually called the parts of the graph. In 1974, Gutman [20] presented the following lower bound on energy of bipartite graph G:

Theorem 2.13. [20] *Let G be a bipartite graph of order n with m edges. Then*

$$\mathcal{E}(G) \geq \sqrt{4m + n(n-2)(\det\,\mathbf{A})^{\frac{2}{n}}}\,, \tag{12}$$

where $\det\,\mathbf{A}$ is the determinant of the adjacency matrix of graph G.

The authors in [16] characterized the extremal graphs for the above lower bound in the following theorem:

Theorem 2.14. [16] *Let G be a bipartite graph of order n with m edges. Then inequality* (12) *holds with equality holding if and only if $G \cong n\,K_1$ or $G \cong K_{p,\,q} \cup (n-p-q)\,K_1$, $p \leq q$, $p+q \leq n$, $1 \leq p \leq \lfloor \frac{n}{2} \rfloor$.*

In the same paper [20], Gutman presented the following upper bound on energy $\mathcal{E}(G)$:

Theorem 2.15. [20] *Let G be a connected graph of order n with m edges. Then*

$$\mathcal{E}(G) \leq \sqrt{2\,m\,n - 4\,m + 2\,n\,(\det \mathbf{A})^{\frac{2}{n}}}\,, \tag{13}$$

where $\det\ \mathbf{A}$ *is the determinant of the adjacency matrix of graph G.*

This upper bound is true for bipartite graphs with even n, but in the general case, it is not true for bipartite graphs with odd n. Simple examples for the failure of (13) are P_3 and P_5, the paths of order 3 and 5. The correct upper bound for bipartite graphs with odd number of vertices is $\mathcal{E}(G) \leq \sqrt{2mn - 2m}$. In the following theorem, the authors in [16] characterized the extremal graphs for the above upper bound (13), of course for the case of even n.

Theorem 2.16. [16] *Let G be a bipartite graph of even order n with m edges. Then inequality* (13) *holds with equality holding if and only if $G \cong n\,K_1$ or $G \cong \frac{n}{2}\,K_2$.*

3. On Laplacian energy of graphs

In 2006, Gutman and Zhou [24] defined the Laplacian energy of a graph as the sum of the absolute deviations (i.e., distance from the mean) of the eigenvalues of its Laplacian matrix, that is,

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

Let σ $(1 \leq \sigma \leq n)$ be the largest positive integer such that

$$\mu_\sigma \geq \frac{2m}{n}. \tag{14}$$

Then from [11], we have

$$LE(G) \;=\; \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| = 2S_\sigma(G) - \frac{4m\sigma}{n},$$

where

$$S_\sigma(G) = \sum_{i=1}^{\sigma} \mu_i.$$

In the following, we present another equality for Laplacian energy $LE(G)$ of graph G.

Lemma 3.1. [11] *Let G be a graph of order n with m edges. Then*

$$LE(G) = 2S_\sigma(G) - \frac{4m\sigma}{n} = \max_{1\le i\le n-1}\left\{2S_i(G) - \frac{4mi}{n}\right\}.$$

First we deal with the lower bounds on the Laplacian energy of graphs. In [46], Zhou gave the following lower bound:

Theorem 3.2. [46] *Let G be a graph of order n with m edges. Then*

$$LE(G) \ge \frac{4m}{n} \tag{15}$$

with equality if and only if G is isomorphic to a regular complete k-partite graph $(1 \le k \le n)$.

In [24], Gutman and Zhou obtained the following lower bound:

Theorem 3.3. [24] *Let G be a graph of order n with m edges and degree sequence $(d) = (d_1,\, d_2,\, \ldots, d_n)$. Then*

$$LE(G) \ge 2\sqrt{m + \frac{1}{2}\sum_{i=1}^{n}\left(d_i - \frac{2m}{n}\right)^2} \tag{16}$$

with equality if and only if G is isomorphic to a complete bipartite graph $K_{\frac{n}{2},\,\frac{n}{2}}$.

In [11], the authors found the following lower bound in terms of n, m and Δ.

Theorem 3.4. [11] *Let G be a connected graph of order n with m edges and maximum degree Δ. Then*

$$LE(G) \ge 2\left(\Delta + 1 - \frac{2m}{n}\right) \tag{17}$$

with equality holding in (17) if and only if $G \cong K_{1,\,n-1}$.

Remark 3.5. *In [11], it was mentioned that the result in (17) is better than the result in (15) for any tree except path P_n. Moreover, the result in (17) is better than the result in (16) for any tree T of order n with $\Delta(T) \ge \frac{n}{\sqrt{2}} + 1$.*

So et al. [39] obtained a lower bound for bipartite graph as follows:

Theorem 3.6. [39] *Let G be a bipartite graph of order n with m edges and degree sequence $(d) = (d_1,\, d_2, \ldots,\, d_n)$. Then*

$$LE(G) \ge \sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|. \tag{18}$$

In [13], the authors presented a lower bound on LE of connected graph G that always is better than the lower bound in (18). Moreover, this lower bound is true for any connected graphs.

Theorem 3.7. [13] *Let G be a connected graph of order n with m edges. Then*

$$LE(G) \ge 2 + \sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|.$$

We now deal with the upper bounds on the Laplacian energy of graphs. In [24], Gutman and Zhou obtained the following three upper bounds:

Theorem 3.8. [24] *Let G be a graph of order n with m edges and the first Zagreb index $M_1(G)$. Then*

$$(i) \qquad LE(G) \leq 2m + M_1(G) - \frac{4m^2}{n}\,. \tag{19}$$

$$(ii) \qquad LE(G) \leq \sqrt{n\left(2m + M_1(G) - \frac{4m^2}{n}\right)}\,. \tag{20}$$

$$(iii) \qquad LE(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m + M_1(G) - \frac{4m^2}{n} - \frac{4m^2}{n^2}\right)}\,. \tag{21}$$

Remark 3.9. *In* [11]*, the authors mentioned that the upper bound on LE in* (20) *is better than the upper bound in* (19)*. Moreover, they showed that the upper bound on LE in* (21) *is better than the upper bound in* (20).

The following upper bound is obtained in [11].

Theorem 3.10. [11] *Let G be a graph of order n with $m \geq \frac{n}{2}$ edges and maximum degree Δ. Then*

$$LE(G) \leq 4m - 2\Delta - \frac{4m}{n} + 2 \tag{22}$$

with equality holding in (22) *if and only if $G \cong K_{1,\,n-1}$ or $G \cong K_{1,\,\Delta} \cup \overline{K}_{n-\Delta-1}$ $(\frac{n}{2} \leq \Delta \leq n-2)$.*

Corollary 3.1. [37] *Let G be a graph of order n with $m > 0$ edges. Then*

$$LE(G) \leq 4m\left(1 - \frac{1}{n}\right)$$

with equality if and only if $G \cong K_2 \cup \overline{K}_{n-2}$.

Remark 3.11. *Let T be a tree of order n with maximum degree $\Delta \geq \frac{n}{2}$ $(n \geq 37)$. In* [11]*, the authors showed that the upper bound in* (22) *is better than the upper bound in* (21) *for any tree T.*

We begin by recalling that a 2-(ν, k, λ)-design is a collection of k-subsets or blocks of a set of ν points, such that each 2-set of points lies in exactly k blocks. The design is called symmetric (or square) in case the number of blocks b equals ν. The incidence matrix B of a 2-(ν, k, λ)-design is the $\nu \times b$ matrix defined by setting, for each x a point and S a block, $B_{x,\,s} := 0$ if $x \notin S$ and $B_{x,\,S} := 1$ otherwise. The incidence graph of a design is defined to be the graph with adjacency matrix

$$\begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix}.$$

Note that the incidence graph of a symmetric 2-(ν, k, λ)-design with $v > k > \lambda > 0$ has eigenvalues k, $\sqrt{k-\lambda}$ (with multiplicity $\nu - 1$), $-\sqrt{k-\lambda}$ (with multiplicity $\nu - 1$), and $-k$. The following two upper bounds have been presented in [16].

Theorem 3.12. [16] *Let G be a bipartite graph of order n with m edges. Then*

$$LE(G) \leq \frac{4m}{n} + \sqrt{(n-2)\left(2\,M - \frac{8m^2}{n^2}\right)}\,,$$

where

$$M = m + \frac{M_1(G)}{2} - \frac{2m^2}{n}\,.$$

Moreover, the equality holds if and only if $G \cong K_1 \cup K_2$ or $G \cong n\,K_1$ or $G \cong m\ K_2$ $(n = 2m)$ or $G \cong K_{\nu,\,\nu}$ $(n = 2\nu)$, or G is the incidence graph of a symmetric 2-$(\nu,\,k,\,\lambda)$-design with $k = \frac{2m}{n}$ and $\lambda = \frac{k\,(k-1)}{\nu-1}$.

Theorem 3.13. [16] *Let G be a bipartite graph of order n with m edges and p connected components. Then*

$$LE(G) \leq \max\left\{\frac{4m}{n}p,\ \frac{2m}{n}(p+1) + \sqrt{(n-p-1)\left[2\,M - \left(\frac{2\,m}{n}\right)^2 (p+1)\right]}\right\}.$$

Moreover,

$$LE(G) = \frac{2m}{n}(p+1) + \sqrt{(n-p-1)\left[2\,M - \left(\frac{2\,m}{n}\right)^2 (p+1)\right]}$$

if and only if $G \cong K_1 \cup K_2$ or $G \cong n\,K_1$ or $G \cong m\ K_2$ $(n = 2m)$ or $G \cong K_{p,\,p}$ $(n = 2p)$ or $n = 2\nu$, and G is the incidence graph of a symmetric 2-$(\nu,\,k,\,\lambda)$-design with $k = \frac{2m}{n}$ and $\lambda = \frac{k(k-1)}{\nu-1}$.

Remark 3.14. *In* [24]*, the following result was obtained for a graph G with p connected components:*

$$LE(G) \leq \frac{2m}{n}\,p + \sqrt{(n-p)\ \left[2\,M - p\left(\frac{2m}{n}\right)^2\right]}\,,$$

where

$$M = m + \frac{M_1(G)}{2} - \frac{2m^2}{n}.$$

In [16]*, the authors mentioned that the result in Theorem 3.13 is always better than the above result for bipartite graphs.*

Nordhaus and Gaddum [35] gave bounds for the sum of the chromatic numbers of a graph and its complement. Eventually, numerous Nordhaus-Gaddum-type results for other graph invariants were obtained in the literature. With regard to Laplacian energy, Zhou and Gutman [47] gave the following result:

Theorem 3.15. [47] *Let G be a graph of order n. Then*

$$2(n-1) \leq LE(G) + LE(\overline{G}) < n\sqrt{n^2-1} \tag{23}$$

with left equality holding if and only if $G \cong K_n$ or $G \cong \overline{K}_n$.

In [11], the authors obtained the following bounds on $LE(G) + LE(\overline{G})$:

Theorem 3.16. [11] *Let G be a connected graph of order $n > 1$ with m edges and maximum degree Δ. Then*

$$2(n-1+\Delta-\delta) \leq LE(G) + LE(\overline{G}) \leq 8m - 4\Delta + 2n - \frac{12m}{n} \tag{24}$$

with left equality holding if and only if $G \cong K_n$ or $G \cong \overline{K}_n$ or $G \cong K_{1,\,2}$ or $G \cong (K_2 \cup K_1) \vee K_1$. Moreover, the right equality holding if and only if $G \cong K_{1,\,n-1}$.

Remark 3.17. *Let Γ be the class of graphs of order n with m edges such that $m \leq \frac{n(n-2)}{8}$. The authors in* [11] *mentioned that the upper bound in* (24) *is better that the upper bound in* (23) *for any graph in Γ.*

4. Relation between different graph energies

Gutman et al. [21] to believe that energy of a graph G is always less than or equal to the corresponding Laplacian energy and so, they made the following conjecture.

Conjecture 4.1. *For any graph G,*

$$\mathcal{E}(G) \leq LE(G). \tag{25}$$

Let KK_n be the graph obtained from two copies of the complete graph K_n by joining a vertex from one copy of K_n to two vertices from the other copy of K_n. Stevanović et al. [41] disproved the conjecture by giving an infinite family of graphs G, namely $G \cong KK_n$, for which the reverse inequality holds for all $n \geq 8$. By direct calculation, it can be seen that the inequality (25) is true for all graphs of order $n \leq 6$. For $n = 7$, there is only one graph (see graph H_1 in Fig. 1) for which the reverse inequality holds. Using this graph, Liu and Liu [33] constructed an infinite family of disconnected graphs for which the reverse inequality holds. Although from [33,41], it was clear that conjecture is not true in general, it is of interest to characterize the graphs for which the conjecture holds. Clearly characterizing all the graphs for which (25) holds or does not hold is not an easy task and is still an open problem [19].

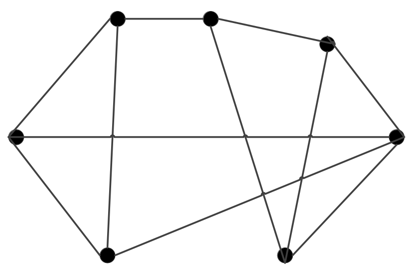

Figure 1. Graph H_1 .

Using Ky Fan Theorem, So et al. [39] presented the following relation between energy and Laplacian energy of graph.

Theorem 4.1. [39] *Let G be a graph of order n with m edges and vertex degrees $d_1,\ d_2,\dots,\ d_n$. Then*

$$LE(G) \le \mathcal{E}(G) + \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right|. \tag{26}$$

In [13], the authors obtained the following relation between energy and Laplacian energy of graphs.

Theorem 4.2. [13] *Let G be a graph of order n with m edges and vertex degrees $d_1,\ d_2,\dots,\ d_n$. Then*

$$LE(G) \le \mathcal{E}(G) + 2\sum_{i=1}^{\sigma} \Big(d_i - \frac{2m}{n} \Big), \tag{27}$$

where σ is the largest positive integer satisfying (14).

Remark 4.3. *In the paper* [13], *it was mentioned that the result in* (27) *is always better than the result in* (26).

We denote a graph H obtained from an isolated vertex joining by two edges to the centers of two stars S_3 and S_4, respectively. For $n \ge 3$, let S_n^+ be an unicyclic graph of order n obtained by adding an edge to S_n. Recently, Abreu et al. [1] obtained the following relation between $\mathcal{E}(G)$, $LE(G)$ and $LE^+(G)$ of graph G:

Theorem 4.4. [1] *Let G be a connected graph of order n with m edges. Then*

$$LE^+(G) + LE(G) \ge \max\left\{ 2\mathcal{E}(G),\ 2\sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right| \right\}. \tag{28}$$

The following result is the relation between $LE^+(G)$, $LE(G)$ and $\mathcal{E}(G)$.

Theorem 4.5. [12] *Let G be a graph of order n with m edges and rank r. Then*

$$LE^+(G) + LE(G) \ge 4\,\mathcal{E}(G) - \frac{4m\,r}{n} \tag{29}$$

with equality holding if and only if $G \cong n\,K_1$ or $G \cong K_2 \cup (n-2)\,K_1$ or $G \cong K_{n/2,\,n/2}$.

Remark 4.6. *In* [12], *the authors mentioned that two results* (28) *and* (29) *are incomparable. Sometimes the result in* (29) *is better than the result in* (28), *but not always. The result in* (29) *is better than the result in* (28) *for graphs H and $K_{3,\,5}$, on the other hand the result in* (28) *is better than the result in* (29) *for graphs S_8 and S_8^+.*

In 2008, Liu and Liu [32] considered a new Laplacian–spectrum–based graph invariant

$$LEL = LEL(G) = \sum_{k=1}^{n-1} \sqrt{\mu_k}$$

and named it *Laplacian–energy–like invariant*. The motivation for introducing LEL was in its analogy to the earlier much studied graph energy [30] and Laplacian energy [24]. For details on LEL see the review [31], the recent papers [8], and the references cited therein. Since both LE and LEL are depend on the Laplacian eigenvalues of graph G, recently, a nice relation between LE and LEL has been obtained in [11]:

Theorem 4.7. [11] *Let G be a connected graph of order n with m edges and maximum degree Δ. Then*

$$n^2\Big(LE(G)-n\Big)^2+8mn\left(LEL(G)-\sqrt{n}\right)^2\le\Big(4mn-4m-n(\Delta+1)\Big)^2$$

with equality holding if and only if $G\cong K_n$ or $G\cong K_{1,\,n-1}$.

A line graph L_G of a simple graph G is obtained by associating a vertex with each edge of the graph G and connecting two vertices with an edge if and only if the corresponding edges of G have a vertex in common. For example, the line graph of star $K_{1,\,n-1}$ is the complete graph K_{n-1}. The line graph L_G of graph G has m vertices and $\frac{1}{2}\,M_1(G)-m$ edges. The relation between $\mathcal{E}(L_G)$ and $LE^+(G)$ of graph G in the following result:

Theorem 4.8. [14] *Let G be a graph of order n with $m\ge 1$ edges.*
(a) For $m<n$,

$$\mathcal{E}(L_G)\le LE^+(G)+\frac{4m}{n}-4$$

with equality holding if and only if $G\cong K_2\cup(n-2)\,K_1$ $(n\ge 2)$ or $G\cong K_3\cup(n-3)\,K_1$ $(4\le n\le 6)$ or $G\cong K_{1,\,i-1}\cup(n-i)\,K_1$ $\left(\left\lceil\frac{n}{2}\right\rceil+1\le i\le n\right)$.
(b) For $m>n$,

$$\mathcal{E}(L_G)\ge LE^+(G)+\frac{4m}{n}-4$$

with equality holding if and only if $G\cong K_4$ or $G\cong K_4\backslash\{e\}$ or $G\cong K_4\cup K_1$ or $G\cong K_4\cup K_2$.
(c) Moreover, $LE^+(G)=\mathcal{E}(L_G)$ if and only if $m=n$.

From Theorem 4.8, the following three results have been obtained in [14]:

Corollary 4.1. [14] *Let G be a graph of order n with $m\ge 1$ edges. Then*

$$\mathcal{E}(L_G)=LE^+(G)+\frac{4m}{n}-4$$

if and only if $m=n$ or $G\cong K_2\cup(n-2)\,K_1$ $(n\ge 2)$ or $G\cong K_3\cup(n-3)\,K_1$ $(4\le n\le 6)$ or $G\cong K_{1,\,i-1}\cup(n-i)\,K_1$ $\left(\left\lceil\frac{n}{2}\right\rceil+1\le i\le n\right)$ or $G\cong K_4$ or $G\cong K_4\backslash\{e\}$ or $G\cong K_4\cup K_1$ or $G\cong K_4\cup K_2$.

Corollary 4.2. [22] *Let G be a graph of order n with $m\ge 1$ edges.*
(a) If $m<n$, then $\mathcal{E}(L_G)<LE^+(G)$.
(b) If $m>n$, then $\mathcal{E}(L_G)>LE^+(G)$.
(c) If $m=n$, then $\mathcal{E}(L_G)=LE^+(G)$.

Corollary 4.3. [14] *Let T be a tree of order n with p pendant vertices. Then*

$$\mathcal{E}(L_T) \leq LE^{+}(T) - 2\Big(1 - \frac{p}{n}\Big).$$

In [14], the authors obtained the lower and upper bounds on $\mathcal{E}(L_G)$ in the following three results:

Theorem 4.9. [14] *Let G be a graph of order n with $m \geq 1$ edges. Then*

$$\mathcal{E}(G) - 2p - 4s \leq \mathcal{E}(L_G) \leq \mathcal{E}(G) + 4m - 4n + 2p + 4s,$$

where p and s are the number of pendant and isolated vertices in G, respectively.

Corollary 4.4. [14] *Let G be a graph of order n with m edges and minimum degree $\delta \geq 1$. Then*

$$\mathcal{E}(G) - 2p \leq \mathcal{E}(L_G) \leq \mathcal{E}(G) + 4m - 4n + 2p,$$

where p is the number of pendant vertices in G.

Corollary 4.5. [14] *Let G be a graph of order n with minimum degree $\delta \geq 2$. Then*

$$\mathcal{E}(G) \leq \mathcal{E}(L_G) \leq \mathcal{E}(G) + 4m - 4n.$$

From Theorems 4.8 (a) and 4.9, the relation between signless Laplacian energy and energy of graphs has been obtained in [14].

Theorem 4.10. [14] *Let G be a graph of order n with m edges $(m < n)$ and p pendant vertices. Then*

$$LE^{+}(G) > \mathcal{E}(G) - \frac{4m}{n} - 2p - 4s + 4.$$

We now give two upper bounds on $\mathcal{E}(L_G)$ in terms of n, m and $M_1(G)$.

Theorem 4.11. [1] *Let G be a connected graph of order n with $m \geq 1$ edges and the first Zagreb index $M_1(G)$. Then*

$$\mathcal{E}(L_G) \leq \frac{M_1(G)}{m} - 2 + \sqrt{(m-1)\left(\left(1 + \frac{4}{m}\right) M_1(G) - \frac{M_1(G)^2}{m^2} - 2\,m - 4\right)}. \tag{30}$$

Theorem 4.12. [14] *Let G be a connected graph of order n with $m \geq 1$ edges and the first Zagreb index $M_1(G)$. Then*

$$\mathcal{E}(L_G) \leq 2m - 2n - 2 + \frac{M_1(G)}{m} + \sqrt{(n-1)\left(\left(1 + \frac{4}{m}\right) M_1(G) - \frac{M_1(G)^2}{m^2} - 6m + 4n - 4\right)} \tag{31}$$

with equality holding in (31) *if and only if $G \cong K_n$ or $G \cong K_{4,\,4}$.*

Remark 4.13. *For connected graph G with $m \geq n$, the upper bound in* (31) *is always better than the upper bound in* (30).

The positive (resp. negative) inertia of the graph G, denoted by ν^+ (resp. ν^-), is the number of the positive (resp. negative) eigenvalues of $A(G)$. The rank of a graph G is the rank of its adjacency matrix $A(G)$, equal to $\nu^+ + \nu^-$. Recall that $\nu^+ \geq 1$ holds if and only if the underlying graph has at least one edge. The relation between $\mathcal{E}(L_G)$ and $\mathcal{E}(G)$ is the following:

Theorem 4.14. [15] *Let G be a connected graph of order n with positive inertia $\nu^+ \geq 1$. Then*

$$\mathcal{E}(L_G) \geq 2\Big(\mathcal{E}(G) - 2\nu^+\Big) \tag{32}$$

with equality holding if and only if $G \cong C_4$ or $G \cong K_i$, $i = 2, 3, 4$.

The same result (32) holds for any graph:

Theorem 4.15. [15] *Let G be a graph of order n with positive inertia $\nu^+ \geq 1$. Then inequality (32) holds with equality if and only if $G \cong aK_2 \cup bK_3 \cup cK_4 \cup fC_4 \cup (n-2a-3b-4c-4f)K_1$, $a, b, c, f \geq 0$.*

The size of a maximal matching of G, that is, the maximum number of independent edges in G, is called the matching number of G, and will be denoted by $\beta(G)$. It is well known that $\nu^+(T) = \beta(T)$ for any tree T. The independence number of a graph G, denoted by $\alpha = \alpha(G)$, is the largest number of pairwise non-adjacent vertices in G. A forest is an acyclic graph, that is, a graph without any graph cycles. In [15], the authors mentioned the following three results:

Corollary 4.6. [15] *Let F be a forest of order n with matching number $\beta \geq 1$. Then*

$$\mathcal{E}(L_F) \geq 2\Big(\mathcal{E}(F) - 2\,\beta\Big)$$

with equality holding if and only if $G \cong aK_2 \cup (n-2a)K_1$, $a \geq 1$.

Corollary 4.7. [15] *Let G be a graph of order n with at least one edge and independence number α. Then*

$$\mathcal{E}(L_G) \geq 2\Big(\mathcal{E}(G) - 2n + 2\alpha\Big)$$

with equality holding if and only if $G \cong aK_2 \cup (n-2a)K_1$.

Corollary 4.8. [15] *Let G be a bipartite graph of order n with $m \geq 1$ edges and rank r. Then*

$$\mathcal{E}(L_G) \geq 2\Big(\mathcal{E}(G) - r\Big)$$

with equality holding if and only if $G \cong aK_2 \cup fC_4 \cup (n-2a-4f)K_1$, $a, f \geq 0$.

Remark 4.16. *In* [15], *it was mentioned that*

$$\mathcal{E}(L_G) \geq \max\left\{\mathcal{E}(G) + \frac{4m}{n} - 4\,,\ 2(\mathcal{E}(G) - r)\right\}$$

for bipartite graph G.

In [15], the authors obtained some bounds on $\mathcal{E}(L_G)$ in terms of n, m, p, s, and $\mathcal{E}(G)$.

Theorem 4.17. [15] *Let G be a graph of order n with $m > 1$ edges. Then $\mathcal{E}(L_G) \leq 4m - 2n$.*

Theorem 4.18. [15] *Let G be a graph of order n with $m \geq n$ edges. Then*

$$\mathcal{E}(L_G) \geq 4m - 4n + 2p + 4s,$$

where p and s are the number of pendent and isolated vertices.

The energy of the n-vertex complete graph K_n is equal to $2(n-1)$. A graph G on n vertices is said to be hyperenergetic if $\mathcal{E}(G) > 2n - 2$. The first systematic construction of hyperenergetic graphs was proposed by Walikar et al. [43], who showed that the line graphs of K_n $(n \geq 5)$ and of $K_{n/2,\, n/2}$ $(n \geq 8)$ are hyperenergetic. Hou et al. [25] showed that the line graph of any $(n,\, m)$-graph $(n \geq 5,\, m \geq 2n)$ is hyperenergetic. Here we mention another necessary condition for hyperenergetic graph.

Corollary 4.9. [15] *Let G be a graph of order n with m edges and p pendent vertices. If $m > 2n - p - 1$, then L_G is hyperenergetic.*

Remark 4.19. *The result in* Corollary 4.9 *was more stronger than the previous result (for $m \geq 2n$, L_G is hyperenergetic).*

Two nonisomorphic graphs are said to be equienergetic if they have the same energy. There exist numerous pairs of graphs with identical spectra, so-called cospectral graphs. In a trivial manner, such graphs are equienergetic. So it is interesting only in noncospectral equienergetic graphs. The concept of equienergetic graphs was put forward independently and almost simultaneously by Brankov et al. [6] and Balakrishnan [3]. Characterize a large class of equienergetic graphs in the following result:

Theorem 4.20. [15] *Let G be a graph of order $n > 2$ with m edges and minimum degree δ. If $\delta \geq \frac{n}{2} + 1$, then the energy of L_G is $4(m-n)$. Thus, the line graphs of all (n, m)-graphs with property $\delta \geq \frac{n}{2} + 1$ are mutually equienergetic.*

Corollary 4.10. [15] *Let G be a graph of order n and minimum degree δ. If $\delta \geq \frac{n}{2} + 1$, then*

$$\mathcal{E}(L_G) \geq \begin{cases} n^2 - 2n, & \text{if } n \text{ is even;} \\ n^2 - n, & \text{if } n \text{ is odd.} \end{cases}$$

In both cases, equality holds if and only if L_G is an $\left(\lceil \frac{n}{2} \rceil + 1\right)$-regular graph.

In Corollary 4.9, the result related to a class of graphs are hyperenergetic. We now mention another result of this kind.

Theorem 4.21. [15] *Let T be a tree. Then L_T is non-hyperenergetic, i.e.,*

$$\mathcal{E}(L_T) \leq 2\Big(|V(L_T)| - 1\Big).$$

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Bounds of the Estrada Index and the Laplacian Estrada Index

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Contents

1. Introduction

Given an n-vertex graph $G = (\{v_1, v_2, \ldots, v_n\}, E(G))$, the $n \times n$ matrix $A = A(G)$, whose entry in the i-th row and j-th column is

$$A_{i,j} = \begin{cases} 1 & \text{if } \{v_i, v_j\} \in E(G), \\ 0 & \text{otherwise} \end{cases}$$

for any $i, j \in \{1, 2, \ldots, n\}$, is known as the adjacency matrix of G. The eigenvalues of $A(G)$ are also called eigenvalues of G. Throughout this chapter, unless otherwise mentioned, G will be considered to have n vertices, m edges and eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. We will use popular notation such as S_n, P_n and K_n for the n-vertex star, path and complete graph, respectively.

The k-th spectral moment of G is defined by

$$\mathrm{M}_k(G) = \lambda_1^k + \lambda_2^k + \cdots + \lambda_n^k,$$

which coincides with the trace of A^k, and thus it is equal to the number of closed walks of length k in G.

In 2000, Estrada considered [1–3] the adjacency matrices of iterated line graphs of molecular graphs, he replaced the diagonal entries with the cosine of the dihedral angles in the corresponding molecules, then he studied the sum of the k-th spectral moment normalized by $k!$ of the resulting matrices. The parameter is then used to measure the 3D folding of molecules. If B is the matrix with eigenvalues $\beta_1, \beta_2, \ldots, \beta_n$, Estrada define the parameter

$$\mathrm{I}(B) = \frac{1}{n} \sum_{k \geq 0} \frac{M_k(B)}{k!} = \frac{1}{n} \sum_{k \geq 0} \frac{\beta_1^k + \beta_2^k \cdots + \beta_n^k}{k!} = \frac{1}{n} \sum_{i=1}^{n} e^{\beta_i}.$$

Later the Estrada index $\mathrm{EE}(G)$ of any graph G with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, is defined to be

$$\mathrm{EE}(G) = e^{\lambda_1} + e^{\lambda_2} + \cdots + e^{\lambda_n}.$$

Still in the 2000s, more applications of EE has been attempted. It has been used to measure bipartivity [4] and subgraph centrality [5] of complex structures such as communication, social and metabolic networks. Estrada, Rodríguez-Velázquez and Randić also used [6] EE to measure atomic branching in molecules. See also [7] for more structure-dependence of EE.

It is well known [8] that the k-th spectral moment of A coincides with the number closed walks of length k in G. This immediately implies that the Estrada index increases if a new edge is added to a graph. Therefore, for any n-vertex graph G which is not the edgeless graph E_n nor the complete graph K_n,

$$0 = \mathrm{M}_k(E_n) < M_k(G) < M_k(K_n) = (n-1)^k + (n-1)(-1)^k$$

for any $k \geq 2$, and thus

$$\mathrm{EE}(E_n) < \mathrm{EE}(G) < \mathrm{EE}(K_n).$$

Given a class of graph $\mathbb{G}$, determining a lower and/or an upper of $\mathrm{EE}(G)$ for $G \in \mathbb{G}$, and finding extremal graphs who achieve the bounds is a common problem that has been treated in the study of EE. This chapter aims at bringing together reported results on such problems. An effort was made to include key lemmas or descriptions of the techniques used that lead to the main results.

The next six sections are devoted to discussing bounds of the Estrada index in various classes of graphs. In the last section, after a list of definitions of other types of the Estrada index, details on the known bounds of the Laplacian Estrada index are provided.

2. (n, m)-type bounds

We call an (n, m)-graph, a graph with n vertices and m edges.

If G is a bipartite (n, m)-graphs, and eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{\lfloor n/2 \rfloor} \geq 0$ and $0 \geq \lambda_{\lceil n/2 \rceil} = -\lambda_{\lfloor n/2 \rfloor} \geq \lambda_{\lceil n/2 \rceil + 1} = -\lambda_{\lfloor n/2 \rfloor - 1} \geq \cdots \geq \lambda_n = -\lambda_1$. Since $\cosh(x) = (e^x + e^{-x})/2$, we can write [4]

$$\mathrm{EE}(G) = n_0(G) + 2 \sum_{+} \cosh \lambda_i, \tag{1}$$

where $n_0(G)$ is the nullity of G and $\sum_+$ is a summation over all positive eigenvalues of G. In view of the analogy between (1) and the formula of the energy $\mathrm{E}(G) = 2 \sum_+ \lambda_i$, Gutman and Radenković used the Lagrange multiplier technique and deduced a McClelland-type bound [9]

$$\mathrm{EE}(G) \geq n_0(G) + (n - n_0(G)) \cosh \sqrt{\frac{2m}{n - n_0(G)}} \; . \tag{2}$$

for any bipartite graphs G.

Introducing auxiliary quantities

$$\mathrm{EE}^-(G) = \sum_{i=1}^{n} e^{-\lambda_i} \qquad \text{and} \qquad \mathrm{ee}(G) = \sum_{i=1}^{n} \cosh \lambda_i,$$

which satisfy

$$\mathrm{EE}(G) - \mathrm{EE}^-(G) = 2 \sum_{k \geq 0} \frac{M_{2k+1}}{(2k+1)!} \geq 0$$

(with equality if and only if G is bipartite), and thus

$$\mathrm{EE}(G) \geq \frac{\mathrm{EE}(G) + \mathrm{EE}^-(G)}{2} = \mathrm{ee}(G),$$

Gutman used again the Lagrange-multiplier technique and study

$$\mathrm{ee}(G) - \frac{\alpha}{2} \left(\sum_{i=1}^{m} \lambda_i^2 - 2m \right)$$

to obtain the following theorem:

Theorem 1 ([10]).

$$\mathrm{EE}(G) \geq q + (n - q) \cosh \sqrt{\frac{2m}{n - q}}$$

for any (n, m)-graph G with exactly q ($< n$) isolated vertices, where the equality holds if and only if each of the connected components of G is a K_i for some $i \in \{1, 2\}$.

Theorem 2 (cf. [11, 12]). *Let G be an (n, m)-graph G with $m \neq 0$, then*

$$\sqrt{n^2 + 2nm + 2nt} \leq \mathrm{EE}(G) < n - 1 + e^{\sqrt{2m-1}}, \tag{3}$$

where t is the number of triangles in G. The lower bound is reached if and only if G has no edge.

The first inequality is obtained using the first four terms of the Maclaurin series of e^x. The second inequality improves the upper bounds [13]

$$\sqrt{n^2+4m+8t} \le \mathrm{EE}(G) = \sum_{n=1}^{n}\sum_{k\ge 0}\frac{\lambda_i^k}{k!} \le n + \sum_{n=1}^{n}\sum_{k\ge 1}\frac{|\lambda_i|^k}{k!} \tag{4}$$

$$\le n + \sum_{k\ge 1}\frac{1}{k!}\left(\sum_{n=1}^{n}\lambda_i^2\right)^{\frac{1}{2}} = n-1+\sum_{k\ge 0}\frac{(\sqrt{2m})^k}{k!} = n-1+e^{\sqrt{2m}}.$$

See [14] for a more general version of the upper bound in (3), provided for weighted graphs.

If furthermore G is bipartite, then $\lambda_1^{2k+1}+\lambda_2^{2k+1}+\cdots+\lambda_n^{2k+1} = 0$ for any non-negative integer k and one can use (1) to obtain

$$\mathrm{EE}(G) = n_0(G) + 2\sum_{+}\sum_{k\ge 0}\frac{\lambda_i^{2k}}{(2k)!} = n + 2\sum_{k\ge 1}\frac{1}{(2k)!}\sum_{+}(\lambda_i^2)^k \le n + 2\sum_{k\ge 1}\frac{1}{(2k)!}\left(\sum_{+}\lambda_i^2\right)^k$$

$$= n + 2\sum_{k\ge 1}\frac{m^k}{(2k)!} = n-2+2\sum_{k\ge 0}\frac{(\sqrt{m})^{2k}}{(2k)!} = n-2+2\cosh(\sqrt{m}). \tag{5}$$

Combined with (2), this leads to the following:

Theorem 3 (cf. [13,15])**.** *If G is a bipartite (n,m)-graph whose zero eigenvalue has multiplicity $n_0(G)$, then*

$$n_0(G) + (n-n_0(G))\cosh\sqrt{\frac{2m}{n-n_0(G)}} \le \mathrm{EE}(G) \le n-2+2\cosh(\sqrt{m}).$$

Equality on the upper bound holds for graphs obtained by adding c isolated vertex to the complete bipartite graph $K_{a,b}$, where $a+b+c=n$ and $ab=m$

In Theorem 2 of [13] the upper bound reads $n-2+2\cosh(\sqrt{2m})$, but in the proof it is actually $n-2+2\cosh(\sqrt{m})$.

Zhao and Jia [16] used similar argument to obtain upper and lower bounds in terms of n, m and λ_1:

$$n_0(G) + \cosh\sqrt{m-\lambda_1^2} + (n-n_0(G)-2)\cosh\sqrt{\frac{2m}{n-n_0(G)-2}}$$

$$\le \mathrm{EE}(G) \le n-4+\cosh\lambda_1+\cosh\sqrt{m-\lambda_1^2}. \tag{6}$$

for any bipartite (n,m)-graph G.

Arithmetic-Geometric Mean Inequality gives [17]

$$\mathrm{EE}(G) \ge e^{\lambda_1} + (n-1)\left(\prod_{i=2}^{n} e^{\lambda_i}\right)^{\frac{1}{n-1}} = e^{\lambda_1} + (n-1)e^{-\frac{\lambda_1}{n-1}} \tag{7}$$

for any (n,m) -graph G. Let χ be the chromatic number of G. From the observation that [18] $\lambda_1 \ge \chi - 1$ and that $f(x) = e^x + (n-1)e^{-\frac{x}{n-1}}$ is an increasing function of x, Das and Lee deduce that [17]

$$\mathrm{EE}(G) \ge e^{\chi-1} + (n-1)e^{-\frac{\chi-1}{n-1}},$$

with equality if and only if G is a complete graph or it has no edge.

Using [8] $\lambda_1 \geq \frac{2m}{n}$, essentially similar idea as above but slightly more technical leads to [17]

$$\mathrm{EE}(G) \geq e^{\frac{2m}{n}} + e^{-\frac{2m}{n}} + n - 2 \geq n + \left(\frac{2m}{n}\right)^2 + \frac{1}{12}\left(\frac{2m}{n}\right)^4.$$

It is worth to be pointed out that since (see Theorem 3)

$$\mathrm{EE}(K_{n_1,n_2}) = n_1 + n_2 - 2 + 2\cosh\sqrt{n_1 n_2},$$

it follows that [19]

$$\mathrm{EE}(K_{1,n-1}) < \mathrm{EE}(K_{2,n-2}) < \cdots < \mathrm{EE}(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}).$$

$K_{p,n-p}$ is the unique bipartite graph with n vertices p matching number and have maximum Estrada index, for any given $1 \leq p \leq \lfloor \frac{n}{2} \rfloor$; it is also the unique bipartite n-vertex graph with connectivity or edge connectivity p and maximum EE if $\frac{n-2}{2} \leq p \leq \lfloor \frac{n}{2} \rfloor$. See [19] for detailed proofs.

The next few bounds establish some relations between EE and other well studies graph invariants. Let n_- (resp. n_+) be the numbers of positive (resp. negative) eigenvalues of G, then [12]

$$\begin{aligned}\mathrm{EE}(G) &\leq n - n_+ + \sum_{i=1}^{n_+} e^{\lambda_i} = n - n_+ + \sum_{i=1}^{n_+}\sum_{k\geq 1}\frac{\lambda_i^k}{k!} = n - n_+ + \sum_{k\geq 1}\frac{1}{k!}\sum_{i=1}^{n_+}\lambda_i^k \\ &\leq n - n_+ + \sum_{k\geq 1}\frac{1}{k!}\left(\sum_{i=1}^{n_+}\lambda_i\right)^k = n - 1 + e^{\frac{\mathrm{E}(G)}{2}}. \end{aligned} \tag{8}$$

One can also get the lower bound [20]

$$\begin{aligned}\mathrm{EE}(G) &= n_0(G) + \sum_{\substack{1\leq i\leq n\\ \lambda_i>0}} e^{\lambda_i} + \sum_{\substack{1\leq i\leq n\\ \lambda_i<0}} e^{\lambda_i} \geq n_0(G) + n_+\left(\prod_{\substack{1\leq i\leq n\\ \lambda_i>0}} e^{\lambda_i}\right)^{1/n_+} + n_-\left(\prod_{\substack{1\leq i\leq n\\ \lambda_i<0}} e^{\lambda_i}\right)^{1/n_-} \\ &= n_0(G) + n_+\left(e^{\mathrm{E}(G)/2}\right)^{1/n_+} + n_-\left(e^{-\mathrm{E}(G)/2}\right)^{1/n_-} = n_0(G) + n_+ e^{\frac{\mathrm{E}(G)}{2n_+}} + n_- e^{-\frac{\mathrm{E}(G)}{2n_-}} \end{aligned} \tag{9}$$

and [12]

$$\mathrm{EE}(G) \geq \frac{1}{2}\,\mathrm{E}(G)(e-1) + n - n_+. \tag{10}$$

The bound in (9) is proven [21] sharp, it can be improved involving λ_1 as follows [11]

$$\mathrm{EE}(G) \geq e^{\lambda_1} + n_0(G) + (n_+ - 1)e^{\frac{\mathrm{E}(G)/2-\lambda_1}{n_+-1}} + n_- e^{-\frac{\mathrm{E}(G)}{2n_-}}.$$

Improved version of the bounds in (8) and (10) for strongly quotient graphs can be found in [22].

Theorem 4 ([12]). *For any r-regular n-vertex graph G with $r \neq 0$,*

$$e^r + (n-1)e^{\frac{-r}{n-1}} \leq \mathrm{EE}(G) < n - 2 + e^r + e^{\sqrt{r(n-r)-1}}.$$

If, additionally, G is bipartite then

$$2\cosh(r) + n - 2 \leq \mathrm{EE}(G) \leq n - 3 + 2\cosh(r) + 2\cosh\sqrt{nr/2 - r^2}. \tag{11}$$

Equalities in both sides of (11) *hold if* $r = \frac{n}{2}$.

Using the Arithmetic-Geometric Means Inequality and well known formulas such as $\lambda_1 + \lambda_2 + \cdots + \lambda_n = 0$ and $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2m$, Zhou [23] derived bounds of EE in terms of weighted sums of spectral moments:

Theorem 5 ([23])**.** *For any (n, m)-graph G and $k_0 \geq 2$,*

$$\sqrt{n^2 + \sum_{k=2}^{k_0} \frac{2^k \operatorname{M}_k(G)}{k!}} \leq \operatorname{EE}(G) \leq n - 1 - \sqrt{2m} + \sum_{k=2}^{k_0} \frac{\operatorname{M}_k(G) - (\sqrt{2m})^k}{k!} + e^{\sqrt{2m}}$$

where equality holds (in both sides) if and only if $m = 0$.

Given the fact that

$$\lambda_1 \geq \sqrt{\frac{\sum_{v \in V(G)} (\deg(v))^2}{n}} \qquad \text{and} \qquad \lambda_1 \geq \frac{2m}{n},$$

the bound in (7) can be improved by replacing λ_1 by $\sqrt{\frac{\sum_{v \in V(G)} (\deg(v))^2}{n}}$ or $2m/n$. The first case also provides a relation between $\operatorname{EE}(G)$ and the first Zagreb index $\operatorname{Zg}(G) = \sum_{v \in V(G)} (\deg(v))^2$. For a bipartite (n, m)-graph G, the upper bound

$$\operatorname{EE}(G) \leq \frac{24n + 22m + \operatorname{Zg}(G) + 8q}{24} + \frac{8m^3}{90(n - n_0(G))^2} e^{\sqrt{\frac{2m}{n - n_0(G)}}}$$

was determined recently [24], where q is the number of quadrangles in G. An upper bound depending on λ_1 is also known:

$$\operatorname{EE}(G) \leq n - 2 - \lambda_1 - \sqrt{2m - \lambda_1^2} + e^{\lambda_1} + e^{\sqrt{2m - \lambda_1^2}},$$

see [23] for more variations of this bound.

Applied to G and its complement $\overline{G}$, (7) leads to the Nordhaus-Gaddum type bound [23]

$$\begin{aligned} \operatorname{EE}(G) + \operatorname{EE}(\overline{G}) &\geq e^{\lambda_1} + e^{\overline{\lambda_1}} + (n-1)\left(e^{-\frac{\lambda_1}{n-1}} + e^{-\frac{\overline{\lambda_1}}{n-1}}\right) \geq 2e^{\frac{\lambda_1 + \overline{\lambda_1}}{2}} + 2(n-1)e^{\frac{\lambda_1 + \overline{\lambda_1}}{2(n-1)}} \\ &\geq e^{\frac{n-1}{2}} + 2(n-1)e^{-\frac{1}{2}} \qquad \text{since} \lambda_1 + \overline{\lambda_1} \geq n - 1. \end{aligned}$$

3. Trees

We denote by $\mathbb{T}_n$ the set of all trees with n vertices. Many characterisations of extremal trees with respect to EE corresponding to various subsets of $\mathbb{T}_n$ are obtained by first determining if a pertinently chosen graph transformation increases or decreases EE. Then apply the transformation iteratively.

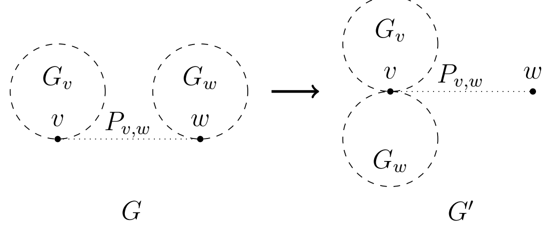


Figure 1. Transformation from G to G' of Lemma 1.

Lemma 1 ([25]). *Let v and w be vertices of a graph G that consists of two connected graphs G_v and G_w and a path $P_{v,w}$ joining two vertices v and w in G_v and G_w respectively. Let $w_1, w_2, \ldots, w_l$ be the neighbours of w that are not on the path $P_{v,w}$, and define*

$$G' = G - ww_1 - ww_2 - \cdots - ww_l + vw_1 + vw_2 + \cdots + vw_l,$$

as in Figure 1. Then

$$\mathrm{M}_{2k}(G) \leq \mathrm{M}_{2k}(G')$$

for every integer $k \geq 0$. The inequality is strict if $k \geq 2$ and both G_v and G_w consist of more than one vertex.

Iterative application of the transformation in Figure 1, by always choosing $P_{u,v}$ to be a P_2, one obtains a star. Repetitive application of the reverse transformation leads to a path. This observation was pointed out in [26], confirming a conjecture [13] that the path P_n and the star S_n are respectively the n-vertex tree with minimum and maximum Estrada index. Furthermore, Deng also proved in the same paper [26] that P_n has the minimum Estrada index among all connected graph with order n.

3.1 Trees with degree sequence conditions

We start with the case of trees with prescribed degree sequence.

Definition 1. *With given vertex degrees, the greedy tree is achieved through the following "greedy algorithm":*

i) Label the vertex with the largest degree as v (the root);

ii) Label the neighbours of v as $v_1, v_2, \ldots,$ assign the largest degrees available to them such that $\deg(v_1) \geq \deg(v_2) \geq \ldots$*;*

iii) Label the neighbours of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that they take all the largest degrees available and that $\deg(v_{11}) \geq \deg(v_{12}) \geq \ldots$*, then do the same for $v_2, v_3, \ldots$;*

iv) Repeat (iii) for all the newly labelled vertices, always start with the neighbours of the labelled vertex with largest degree whose neighbours are not labelled yet.

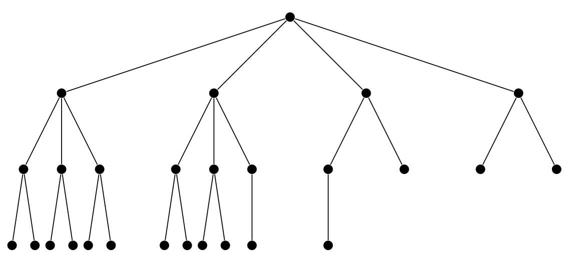


Figure 2. An example of a greedy tree.

We denote by $\mathbb{T}_D$ the set of all trees with degree sequence D, and G_D the greedy tree with degree sequence D.

Theorem 6 ([27]). *Let D be a degree sequence of a tree. For any non-negative integer k and all $T \in \mathbb{T}_D$, we have*

$$\mathrm{M}_k(T) \leq \mathrm{M}_k(G_D).$$

For sufficiently large even k, the inequality is strict unless T and G_D are isomorphic. Hence, we also have

$$\mathrm{EE}(T) \leq \mathrm{EE}(G_D)$$

with equality if and only if $T = G_D$.

A sequence $S = (s_1, s_2, \ldots, s_n)$ majorizes $R = (r_1, r_2, \ldots, r_n)$, and we write $S \preccurlyeq R$, if $s_1 + s_2 + \cdots + s_k \leq r_1 + r_2 + \cdots + r_k$ for any $k \in \{1, 2, \ldots, n\}$.

Theorem 7 ([27]). *Let $D = (d_1, \ldots, d_n)$ and $B = (b_1, \ldots, b_n)$ be degree sequences of trees of the same order such that $B \preccurlyeq D$. Then for any integer $k \geq 0$ we have*

$$\mathrm{M}_k(G_B) \leq \mathrm{M}_k(G_D).$$

If $B \neq D$ and k is even and ≥ 4, then the inequality is strict. Consequently, we also have

$$\mathrm{EE}(G_B) < \mathrm{EE}(G_D)$$

if $B \neq D$.

Let $\mathbb{S} \subseteq \mathbb{T}_n$ such that there exists a degree sequence D of an n-vertex tree which majorizes any degree sequence of an element in $\mathbb{S}$. Then for any $T \in \mathbb{S}$, we obtain

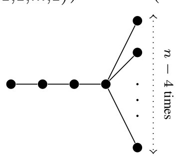
$$\mathrm{M}_k(T) \leq \mathrm{M}_k(G_D) \text{ for all } k \geq 0, \text{ and thus } \mathrm{EE}(T) \leq \mathrm{EE}(G_D).$$

For example, if we take $\mathbb{S} = \mathbb{T}_n$, then we can choose $D = (n-1, 1, \ldots, 1)$ so that $G_D = K_{1,n-1} = S_n$ is the n-vertex star, and one can obtain [26]:

Corollary 1. *For any n-vertex tree $T \neq S_n$, we have $\mathrm{M}_k(T) \leq \mathrm{M}_k(S_n)$ for all $k \geq 0$ and $\mathrm{EE}(T) < \mathrm{EE}(S_n)$.*

Note that Corollary 1 can also be deduced easily from Theorem 3, since all trees are bipartite. The six trees with $n \geq 6$ vertices and largest Estrada index are known [16,28], five of which are greedy trees: They are

$$\mathrm{EE}(G_{(n-1,1,\ldots,1)}) > \mathrm{EE}(G_{(n-2,2,1,\ldots,1)}) > \mathrm{EE}(G_{(n-3,3,1,\ldots,1)}) > \mathrm{EE}(G_{(n-4,2,2,1,\ldots,1)})$$

$> \mathrm{EE}\Bigg($ 

$\Bigg) > \mathrm{EE}(G_{(n-4,4,1,\ldots,1)}).$

Corollary 2. *Among trees T of order n with s leaves, $\mathrm{M}_k(T)$ is maximized by the greedy tree $G(s, 2, 2, \ldots, 2, 1, 1, \ldots, 1)$ (the number of 2s is $n - s - 1$, the number of 1s is s) for any $k \geq 0$.*

Corollary 3. *Among trees T of order n with independence number $\alpha \geq n/2$ and among all trees T with matching number $n - \alpha \leq n/2$, $\mathrm{M}_k(T)$ is maximized by the greedy tree $G(\alpha, 2, 2, \ldots, 2, 1, 1, \ldots, 1)$ (the number of 2s is $n - \alpha - 1$, the number of 1s is α) for any $k \geq 0$.*

The tree $G(\alpha, 2, 2, \ldots, 2, 1, 1, \ldots, 1)$ in Corollary 3 also has the maximum Estrada index among all trees with domination number $n - \alpha$, see [29].

Corollary 4. *Among trees T of order n and maximum degree Δ, $\mathrm{M}_k(T)$ is maximized by the the Volkmann tree G_D for $D = (\Delta, \ldots, \Delta, r, 1, \ldots, 1)$ for some $1 \leq r < \Delta$ for any $k \geq 0$.*

In each of the Corollaries 2, 3, 4, M_k can be replaced by EE. They are obtained in [30] using different approach. Corollary 4 was conjectured [31] by Ilić and Stevanović in 2009. In [32], Gutman et al. approximated the Estrada index of chemical trees (with maximum degree 4) by an expression that increases with the Zagreb index and the spectral radius. This finding is in favour of the conjecture of Ilić and Stevanović, because the Volkmann tree with maximum degree 4 clearly have maximum Zagreb index among fixed order chemical trees.

For a given vertex v of a graph G, we denote by $\mathrm{M}_k(G, v)$ the number of closed walks of length k starting from v in G. The following lemma appears to help to find trees with minimum Estrada index.

Lemma 2 ([31]). *Let $v_1, v_2, \ldots, v_n$ be the vertices from one end to the other end of a path P. Let v be a vertex of a connected graph G with $|V(G)| \geq 2$, and G_i^n is obtained by merging v with the vertex v_i of P. Then*

$$\mathrm{M}_{2k}(P, v_1) \leq \mathrm{M}_{2k}(P, v_2) \leq \cdots \leq \mathrm{M}_{2k}(P, v_{\lfloor n/2 \rfloor})$$

and

$$\mathrm{M}_{2k}(G_1^n) \leq \mathrm{M}_{2k}(G_2^n) \leq \cdots \leq \mathrm{M}_{2k}(G_{\lfloor n/2 \rfloor}^n),$$

for any integer $k \geq 0$. The inequalities are strict for large enough k.

See [33] for a slightly stronger version of Lemma 2, considering the case where the graph G is allowed to be in contact with two consecutive vertices in the path P. Let $G_{u,v}(a, b)$ be the graph obtained by attaching pendent path P_a and P_b at the two vertices u and v of a graph G, respectively. Zhibin Du established the following edge grafting theorem.

Theorem 8 ([34]). *Suppose that x is a pendent vertex in $G_{u,v}(1, 0)$ attached at u,*

$$\mathrm{M}_k(G_{u,v}(1, 0), x) \leq \mathrm{M}_k(G_{u,v}(1, 0), v) \quad \textit{for all integers } k \geq 0,$$

and there exists k for which the inequality is strict. Then for any integers $s \geq t + 2 \geq 2$,

$$\mathrm{EE}(G_{u,v}(s, t)) < \mathrm{EE}(G_{u,v}(t + 1, s - 1)).$$

Let $3 \leq d \in \mathbb{N}$. A d-starlike (or simply starlike) tree is a tree which has only one vertex of degree greater than 2, and it has degree d. A starlike tree with branching vertex v is called a balanced starlike tree if the difference between the lengths of any two branches of v is at most 1.

Theorem 9 ([31]). *The balanced Δ-starlike tree has maximum even spectral moments and maximum* EE *among Δ-starlike trees of order n.*

The fact that the path has minimum Estrada index among trees of given order follows immediately from Lemma 2. Ilić and Stevanović used it for more classes of trees. Let T be a tree and v is one of its vertex with largest degree. By moving a part of T along a path one step toward the closest leaf without modifying the degree of v, as long as this is possible, one will end with a starlike graph with branches of length 1 except possibly one. Let $B(n, i)$ be the tree which has exactly i leaves, one branching vertex v, such that each branch of v has length 1 except possibly one. Such trees are usually called a broom or a comet. For $n \geq i + 2$, define $B'(n, i)$ to be the graph obtained from $B(n, i)$ by moving the branching vertex one step closer to the center of the longest path.

Theorem 10 ([31]). *For any tree $T \neq B(n, \Delta), B'(n, \Delta)$ with maximum degree $\Delta \geq 3$ and $n \geq \Delta + 3$ vertices,*

$$\mathrm{EE}(B(n, \Delta)) < \mathrm{EE}(B'(n, \Delta)) < \mathrm{EE}(T).$$

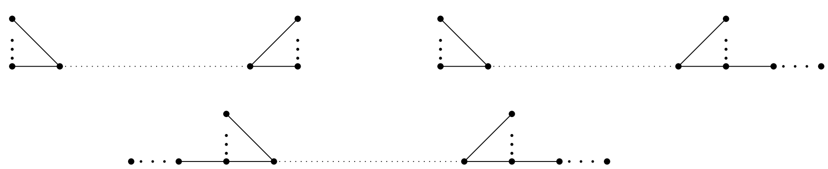
Theorem 11 ([31]). *Among all trees T with $n \geq 2\Delta$ vertices, which have a perfect matching and a maximum degree Δ, the minimum Estrada index is reached by the Δ-starlike tree obtained by merging one end vertex from each of $P_{n-2\Delta+3}$, P_2 and $\Delta - 2$ P_3.*

Li et al. continued this line of research. They studied the trees which have exactly two vertices with maximum degree. The following lemma describes the key graph transformation used.

Lemma 3. *[35] Let $u_0, u_1, \ldots, u_{s+1}$ be the vertices of a path $P = P_{s+2}$, from one end to the other. Let v and w be vertices from two connected graphs A and B, respectively. Define G_1 to be the graph obtained by merging v and u_0, w and u_{s+1}, and u_i with an end vertex of a path P_{ℓ_i} for any $i \in \{1, 2, \ldots, s\}$; and G_2 is obtained by merging v and w, respectively to the ends of a path $P_{s+2+\sum_{i=1}^{s} \ell_i}$. If G_1 and G_2 are not isomorphic, then*

$$\mathrm{EE}(G_2) < \mathrm{EE}(G_1).$$

The two Lemmas 2 and 3 imply that if we replace a branch or a part between two vertices of a tree by a path, then we obtain a tree with Estrada index smaller or equal to that of the original tree. By iteratively performing such a transformation, while avoiding to change the two largest degrees, we necessarily end with one of the following three types of trees:



Furthers comparison of the EE of these trees leads to Theorem 12.

For any $n, d, d' \in \mathbb{N}$ with $n \geq d + d'$, we denote by $BB(n, d, d')$ the tree obtained by merging the centres of the stars S_{d+1} and $S_{d'+1}$ with the ends of $P_{n-d-d'+2}$, respectively. See Figure 3.

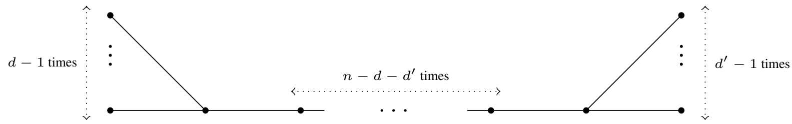


Figure 3. $B(n, d, d')$.

Theorem 12 ([35]). *If T is an n-vertex tree, $u, v \in V(T)$ and $\deg(u) = d \geq d' = \deg(v) > \deg(w)$ for all $w \in V(T) \setminus \{u, v\}$, then*

$$\mathrm{EE}(T) \geq \mathrm{EE}(BB(n, d, d')).$$

$BB(d+d', d, d')$ is also proven [36] to have maximum k-th spectral moment for any $k \in \mathbb{N}$, and thus maximum EE, among all trees with (d, d')-bipartition.

Let $SB(n, \Delta)$ be the tree obtained by merging a leaf of $BB(2\Delta, \Delta, \Delta)$ and an end of a $P_{n-2\Delta+1}$ path. Left as a conjecture in [35], the following result was soon confirmed:

Theorem 13 ([29]). *Let $n \geq 2\Delta + 1 \geq 7$ be integers, and T a tree which has two adjacent vertices with maximum degree Δ, then $\mathrm{EE}(T) \geq \mathrm{EE}(SB(n, \Delta))$, with equality only if G and $SB(n, \Delta)$ are isomorphic.*

3.2 Trees with perfect matching

Let $\mathbb{P}_{2n}$ be the set of all $2n$-vertex tree with perfect matching. Since for any $n \in \mathbb{N}$ the path P_{2n} has a perfect matching, it is the element of $\mathbb{P}_{2n}$ which has minimum Estrada index. Using the notation of Lemma 2, for any vertex v in a connected graph G and integer $n \geq 2$, if G_i^n has a perfect matching for some i then so is G_1^n. Therefore, the element of $\mathbb{P}_{2n} \setminus \{P_{2n}\}$ with minimum Estrada index has to be a 3-starlike tree. After further comparison, Zhai and Wang obtained the appropriate lengths of the branches:

Theorem 14 ([37]). *Let $n \in \mathbb{N}$ and $T \in \mathbb{P}_{2n} \setminus \{P_{2n}, {}^2T_1^{2n-4}\}$, where ${}^2T_1^{2n-4}$ is the tree obtained by merging one end vertex from each of P_2, P_3 and P_{2n-3}. Then*

$$\mathrm{EE}(T) > \mathrm{EE}({}^2T_1^{2n-4}).$$

In addition to other popular lemmas, the following lemma plays key role to obtain characterisation of trees with perfect matching and large Estrada index.

Lemma 4 ([38]). *Let G and H be two vertex-disjoint connected graphs with $|V(G)| \geq 4$ and $|V(H)| \geq 2$. Let $z \in V(H)$ and $v, v_1, v_2 \in V(G)$, where $\deg_G(v) = 1$, $\deg_G(v_1) = 2$, and $\deg_G(v_2) \geq 2$, and v_1 is adjacent to v and v_2. We have $\mathrm{M}_k(G; v_2) \geq \mathrm{M}_k(G; v_1)$ for all positive k. Furthermore, if there exists at least one k such that $\mathrm{M}_k(G; v_2) > \mathrm{M}_k(G; v_1)$, then $\mathrm{EE}(G_1) > EE(G_2)$, where G_i is obtained from G and H by identifying v_i to z, for any given $i \in \{1, 2\}$.*

Define F_{2n} to be the tree obtained by attaching a pendent vertex to each vertex of the star S_n, and B_{2n} is the tree obtained by merging one end vertex of a P_3 path with a vertex of degree 2 in F_{2n-2}.

Theorem 15 ([38]). *Let $T \in \mathbb{P}_{2n} \setminus \{F_{2n}, B_{2n}\}$ with $n \geq 5$, then*

$$\mathrm{EE}(F_{2n}) > \mathrm{EE}(B_{2n}) > \mathrm{EE}(T).$$

For $n \geq 4$ and $n = 2$ the unicyclic graph which has $2n$ vertices, a perfect matching and maximum Estrada index is [39] obtained by merging a vertex of C_3 with the branching vertex of $F_{2(n-1)}$.

3.3 Trees with fixed diameter

Let $P = P_{d+1}$ be a path with maximum length in a tree T with diameter d. It is clear from Lemma 1 that if we replace each branch attached to a vertex in P, by a start of the same number of vertices, to get T', then we have

$$\mathrm{M}_k(T) \leq \mathrm{M}_k(T') \quad \text{for all } k \in \mathbb{N} \text{ and } \mathrm{EE}(T) < \mathrm{EE}(T') \quad \text{unless } T = T'.$$

Zhang et al. [30] further observed that, in the caterpillar T', if the star branch furthest from the center of P and has no edges from P is moved to the next branching vertex closer to the center, then each spectral moment will not decrease and the Estrada index increases. After finite steps of such transformation, one will obtain a tree T'' with only one branching vertex. Combined with Lemma 5 in Section 4, this leads to the following theorem:

Theorem 16. *[30] Let T be a n-vertex tree with diameter d. Define $D(n, d)$ to be the tree obtained by attaching $n - d - 1$ pendent leaves to a center vertex of a path with length d. Then*

$$\mathrm{M}_k(T) \leq \mathrm{M}_k(D(n,d)) \qquad \textit{for all } k \in \mathbb{N} \textit{ and } \mathrm{EE}(T) < \mathrm{EE}(D(n,d))$$

unless T is isomorphic to $D(n, d)$.

3.4 Trees with segment sequence conditions

A segment of a tree T is a path whose end vertices have degree 1 or at least 3, and all its internal vertices have degree 2. In analogy to the degree sequence, the segment sequence of T is the non-increasing sequence of the lengths of its segments. We denote by $S(l_1, l_2, \ldots, l_m)$ the m-starlike graph where the lengths of the m branches are $l_1, l_2, \ldots, l_m$, respectively. The balanced m-starlike with n vertices is denoted by $ST(n, m)$.

The characterisation of the tree with given segment sequence and has maximum EE, can be obtained easily from Lemma 1.

Theorem 17. *[25] If T is a tree with segment sequence $(l_1, \ldots, l_m)$, then*

$$\mathrm{M}_{2k}(S(l_1, \ldots, l_m)) \geq \mathrm{M}_{2k}(T)$$

for any integer $k \geq 0$.

Furthermore, the inequality is strict if $T \neq S(l_1, \dots, l_m)$ and $k \geq 2$. Thus, in this case

$$\mathrm{EE}(S(l_1, \dots, l_m)) > \mathrm{EE}(T) .$$

The following majorisation theorem follows from Lemma 2.

Theorem 18. *[25] Given two segment sequences τ and τ' such that $\tau' \preccurlyeq \tau$, we have*

$$\mathrm{M}_{2k}(S(\tau)) \leq \mathrm{M}_{2k}(S(\tau'))$$

for every integer $k \geq 0$.

Combining Theorem 17 and Theorem 18, it follows that the balanced starlike $ST(n, m)$ maximizes all even spectral moments and thus the Estrada index among tree with at most m segments.

Corollary 5 (cf. [25, 29]). *If T is a tree with at most m segments and n vertices or at most m leaves, then*

$$\mathrm{M}_{2k}(T) \leq \mathrm{M}_{2k}(ST(n, m))$$

for every integer $k \geq 0$, and hence

$$EE(T) \leq EE(ST(n, m)).$$

The broom is again maximal among trees with bounded length of segments.

Corollary 6 ([25]). *If T is a tree of order n whose longest segment consists of L edges, then*

$$\mathrm{M}_{2k}(T) \leq \mathrm{M}_{2k}(B(n, n - L))$$

for every integer $k \geq 0$, and hence

$$EE(T) \leq EE(B(n, n - L)).$$

3.5 *k*-trees

For a given $k \in \mathbb{N}$, a graph is called a k-tree if it is the complete graph K_k or it can be obtained from a smaller k-tree G by adding a new vertex and k edges to join it to a k-clique in G. A k-tree is only a tree if $k = 1$. A vertex v of degree k in a k-tree G, whose neighbours form a k-cliques is called a simplicial vertex G. The k-tree K_k has no simplicial vertex. The k-tree of order $k + 1$ is usually considered to have one simplicial vertex, although each of its $k + 1$ vertices satisfies the condition to be a simplicial vertex. Let $\mathbb{T}_n^k$ be the set of all k-tree of order n. The $(k; n)$-star $S_{k,n-k}$ is the only one element of $\mathbb{T}_n^k$ which has $n - k$ simplicial vertices. Let $u_1, u_2, \dots, u_{n-k}$ be the simplicial vertices of $S_{k,n-k}$, and $v_1, v_2, \dots, v_k$ the other remaining vertices. Define

$$S'_{k,n-k} = S_{k,n-k} - u_1 v_1 + u_1 u_2.$$

It easy to check that $S'_{k,n-k} \in \mathbb{T}_n^k$. Huang and Wang observed [40] that whenever $T \in \mathbb{T}_n^k$ has fewer than $n - k$ simplicial vertices, there exists $T' \in \mathbb{T}_n^k$ with more simplicial vertices and larger Estrada index. This helped to find the two elements of $\mathbb{T}_n^k$ with largest EE.

Theorem 19 ([40]). *For any integers $n > k \geq 1$ and $T \in \mathbb{T}_n^k \setminus \{S_{k,n-k}, S'_{k,n-k}\}$, one has*

$$\mathrm{EE}(T) < \mathrm{EE}(S'_{k,n-k}) < \mathrm{EE}(S_{k,n-k}).$$

4. Unicyclic, bicyclic and tricyclic graphs

A connected graph G is a c-cyclic if $|E(G)| = |V(G)| - 1 + c$. For $c = 1, 2, 3$, G is a unicyclic, bicyclic and tricyclic respectively. This section contains bounds of the Estrada index in those classes of graphs, and related results.

In Lemma 1, the graphs G_v and G_w do not have to be a tree. We can use the lemma for unicyclic graph. Hence, an n-vertex unicyclic graph with maximum Estrada index must be a graph obtained by attaching pendent vertices to vertices of a cycle. Let $\mathbb{U}_{n,m}$ be the set of such unicyclic graphs which have n vertices and a cycle of length m.

The following exchange lemma by Wang and Xu is useful to the study of graphs which have cycles. In particular, it suggests that there is always a way to transform a graph which has more than one cut vertices to a graph with fewer cut vertices and larger Estrada index.

Lemma 5 ([41]). *Let G, G' and G'' be three disjoint connected graphs, $u, v \in V(G)$, $u' \in V(G')$, and $u'' \in V(G'')$. Let G_1, G_2 and G_3 be three graphs constructed from G, G' and G'', where G_1 is obtained by identifying u with u' and v with u'', G_2 by identifying u, u' with u'', and G_3 by identifying v, u' with u'' . Then $\mathrm{EE}(G_2) \geq \mathrm{EE}(G_1)$ or $\mathrm{EE}(G_3) \geq \mathrm{EE}(G_1)$. Furthermore, suppose that $\min\{|V(G')|, |V(G')|\} \geq 2$, then $\mathrm{EE}(G_2) > \mathrm{EE}(G_1)$ if $\deg_G(u) \geq \deg_G(v)$ or $\mathrm{EE}(G_3) > \mathrm{EE}(G_1)$ if $\deg_G(v) \geq \deg_G(u)$.*

It is clear from Lemma 5 that an element of $\mathbb{U}_{n,m}$ with maximum EE must have all its pendent vertices attached to one vertex.

A special case of the following theorem appears in [42], it compares unicyclic graphs with different cycle length.

Lemma 6 ([41]). *Let $l \geq 5$ be an integer, $u_1, u_2, \ldots, u_l$ be the consecutive vertices of a cycle C_l in a graph G. If there exists one vertex (denoted by u_l) in C_l of degree 2 and u_{l-2} is not adjacent to u_1, then there exists another graph $G = G - u_1u_l + u_1u_{l-2}$ with a cycle C_{l-2} such that $\mathrm{EE}(G) > \mathrm{EE}(G)$.*

The lemma implies that the n-vertex unicyclic graph with maximum EE has to be an element of $\mathbb{U}_{n,3}$. Bipartite unicyclic graph must have even girth, the corresponding maximal graph must have a cycle of length 4. Theorem 20 is obtained after comparison of the elements of $\mathbb{U}_{n,3} \cup \mathbb{U}_{n,4}$.

Let $C_m(k)$ be the graph obtained by attaching k pendent vertices to one vertex of C_m.

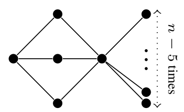
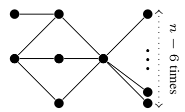
Theorem 20 (cf. [42, 43]).
i) Let G be a bipartite unicyclic graph on $n \geq 6$ vertices which is not $C_4(n-4)$ and $C_4(n-5,1)$, where $C_4(n-5,1)$ is obtained by attaching a pendent vertex to a degree 2 neighbour of the branching vertex of $C_4(n-5)$. Then $\mathrm{EE}(G) < \mathrm{EE}(C_4(n-5,1)) < \mathrm{EE}(C_4(n-4))$.

ii) Let G be an unicyclic graph on $n \geq 3$ vertices. Then

$$\min\{\mathrm{EE}(C_n), \mathrm{EE}(C_{n-1}(1))\} \leq \mathrm{EE}(G) \leq \mathrm{EE}(C_3(n-3)),$$

where the first inequality is strict if $G \notin \{\mathrm{EE}(C_n), \mathrm{EE}(C_{n-1}(1))\}$ and equality in the second inequality only occurs if $G = C_3(n-3)$.

The first four n-vertex bipartite unicyclic with largest EE, for $n \geq 28$, have girth 4, although some are not in $\mathbb{U}_{n,4}$, see [44]. The maximality of $C_4(n-4)$ and $C_3(n-3)$ are also proven in [41], where bicyclic graphs with maximum Estrada index are described. In [43], it is shown that the complements of the two bipartite unicyclic graphs of order $n \geq 6$ with maximum Estrada index have maximum Kirchhoff index among all complements of n-vertex bipartite unicyclic graphs. Similar work has been done in [45] for bipartite bicyclic graph of fixed order n; for this case the two graphs with maximum EE are

EE () > EE ()

for $n \geq 23$.

Let B_4 be the only bicyclic graph of order 4, it is obtained by adding one more edge to C_4. $E_n^{3,3}$ is defined as the graph obtained by attaching $n-4$ pendent vertices to one vertex of degree 3 in B_4.

Theorem 21 ([41, 46]). *Let B be an n-vertex bicyclic graphs. Then*

$$\mathrm{EE}(B) \leq \mathrm{EE}(E_n^{3,3}),$$

where the equality only occurs if the two graphs compared are isomorphic.

The authors of [41] noted that in a graph which does not have an even cycle, no two odd cycles share an edge. This leads to the finding that, for $n \leq m \leq 3(n-1)/2$, a connected graph of such type, with n vertices, m edges and maximum EE is obtained by merging one vertex from $m-n+1$ triangles and $3n-3-2m$ 2-vertex paths.

A cactus is a connected graph where no two cycles have a common edge, i.e any two of its cycles have at most one vertex in common. Shan et al. proved weaker versions of Lemmas 5 and 6 and used them to show [47] that the graph obtained by merging one vertex from each of k disjoint triangles and then attaching $n-2k-1$ pendent vertices to the resulting vertex has maximum Estrada index among all cacti with n vertices and k cycles. The case of cacti graphs with fixed number of cut edges is also discussed in the paper. See also [48] for further use of Lemma 5 to obtain that the 3-uniform linear star S_m^3 with m hyperedges has maximum EE among all 3-uniform linear hypergraphs with m edges, and

$$\mathrm{EE}(S_m^3) = \frac{m}{e} + (m-1)e + e^{(1+\sqrt{8m+1})/2} + e^{(1-\sqrt{8m+1})/2}.$$

Define T_n, for $4 \leq n \in \mathbb{N}$, to be the graph obtained by attaching $n-4$ pendent vertices to one vertex of the complete graph K_4, and for $5 \leq n \in \mathbb{N}$ T_n' is the graph obtained from the star S_n by adding three more edges to join one leaf to three other leaves.

Theorem 22 ([49])**.** *Let G be a tricyclic graph with n vertices.*

i) If $4 \leq n \leq 9$, then $\mathrm{EE}(G) \leq \mathrm{EE}(T_n)$, with equality only if G and T_n are isomorphic.

ii) If $n \geq 10$, then $\mathrm{EE}(G) \leq \mathrm{EE}(T'_n)$, with equality only if G and T'_n are isomorphic.

Studies of the case of 3-cactus graphs, where all cycles are triangles and there is no cut edges, are reported in [50]. Let $\mathbb{H}_t$ be the set of all 3-cactus graphs which have exactly t triangles. P_t^3 is the only element of $\mathbb{H}_t$ where no vertex has degree greater than 4, it is just a string of t triangles. S_t^3 is the only element of $\mathbb{H}_t$ where there is a central vertex shared by all t triangles. For $t \geq 3$, F_t^3 is the element of $\mathbb{H}_t$ obtained by attaching a triangle to a vertex of degree 2 in S_{t-1}^3.

Theorem 23 ([50])**.** *For any $G \in \mathbb{H}_t \setminus \{P_t^3, S_t^3, F_t^3\}$, one has*

$$4.28757879466(2t+1) - 4.80813993325 \approx \mathrm{EE}(P_t^3) < \mathrm{EE}(G) \leq \mathrm{EE}(F_t^3) < \mathrm{EE}(S_t^3).$$

Moreover, theorems on 3-cactus graphs with similar type as edge grafting can be found in [50], where the branches exchange a triangle instead of just an edge. As an application, the 3-cactus graph with t triangles, maximum degree Δ and minimum EE is characterised in the same paper.

5. Graphs with bounded degree

It is not difficult to deduce

$$\mathrm{EE}(G) = \mathrm{M}_0(G) + \mathrm{M}_1(G) + \frac{\mathrm{M}_2(G)}{2} + \frac{\mathrm{M}_3(G)}{3!} + \sum_{k \geq 4} \frac{\mathrm{M}_2(G)}{k!} = n + m + t + \sum_{k \geq 4} \frac{\mathrm{M}_2(G)}{k!}$$

where t is the number of triangles in G, and [51]

$$\begin{aligned}
&\mathrm{M}_k(G) \leq n\Delta^{k-1}, \\
&\mathrm{M}_k(G) \leq 2m\Delta^{k-2}, \\
&\mathrm{M}_k(G) \leq \Delta^{k-3} \sum_{v \in V(G)} \deg^2(v), \\
&\mathrm{M}_k(G) \leq \Delta^{k-4} 2 \sum_{uv \in E(G)} \deg(u)\deg(v), \\
&\mathrm{M}_k(G) \leq \sum_{v \in V(G)} \deg^{k-1}(v)
\end{aligned}$$

for any integer $k \geq 3$, where $\Delta = \max\{\deg(v) : v \in V(G)\}$. These in turn imply bounds for Estrada index:

Theorem 24. *[51] If G is an (n,m)-graph, with exactly t triangles and Δ maximum degree, then*

$$
\begin{aligned}
&\mathrm{EE}(G) < \frac{n}{\Delta}(e^{\Delta} - 1),\\
&\mathrm{EE}(G) < n + \frac{2m}{\Delta^2}(e^{\Delta} - 1 - \Delta),\\
&\mathrm{EE}(G) < n + m + \frac{\sum_{v\in V(G)} \deg^2(v)}{\Delta^3}\left(e^{\Delta} - 1 - \Delta - \frac{\Delta^2}{2}\right),\\
&\mathrm{EE}(G) < n + m + t + \frac{2\sum_{uv\in E(G)} \deg(u)\deg(v)}{\Delta^4}\left(e^{\Delta} - 1 - \Delta - \frac{\Delta^2}{2} - \frac{\Delta^3}{6}\right),\\
&\mathrm{EE}(G) < \sum_{v\in V(G)} \frac{e^{\deg(v)} - 1}{\deg(v)}.
\end{aligned}
$$

If G is bipartite, then

$$
\begin{aligned}
&\mathrm{EE}(G) < n + \frac{n}{\Delta}(\cosh(\Delta) - 1),\\
&\mathrm{EE}(G) < n + \frac{2m}{\Delta^2}(\cosh(\Delta) - 1),\\
&\mathrm{EE}(G) < n + m + \frac{\sum_{v\in V(G)} \deg^2(v)}{\Delta^3}\left(\cosh(\Delta) - 1 - \frac{\Delta^2}{2}\right),\\
&\mathrm{EE}(G) < n + m + \frac{2\sum_{uv\in E(G)} \deg(u)\deg(v)}{\Delta^4}\left(\cosh(\Delta) - 1 - \frac{\Delta^2}{2}\right),\\
&\mathrm{EE}(G) < n + \sum_{v\in V(G)} \frac{\cosh(\deg(v)) - 1}{\deg(v)}.
\end{aligned}
$$

Bounds for directed graph are also provided in the same paper.

6. Random graphs

Let $G_n(p)$ denote a random graph obtained from the Erdös-Reényi model, that is to start from n vertices and independently add an edge at probability $p \in (0,1)$ between each pair of vertices. The asymptotic estimate [52]

$$\mathrm{EE}(G_n(p)) = e^{np}\left(e^{O(\sqrt{n})+o(1)}\right) \quad a.s. \tag{12}$$

is better than the (n,m)-type lower bound $\sqrt{n^2+4m}$ and the upper bound $n - 1 + e^{\mathrm{E}(G)/2}$ in (8). (12) can be deduced from the asymptotic bounds [53]

$$
\begin{aligned}
e^{-(2+o(1))\sqrt{np}}\big(e^{(n-1)p} + (n-1)e^{-p}\big) &\le \mathrm{EE}(G_n(p))\\
&\le e^{(2+o(1))\sqrt{np}}\big(e^{(n-1)p} + (n-1)e^{-p}\big) \quad a.s.,
\end{aligned} \tag{13}
$$

later found by Shan. (13) is in turn a special case of the bounds [53]

$$e^{-2(2+o(1))\sqrt{\Delta}} \sum_{k=1}^{n} e^{\nu_k} \le \mathrm{EE}(G_n(P(n))) \le e^{-2(2+o(1))\sqrt{\Delta}} \sum_{k=1}^{n} e^{\nu_k} \quad a.s.,$$

which holds for $\Delta \gg \ln^4 n$; where Δ is the maximum degree in $G_n(P(n))$, $P(n)$ is an $n \times n$ matrix with entries in $[0,1]$ and $G_n(P(n))$ is the edge-independent random graph with vertices $v_1, v_2, \dots, v_n$ such that the probability to have an edge between v_i and v_j is $(P(n))_{i,j}$ for any $1 \leq i, j \leq n$.

Define the n-vertex random m-partite graph $G = G_{n,\nu_1,\nu_2,\dots,\nu_m}(p)$ to be such that $V(G) = V_1 \cup V_2 \cup \dots \cup V_m$ is a partition of its set of vertices, $|V_i| = n\nu_i$ for all i, and the probability to have an edge between any $u \in V_i$ and $v \in V_j$ for any $i \neq j$ is p. Applications of the Weyl inequality [8] to adjacency matrices of random graphs leads to asymptotic lower and upper of the Estrada index of $G_{n,\nu_1,\nu_2,\dots,\nu_m}(p)$.

Theorem 25 ([52]).

$$e^{np(1-\max\{\nu_1,\nu_2,\dots,\nu_m\})}\left(e^{O(\sqrt{n})} + o(1)\right) \leq \mathrm{EE}(G_{n,\nu_1,\nu_2,\dots,\nu_m}(p)) \leq e^{np}\left(e^{O(\sqrt{n})} + o(1)\right) \quad a.s.$$

A better upper bound than what is in Theorem 25 is known for the case of bipartite graphs.

Theorem 26 ([54]).

$$e^{n\nu_2 p}(e^{O(\sqrt{n})} + o(1)) \leq \mathrm{EE}(G_{n,\nu_1,\nu_2}) \leq e^{n\nu_1 p}(e^{O(\sqrt{n})} + O(1)) \quad a.s.$$

provided that $\lim_{n\to\infty} \nu_2/\nu_1 \in (0,1]$.

Theorem 26 is a considerable step toward the proof of the conjecture [52]

$$\mathrm{EE}(G_{n,\nu_1,\nu_2}) = e^{\frac{n}{2}p}(e^{O(\sqrt{n})} + O(1)) \quad a.s.$$

Let $\mathbb{T}_n^{\Delta}$ be the set of all tree with n vertices each of which has degree at most equal to Δ. We say that almost every tree in $\mathbb{T}_n^{\Delta}$ satisfies some given property Q if, assuming that every element of $\mathbb{T}_n^{\Delta}$ has the same probability to be picked up, the probability to get an element of $\mathbb{T}_n^{\Delta}$ with the property Q tends to 1 as n tend to infinity.

Theorem 27. *[55] There exists a constant μ_Δ such that for any given $\epsilon > 0$ almost every element T of $\mathbb{T}_n^{\Delta}$ satisfies*

$$(\mu_\Delta - \epsilon)n < \mathrm{EE}(T) < (\mu_\Delta + \epsilon)n.$$

7. Graphs with given number of cut vertices or number of cut edges

Say we have a graph M with n vertices r cut edges and maximum EE. Then M must be edge saturated, in the sense that after removing the cut edges from M one obtain a graph whose components are complete graphs. By Lemma 1, all the cut edges have to be pendent. In view of Lemma 5, we know that one can group the pendent vertices to one vertex without reducing the Estrada index.

Theorem 28 ([56]). *Let G be a graph with n vertices and r cut edges. Let $G_{n,r}$ be the graph obtained by attaching r pendent vertices to a vertex of the complete graph K_{n-r}. Then $\mathrm{EE}(G) \leq \mathrm{EE}(G_{n,r})$, with equality only if G and $G_{n,r}$ are isomorphic.*

Du, Zhou and Xing continued this research by studying the case of graphs with given number of cut vertices. Let G be an n-vertex graph, which has exactly r cut vertices, and maximum Estrada index. Then G has to be edge saturated, in the sense that no more edge can be added to G without reducing its number of cut vertices. Thus G has to be connected, otherwise one can add an edge between two cut vertices from different components or join a cut vertex in one component to all vertices of a component which has no cut vertex; this would increase the Estrada index and keep the number of cut vertices unchanged. Each cut vertex in G is contained in exactly two blocks. Further investigation of the structure of G leads to Theorem 29.

For $0 \le r \le n-2$, denote by $G_{n,r}$ the graph which contain a complete graph $K = K_{n-r}$, such that if all the edges of K are removed from G then one obtain $n-r$ path $P_{t_1}, P_{t_2}, \dots, P_{t_{n-r}}$, where $|t_i - t_j| \le 1$ for any i, j.

Theorem 29 ([57]). *Among n-vertex graphs with r cut vertices with $0 \le r \le n-2$, $G_{n,r}$ is the unique graph with maximum Estrada index.*

Let H_{n_1,n_2,n_3} be the graph obtained by adding all possible edges between $K_{n_1} \cup K_{n_2}$ and K_{n_3}. By similar reason as above, the graph with n vertex and connectivity κ (resp. edge connectivity κ') has to be of the form $H_{n_1,n_2,\kappa}$ (resp. $H_{n_1,n_2,\kappa'}$) for some n_1 and n_2.

Theorem 30 ([57]). *Among n-vertex graphs with connectivity $\kappa \le n-2$ (resp. edge connectivity $\kappa' \le n-2$), $H_{n-\kappa-1,1,\kappa}$ (resp. $H_{n-\kappa'-1,1,\kappa'}$) is the unique tree with maximum Estrada index.*

8. Generalisations and variations of the Estrada index

As part of the growing literature on the Estrada index, generalisations and variations were attempted.

Recall that if $A = A(G)$ is the adjacency matrix of an n-vertex graph

$$G = (\{v_1, v_2, \dots, v_n\}, E(G)),$$

and $D = D(G)$ the $n \times n$ diagonal matrix with $D_{i,i} = \deg(v_i)$ for all i, then the Laplacian matrix of G is $L = L(G) = D - A$, its signless Laplacian matrix is $L^+ = L^+(G) = D + A$, and its normalized Laplacian matrix $N = N(G)$ is defined by

$$N_{i,j} = \begin{cases} 1 & \text{if } i = j \text{ and } \deg(v_i) \neq 0, \\ \frac{-1}{\sqrt{\deg(v_i)\deg(v_j)}} & \text{if } \{v_i, v_j\} \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

For any pair $v_i, v_j \in V(G)$, $d_G(v_i, v_j)$ is the length of the shortest path in G which joins v_i to v_j, it is set to be ∞ if there is no such path. $d_G(v_i, v_j)$ is called the distance between v_i and v_j in G. The distance matrix $M = M(G)$ of G and its Harary matrix $H = H(G)$ are the $n \times n$ matrices defined by $M_{i,j} = d_G(v_i, v_j)$ and $H_{i,j} = 1/d_G(v_i, v_j)$ for any $1 \le i, j \le n$. A, L, L^+, N and M are all real symmetric matrices, thus their eigenvalues are all real numbers. Throughout this section, $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$ denote the eigenvalues of L, $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$ those of L^+, $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$ are those of M and $\tau_1 \geq \tau_2 \geq \ldots \tau \geq \tau_n$ those of N.

The Laplacian Estrada index of G is defined as [58] $\mathrm{LEE}(G) = e^{\mu_1} + e^{\mu_2} + \cdots + e^{\mu_n}$. Analogously, the signless Laplacian Estrada index is [59] $\mathrm{SLEE}(G) = e^{\nu_1} + e^{\nu_2} + \cdots + e^{\nu_n}$ and the distance Estrada index is [60] $\mathrm{LEE}(G) = e^{\delta_1} + e^{\delta_2} + \cdots + e^{\delta_n}$. The Seidel-Estrada index [61], Harary Estrada index [62] and the Randić Estrada index [63] are defined in a similar manner, using the Seidel matrix $S(G) = J_n - 2A - I_n$, Harary matrix and the Randić matrix respectively, where J_n is the $n \times n$ matrix with $(J_n)_{i,j} = 1$ for all i and j. The resolvent Estrada index is defined [64–66] in terms of the eigenvalues of the resolvent $\left(I_n - \dfrac{1}{n-1}A\right)^{-1}$ and is given by

$$\mathrm{EE}_r(G) = \operatorname{tr}\left(I_n - \frac{1}{n-1}A\right)^{-1} = \sum_{i=1}^{n}\left(1 - \frac{\lambda_i}{n-1}\right)^{-1} = \sum_{k=0}^{\infty} \frac{\mathrm{M}_k(G)}{(n-1)^k}.$$

This is one special case of the generalisation of the Estrada index [66] as

$$\mathrm{EE}(G, c) = \sum_{k=0}^{\infty} c_k \, \mathrm{M}_k(G).$$

The normalized Laplacian Estrada index is [67] $\mathrm{NLEE}(G) = e^{\tau_1 - 1} + e^{\tau_2 - 1} + \cdots + e^{\tau_n - 1}$. See also [68] for the Laplacian Estrada index like, and [69] for a generalisation of the Estrada index to be defined for Hermite matrices.

This section focuses in the Laplacian Estrada index. SLEE and NLEE are treated in another chapter of this book. The reader is referred to [60, 70–73] for the distance Estrada index, [63, 74] for the Randić Estrada index, [65, 75] for the resolvent Estrada index, [61] for the Seidel-Estrada index, and [62, 76] for the Harary Estrada index.

8.1 (n, m)-graphs

Arithmetic-Geometric Mean Inequality, estimates of $\sum_{i=1}^{n} \mu_i^k/(k!)$ and the relation $\mu_1 \geq 1 + \max\{\deg(v) : v \in V(G)\}$ lead to the following (n, m)-type bounds:

Theorem 31 (cf. [21, 58, 77–79])**.** *For any (n, m)-graph G one has*

i) $\mathrm{LEE}(G) \geq ne^{2m/n}$ *with equality if and only if G has no edge,*

ii) $\mathrm{LEE}(G) \geq 1 + (n-1)e^{2m/(n-1)}$ *with equality if and only if $m = 0$,*

iii) $\sqrt{n(n-1)e^{4m/n} + n + 8m + 2\,\mathrm{Zg}(G)} \leq \mathrm{LEE}(G) \leq n - 1 + e^{2m} + m - 2m^2 + \dfrac{\mathrm{Zg}(G)}{2}$ *with equality on both sides if and only if G has no edge,*

iv) If G has no isolated vertex, then

$$\mathrm{LEE}(G) \leq \left\lfloor \frac{2m}{n} \right\rfloor e^n + n - \left\lfloor \frac{2m}{n} \right\rfloor - 1 + e^{2m - n\lfloor 2m/n \rfloor}$$

with equality if and only if $m \in \{(n^2 - n)/2, (n^2 - n)/2 - 1\}$.

v) if G is r-regular then

$$\max\Big\{1+\sqrt{n-2+2nr+4r-4r^2+e^{-2r}+(n-1)(n-2)e^{2r/(n-1)}},\\ 1+(n-1)e^{nr/(n-1)}\Big\} \leq e^{-r}\,\mathrm{LEE}(G) \leq n-1-r^2+\frac{nr}{2}+e^r$$

vi) If Δ is the maximum degree in G, then

$$\mathrm{LEE}(G) \geq e^{\Delta+1-2m/n}+(n-2)\big(e^{4m/n-\Delta-1}\big)^{1/(n-2)}+e^{-2m/n}$$

and

$$\mathrm{LEE}(G) \geq e^{-2m/n}\Big(e^{\Delta+1}+e^{4m/(n-1)-\Delta-1}+(n-3)e^{2m/(n-1)}+1\Big).$$

The two lower bounds are sharp, they are reached when $G = K_n$ for example.

Note that for an r-regular bipartite graph G, the relation $e^{-r}\,\mathrm{LEE}(G) = \mathrm{EE}(G)$ holds. In this case, bounds for LEE can be derived easily from known bounds of EE.

The Nordhaus-Gaddum inequality

$$\mathrm{LEE}(G)+\mathrm{LEE}(\overline{G}) \geq 2+2(n-1)e^{n/2}$$

follows directly from Theorem 31 ii). If the number of connected components of G is c, then G has c zero eigenvalues, and in the same way as how to obtain Theorem 31 ii) one also get [21] $\mathrm{LEE}(G) \geq c+(n-c)e^{2m/(n-c)}$. If furthermore the maximum degree Δ of G is known, then the bound can be improved [80] to have

$$\mathrm{LEE}(G) \geq c+e^{\Delta+1}+(n-c-1)e^{\frac{2m-\Delta-1}{n-c-1}}.$$

Further useful inequalities are $\mu_1 \geq 2m/(n-1)$, and [81]

$$\left(\frac{1}{p}\sum_{i=1}^{p}a_i^{\ell}\right)^{1/\ell} \leq \left(\frac{1}{p}\sum_{i=1}^{p}a_i^{h}\right)^{1/h}$$

for non-negative numbers $a_1, a_2, \ldots, a_p$ and $\ell \leq h$ with $\ell, h \neq 0$. For example, they were used to obtain the next theorem.

Theorem 32 ([79]). *For any (n,m)-graph G with $n \geq 2$,*

$$\max\Big\{2+\sqrt{n(n-1)e^{4m/n}+4-3n-4m},\\ 1+2m-\sqrt{(n-1)(\mathrm{Zg}(G)+2m)}+(n-1)e^{\sqrt{(\mathrm{Zg}(G)+2m)/(n-1)}}\Big\}\\ \leq \mathrm{LEE}(G) \leq e^{\frac{2m}{n}}\left(n-1-\mathrm{LE}(G)-\frac{\mathrm{LE}^2(G)}{2}+\frac{\mathrm{Zg}(G)}{2}+m-\frac{2m^2}{n}+e^{\mathrm{LE}(G)}\right),$$

where $\mathrm{LE}(G) = \sum_{i=1} n|\mu_i - 2m/n|$ is the Laplacian energy. Both upper and lower bounds are sharp, they are reached when $m = 0$.

Another straightforward lower bound in terms of LE [82]

$$\mathrm{LEE}(G) \geq \Big(\ell + \ell_+ e^{\mathrm{LE}(G)/(2\ell_+)} + \ell_- e^{-\,\mathrm{LE}(G)/(2\ell_-)}\Big) e^{2m/n},$$

where ℓ_+ (resp. ℓ_-) is the number of positive (resp. negative) eigenvalues of $L(G)$ and ℓ its nullity.

Zhou studied [83] the Laplacian spectral moment $t_k = \sum_{k=1}^{n} \mu^k$, and observed that for a graph G with degree sequence $(d_1, d_2, \ldots, d_n)$,

$$t_k(G) \geq (d_1+1)^k + (d_n-1)^k + \sum_{i=2}^{n-1} d_i^k$$

for any integer $k \geq 0$, with equality for $k = 0, 1$ (in which cases $t_1(G) = n$, $t_2(G) = d_1 + d_2 + \cdots + d_n$), and the equality occurs for $k \geq 2$ if and only if G is the start S_n. This leads to the sharp upper bound [83]

$$\begin{aligned}\mathrm{LEE}(G) = \sum_{k\geq 0} \frac{t_k(G)}{k!} &\geq \sum_{k\geq 0} \frac{(d_1+1)^k + (d_n-1)^k + \sum_{i=2}^{n-1} d_i^k}{k!} \\ &= e^{d_1+1} + e^{d_n-1} + \sum_{i=2}^{n-1} e^{d_i}\end{aligned}$$

for a graph G with at least two vertices. Below are more lower bounds deduced from previously known lower bounds of the Laplacian spectral moments: If G has $n \geq 2$ vertices then [83]

$$\mathrm{LEE}(G) \geq n + \sum_{i=1}^{n} \frac{d_i}{1+d_i}(e^{1+d_i} - 1)$$

with equality if and only if G is a vertex-disjoint union of complete graphs, and

$$\begin{aligned}\mathrm{LEE}(G) &\geq 1 + e^{1+d_1} + (n-2)e^{\frac{2m-1-d_1}{n-2}} \\ \mathrm{LEE}(G) &\geq 1 + e^{1+d_1} + (n-2)e^{\left(\frac{s(G)n}{1+d_1}\right)^{\frac{1}{n-2}}}\end{aligned}$$

,

with equality if and only if G is S_n or K_n, where $s(G)$ is the number of spanning trees of G.

8.2 Trees and unicyclic graphs

Recall that the line graph of a graph G is defined by

$$\mathcal{L}(G) = \Big(E(G), \big\{\{e, e'\} \subseteq E(G) : e \neq e' \text{and } e \cap e' \neq \emptyset\big\}\Big).$$

For any bipartite graph (and thus for any tree) G, the following relation holds

$$\mathrm{LEE}(G) = n - m + e^2 \cdot \mathrm{EE}(\mathcal{L}(G)). \tag{14}$$

Since $\mathcal{L}(P_n) = p_{n-1}$ and $\mathcal{L}(S_n) = K_{n-1}$, and for any n-vertex tree T the line graph $\mathcal{L}(T)$ is some graph with $n-1$ vertices, the following theorem follows from the fact that P_n (resp. K_n) is the connected graph with n vertices and minimum (resp. maximum) EE.

Theorem 33 ([84]). *For any tree $T \in \mathbb{T}_n \setminus \{P_n, S_n\}$ we have*

$$\mathrm{LEE}(P_n) < \mathrm{LEE}(T) < \mathrm{LEE}(S_n).$$

Lemma 7 ([84]). *Let v be a vertex of degree $d \geq 2$ in a graph G. Let $u, v_1, v_2, \ldots, v_{d-1}$ be the neighbours of v in G. Assume that $\deg(v_i) = 1$ for all $i \in \{1, 2, \ldots, d-1\}$. Then*

$$\mathrm{LEE}(G - vv_1 - vv_2 - \cdots - vv_{d-1} + uv_1 + uv_2 + \cdots + uv_{d-1}) \geq \mathrm{LEE}(G),$$

where the equality only occurs if G is a star, in which case the two graphs are isomorphic.

It is clear from Lemma 7 that the n-vertex tree with second maximum LEE should be a double $S(a, n-a)$ where the only two vertices of degree greater than 1 have degree a and $n-a$, respectively. Further investigation of the Laplacian Estrada index of $S(a, n-a)$ leads to the conclusion [84] that $S(2, n-2)$ is the element of $\mathbb{T}_n$ with second maximum Laplacian Estrada index for $n \geq 4$. Du continued the work and obtained Theorem 34. Let v_0, v_1, v_2, v_3, v_4 be the vertices of P_5 from one end to the other. Define $P(n_1, n_2, n_3)$ the tree obtained P_5 by attaching n_i pendent vertices to v_i for $i = 1, 2, 3$.

Theorem 34 ([82]). *For any*

$$T \in \mathbb{T}_n \setminus \Big(\{S(i, n-i) : 2 \leq i \leq 4\} \cup \{S_n, P(0, n-5, 0), P(n-5, 0, 0)\}\Big)$$

with $n \geq 8$

$$\begin{aligned}\mathrm{LEE}(S_n) > \mathrm{LEE}(S(2, n-2)) > \mathrm{LEE}(S(3, n-3)) > \mathrm{LEE}(P(0, n-5, 0))\\ > \mathrm{LEE}(P(n-5, 0, 0)) > \mathrm{LEE}(S(4, n-4)) > \mathrm{LEE}(T).\end{aligned}$$

The double star $S(a, n-a)$ is also proven [82] to be the tree with $(a, n-a)$-bipartition with maximum LEE.

LEE obeys an edge grafting theorem (see Theorem 5.1 in [33]), hence the following natural consequences:

Theorem 35 ([33]). *i) For any tree $T \in \mathbb{T}_n$ with maximum degree Δ, if T is not isomorphic to the broom $B(n, \Delta)$ then* $\mathrm{LEE}(T) > \mathrm{LEE}(B(n, \Delta))$.

ii) Let $T \in \mathbb{T}_n \setminus \{P_n, B(n, 3)\}$, then $\mathrm{LEE}(T) > \mathrm{LEE}(B(n, 3))$.

In analogy to Theorem 16 and Corollary 5 respectively, $D(n, d)$ is also proven the unique element of $\mathbb{T}_n$ with diameter d and maximum LEE, and the balanced starlike tree $ST(n, m)$ is the unique n-vertex tree with m leaves and maximum EE. See [33, 85] for more Corollaries related to these, such as the maximal trees with given matching number, independence number or domination number.

The maximal unicyclic graphs with $n \geq 9$ vertices with respect to EE and LEE also coincide:

Theorem 36 ([86]). *For any $n \geq 9$, and any n-vertex unicyclic graph $G \neq C_3(n-3)$*

$$\mathrm{LEE}(G) < \mathrm{LEE}(C_3(n-3)) = e^n + e^3 + (n-3)e + 1.$$

See Theorem 2 in [78] and Theorem 2 in [87] for a natural continuation of Theorem36, considering the case of graphs G with $n + 1 \leq |E(G)| \leq 2n - 4$.

8.3 Miscellaneous

The connected n-vertex (not necessary a tree) with matching number β and maximum LEE is determined in [88]: it is the complete graph K_n if $\beta = \lfloor n/2 \rfloor$, and the $(\beta; n)$-star $S_{\beta,n-\beta}$ if $1 \leq \beta < \lfloor n/2 \rfloor$, where $\mathrm{LEE}(K_n) = (n-1)e^n + 1$ and $\mathrm{LEE}(S_{\beta,n-\beta}) = 1 + \beta e^n + (n - \beta - 1)e^{\beta}$. $S_{\beta,n-\beta}$ is also the unique n-vertex graph with independence number $n - \beta$ and maximum LEE, see [85].

If G is not a complete graph, and $G + e$ is obtained by adding one more edge e to G, then [89]

$$\mu_1(G+e) \geq \mu_1 \geq \mu_(G+e) \geq \mu_2 \geq \cdots \geq \mu_n(G+e) \geq \mu_n = 0,$$

where the $\mu_i(G+e)$ are the Laplacian eigenvalues of $G + e$, and

$$\sum_{i=1}^{n} \mu_i(G+e) - \sum_{i=1}^{n} \mu_i = 2.$$

These imply the following useful inequality [88]

$$\mathrm{LEE}(G+e) > \mathrm{LEE}(G).$$

It for instance imply that a graph with given order and connectivity κ (or edge connectivity κ') must be edge saturated. Using the notation of Theorem 30, we have [88]

$$\mathrm{LEE}(G) < \mathrm{LEE}(H_{n-\kappa-1,1,\kappa}) = ke^n + (n-k-2)e^{n-1} + e^k + 1$$

for any n-vertex graph $G \neq H_{n-\kappa-1,1,\kappa}$ with connectivity κ or edge connectivity κ.

For graphs with fixed chromatic numbers, the maximal graphs are complete multipartite. Recall that the Turan graph $T_{n,\chi}$ is the complete multipartite graph $K_{n_1,n_2,\ldots,n_\chi}$, where $|n_i - n_j| \leq 1$ for any i and j.

Theorem 37 ([78]). *Suppose that G is a graph with $n \geq 8$ vertices and chromatic number $\chi \geq 2$. Then*

$$\mathrm{LEE}(G) \leq (\chi-1)e^n + (n-\chi)e^{n-2} + (2\chi-2)e^{n-1} + 1 \qquad \text{if } \chi \leq n < 2\chi, \tag{15}$$

$$\mathrm{LEE}(G) \leq (\chi-1)e^n + 2(n-2\chi)e^{n-3} + (3\chi-n)e^{n-2} + 1 \qquad \text{if } 2\chi \leq n < 2\chi+3, \tag{16}$$

and

$$\mathrm{LEE}(G) \leq (\chi-1)(e^n + e^{n-2}) + (n-2\chi+1)e^{2\chi-2} + 1 \qquad \text{if } n \geq 2\chi+4. \tag{17}$$

Bounds in all three cases are sharp: Equalities in (15) *and* (16) *hold if and only if $G = T_{n,\chi}$, and the equality in* (17) *holds if and only if $G = K_{n-2\chi+2,2,2,\ldots,2}$.*

Further results for the case of $2 \leq \chi \leq n$ are reported in [85], where the series of lower bounds below are also obtained. Recall that $G_1 \vee G_2$ is the graph obtained by adding all possible edges between G_1 and G_2.

Theorem 38. *[85] Let G be a connected graph with $n \geq 3$ vertices and m edges.*

i) If $G \neq K_n$ then

$$\mathrm{LEE}(G) \geq 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}},$$

where Δ and δ are respectively the maximum and minimum degree in G. The equality holds if and only if $G = 2K_1 \vee K_{n-2}$ or $G = S_n$ or $G = (K_1 \cup K_{n-2}) \vee K_1$.

If, furthermore, the complement $\overline{G}$ of G is also connected, then the following Nordhaus-Gaddum inequality holds

$$\mathrm{LEE}(G) + \mathrm{LEE}(\overline{G}) > e^{\Delta+1} + e^{n-1-\Delta} + e^{\delta} + e^{n-\delta} + 2(n-3)e^{n/2} + 2$$

ii) If $\omega \geq 2$ is the clique number of G and Δ is the maximum degree, then

$$\mathrm{LEE}(G) \geq 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + (\Delta-\omega+1)e,$$

where the equality holds if G is the graph $K_\omega^{n-\omega}$ obtained by attaching $n-\omega$ pendent vertices to one vertex of K_ω.

$K_\omega^{n-\omega}$ is also proven [87] to be the n-vertex graph with exactly $n-\omega$ pendent vertices and maximum LEE.

Theorem 39 ([90]). *Let $G_{n,\nu_1,\nu_2,\ldots,\nu_k}(p)$ be the random multipartite graph as defined in Theorem 25, such that* $\lim_{n\to\infty} \beta_i/\beta_j = 1$, $1 \leq i, j \leq k$. *Then almost surely*

$$\begin{aligned}\left(\frac{2\sqrt{2p(1-p)}}{3} - \sqrt{\frac{2p-p^2}{k}} + o(1)\right) n^{3/2} &\leq \mathrm{EE}(G_{n,\nu_1,\nu_2,\ldots,\nu_m}(p)) \\ &\leq \left(\sqrt{2p-p^2}\left(1 + \frac{1}{\sqrt{k}}\right) + o(1)\right) n^{3/2}.\end{aligned}$$

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Extremal Trees With Respect to the Atom-Bond Connectivity Index

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Abstract

One of the most current and demanding problems in chemical graph theory is the problem of characterizing trees with minimal atom-bond connectivity index (minimal-ABC trees). Although this problem is still open, there was significant progress in the last several years heading towards its final solution. Here, we give an overview of the related theoretical results as well as an overview of some computational approaches that help us to better understand the structure of the minimal-ABC trees.

Contents

1. Introduction

Let $G = (V, E)$ be a simple undirected graph of order $n = |V|$ and size $m = |E|$. For $v \in V(G)$, the degree of v, denoted by $d(v)$, is the number of edges incident to v. The *atom-bond connectivity (ABC) index* of G is defined as

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{(d(u) + d(v) - 2)}{d(u)d(v)}}.$$

The ABC index was introduced in 1998 by Estrada, Torres, Rodríguez and Gutman [23], who showed that it can be a valuable predictive tool in the study of the heat of formation in alikeness. Ten years later Estrada [22] elaborated a novel quantum-theory-like justification for this topological index. After that revelation, the interest of ABC-index has grown rapidly. Accordingly, the physico-chemical applicability of the ABC index was confirmed and extended in several studies [4, 10, 15, 32, 36, 42, 55].

As a new and well-motivated graph invariant, the ABC index has attracted a lot of interest in the last several years both in the mathematical and chemical research communities. Due to this interest, numerous results, structural properties and few variants of ABC index were established [6–9, 11–14, 17, 21, 24–26, 28–31, 33, 35, 37, 44, 45, 47, 50, 52–54, 56].

In the sequel, we present some additional results and notation that will be used in the rest of the chapter. A vertex of degree one is a *pendant vertex*. A vertex is *big*, if its degree is at least 3 and it is not adjacent to a vertex of degree 2. As in [35], a sequence of vertices of a graph G, $S_k = v_0\, v_1 \dots v_k$, will be called a *pendant path* if each two consecutive vertices in S_k are adjacent in G, $d(v_0) > 2$, $d(v_i) = 2$, for $i = 1, \dots k-1$, and $d(v_k) = 1$. The length of the pendant path S_k is k. If $d(v_k) > 2$, then S_k is an *internal path* of length $k-1$.

A B_1-branch is a path of length 2. A B_k-branch, $k \geq 2$ is a (sub)graph comprised of vertex v of degree $k+1$ and of k pendant paths of length 2 that all have v as a common vertex. Illustrations of B_k-branches, $k \geq 1$, as well as of B_2^*, B_3^*, $B_3^{**}-$branches are given in Figure 1.

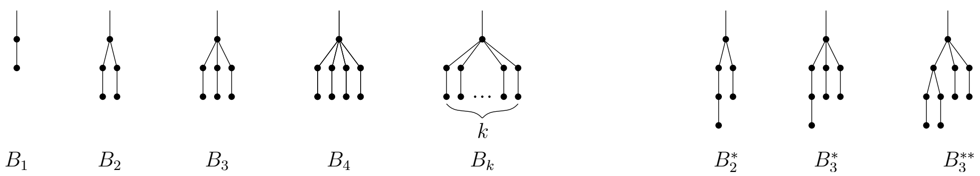

Figure 1. B_k and B_k^*-branches, $k \geq 1$.

A *k-terminal vertex* of a rooted tree is a vertex that has at least two children and all its (direct and indirect) children induce $B_{\geq 1}$-branches and maybe one B_1^*-branch. The (sub)tree induced by a *k-terminal vertex* and all its (direct and indirect) children vertices, we denote as a *k-terminal branch*. If the k-terminal vertex has at least one child with degree at least 3, then we say that the k-terminal branch is *proper*. Notice that B_k-branches are T_k-branches, but not proper T_k-branches, and the only proper T_k-branch in Figure 1 is the B_3^{**}-branch.

A sequence $D = (d_1, d_2, \dots, d_n)$ is *graphical* if there is a graph whose vertex degrees are d_i, $i = 1, \dots, n$. If in addition $d_1 \geq d_2 \geq \dots \geq d_n$, then D is a *degree sequence*.

In [51] Wang defined a *greedy tree* as follows.

Definition 1.1 ([51]). *Suppose the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following 'greedy algorithm':*

1. *Label the vertex with the largest degree as v (the root).*

2. *Label the neighbors of v as $v_1, v_2, \ldots,$ assign the largest degree available to them such that $d(v_1) \geq d(v_2) \geq \ldots$*

3. *Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq$ ... then do the same for $v_2, v_3, \ldots$*

4. *Repeat 3. for all newly labeled vertices, always starting with the neighbors of the labeled vertex with largest whose neighbors are not labeled yet.*

The rest of the chapter is structured as follows. In Section 2 we give an overview of the theoretical and in Section 3 an overview of the computational results related to the minimal-ABC trees. Concluding remarks are presented in Section 4.

2. Known structural properties of the minimal–ABC trees

The fact that adding an edge in a graph strictly increases its ABC index [12] (or equivalently that deleting an edge in a graph strictly decreases its ABC index [7]) has the following two immediate consequences.

Corollary 2.1. *Among all connected graphs with n vertices, the complete graph K_n has maximal value of ABC index.*

Corollary 2.2. *Among all connected graphs with n vertices, the graph with minimal ABC index is a tree.*

Although it is fairly easy to show that the star graph S_n is a tree with maximal ABC index [26], the characterization of trees with minimal ABC index (also refereed as minimal-ABC trees) still remains an open problem, despite the numerous attempts in the last years to come to a conclusion. A thorough overview of some initial known structural properties of the minimal-ABC trees was given in [34].

To determine the minimal-ABC tress of order less than 10 is a trivial task, and those trees are depicted in Figure 2. To simplify the exposition in the rest of the paper, we assume that the trees of interest are of order at least 10.

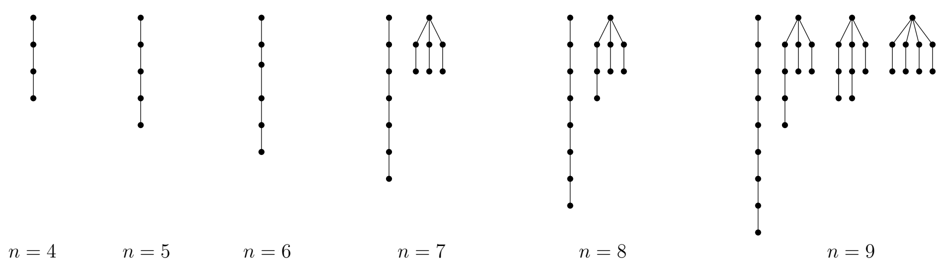

Figure 2. Minimal-ABC trees of order n, $4 \leq n \leq 9$.

In [35], Gutman, Furtula and Ivanović obtained the following results.

Theorem 2.1. *The n-vertex tree with minimal ABC-index does not contain internal paths of any length $k \geq 1$.*

Theorem 2.2. *The n-vertex tree with minimal ABC-index does not contain pendant paths of length $k \geq 4$.*

An immediate, but important, consequence of Theorem 2.1 is the next corollary.

Corollary 2.3. *Let T be a tree with minimal ABC index. Then the subgraph induced by the vertices of T whose degrees are greater than two is also a tree.*

The following result by Gan, Liu and You [29] characterizes the trees with minimal ABC index with prescribed degree sequences. The same result, using slightly different notation and approach, was obtained by Xing and Zhou [52].

Theorem 2.3. *Given the degree sequence, the greedy tree minimizes the ABC index.*

The next result was obtained in [34]. Alternatively, it can be obtained as a corollary of Theorem 2.3.

Theorem 2.4. *If a minimal-ABC tree possesses three mutually adjacent vertices v_1, v_2, v_3, such that*

$$d(v_1) \geq d(v_2) \geq d(v_3),$$

then v_3 must not be adjacent to both v_1 and v_2.

The following four results give us more precise description of the structure of minimal-ABC trees by excluding some configuration as well as giving us some bounds on the number of T_k- and B_4-branches.

Theorem 2.5 ([17]). *A minimal-ABC tree does not contain a B_k-branch, $k \geq 5$.*

Lemma 2.1 ([17]). *A minimal-ABC tree does not contain*

(a) a B_1-branch and a B_4-branch,

(b) a B_2-branch and a B_4-branch,

that have a common parent vertex.

Theorem 2.6 ([17]). *A minimal-ABC tree does not contain more than four B_4-branches.*

Proposition 2.1 ([18]). *A minimal-ABC tree can contain at most one proper T_k-branch, $k \geq 2$.*

Next result is an improvement of Theorem 2.5.

Lemma 2.2 ([20]). *A minimal-ABC tree does not contain B_k or B^*_k-branches, $k \geq 4$.*

An improvement of Theorem 2.2 is the following result by Lin, Lin, Gao and Wu [45].

Theorem 2.7. *Each pendant vertex of an n-vertex tree with minimal ABC index belongs to a pendant path of length k, $2 \leq k \leq 3$.*

A further improvement was obtained by the next theorem.

Theorem 2.8 ([35]). *The n-vertex tree with minimal ABC-index contains at most one pendant path of length 3.*

The following five results consider the configurations of the minimal-ABC trees that contain a pendent path of length 3.

Theorem 2.9 ([20]). *Suppose that T is a minimal-ABC tree of order $n > 18$. If T contains a pendent path of length 3, then two B_2-branches cannot be attached to the same vertex in T.*

Corollary 2.4 ([20]). *Suppose that T is a minimal-ABC tree of order $n > 18$. If T contains a pendent path of length 3, then there are at most two B_2-branches in T.*

Theorem 2.8 says that there is at most one pendent path of length 3 in the tree with minimal ABC-index. It was already observed in [40] that the position of the path of length $k \geq 3$ does not have an influence on the value of the ABC index. The following result was strengthened with Theorem 2.12.

Theorem 2.10 ([20]). *A minimal-ABC tree of order $n > 18$ with a pendent path of length 3 does not contain more than one B_2-branch.*

Theorem 2.11 ([19]). *A minimal-ABC tree of order $n > 18$ with a pendent path of length 3 does not contain B_1-branch (B_1^*-branch).*

Theorem 2.12 ([19]). *A minimal-ABC tree of order $n > 18$ with a pendent path of length 3 may contain a B_2-branch if and only if it is of order 161 or 168. Moreover, in this case a minimal-ABC tree is comprised of a single central vertex, B_3-branches and one B_2, including a pendent path of length 3 that may belong to a B_3^*-branch or B_2^*-branch.*

To the best of our knowledge, the above-mentioned results seem to be the only proven and published properties of the minimal-ABC trees. For complete characterization of the minimal-ABC trees, besides the theoretically proven properties, computer supported search can be of enormous help. Therefore, in the next section we present the existing computational approaches.

3. Computation of the minimal–ABC trees

3.1 Brute–force approach

A first significant example of using computer search was done by Furtula, Gutman, Ivanović and Vukičević [27], where the trees with minimal ABC index of up to the size of 31 were computed, and an initial conjecture of the general structure of the minimal-ABC trees was set. There, a brute-force approach of generating all trees of a given order, accelerated by using a distributed computing platform, was applied. The plausible structural computational model and its refined version presented there was based on the main assumption that the minimal ABC tree posseses a single *central vertex*, or said with other words, it is based on the assumption that the vertices of a minimal ABC tree of degree ≥ 3 induce a star graph. This assumption was shattered by counterexamples presented in [1–3, 16]. In this context, it is worth to mention that for a special class of trees, so-called *Kragujevac trees*, that are comprised of a central vertex and B_k-branches, $k \geq 1$, the minimal-ABC tress were fully characterized by Hosseini, Ahmadi and Gutman [40].

3.2 Approach by enumerating degree sequences of trees

There exist several algorithms for enumerating degree sequences of graphs. A comprehensive source of references of such algorithms can be found in [41]. Clearly, each of those algorithms can be used for enumerating degree sequences of trees just by considering only the degree sequences with sum of degrees equals to $2n-2$, where n is the length of the degree sequences. However, this is not an efficient approach, because most of the generated degree sequences are not degree sequences of trees. For an illustration, the number of all degree sequences of length 29 is $2\,022\,337\,118\,015\,338$ [49], while the number of degree sequences that correspond to trees of order 29 is 3010. Thus, it is not a surprise that the largest reported enumerated degree sequences of graphs was only of length 29, with running time of 6733 days, distributed to 200 PCs containing about 700 cores [41].

3.2.1 Enumerating degree sequences of trees based on the Havel–Hakim recursive characterization

In [16] by considering only the degree sequences of trees and some known structural properties of the trees with minimal ABC index all trees with minimal ABC index of up to size of 300, within 15 days, were computed. The enumeration of the degree sequences of trees in [16] is related to the enumeration of the degree sequences of graphs by Ruskey et al. [48]. It is based on the Havel-Hakimi's recursive characterization of the degree sequences of grpahs [38, 39], and exploits the so called "reverse search", a term originated by Avis and Fukuda [5]. The main result, on which our algorithm is based, is the following characterization of a degree sequence of a tree.

Theorem 3.1. *A sequence of integers $D = (d_1, d_2, \cdots, d_n)$, with $n-1 \geq d_1 \geq d_2 \geq \cdots \geq d_{n-m} > d_{n-m+1} = \cdots = d_n = 1$, is the degree sequence of a tree if and only if $C = (c_1, c_2, \cdots, c_{n-d_{n-m}+1})$ is the degree sequence of a tree, where*

$$c_i = \begin{cases} d_i & i \leq n-m-1; \\ 1 & otherwise. \end{cases} \tag{1}$$

Proof. Let T_C be a tree with degree sequence $C = (c_1, c_2, \cdots, c_{n-d_{n-m}+1})$, with $c_1 \geq c_2 \geq \cdots \geq c_{n-m-1} > c_{n-m} = \cdots = c_{n-d_{n-m}+1} = 1$ and $c_{n-m-1} \geq d_{n-m} \geq 2$, satisfying (1).

To prove the easier direction of the equivalence, just add $d_{n-m} - 1$ pendant vertices to a pendant vertex of T_C, obtaining a tree T_D. The degree sequence that corresponds to T_D is $D = (d_1, d_2, \cdots, d_n)$, with $n - 1 \geq d_1 \geq d_2 \geq \cdots \geq d_{n-m} > d_{n-m+1} = \cdots = d_n = 1$.

The other direction of the equivalence, we prove as follows. Let $D = (d_1, d_2, \cdots, d_n)$, with $n-1 \geq d_1 \geq d_2 \geq \cdots \geq d_{n-m} > d_{n-m+1} = \cdots = d_n = 1$, be a degree sequence of a tree T_D. Let v_{n-m} be the vertex with degree d_{n-m}. If v_{n-m} has $d_{n-m} - 1$ pendant vertices, then delete them obtaining the tree T_C. If this is not a case, i.e., v_{n-m} has $d > 1$ adjacent vertices of a degree bigger than one that comprised a set $U = \{u_1, u_2, \ldots, u_d\}$. Let U_1 be a set of adjacent vertices to u_1. First, delete all edges between u_1 and vertices in $U_1 \setminus \{v_{n-m}\}$ and add edges between vertices in $U_1 \setminus \{v_{n-m}\}$ and a pendant vertex whose distance to u_1 is bigger than its distance to any other vertex in U. Notice that T_D has more than d_{n-m} pendant vertices, therefore such pendant vertex must exists. Repeat the same as for u_1, for the rest of the vertices $u_2, u_3, \ldots, u_d$, considering one vertex per step until v_{n-m} has $d_{n-m} - 1$ pendant vertices, obtaining a tree T'_D. Observe that T'_D has the same degree sequence as T_D. Finally, in T'_D delete all $d_{n-m} - 1$ pendant vertices adjacent to v_{n-m}, obtaining the tree T_C. ■

Let $\mathbf{S_i}$ be the set of all sequences $D_i = (d_1, d_2, \cdots, d_i)$, with fixed length i , where $1 < i \leq n$ and $n - 1 \geq d_1 \geq d_2 \geq \cdots \geq d_{h_i} > d_{h_i+1} = \cdots = d_i = 1$. Notice that, d_{h_i} denotes the smallest degree in D_i larger than one. Define a function $f_i : \mathbf{S_i} \times d_{h_i} \to \mathbf{S_{i-d_{h_i}+1}} \times d_{h_i-1}$ such that for a given $D_i \in \mathbf{S_i}$, and $C = (c_1, c_2, \cdots, c_{i-c_{h_i}+1})$, it holds that $(C, c_{h_i-1}) = f_i(D_i, d_{h_i})$ if

$$c_k = \begin{cases} d_k & k \leq h_i - 1; \\ 1 & otherwise. \end{cases}$$

By Theorem 3.1 and definition od the function f_i, we have the following two corollaries.

Corollary 3.1. *For $i > 0$ and $D_i \in \mathbf{S_i}$, the sequence $D_i \in \mathbf{D_i}$ if and only if $f_i(D_i, d_{h_i}) = (D_{i-d_{h_i}+1}, d_{h_i-1}) \in \mathbf{D_{i-d_{h_i}+1}}$.*

Corollary 3.2. *Let $C = (c_1, c_2, \ldots, c_{h_i} \ldots, c_{i-z}, c_{i-z+1}) \in \mathbf{D_{i-z+1}}$, with c_{h_i} the smallest degree bigger than 1, and $2 \leq z \leq c_{h_i}$. The sequence $D_i = (d_1, d_2, \ldots, d_i) \in f_i^{-1}(C, c_{h_i})$ if and only if*

$$d_k = \begin{cases} c_k & k \leq h_i; \\ z & k = h_i + 1; \\ 1 & otherwise. \end{cases}$$

The following example illustrates Corollary 3.2:

$$f^{-1}(65111111111) \supseteq \{655111111111111, 65411111111111, 6531111111111, 652111111111\}.$$

One may straightforwardly implement Corollary 3.2 using recursion to enumerate degree sequences of trees.

Having all degree sequences of a particular length, it is easy to determine the trees with minimal ABC index. An algorithm of identifying trees with minimal ABC index of order n, comprised of three consecutive steps is presented below.

Algorithm 1 MINABCTREES(n). Algorithm based on the degree sequences that identifies the minimal-ABC trees.

Input: An order n of a tree
Output: A tree with the minimal ABC index
1. Enumerate the degree sequences based on the Havel-Hakim recursive characterization, satisfying in addition some known properties of the minimal-ABC trees.
2. Find corresponding 'greedy trees' for each generated degree sequence applying Theorem 2.3.
3. Calculate the ABC index of each 'greedy tree' and select the tree with minimal value.

3.2.2 Enumerating degree sequences of trees based on integer partitioning

Due to the nature of the recursive relation used in the first step of Algorithm 1, the same degree sequences were generated several times. That disadvantage was improved in [43], where the appropriate degree sequences were enumerated by applying an integer partitioning argument. Together with combing the known properties of the minimal-ABC, the number and the length of the candidate degree sequences was reduced. Thus, in [43], using a similar single computer platform as in [16], all minimal-ABC tree of up to size of 350 within 8 days were identified.

Another advantage of applying integer partitioning for enumeration of the degree sequences is that such enumeration can be easily parallelized. In [46], the above variant of the degree sequences' based algorithm, was implemented with MPI + OpenMP, and minimal-ABC trees of up to size of 400 within 23 hours, on a workstation group with 36 CPU cores, were identified.

Trees of order n, $7 \leq n \leq 400$, with minimal ABC index obtained by computer search are presented in Figures 3 and 4.

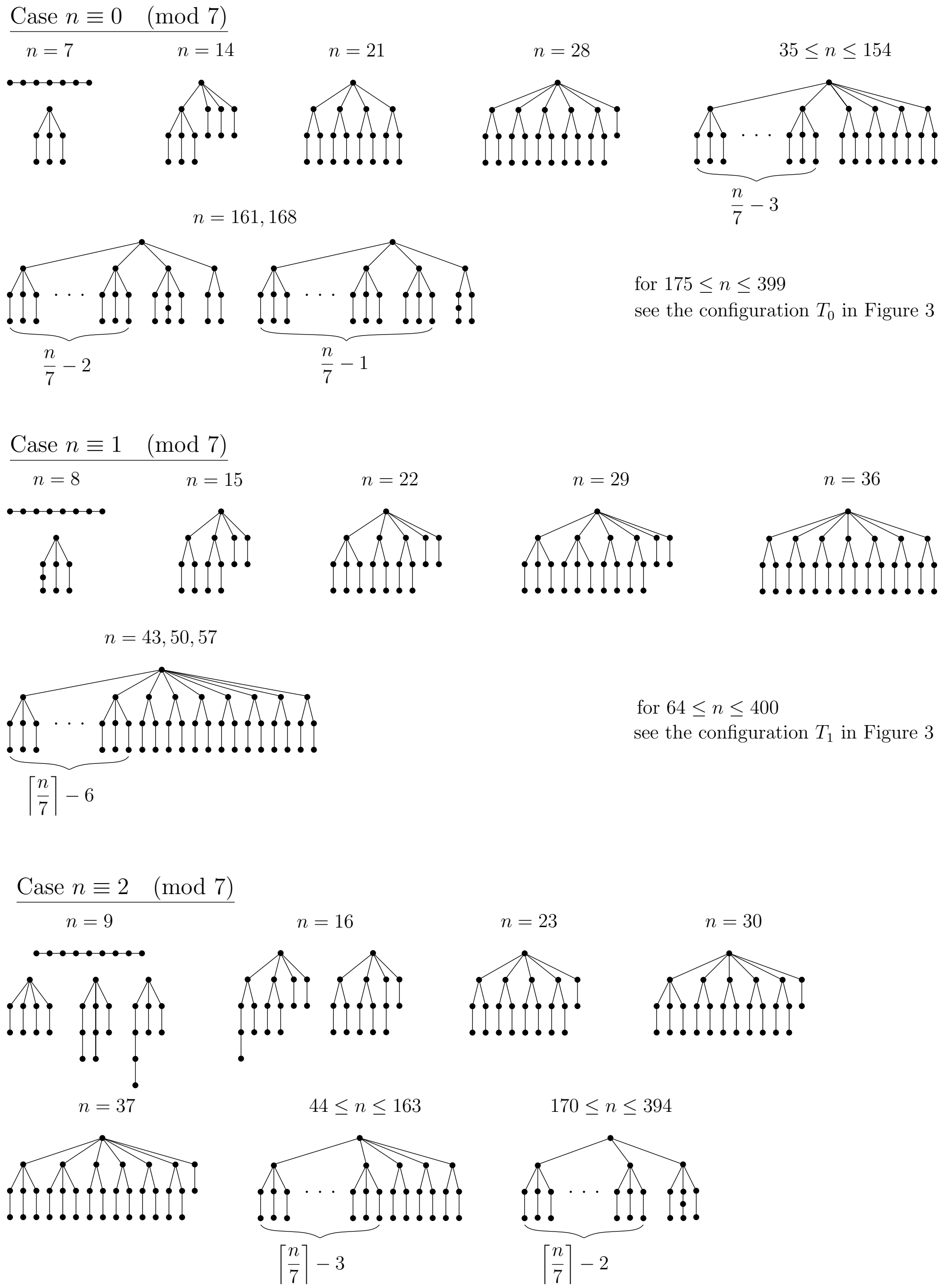

Figure 3. Trees of order n, $7 \leq n \leq 400$, with minimal ABC index obtained by computer search - cases $n \equiv 0, 1, 2 \pmod 7$.

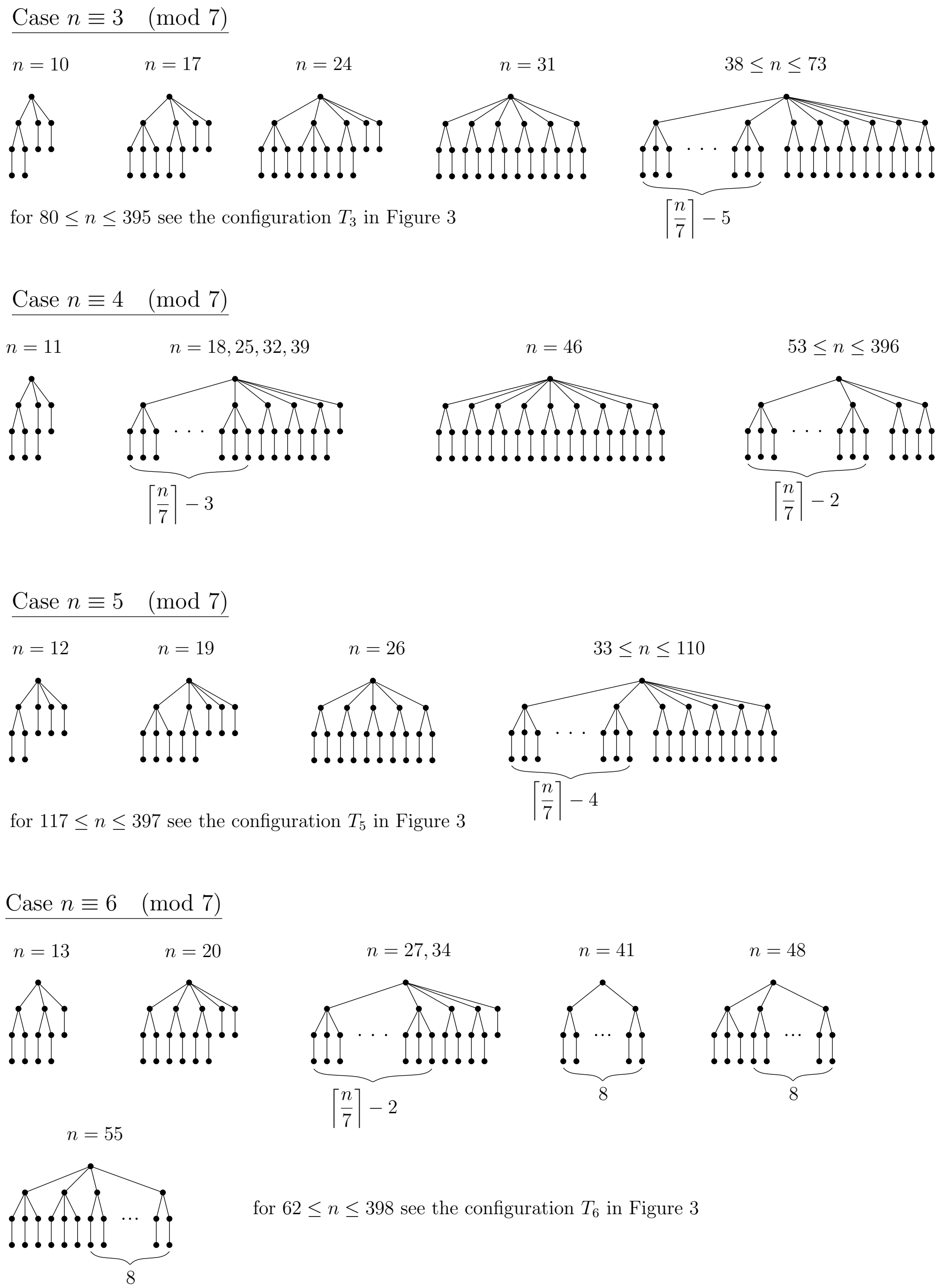

Figure 4. Trees of order n, $7 \leq n \leq 400$, with minimal ABC index obtained by computer search - cases $n \equiv 3, 4, 5, 6 \pmod 7$.

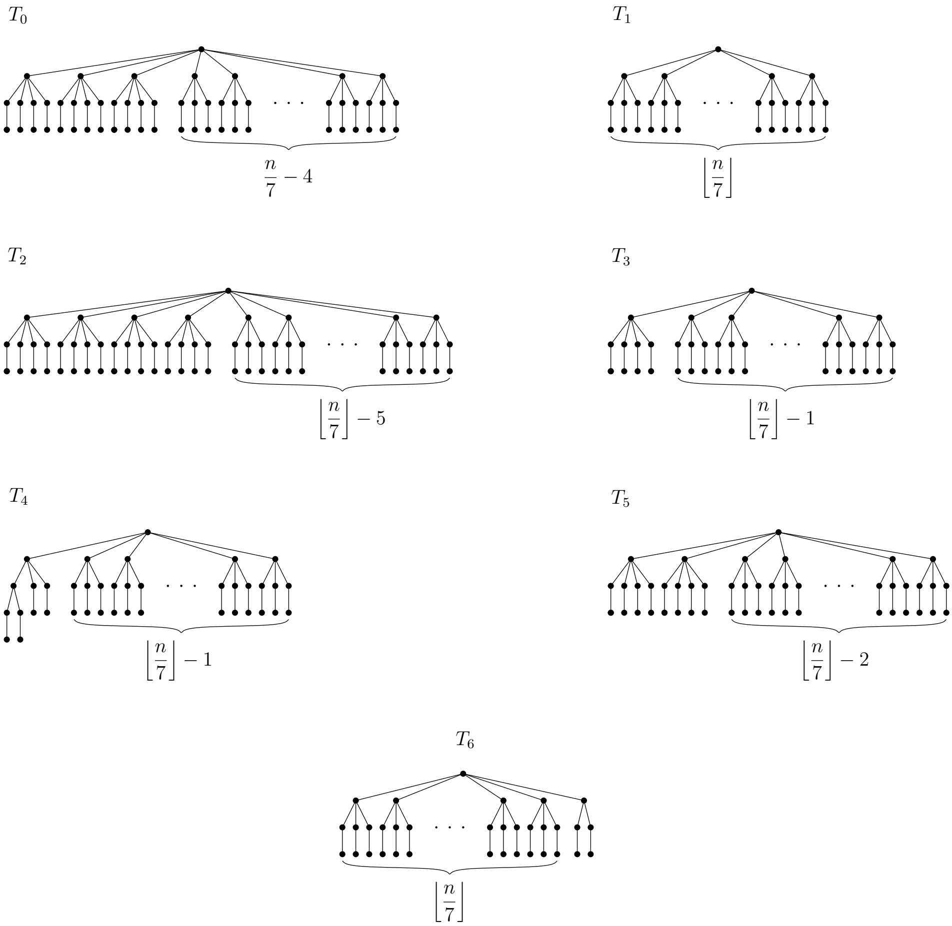

Figure 5. Types of trees with minimal ABC index based on the existing theoretical and computational results.

4. Concluding comments

As a consequence of the theoretically proven and computational results, one could modify the conjecture by Gutman and Furtula [33] about the trees with minimal ABC index, with hope that it is a correct one. The newly conjectured structure is depicted in Figure 5. However, note that this structure is computationally supported in the cases when the order of a tree is up to 400 and indeed, it was shown that it does not hold for a larger n. In [1] several counterexamples were shown and one of them is given in Figure 6. So, the exciting journey of complete characterization of the minimal-ABC trees continues and we hope that the newly emerging theoretical and computational results will help us to reach the final destination.

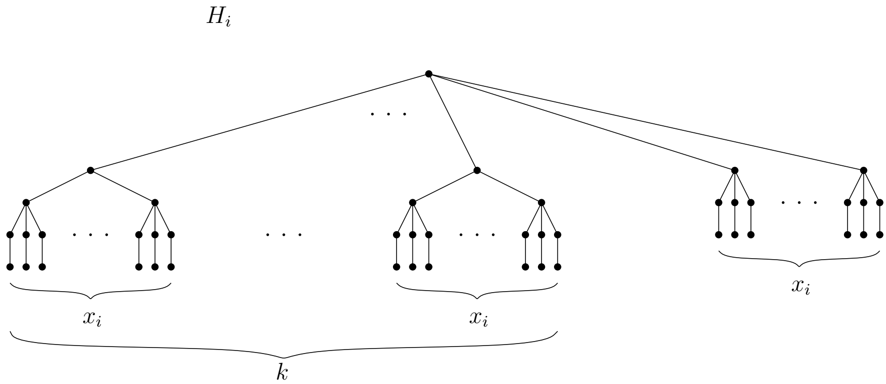

Figure 6. Graph H_i, $i = 0, 1, \ldots, 6$ that for enough large n has smaller ABC-index than its corresponding graph T_i from Figure 5, for $i = 0, 2, 3, 4, 5, 6$, $k = (i + 6) \mod 7$, and $k = 7$, for $i = 1$.

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Relations Between the First and Second Zagreb Indices of Graphs

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Abstract

For a graph $G = (V, E)$, the first Zagreb index M_1 and the second Zagreb index M_2 are defined as: $M_1(G) = \sum_{u \in V(G)} (d_G(u))^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$, where $d_G(u)$ is the degree of vertex u in G. In 2007, it was conjectured that for each simple graph G with n vertices and m edges, the inequality $M_2(G)/m \geq M_1(G)/n$ holds. Although this conjecture does not hold in general, it was the beginning of a long series of studies in which the validity or non-validity of this inequality for various classes of graphs. This chapter concentrates on the above inequality and its generalization. Moreover, the difference between Zagreb indices is discussed.

Contents

1. Introduction

Let $G = (V, E)$ be a connected graph with vertex set $|V(G)| = n$ and edge set $|E(G)| = m$. Denote by $d_G(u)$, the degree of the vertex u of G. A pendant vertex is a vertex of degree one. An edge of a graph is said to be pendant if one of its end vertices is a pendant vertex. For $v \in V(G)$, $N_G(v)$ denotes the neighbors of v. The maximum and minimum degree of G are denoted by Δ and δ. The average of the degrees of the vertices adjacent to a vertex u is denoted by $\mu_G(u)$. The path, star, cycle, complete graph of order n are denoted by P_n, S_n, C_n and K_n, respectively. A regular graph is a graph where each vertex has the same degree. A regular graph with vertices of degree k is called a k-regular graph. A cut edge in a graph G is an edge whose removal increases the number of connected components of G. The cyclomatic number of a connected graph is equal to $\nu = m - n + 1$, i. e., its number of independent cycles. If $\nu > 1$ for a graph G then it is called cyclic graph. If a graph G has $\nu = 0$, $\nu = 1$ and $\nu = 2$, then it is called tree, unicyclic and bicyclic, respectively.

The classical first Zagreb index M_1 and second Zagreb index M_2 of graph G are among the oldest and the most famous topological indices and they are defined as

$$M_1(G) = \sum_{u\in V(G)} (d_G(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)\ .$$

In 1972, the quantities the Zagreb indices were found to occur within certain approximate expressions for the total π-electron energy [26]. In 1975, these graph invariants were proposed to be measures of branching of the carbonatom skeleton [25]. For details of the mathematical theory and chemical applications of the Zagreb indices, see [9, 16, 18, 19, 23, 24, 37, 39, 43, 46, 55] and the references cited therein. The Zagreb indices were independently studied in the mathematical literature under other names [7, 8, 10, 14, 21, 22, 44, 45]. Zagreb indices have been generalized to variable first and second Zagreb indices in [41], where they defined as

$${}^{\lambda}M_1(G) = \sum_{u\in V(G)} (d_G(u))^{2\lambda} \quad \text{and} \quad {}^{\lambda}M_2(G) = \sum_{uv\in E(G)} (d_G(u))^{\lambda}\,(d_G(v))^{\lambda}\ .$$

A natural issue is to compare the values of the Zagreb indices on the same graph. Observe that, for general graphs, the order of magnitude of M_1 is $O(n^3)$ while the order of magnitude of M_2 is $O(mn^2)$. This suggests comparing $M_1(G)/n$ and $M_2(G)/m$ instead of $M_1(G)$ and $M_2(G)$. Using the AutoGraphiX system, Caporossi and Hansen [11, 12] proposed the following conjecture:

Conjecture 1.1. *For all simple connected graphs G,*

$$\frac{M_2(G)}{m} \geq \frac{M_1(G)}{n} \tag{1}$$

and the bound is tight for complete graphs.

Although this conjecture is disproved for general graphs [27], it was just the beginning of a long series of studies in which the validity or non-validity of (1) was considered for various classes of graphs. This chapter outlines previously established results on the inequality (1) and generalization of Conjecture 1.1 for the variable Zagreb indices.

2. Zagreb indices inequality

In 2007, Hansen and Vukičević [27] showed that the Conjecture 1 does not hold in general and it is true for chemical graphs, i.e. for graphs with maximum degree at most four.

Theorem 2.1. [27] Inequality (1) holds for all chemical graphs. Moreover, the bound is tight if and only if all edges uv have the same pair $(d(u), d(v))$ of degrees or if the graph is composed of disjoint stars S_5 and cycles $C_p, C_q, \ldots$ of any length.

Although Conjecture 1 is disproved for general graphs, Vukičević and Graovac showed that it is true for all trees.

Theorem 2.2. [52] Let T be a tree with n vertices and m edges. Inequality (1) holds with equality if and only if T is isomorphic to $K_{1,\,n-1}$.

In [38], Liu proved that Inequality (1) holds for all unicyclic graphs.

Theorem 2.3. [38] Let G be a unicyclic graph with n vertices and m edges. Then Inequality (1) holds with equality if and only if G is isomorphic to C_n.

Sun and Wei [49] showed that Inequality (1) holds for bicyclic graphs except one class and characterized the extremal graph. Moreover, counter-examples of connected bicyclic graphs are constructed from the excluded class. A hook is the unique neighbor of a pendant vertex. Denote the set of hooks of G by $H(G)$. For any vertex $u \in H(G)$, $N_G(u) = v_1, \ldots, v_k$ $(k \geq 2)$. Let $\mathbb{A} = \{G : d_G(v_1) = 2, d_G(v_i) = 1, i = 2, 3, \ldots, k\}$.

Theorem 2.4. [49] If $G \notin \mathbb{A}$ is a connected bicyclic graph with n vertices and m edges, then Inequality (1) is obtained with equality holding if and only if G is isomorphic to $K_{2,3}$.

Denote by $\mathcal{G}_\nu$, the class of connected graphs with cyclomatic number ν. If $\nu \leq 1$, then Conjecture 1 is true all graphs G in $\mathcal{G}_\nu$ by Theorem 2.2 and Theorem 2.3. Horoldagva and Lee gave the following result when $\nu \geq 2$.

Theorem 2.5. [34] If $\nu \geq 2$ then there exists a graph G in $\mathcal{G}_\nu$ for which Conjecture 1 does not hold.

Alternative and simple proofs of Theorem 2.2-2.4 were given in [4] and [34]. See [2, 3, 13, 27, 34, 49, 52] for various examples of graphs dissatisfying Conjecture 1. Of course, it is a very natural aim to characterizing the class of graphs for satisfying or dissatisfying inequality (1). Many researchers are still working on this problem and we introduce known results. In the current mathematico-chemical literature, the relation (1) is usually referred to as the Zagreb indices inequality. The subdivision graph of a graph G is obtained by inserting new vertices of degree two on each edge of G. If a graph G has n vertices and m edges then clearly the subdivision of G has $n + m$ vertices and $2m$ edges.

Theorem 2.6. [35] Let $S(G)$ be the subdivision graph of G. Then Zagreb indices inequality holds for $S(G)$ with equality if and only if G is a regular graph.

The join, $G_1 \vee G_2$, of G_1 and G_2 is the graph obtained from $G_1 + G_2$ by adding new edges from each vertex of G_1 to every vertex of G_2 . Then we have $|V(G_1 \vee G_2)| = |V(G_1)| + |V(G_2)|$ and $|E(G_1 \vee G_2)| = |E(G_1)| + |E(G_2)| + |V(G_1||V(G_2)|$.

Theorem 2.7. [15] Let G be a graph of n vertices with m edges. If the Zagreb indices inequality holds for G, then it also holds for $G \vee G$.

Theorem 2.8. [15] Let G be a graph of n vertices with m edges. If the Zagreb indices inequality does not hold for G, then it holds for $\overline{G}$.

Let $G = (V, E)$ be a simple graph of order n with m edges. If we put two similar graphs G side by side, and any vertex of the first graph G is connected by edges with the corresponding vertices of the second graph G and the resultant graph is $\hat{G}$. Then $|V(\hat{G})| = 2n$ and $|E(\hat{G})| = 2m + n$.

Theorem 2.9. [15] If the Zagreb indices inequality holds for G, then it also holds for $\hat{G}$.

Let $G = (V, E)$ be a graph of order n with m edges. If we take two copies of G, and any vertex of the first copy is connected by edges to the vertices that are adjacent to the corresponding vertex of the second copy, the resultant graph is $\tilde{G}$. Then we have $|V(\tilde{G})| = 2n$ and $|E(\tilde{G})| = 4m$

Theorem 2.10. [15] If the Zagreb indices inequality holds for G, then it also holds for $\tilde{G}$.

The cartesian product $G_1 \times G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $(u, x)(v, y)$ is an edge of $G_1 \times G_2$ if $u = v$ and $xy \in E(G_2)$, or $uv \in E(G_1)$ and $x = y$.

Theorem 2.11. [31] Let G_1 and G_2 be two graphs with $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1, 2$. If the Zagreb indices inequality holds for G_1 and G_2, then it also holds for $G_1 \times G_2$.

Let G be a graph with vertex set V and edge set E. Let $\overline{V}$ be a copy of V, $\overline{V} = \{\overline{x} : x \in V\}$. Then denoted by G', is the graph with vertex set $V \cup \overline{V}$ and edge set $E' = E \cup \{x\overline{y} : xy \notin E\}$.

Theorem 2.12. [31] Let G be a simple graph of n vertices with m edges. Then the Zagreb indices inequality must hold for G'.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple graphs with $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1, 2$. Then the tensor product $G_1 \otimes G_2$ of graphs G_1 and G_2 is a graph such that the vertex set of $G_1 \otimes G_2$ is the Cartesian product $V(G_1) \times V(G_2)$, and any two vertices (v'_i, v''_j) and (v'_p, v''_q) are adjacent in $G_1 \otimes G_2$ if and only if v''_j is adjacent with v''_q and v'_i is adjacent with v'_p. Then we have $|V(G_1 \otimes G_2)| = n_1 n_2$. Denote by $d_{i,j}$, $1 \leq i \leq n_1$, $1 \leq j \leq n_2$, is the degree of the (v'_i, v''_j) vertex of $G_1 \otimes G_2$. Then $d_{i,j} = d'_i \cdot d''_j$, where d'_i is the degree of the v'_i vertex of G_1 and d''_j is the degree of the v''_j vertex of G_2. Then we have

$$2|E(G_1 \otimes G_2)| = \sum_{1 \leq i \leq n_1, 1 \leq j \leq n_2} d_{i,j} = \sum_{i=1}^{n_1} d'_i \sum_{j=1}^{n_2} d''_j = 4m_1 m_2 \,,$$

that is,

$$|E(G_1 \otimes G_2)| = 2m_1 m_2 \,.$$

Theorem 2.13. [31] If the Zagreb indices inequality holds for G_1 and G_2, then it also holds for $G_1 \otimes G_2$.

Threshold graph is a graph that can be constructed from a one-vertex graph by repeated applications of the following two operations: (i) Addition of a single isolated vertex to the graph. (ii) Addition of a single dominating vertex to the graph, i.e., a single vertex that is connected to all other vertices.

Theorem 2.14. [31] The Zagreb indices inequlaity holds for all threshold graphs.

It was proved in [28] that, if T is not a star, then $nM_2(T) - mM_1(T) \geq 2(n-3)$. Stevanović and Milanič [48] improved this inequality. A Broom is a graph of order n, which have a path P_d and $n-d$ pendant vertices, all of these being adjacent to either the origin or the terminus of the path P_d

Theorem 2.15. [48] Let T be a tree with n vertices, $m = n-1$ edges and maximum degree Δ. If T is not a star, then

$$nM_2(T) - mM_1(T) \geq 2(n-3) + (\Delta - 1)(\Delta - 2)$$

with equality if and only if T is a broom.

Sun and Chen [50] showed that any graph G with $\Delta(G) - \delta(G) \leq 2$ satisfies Zagreb indices inequality.

Theorem 2.16. [50] If G is a graph with n vertices, m edges and $\Delta(G) - \delta(G) \leq 2$, then the Zagreb indices inequality holds with the equality if and only if all edges uv have the same pair (d_u, d_v) of degrees.

Let $D(G)$ be the set of the vertex degrees of G. A set S of integers is good if for every graph G with $D(G) \subseteq S$, the Zagreb indices inequality holds. Otherwise, S is a bad set. Thus, any interval of length three is good by Theorem 2.16. One can generalize this result in the following.

Theorem 2.17. [3] Let $s, x \in N$. For every graph G with n vertices, m edges, and $D(G) \subseteq \{x - s, x, x+s\}$, the Zagreb indices inequality holds. i.e., $D \subseteq \{x-s, x, x+s\}$ is good.

Andova at. al. [3] show that there are arbitrarily long intervals $[a, b]$ such that a graph with minimal degree at least a and maximum degree at most b satisfies the Zagreb indices inequality.

Theorem 2.18. [3] For every integer c, the interval $[c, c + \lceil \sqrt{c}\ \rceil]$ is good.

Andova at. al. [2] determined when a graph with vertices degrees in the interval $[a, a+n]$, satisfies the Zagreb indices inequality. On the other hand there are graphs that do not satisfy the inequality, even more, there is an infinite family of graphs of maximum degree at least 5 such that the inequality does not hold.

Theorem 2.19. [2] For every positive integer n, the interval $[a, a+n]$ is good if and only if $a \geq n(n-1)/2$ or $[a, a+n] = [1, 4]$.

Consider the function

$$f(i,j,k,l) = (ij - kl)\left(\frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j}\right).$$

Theorem 2.20. [2] If $f(i,j,k,l) < 0$ for some positive integers $i, j, k, l \in [a, b]$, then $[a, b]$ is a bad interval.

Easy verification shows that the Zagreb indices equality holds for regular graphs and stars. In [54] it was shown that the Zagreb indices equality holds for the subdivision graph $S(G)$ of r-regular graph, union of complete graphs that have same cardinality, union of p-complete graph and q-cycle graph for $p = 3$, $q \geq 3$, union of p-path graph and q-path graph for $p = q = 2$, and $p = q = 3$, union of p-cycle graph and complete bipartite graph $K_{a,b}$, $a \leq b$ only for $p \geq 3$, $a = b = 2$ and $p \geq 3$, $a = 1$, $b = 4$. The graph G is biregular if its vertex degrees assume exactly two distinct values. Distinguish between two types of biregular graphs: biregular graphs of class 1 have the property that no two vertices of the same degree are adjacent. In biregular graphs of class 2 at least one edge connects vertices of equal degree. Abdo, Dimitrov and Gutman [1] studied some class of graphs satisfying the Zagreb indices equality.

Theorem 2.21. [1] There exist infinitely many connected graphs G of maximum degree $\Delta \geq 5$ that are neither regular nor biregular of class 1 that satisfy the Zagreb indices equality.

Theorem 2.22. [1] Let G be a graph with $D(G) \subseteq [a, a + p]$, $a \geq p(p - 1)/2$ or $D(G) \subseteq [1, 4]$. Then, G satisfies the Zagreb indices equality if

(a) G is regular graph,

(b) G is biregular graph of class 1,

(c) G is disjoint union of $(p - 1)(p + 1)/2$-regular graphs and biregular graph of class 1 with degree of vertices $(p - 1)p/2$ and $p(p + 1)/2$, where p is odd, or

(d) G is disjoint union of stars S_5 and cycles of arbitrary length.

Conjecture 2.1. [1] Let I be an interval such that $I = [a, a + p], a \geq p(p - 1)/2$, or $I = [1, 4]$. Then, for any other interval $I_n \nsubseteq I$ there exist infinitely many graphs G with $D(G) \subseteq I_n$ such that G satisfies the Zagreb indices equality.

3. Difference of Zagreb indices

In the previous section we discussed the Zagreb indices inequality, but direct comparisons have been studied only to a limited extent, namely for trees [17, 48] and cyclic graphs [13]. Furtula, Gutman and Ediz [20] studied the difference of the classical first and second Zagreb indices of a graph G and determined a few basic properties of it. In [20], the authors mentioned that an obvious reason why the difference of the two Zagreb indices was not considered is that for structurally similar graphs it may assume negative, zero, or positive values and they gave a characteristic example. For a star S_n, we have $M_2(S_n) - M_1(S_n) = 1 - n$. The following lower bounds on the difference of Zagreb indices were given in [42].

Proposition 3.1. [42] If a connected graph G is not a star, then $M_2(G) - M_1(G) \geq -2$.

Proposition 3.2. [42] If G is a connected graph that is neither a tree nor a cycle, then $M_2(G) - M_1(G) \geq 1$.

Furtula et al. [20] showed that the difference of the Zagreb indices is closely related to the vertex-degree-based graph invariant

$$MR_2(G) = \sum_{uv\in E(G)} (d_G(u)-1)(d_G(v)-1)$$

and determined a few basic properties of MR_2. They proposed that RM_2 be called the reduced second Zagreb index. Let D be a positive integer, $D \geq 2$. Let S_{D+1} be the star on $D+1$ vertices, and let $v_1, v_2, \ldots, v_D$ be its pendant vertices. For $i = 1, 2, \ldots, D$, let r_i be non-negative integers, labeled so that $r_1 \geq r_2 \geq \cdots \geq r_D$. Construct the tree $T(r_1, r_2, \ldots, r_D)$ by attaching r_i pendant vertices to the vertex v_i of S_{D+1}, and by doing this for $i = 1, 2, \ldots, D$. The tree $T(r_1, r_2, \ldots, r_D)$ has thus $n = 1 + D + \sum_{i=1}^{D} r_i$ vertices. For given values of $D \geq 2$ and $n \geq D+1$, the set of all trees $T(r_1, r_2, \ldots, r_D)$ constructed in the above described manner is denoted by $T(n, D)$. Furtula et al. [20] characterized the n-vertex trees with maximal RM_2-values.

Theorem 3.3. [20] Let T be a tree of order n.
(i) If n is even, then $RM_2(T) \leq \frac{1}{4}(n-2)^2$ with equality if and only if $T \in \mathcal{T}(n, n/2)$.
(ii) If n is odd, then $RM_2(T) \leq \frac{1}{4}(n-1)(n-3)$ with equality if and only if $T \in \mathcal{T}(n, \lceil n/2 \rceil) \cup \mathcal{T}(n, \lfloor n/2 \rfloor)$.

Wang and Yuan [56] studied the maximum $M_2 - M_1$ for trees of given order and also considered the maximum $M_1 - M_2$. From Proposition 3.1 and Theorem 3.3, the following result follows.

Theorem 3.4. [20,28,56] If T is a tree of order n, then

$$1 - n \leq M_2(T) - M_1(T) \leq \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil + 1 - n\,.$$

Equality on the left-hand side holds if and only if $T \cong S_n$. Equality on the right-hand side holds if and only if $T \in \mathcal{T}(n, n/2)$ for even n and $T \in \mathcal{T}(n, \lceil n/2 \rceil) \cup \mathcal{T}(n, \lfloor n/2 \rfloor)$ for odd n.

Theorem 3.5. [56] Among all trees with diameter at least 3, the path achieves the maximum $M_1 - M_2 = 2$.

Theorem 3.6. [56] If there is an edge uv with $d_T(u), d_T(v) \geq 3$ in a tree T, and neither u or v is adjacent to a pendant vertex, then $M_1(T) - M_2(T) < 0$.

If G is a unicyclic graph different from C_n then $M_2(G) - M_1(G) \geq 1$ by Proposition 3.1. Lower bounds on $M_2 - M_1$ for unicyclic graphs in terms of cycle length and maximum degree were established in [32]. Denote $\mathcal{S} = \{S(m_1, m_2, \ldots, m_k) |\, m_{i-1} = m_{i+1} = 0 \text{ for } m_i \neq 0\,,\ 2 \leq i \leq k, \text{ where } m_{k+1} = m_1\}$.

Theorem 3.7. [32] Let G be a unicyclic graph with cycle length k. Then

$$M_2(G) - M_1(G) \geq \sum_{u\in V(C(G))} d_G(u) - 2k \tag{2}$$

with equality if and only if $G \in \mathcal{S}$.

Let B_n^k ($k \leq n$) be the unicyclic graph with $n-k$ pendant vertices and its each pendant vertex is adjacent to one vertex of C_k. In particular, $B_n^n = C_n$, a cycle of order n. Denote by $C_{n,\Delta}^k$ ($\Delta \geq 4$), a unicyclic graph obtained by identifying two pendant vertices of the path $P_{n-\Delta-k+2}$ with the center of star $K_{1,\Delta-1}$ and one vertex of cycle C_k, respectively. Denote $\mathcal{C}_\Delta = \{C_{n,\Delta}^k \mid 3 \leq k \leq n-\Delta-1\}$.

Theorem 3.8. [32] Let G be a unicyclic graph of order n with maximum degree Δ. Then

$$M_2(G) - M_1(G) \geq \begin{cases} \Delta - 2 & \text{if} \quad d = 0 \\ \Delta & \text{if} \quad d = 1 \\ 2 & \text{if} \quad d > 1\,, \end{cases} \tag{3}$$

where d is the length of the shortest path from the maximum degree vertex u to the cycle $C(G)$. The equalities hold in (3) if and only if $G \cong B_n^k$, $G \cong C_{n,\Delta}^k$, $\Delta + k = n$, and $G \in \mathcal{C}_\Delta$, respectively.

Let N be positive integer, $N \geq 2$. K_N be a complete graph of order N, and let $v_1, v_2, \ldots, v_N$ be its vertices. For $i = 1, 2, \ldots, N$, let r_i be non-negative integers, labeled so that $r_1 \geq r_2 \geq \cdots \geq r_N$. Construct the graph $G(r_1, r_2, \ldots, r_N)$ by attaching r_i pendant vertices to the vertex v_i of K_N. The graph $G(r_1, r_2, \ldots, r_N)$ has thus $n = N + \sum_{i=1}^N r_i$ vertices. For nonnegative integers n and k with $0 \leq k < n-1$, denote by $\mathcal{G}_n^k$ the set of connected cyclic graphs of order n with k cut edges. The graphs having maximum and minimum reduced second Zagreb index in $\mathcal{G}_n^k$ were studied in [29].

Theorem 3.9. [29] Let G be a graph in $\mathcal{G}_n^k$. If $M_2(G) - M_1(G)$ or $RM_2(G)$ is maximum then $G \cong G(r_1, r_2, \ldots, r_{n-k})$, where $\mid r_p - r_q \mid \leq 1$ for $1 \leq p, q \leq n-k$.

We denote by $\mathcal{A}_n^2$, a class of unicyclic graphs of order n obtained by attaching two pendant edges to the two non-adjacent vertices of the cycle C_{n-2}.

Theorem 3.10. [29] Let G be a graph in $\mathcal{G}_n^k$. Also let $M_2(G) - M_1(G)$ or $RM_2(G)$ be minimum.
(i) If $k = 0$, then $G \cong C_n$.
(ii) If $k = 1$, then $G \cong B_n^{n-1}$.
(iii) If $k = 2$, then $G \cong C_{n,2}^{n-1}$, $G \cong B_n^{n-2}$, or $G \in \mathcal{A}_n^2$
(iv) If $k \geq 3$, then $G \in \mathcal{U}_n^{n-k}$.

Corollary 3.1. [29] Let G be a cyclic graph. Then
(i) $M_2(G) - M_1(G) = 0$ if and only if $G \cong C_n$.
(ii) $M_2(G) - M_1(G) = 1$ if and only if $G \cong B_n^{n-1}$.
(iii) $M_2(G) - M_1(G) = 2$ if and only if $G \cong C_{n,2}^{n-1}$, $G \cong B_n^{n-2}$, $G \in \mathcal{A}_n^2$ or $G \in \mathcal{U}_n^{n-k}$.

Theorem 3.11. [13] Let G be a simple connected graph with ν independent cycles, $n \geq 5(\nu - 1)$ vertices, $m = n + \nu - 1$ edges, Zagreb indices M_1 and M_2. Then,

$$M_2 - M_1 \geq 6(\nu - 1) = 6(m - n)\,.$$

Moreover, the bound is tight and is attained if and only if G is a graph with vertices of degree 2 and 3 only and the vertices of degree 3 form an independent set.

Theorem 3.12. [13] Let G be a simple and connected graph with n vertices, $m(\geq n)$ edges and Zagreb indices M_1 and M_2. Then,

$$M_2 - M_1 \geq 11(\nu - 1) - n = 11m - 12n\,.$$

Moreover, the bound is tight and is attained if G is a graph with vertices of degree 2 and 3 only and, when $n \leq 5(\nu - 1)$, no pair of vertices of degree 2 are adjacent.

Given n and $n_1, n_2, \ldots, n_d$ ($d \geq 2$) are positive integers such that $1 + \sum_{i=1}^{d} n_i \leq n$ and $1 \leq n_1 \leq n_2 \leq \cdots \leq n_d$. Denote by $\mathbb{T}_n(n_1, n_2, \ldots, n_d)$, the set of trees T of order n with a vertex v and adjacent vertices of v have degrees $n_1, n_2, \ldots, n_d$, and each connected component of $T - v$ is star or broom with origin w, $vw \in E(T)$. Let Γ be a class of graphs $H = (V, E)$ of order n such that $H \ncong \{C_n, P_n, K_{1,n-1}, T(1, 1, 3), T(1, 1, 1, 3)\}$ and $H \notin \{B_n, \mathbb{T}_n(1, 2, 2), \mathbb{T}_n(2, 2, 2), \mathbb{T}_n(1, 2, 3), \mathbb{T}_n(1, 1, 2, 2), \mathbb{T}_n^*\}$. Furtula, Gutman and Ediz [20] mentioned a problem to characterize the graphs for which $M_1(G) > M_2(G)$ or $M_1(G) < M_2(G)$ or $M_1(G) = M_2(G)$. Horoldagva, Das and Selenge [33] completely solved this problem.

Theorem 3.13. [33] Let G be a connected graph of order $n \geq 3$. Then
(i) $M_1(G) = M_2(G)$ if and only if $G \cong C_n$ or $G \cong T(1, 1, 1, 3)$ or $G \in \{\mathbb{T}_n(2, 2, 2), \mathbb{T}_n(1, 2, 3), \mathbb{T}_n(1, 1, 2, 2), \mathbb{T}_n^*\}$.
(ii) $M_1(G) > M_2(G)$ if and only if $G \cong K_{1,n-1}$ or $G \cong P_n$ or $G \cong T(1, 1, 3)$ or $G \in B_n$ or $G \in \mathbb{T}_n(1, 2, 2)$.
(iii) $M_1(G) < M_2(G)$ if and only if $G \in \Gamma$.

4. Comparing variable Zagreb indices

Vukičević and Graovac pointed out that inequality (1) can be generalized to the variable Zagreb indices, namely for which λ it holds that

$$\frac{{}^{\lambda}M_1(G)}{n} \leq \frac{{}^{\lambda}M_2(G)}{m}\,, \tag{4}$$

where λ is any real number. Inequality (4) is known as generalized Zagreb indices inequality.

Vukičević [51] proved that inequality (4) holds for all graphs G and $\lambda \in [0, \frac{1}{2}]$. Later, Andova and Petruevski [5] gave a complete proof using Karamata's inequality.

Theorem 4.1. [5, 51] Inequality (4) holds for all graphs and for all $\lambda \in [0, \frac{1}{2}]$.

We know from the previous section that the Zagreb indices inequality holds for chemical graphs, trees, unicyclic graphs and graphs with small difference between the maximum and minimum vertex degrees. The generalized Zagreb indices inequality also holds for these mentioned class of graphs when $\lambda \in [0, 1]$.

Theorem 4.2. [51] Inequality (4) holds for all chemical graphs and all $\lambda \in [0, 1]$.

Theorem 4.3. [53] Inequality (4) holds for all trees and all $\lambda \in [0, 1]$.

Theorem 4.4. [30] Inequality (4) holds for all unicyclic graphs and for all $\lambda \in [0, 1]$.

Theorem 4.5. [40] Inequality (4) holds for all graphs with $\Delta - \delta \leq 2$ and for all $\lambda \in [0, 1]$.

Theorem 4.6. [40] Inequality (4) holds for all graphs with $\Delta - \delta \leq 3$ ($\delta \neq 2$) and for all $\lambda \in [0, 1]$.

If $\lambda > 1$, then two examples where given in [57] for unicyclic graphs such that ${}^\lambda M_1(G)/n >^\lambda M_2(G)/m$ and ${}^\lambda M_1(G)/n <^\lambda M_2(G)/m$. Huang at. al. [36] proved that opposite inequality of (4) holds for all $\lambda \in (-\infty, 0)$ and all graphs G.

Theorem 4.7. [36] Let G be a graph with n vertices and m edges. Then ${}^\lambda M_1(G)/n \geq^\lambda M_2(G)/m$ holds for all $\lambda \in (-\infty, 0)$. Moreover, equality holds if and only if G is a regular graph.

Vukičević [51] characterized some class of graphs and intervals in which inequality (4) does not hold and proposed an open problem: Identify $\lambda \in (1/2, \sqrt{2}/2]$ such that ${}^\lambda M_1(G)/n >^\lambda M_2(G)/m$ for all graphs G.

Theorem 4.8. [51] If $\lambda \in R \setminus [0, 1)$ then inequality (4) does not hold for all complete unbalanced bipartite graphs.

Theorem 4.9. [51] Let $\lambda \in (\sqrt{2}/2, 1)$. Then there is a graph such that inequality (4) does not hold.

Bogoev [6] gave a complete answer to Vukičević's open problem.

Theorem 4.10. [6] For all graphs G and $\lambda \in (1/2, \sqrt{2}/2]$, inequality (4) holds.

The difference of the variable Zagreb indices for cyclic graphs were studied in [47]. Let Γ be a class of graphs $H = (V, E)$ in $\mathcal{G}_\nu$ such that $2 \leq d_i \leq 3$ (there exists a vertex v_k in H such that $d_k = 3$) for all $v_i \in V(H)$ and the set of vertices of degree three is an independent set in H.

Theorem 4.11. [47] Let G be a graph in $\mathcal{G}_\nu$ and $\lambda \in (0, 1]$. Then

$$ {}^\lambda M_2(G) - {}^\lambda M_1(G) \geq (\nu - 1) \left(3^{\lambda+1}\, 2^{\lambda+1} - 2 \cdot 3^{2\lambda} - 3 \cdot 2^{2\lambda}\right) \tag{5} $$

with equality holding if and only if $G \cong C_n$ or $G \in \Gamma$.

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Inequalities between Kirchhoff Index and Laplacian–Energy–Like Invariant

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Contents

1. Introduction

Let G be a simple graph with n vertices and m edges. The cyclomatic number of G is $c = m - n + 1$. For example, if $c = 0$ then a connected graph G is called a tree. If $c = 1, 2, 3, 4$, then G is said to be a unicyclic, bicyclic, tricyclic, and tetracyclic graph, respectively. Let d_i be the degree of a vertex v_i in G. The maximum and minimum vertex degrees in G are denoted by Δ and δ, respectively. A chemical graph is a connected graph with the maximum vertex degree at most 4. The Laplacian matrix of G is defined as $L = D - A$, where A is the adjacency matrix of G and $D = diag(d_1, d_2, \dots, d_n)$ is the diagonal matrix of vertex degrees. The Laplacian spectrum of G is the spectrum of its Laplacian matrix, and consists of the values $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$.

In 1993, Klein and Randić [7] introduced the resistance distance, based on the electrical network theory. The Kirchhoff index [3] is defined as $Kf(G) = \sum\limits_{i<j} r_{ij}$, where r_{ij} is the resistance distance between vertices v_i and v_j. For a connected graph G with $n \geq 2$ vertices, it has been proven [5, 14] that

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

For results on the Kirchhoff index, we only cite recent works [2, 8, 11, 13].

The Laplacian–energy–like invariant [10] of G, denoted by $LEL(G)$, has recently been defined as

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

There are several works about this graph invariant (see [9] and the references therein).

Motivated by [4], in which two sufficient conditions are established for $Kf(G) < LEL(G)$ and nine graphs with $Kf(G) < LEL(G)$ are detected, there are some works on this topic.

This survey outlines results on the comparison between Kirchhoff index and Laplacian–energy–like invariant of graphs. This chapter consists of five sections, followed by detailed list of references on the comparison of Kirchhoff index and Laplacian–energy–like invariant. Section 2 is devoted to some graphs with Kf larger than LEL. The results on Kf smaller than LEL are presented in Section 3. In Section 4, we consider some graph operations on Kf and LEL. In the last section, comparisons between the two invariants of some special graphs are given.

2. Graphs with Kf larger than LEL

Theorem 2.1 [4]. *Let G be a connected graph of order n with m edges and minimum degree δ. If $2m \leq (n-1)n^{2/3} + \delta$, then $Kf(G) > LEL(G)$.*

Corollary 2.2 [4]. *Let T be a tree of order n. Then $Kf(T) > LEL(T)$ for $n > 2$.*

Corollary 2.3 [4]. *Let U be a unicyclic graph of order n. Then $Kf(U) > LEL(U)$ for $n \geq 4$.*

Corollary 2.4 [4]. *Let B be a bicyclic graph of order n. Then $Kf(B) > LEL(B)$ for $n \geq 5$.*

Theorem 2.5 [4]. *Let G be a connected graph of order n with m edges. If $2m \leq (n-1)n^{2/3}$, then $Kf(G) > LEL(G)$.*

The *kite* $Ki_{n,\omega}$ is the graph of order n, obtained by attaching a pendent path on $n-\omega$ vertices to a vertex of the complete graph of order ω. Let $\Gamma_{n,k}$ be the class of graphs of order n obtained by attaching a pendent path on $n-k$ vertices to a vertex of a connected graph of order k. Obviously, $Ki_{n,k} \in \Gamma_{n,k}$.

Theorem 2.6 [4]. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq 1$. If $k^3 < (\frac{3n}{8} - 2)^2(n-k)^2$, then $Kf(G) > LEL(G)$.*

Corollary 2.7 [4]. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq 2$. If $k < \frac{n}{2}$ and $n \geq 12$, then $Kf(G) > LEL(G)$.*

Corollary 2.8 [4]. *Let $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n-k \geq 2$. If $k < \frac{2n}{3}$ and $n \geq 20$, then $Kf(G) > LEL(G)$.*

3. Graphs with Kf smaller than LEL

In [4], an open problem is proposed:

Problem 3.1 [4]. *Is it possible to find a constant* c *(which may depend on the number of vertices and maximum vertex degree* Δ*), such that for any connected graph* G *with* $m \geq c$ *edges ,*
$Kf(G) < LEL(G)$ *?*

Theorems 2.1 and 2.5 immediately imply:

Corollary 3.2 [1]. *Let* G *be a connected graph of order* n*. Let* δ *be the smallest degree of a vertex of* G*. If* $Kf(G) < LEL(G)$*, then* G *must have more than* $\frac{1}{2}[(n-2)n^{2/3} + \delta]$ *edges.*

Corollary 3.3 [1]. *Let* G *be a connected graph of order* n*. If* $Kf(G) < LEL(G)$*, then* G *must have more than* $\frac{1}{2}(n-1)n^{2/3}$ *edges.*

In [1], a weakened variant of Corollary 3.2 was obtained:

Corollary 3.4 [1]. *Let* G *be a connected graph of order* n*. If* $Kf(G) < LEL(G)$*, then* G *must have more than* $\frac{1}{2}[(n-2)n^{2/3} + 1]$ *edges.*

Remark 3.5 [1]. *By combining Corollaries 3.3 and 3.4, if the relation* $Kf(G) < LEL(G)$ *is obeyed, then the graph* G *must possess more than* $\frac{1}{2}min\{(n-1)n^{2/3}, (n-2)n^{2/3}+1\}$ *edges. It is easy to show that* $(n-2)n^{2/3} + 1 < (n-1)n^{2/3}$ *holds for* $n \geq 3$*.*

By using Remark 3.5, the following theorem is attained:

Theorem 3.6 [1]. *Let* $\mathcal{G}(\dagger)$ *be the set of connected graphs with cyclomatic number* c*. For any fixed value of* c*, the number of elements of* $\mathcal{G}(\dagger)$ *for which* $Kf < LEL$ *holds is finite.*

Remark 3.7 [1]. *For* $c = 0, 1, 2, 3, 4$*, connected graphs for which the Kirchhoff index is smaller than the Laplacian–energy–like invariant can possess at most 3, 5, 5, 6, and 7 vertices, respectively.*

Remark 3.8 [4]. *For* $G \cong K_n$*,* $Kf(G) = n - 1 < (n-1)\sqrt{n} = LEL(G)$*.*

Corollary 3.9 [4]. *The only tree for which* $Kf(T) < LEL(T)$ *holds is* K_2*.*

Corollary 3.10 [4]. *The only unicyclic graph for which* $KF(G) < LEL(G)$ *holds is* K_3*.*

Corollary 3.11 [4]. *The only bicyclic graph for which* $Kf(G) < LEL(G)$ *holds is* $K_4 - e$*.*

Corollary 3.12 [1]. *The only tricyclic graphs for which* $Kf(G) < LEL(G)$ *holds are* $G \cong H_1$*–*H_4*, depicted in Fig. 1.*

Corollary 3.13 [1]. *The only tetracyclic graphs for which* $Kf(G) < LEL(G)$ *holds are* $G \cong H_5$*–*H_8*, depicted in Fig. 1.*

Remark 3.14 [1]. *There are 2, 20, and 132 connected tetracyclic graphs with 5, 6, and 7 vertices, respectively. Among the 7-vertex species, no one satisfies the inequality* $Kf < LEL$*.*

The union of simple graphs G_1 and G_2 is the graph $G_1 \cup G_2$ with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. Let $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by connecting all vertices of G_1 to all vertices of G_2.

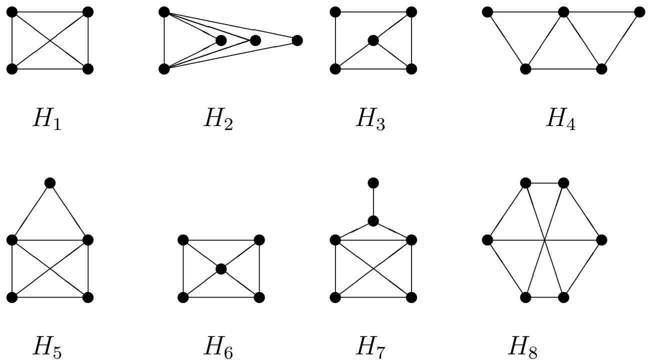


Figure 1. The tricyclic and tetracyclic graphs with $Kf(G) < LEL(G)$.

Let

$$\begin{aligned}
G_1(n) &= K_{n-2} \vee (2K_1) \\
G_2(n) &= K_{n-4} \vee C_4 \\
G_3(n) &= K_{n-3} \vee (K_1 \cup K_2) \\
G_4(n) &= K_{n-6} \vee (C_4 \vee 2K_1) \\
G_5(n) &= K_{n-5} \vee ((K_2 \cup K_1) \vee 2K_1) \\
G_6(n) &= K_{n-4} \vee P_4 \\
G_7(n) &= K_{n-3} \vee (3K_1) \\
G_8(n) &= K_{n-4} \vee (K_1 \cup K_3)\,.
\end{aligned}$$

Then

$$\begin{aligned}
\overline{G_1(n)} &= K_2 \cup (n-2)K_1 \\
\overline{G_2(n)} &= 2K_2 \cup (n-4)K_1 \\
\overline{G_3(n)} &= K_{1,2} \cup (n-3)K_1 \\
\overline{G_4(n)} &= 3K_2 \cup (n-6)K_1 \\
\overline{G_5(n)} &= K_{1,2} \cup K_2 \cup (n-5)K_1 \\
\overline{G_6(n)} &= P_4 \cup (n-4)K_1 \\
\overline{G_7(n)} &= K_3 \cup (n-3)K_1 \\
\overline{G_8(n)} &= K_{1,3} \cup (n-4)K_1\,.
\end{aligned}$$

Theorem 3.15 [4]. *For any graph $G \in \{K_n, G_1(n), \ldots, G_8(n)\}$, the inequality $Kf(G) < LEL(G)$ holds.*

Denote by $\overline{G}$ the complement of G. Let $\overline{G^*(n)}$ be the graph depicted in Fig. 2.

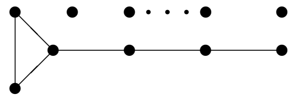


Figure 2. The graph $\overline{G^*(n)}$.

Theorem 3.16 [6]. *Let G be a connected graph with $n \geq 7$ vertices. If $\overline{G}$ is a spanning subgraph of $\overline{G^*(n)}$, then $Kf(G) < LEL(G)$.*

Theorem 3.17 [12]. *Let G be a connected graph with algebraic connectivity $\mu_{n-1} \geq k$ and let m be the number of edges and Δ the maximum degree of G. If*

$$2m > \frac{k(\sqrt{n}+\sqrt{k})}{k+\sqrt{n}+\sqrt{k}} \left(\frac{(n+k)(n-1)}{k} - \frac{(n-1)\sqrt{k(\Delta+1)}}{\sqrt{n}+\sqrt{k}} \right)$$

then $Kf(G) < LEL(G)$.

The following corollary provides a partial answer to Problem 3.1:

Corollary 3.18 [12]. *Let G be a connected graph G with algebraic connectivity $\mu_{n-1} \geq 1$. Let m be the number of edges and Δ the maximum degree of G. If*

$$2m > \frac{\sqrt{n}+1}{\sqrt{n}+2} \left(n^2 - 1 - \frac{(n-1)\sqrt{\Delta+1}}{\sqrt{n}+1} \right)$$

then $Kf(G) < LEL(G)$.

Corollary 3.19 [12]. *Let T be a tree and $\overline{T}$ its complement. If the order of T is $n \geq 7$ and $\Delta(T) \leq n-2$, then $K(\overline{T}) < LEL(\overline{T})$.*

Corollary 3.20 [12]. *Let U be a unicyclic graph and $\overline{U}$ its complement. If the order of U is $n \geq 14$ and $\Delta(U) \leq n-2$, then $Kf(\overline{U}) < LEL(\overline{U})$.*

Corollary 3.21 [12]. *Let B be a bicyclic graph and $\overline{B}$ its complement. If the order of B is $n \geq 15$ and $\Delta(B) \leq n-2$, then $Kf(\overline{B}) < LEL(\overline{B})$.*

Corollary 3.22 [12]. *Let TC be a tricyclic graph and $\overline{TC}$ its complement. If the order of TC is $n \geq 16$ and $\Delta(TC) \leq n-2$, then $Kf(\overline{TC}) < LEL(\overline{TC})$.*

Corollary 3.23 [12]. *Let QC be tetracyclic graph and $\overline{QC}$ its complement. If the order of QC is $n \geq 17$ and $\Delta(QC) \leq n-2$, then $Kf(\overline{QC}) < LEL(\overline{QC})$.*

4. Graph operations on Kf and LEL

Theorem 4.1 [1]. *Let G be a connected graph and e its edge, such that $G-e$ is also connected. If $Kf(G) > LEL(G)$, then $Kf(G-e) > LEL(G-e)$ holds.*

Corollary 4.2 [1]. *If $Kf(G) > LEL(G)$ and if $e_1, e_2, \ldots, e_t$ are edges of G, such that $G - e_1 - e_2 - \cdots - e_t$ is connected, then $Kf(G - e_1 - e_2 - \cdots - e_t) > LEL(G - e_1 - e_2 - \cdots - e_t)$.*

Similar to Theorem 4.1, in [1] it was obtained:

Theorem 4.3 [1]. *Let $G+e$ be the graph obtained by adding a new edge to the connected graph G. If $Kf(G) < LEL(G)$, then $Kf(G+e) < LEL(G+e)$ holds.*

Corollary 4.4 [1]. *If G is a connected graph of order n with cyclomatic number $c \geq 0$, such that $Kf(G) < LEL(G)$, then we can construct a connected graph $G^{\dagger}$ of order n, with cyclomatic number $c^{\dagger}$, $c < c^{\dagger} \leq \frac{(n-1)(n-2)}{2}$, such that $Kf(G^{\dagger}) < LEL(G^{\dagger})$.*

Corollary 4.5 [1]. *If $n \geq 4$, then $Kf(K_n - e) < LEL(K_n - e)$.*

The product of G_1 and G_2 is the graph $G_1 \times G_2$ whose vertex set is the Cartesian product $V(G_1) \times V(G_2)$. Suppose that $v_1, v_2 \in V(G_1)$ and $u_1, u_2 \in V(G_2)$. Then (v_1, u_1) and (v_2, u_2) are adjacent in $G_1 \times G_2$ if and only if one of the following conditions is satisfied: (i) $v_1 = v_2$ and $\{u_1, u_2\} \in E(G_2)$, or (ii) $\{v_1, v_2\} \in E(G_1)$ and $u_1 = u_2$.

Let $H_n = K_p \times K_2$. Then $n = 2p$.

Theorem 4.6 [1]. *Let G be a graph of order $n \geq 8$ (n is even) and let H_n be a subgraph of G. Then $Kf(G) < LEL(G)$.*

Remark 4.7 [1]. *In particular, $H_4 = C_4$, $Kf(C_4) > LEL(C_4)$, and $Kf(H_6) > LEL(H_6)$.*

Let H'_n be the graph of order n $(n = 2p + 1)$ obtained from H_n in such a way that $H'_n = \overline{\overline{H_n} \cup K_1}$, where $H_n = K_p \times K_2$.

Theorem 4.8 [1]. *Let G be a graph of order $n \geq 5$ (n is odd) and let H'_n be a subgraph of G. Then $Kf(G) < LEL(G)$.*

Next results are related to the complement of a graph.

Theorem 4.9 [12]. *If G is a graph for which $\mu_1 < n - n^{2/3}$, then $Kf(\overline{G}) < LEL(\overline{G})$.*

The line graph of G, denoted by $\ell(G)$, is the graph whose vertices correspond to the edges of G, with two vertices of $\ell(G)$ being adjacent if and only if the corresponding edges of G share a common vertex.

Remark 4.10 [12]. *Let t_1 be the maximum vertex degree of the line graph $\mathcal{L}(G)$. By the proof the Theorem 4.9, if $t_1 < n - n^{2/3} - 2$, then $Kf(\overline{G}) < LEL(\overline{G})$.*

Corollary 4.11 [12]. *If $G \in \Gamma_{n,k}$ with $k \geq 4$ and $n - k \geq n^{2/3} + 2$. Then $Kf(\overline{G}) < LEL(\overline{G})$.*

Corollary 4.12 [12]. *Let $G \ncong K_n$ be an r-regular graph with n vertices. If $r < \frac{(n-n^{2/3})}{2}$, then $Kf(\overline{G}) < LEL(\overline{G})$. If $r > \frac{n+n^{2/3}-2}{2}$, then $Kf(G) < LEL(G)$.*

Let KK_n^j be the graph obtained from two copies of complete graphs K_n, by joining a vertex of one copy with j , $1 \leq j \leq n$, vertices of the other copy [12].

Theorem 4.13 [12]. *For $j \geq \frac{n}{4}$, let KK_n^j be a spanning subgraph of the graph of G. Then $Kf(G) < LEL(G)$ for $n \geq 22$.*

Remark 4.14 [12]. *If G is a graph of order n, $(n \equiv 0 (mod\, 8))$ having two cliques of order $\frac{n}{2}$ each, such that there are at least $\frac{n}{8}$ edges between a vertex in one of the cliques and $\frac{n}{8}$ vertices of the other clique, then for $n \geq 44$, $Kf(G) < LEL(G)$.*

Theorem 4.15 [12]. *If $\overline{KK_n^j}$ is a spanning subgraph of a graph G with $2n$ vertices, then $Kf(G) < LEL(G)$ for $n \geq 7$.*

Theorem 4.16 [12]. *For $p \geq 4$, let $K_p \vee \overline{K_r}$, $1 \leq r \leq p$, be a spanning subgraph of a graph G of order $n = p + r$. Then $Kf(G) < LEL(G)$.*

Theorem 4.17 [12]. *If $K_{\frac{n}{2},\frac{n}{2}}$ is a spanning subgraph of a graph G of order n, then $Kf(G) < LEL(G)$ for all $n \geq 5$.*

Similar to Theorem 3.15, the following is an analogous condition on the graph complement.

Theorem 4.18 [12]. *Let G be a connected graph with n vertices, with largest Laplacian eigenvalue $\mu_1 \leq \frac{n}{2}$ and algebraic connectivity $\mu_{n-1} \geq k$. If*

$$2m < \frac{(\Delta+1)(n-\Delta-1)\Big(n(n-1)+(n-1)\sqrt{k(n-k)}\Big)}{n(\sqrt{n-k}+\sqrt{k})+(\Delta+1)(n-\Delta-1)}$$

then $Kf(\overline{G}) < LEL(\overline{G})$.

Corollary 4.19 [12]. *Let T be a tree on $n \geq 41$ vertices with largest Laplacian eigenvalue $\mu_1 \leq \frac{n}{2}$ and algebraic connectivity $\mu_{n-1} \geq 0.1$. Then $Kf(\overline{T}) < LEL(\overline{T})$.*

5. Comparison of Kf and LEL of special graphs

Theorem 5.1 [6]. *Let G be a chemical graph with n vertices. Then $Kf(G) > LEL(G)$ except the graphs H_i $(i = 1, \ldots, 41)$ in Figs. 3–7.*

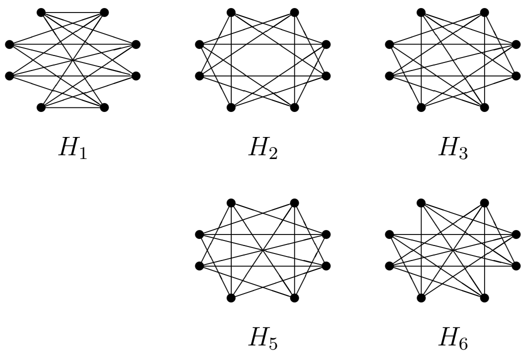


Figure 3. Chemical graphs with $n = 8$ vertices, $\delta = \Delta = 4$ and $Kf < LEL$.

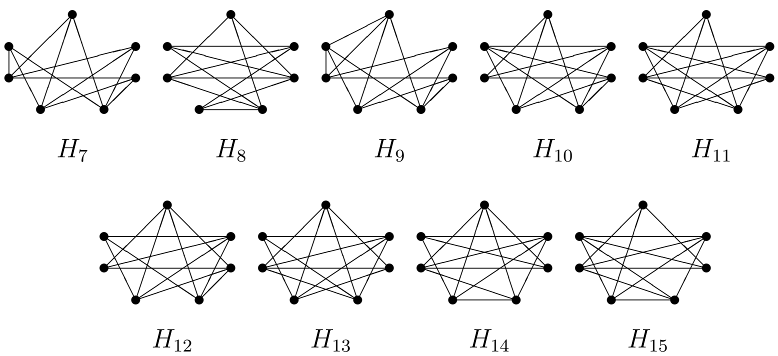


Figure 4. Chemical graphs with degree sequences $(4, 4, 4, 3, 3, 3, 3)$ and $(4, 4, 4, 4, 4, 3, 3)$.

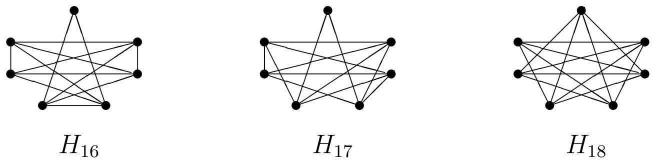


Figure 5. Chemical graphs with degree sequence $(4, 4, 4, 4, 4, 4, 2)$.

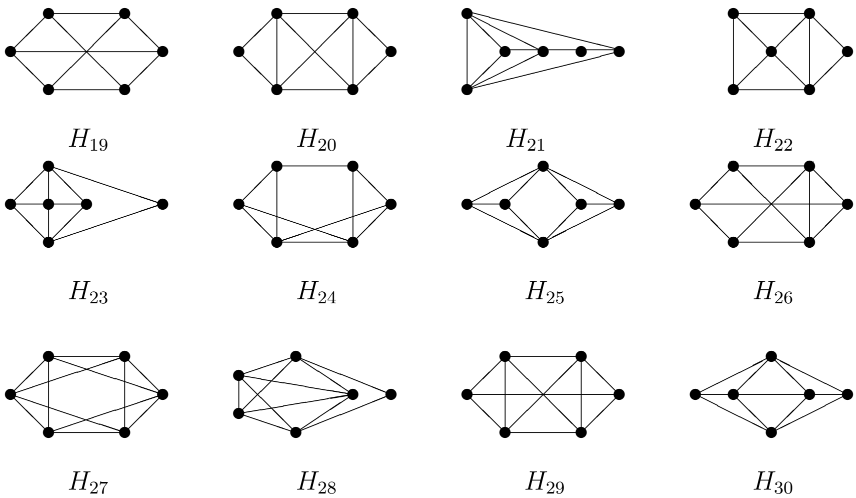


Figure 6. Chemical graphs with $n = 6$ vertices and $Kf < LEL$.

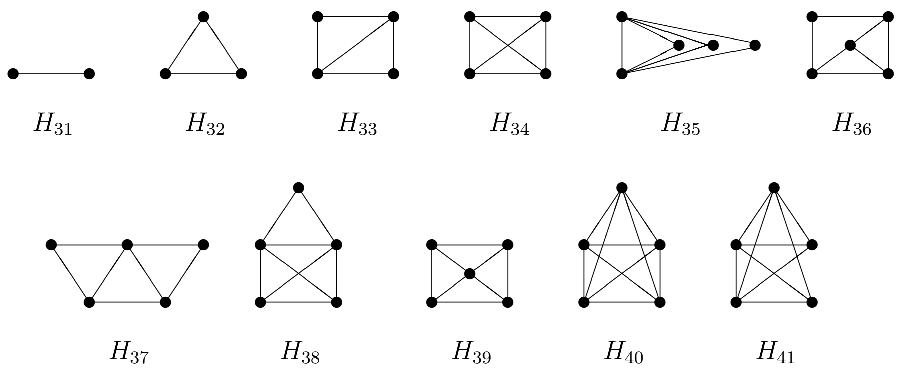


Figure 7. Chemical graphs with $n \leq 5$ vertices and $Kf < LEL$.

Theorem 5.2 [6]. *Let G be a connected r-regular graph with n vertices. If $r \leq (\frac{n-1}{n})n^{2/3}$, then $LEL(G) < Kf(G)$.*

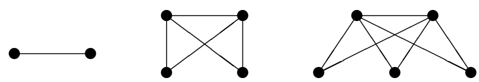
Remark 5.3 [6]. For an r-regular graph with $r = n^{2/3}$, let $r = 4 = 8^{2/3} = n^{2/3}$. It is easy to see that there exist graphs with $LEL(G) > Kf(G)$.

Theorem 5.4 [6]. *Let G be an r-regular graph with $r \leq (\frac{n-1}{n})n^{2/3}$. Then $LEL(\ell(G)) < Kf(\ell(G))$, where $\ell(G)$ is the line graph of G.*

The independence number of a graphs G, denoted by α, is the number of vertices in the largest independent set of G.

Let $\overline{CS}(n, n-\alpha) := K_\alpha \cup (n-\alpha)K_1$.

Theorem 5.5 [6]. *Let G be a connected graph with n vertices and independence number α. If $\alpha > n - \sqrt{n}$, then $LEL(G) < Kf(G)$ holds except for the graphs in Fig. 8.*



S_2 $\quad CS(4,2) \quad CS(5,2)$

Figure 8. Graphs with independence number $\alpha \geq n - \sqrt{n}$ and $Kf < LEL$.

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Bounds for the Kirchhoff and degree Kirchhoff indices

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Contents

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, $E = \{e_1, e_2, \ldots, e_m\}$, be a simple connected graph of order $n \geq 2$ and size m. If vertices i and j are adjacent, we denote it by $i \sim j$. Further, let $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $\Delta = d_1$, $\Delta_2 = d_2$, $\delta = d_n$, be a sequence of vertex degrees, $\mathbf{A}$ the adjacency matrix of G, and $\mathbf{D} = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of vertex degrees. Matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix of G. Eigenvalues of $\mathbf{L}$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, are the Laplacian eigenvalues of graph G. Some well known properties of the Laplacian eigenvalues of graph are (see for example [5] and [13]):

$$\sum_{i=1}^{n-1} \mu_i = \sum_{i=1}^{n} d_i = 2m \qquad \text{and} \qquad \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m,$$

where

$$M_1 = \sum_{i=1}^{n} d_i^2 = \sum_{i \sim j} (d_i + d_j) = \sum_{i=1}^{m} \left(d(e_i) + 2\right),$$

is the first Zagreb index [30]. In the same paper (see also [24, 25, 34, 35]) the second Zagreb index, M_2, and so called forgotten Zagreb index, F, were defined as follows

$$M_2 = M_2(G) = \sum_{i \sim j} d_i d_j \qquad \text{and} \qquad F = F(G) = \sum_{i=1}^{n} d_i^3.$$

Matrix $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ is the normalized Laplacian matrix of G. Its eigenvalues, $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$, represent normalized Laplacian eigenvalues of G. The following is valid for ρ_i, $i = 1, 2, \ldots, n$, (see [13]):

$$\sum_{i=1}^{n-1} \rho_i = n \qquad \text{and} \qquad \sum_{i=1}^{n-1} \rho_i^2 = n + 2R_{-1},$$

where

$$R_{-1} = \sum_{i \sim j} \frac{1}{d_i d_j},$$

is the general Randić index (also called branching index) introduced in [71].

In 1993 [41] a new distance function, named resistance distance, based on the theory of electrical networks was introduced. A graph G was viewed as an electrical network N obtained by replacing each edge of G with a unit resistor. The resistance distance between the vertices i and j of the graph G, denoted by r_{ij}, is then defined to be the effective resistance between the nodes i and j in N. Similar to the long recognized shortest–path distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical properties, but also with a substantial potential for chemical applications.

The Wiener index is the sum of ordinary distances between all pairs of vertices of a (connected) graph; for details and further references see [76]. The *Kirchhoff index* is defined in analogy to the Wiener index as [6, 41]:

$$Kf(G) = \sum_{i<j} r_{ij}.$$

A long time known result for the Kirchhoff index is [29]:

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

In 2007, a closely related graph invariant, named *degree Kirchhoff index*, was put forward in [12]. It is defined as

$$Kf^*(G) = \sum_{i<j} d_i d_j r_{ij}.$$

In analogy with the Kirchhoff index, the degree Kirchhoff index can also be represented as [12]

$$Kf^*(G) = 2m \sum_{i=1}^{n-1} \frac{1}{\rho_i}.$$

The graph invariants Kf and Kf^* are currently much studied in the mathematical and mathematico–chemical literature. In this chapter we give a survey on the bounds for the Kirchhoff and degree Kirchhoff indices. We say that a bound, either of Kirchhoff or degree Kirchhoff index, belongs to a class $I(\alpha)$ if it depends on parameters from the set α. We consider bounds involving either of the following parameters: a number of vertices, n, a number of edges, m, vertex degrees, $d_1, \ldots, d_n$, the first Zagreb index, M_1, general Randić index, R_{-1}, number of spanning trees of a graph, $t = \dfrac{1}{n}\displaystyle\prod_{i=1}^{n-1} \mu_i = \dfrac{\prod_{i=1}^{n} d_i}{2m}\displaystyle\prod_{i=1}^{n-1} \rho_i$.

We will give mutual comparison of the bounds only if they belong to the same class. Before we proceed with the survey, we give exact values of the Kirchhoff and degree Kirchhoff indices for some special classes of graphs.

For the complete graph K_n, complete bipartite graph $K_{r,n-r}$, $1 \leq r \leq \lfloor \frac{n}{2} \rfloor$, and cycle C_n, the following equalities are, respectively, valid:

$$\begin{array}{ll} Kf(K_n) = n-1, & Kf^*(K_n) = (n-1)^3, \\ Kf(K_{r,n-r}) = (n-1)\left(\frac{r}{n-r} + \frac{n-r}{r}\right) - 1, & Kf^*(K_{r,n-r}) = r(n-r)(2n-3), \\ Kf(C_n) = \dfrac{n^3-n}{12}, & Kf^*(C_n) = \dfrac{n^3-n}{3}. \end{array}$$

In a special case when $r = 1$ a star graph $K_{1,n-1}$ is obtained, and

$$Kf(K_{1,n-1}) = (n-1)^2, \qquad Kf^*(K_{1,n-1}) = (n-1)(2n-3).$$

For the complete bipartite graphs where $r = \frac{n}{2}$, n is even, we have

$$Kf(K_{\frac{n}{2},\frac{n}{2}}) = 2n-3, \qquad Kf^*(K_{\frac{n}{2},\frac{n}{2}}) = \frac{n^2}{4}(2n-3).$$

For the path P_n, holds

$$Kf(P_n) = \frac{n^3-n}{6}.$$

Let $G = K_n - e$ be a graph obtained after removing an edge from the complete graph K_n, and $G = K_{n-1} + e$ a graph obtained after adding a vertex to the complete graph K_{n-1} and edge that connects that vertex to an arbitrary vertex from K_{n-1}. The values of Kirchhoff index for these graphs are [17,42]:

$$Kf(K_n - e) = n - 2 + \frac{n}{n-2} \qquad \text{and} \qquad Kf(K_{n-1} + e) = 2n - 1 - \frac{2}{n-1}.$$

In [60] (see also [64]) a class of d-regular graphs Γ_d, $1 \leq d \leq n-1$, was defined as follows. Let $N(i)$ be a set of all neighborhoods 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 all d-regular graphs, $1 \leq d \leq n-1$, with the properties that diameter is $D = 2$ and $|N(i) \cap N(j)| = d$. For any $G_d \in \Gamma_d$ holds

$$Kf(G_d) = \frac{n(n-1)-d}{d} \qquad \text{and} \qquad Kf^*(G_d) = d(n(n-1)-d).$$

The rest of the chapter is organized as follows. In Sections 2 and 3 we provide an overview of lower and upper bounds of the Kirchhoff index, respectively. Sections 4 and 5 are devoted to lower and upper bounds of the degree Kirchhoff index. Open problems are pointed out at various places.

2. Lower bounds for the Kirchhoff index

The following Chebyshev-type inequality [58,59] plays an important role in determining lower bounds of the Kirchhoff index:

$$\sum_{i=k_1}^{n-k_2} p_i \sum_{i=k_1}^{n-k_2} p_i a_i b_i \geq \sum_{i=k_1}^{n-k_2} p_i a_i \sum_{i=k_1}^{n-k_2} p_i b_i, \tag{1}$$

where $1 \leq k_1 \leq n - k_2$, $0 \leq k_2 \leq n-1$, $a = (a_i)$ and $b = (b_i)$ are non-negative real sequences of the same monotonicity, and $p = (p_i)$ are positive real numbers. Equality holds if and only if either of the sequences $a = (a_i)$ or $b = (b_i)$ is constant.

Now we list lower bounds for $Kf(G)$ in various classes obtained using (1).

- For $k_1 = 1$, $k_2 = 1$, $p_i = \mu_i$, $a_i = b_i = \frac{1}{\mu_i}$, $i = 1, 2, \ldots, n-1$, from (1) we get

$$Kf(G) \geq \frac{n(n-1)^2}{2m}. \tag{2}$$

Equality holds if and only if $G \cong K_n$. This inequality, proved in [78] (see also [57]), sets up a lower bound for the $Kf(G)$ in the class $I(n,m)$.

Since $2m \leq n\Delta$, from (2) follows

$$Kf(G) \geq \frac{(n-1)^2}{\Delta}, \tag{3}$$

with equality if and only if $G \cong K_n$. This bound, reported in [86] (see also [64]), belongs to the class $I(n,\Delta)$. In the special case, for d-regular graphs, $1 \leq d \leq n-1$, from (3) follows [66]

$$Kf(G) \geq \frac{(n-1)^2}{d}, \tag{4}$$

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

In [79] the following lower bound for $Kf(G)$ that belongs to the class $I(n,\delta)$ was obtained

$$Kf(G) \geq n - 1 + \frac{n}{\delta} - \frac{\delta+1}{n-1},$$

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

The lower bound for $Kf(G)$ in the class $I(n)$ obtained in [49], (see also [60,81]) has the following form

$$Kf(G) \geq Kf(K_n) = n - 1. \tag{5}$$

This is the best possible bound for the $Kf(G)$ in the class $I(n)$. Let us note that inequality (5) can be easily obtained from (2) and inequalities $2m \leq n(n-1)$, or (3) and $\Delta \leq n-1$.

Since for the planar graphs hold $m \leq 3(n-2)$, from (2) follows

$$Kf(G) \geq \frac{n(n-1)^2}{6(n-2)}, \tag{6}$$

with equality if and only if $G \cong K_3$ or $G \cong K_4$ (see [78]). This represents a lower bound for $Kf(G)$ in the class $I(n)$ for planar graphs.

The graphs G_p, $2 \leq p \leq \lfloor \frac{n}{2} \rfloor$, obtained by removing p edges from a complete graph K_n, were considered in [75]. It was proved that

$$Kf(G_p) \geq n - 1 + \frac{2p}{n-2},$$

with equality if and only if $G_p \cong K_n - pK_2$.

In [41] it was proved that for every tree T holds

$$W(T) \geq W(K_{1,n-1}),$$

where $W = W(G)$ is a Wiener index. Since for any tree $W(T) = Kf(T)$, it means that the lower bound for $Kf(T)$ in the class $I(n)$ is obtained as well, i.e. that

$$Kf(T) \geq (n-1)^2,$$

with equality if and only if $T \cong K_{1,n-1}$.

Since the inequality $2m \leq n(n-1)$ holds if and only if

$$n \geq \frac{1}{2}\left(\sqrt{8m+1}+1\right),$$

from (5) we get

$$Kf(G) \geq \frac{1}{2}\left(\sqrt{8m+1}-1\right),$$

with equality if and only if $G \cong K_n$. This is the best possible lower bound for $Kf(G)$ in the class $I(m)$.

- For $k_1 = 2$, $k_2 = 1$, $p_i = \mu_i$, $a_i = b_i = \frac{1}{\mu_i}$, $i = 2, 3, \ldots, n-1$, from (1) the following inequality is obtained
$$Kf(G) \geq n\left(\frac{1}{\mu_1} + \frac{(n-2)^2}{2m-\mu_1}\right),$$
with equality if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$, i.e. if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n (see [47, 84, 85]).

- For $k_1 = 1$, $k_2 = 2$, $p_i = \mu_i$, $a_i = b_i = \frac{1}{\mu_i}$, $i = 1, 2, \ldots, n-2$, from (1) follows
$$Kf(G) \geq n\left(\frac{1}{\mu_{n-1}} + \frac{(n-2)^2}{2m-\mu_{n-1}}\right),$$
with equality if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-2}$, i.e. if and only if $G \cong K_n$, or $G \cong K_n - e$. Accordingly, we have that
$$Kf(G) \geq n \max\left\{\frac{1}{\mu_1} + \frac{(n-2)^2}{2m-\mu_1}, \frac{1}{\mu_{n-1}} + \frac{(n-2)^2}{2m-\mu_{n-1}}\right\},$$
with equality if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $G \cong K_n - e$.

Consider the function (see [18])
$$f(x) = \frac{1}{x} + \frac{(n-2)^2}{2m-x}.$$
It is monotone increasing when $x \geq \frac{2m}{n-1}$, monotone decreasing when $\frac{2m}{n-1} \geq x$, and has a minimum for $x = \frac{2m}{n-1}$. This means that for any k, $\mu_1 \geq k \geq \frac{2m}{n-1}$ holds
$$Kf(G) \geq n\left(\frac{1}{\mu_1} + \frac{(n-2)^2}{2m-\mu_1}\right) \geq \left(\frac{1}{k} + \frac{(n-2)^2}{2m-k}\right) \geq \frac{n(n-1)^2}{2m},$$

and for any k, $\frac{2m}{n-1} \geq k \geq \mu_{n-1}$,

$$Kf(G) \geq n\left(\frac{1}{\mu_{n-1}} + \frac{(n-2)^2}{2m-\mu_{n-1}}\right) \geq \left(\frac{1}{k} + \frac{(n-2)^2}{2m-k}\right) \geq \frac{n(n-1)^2}{2m}.$$

Consequently, for any k, $\mu_1 \geq k \geq \mu_{n-1}$, holds

$$Kf(G) \geq n\left(\frac{1}{k} + \frac{(n-2)^2}{2m-k}\right), \tag{7}$$

with equality if and only if $k = n$ and $G \cong K_n$, or $k = n$ and $G \cong K_{1,n-1}$, or $k = n$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $k = n-2$ and $G \cong K_n - e$.

The inequality (7) determines a lower bound for $Kf(G)$ in the class $I(n,m,k)$, $\mu_1 \geq k \geq \mu_{n-1}$. The obtained bound is very good since the inequality (7) is strong and is reached for various types of graphs.

Having in mind that for connected graphs hold $\mu_1 \geq 1 + \Delta$ (see [36]), it is easy to show that

$$\mu_1 \geq 1 + \Delta \geq \frac{M_1}{2m} + 1 \geq \frac{2m}{n} + 1 \geq \frac{2m}{n-1} \geq \mu_{n-1}.$$

For $k = \frac{2m}{n-1}$, from (7) the inequality (2) is obtained.

For $k = \frac{2m}{n} + 1$, from (7) follows

$$Kf(G) \geq n^2\left(\frac{1}{2m+n} + \frac{(n-2)^2}{2m(n-1)-n}\right). \tag{8}$$

Equality holds if and only if $G \cong K_n$. This inequality establishes a lower bound for $Kf(G)$ in the class $I(n,m)$. It is better than the one given by (2).

For $k = \frac{M_1}{2m} + 1$, from (7) the following is obtained

$$Kf(G) \geq 2mn\left(\frac{1}{M_1+2m} + \frac{(n-2)^2}{4m^2-M_1-2m}\right), \tag{9}$$

with equality if and only if $G \cong K_n$. On the other hand, in [16] it was proved that

$$Kf(G) \geq \frac{2mn(n-1)(n-2)}{4m^2-M_1-2m}, \tag{10}$$

with equality if and only if $G \cong K_n$. Both (9) and (10) set up a lower bound for $Kf(G)$ in the class $I(n,m,M_1)$. However, bound (10) is better than (9).

Since $M_1 \geq \frac{4m^2}{n}$ (see [20]), from (10) follows

$$Kf(G) \geq \frac{n^2(n-1)(n-2)}{2m(n-1)-n},$$

with equality if and only if $G \cong K_n$. This inequality is stronger than (2).

For $k = 1 + \Delta$ from (7) the inequality

$$Kf(G) \geq n\left(\frac{1}{1+\Delta} + \frac{(n-2)^2}{2m-\Delta-1}\right), \tag{11}$$

is obtained [84] (see also [85]). Equality holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

In [60] (see also [83, 84]) the following lower bound for $Kf(G)$ was determined

$$Kf(G) \geq n - 1 + \frac{n(n-1) - 2m}{\Delta}, \tag{12}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n, or $G \in \Gamma_d$.

Lower bounds (11) and (12) belong to the same class $I(n, m, \Delta)$, but are not comparable and, hence, none of them is the best possible in the class.

From (11) it follows that for regular graphs of degree d, $1 \leq d \leq n-1$, hold

$$Kf(G) \geq n\left(\frac{1}{1+d} + \frac{(n-2)^2}{nd-d-1}\right), \tag{13}$$

with equality if and only if $G \cong K_n$ (see [2] and [66]).

In [11] (see also [17]) the following lower bound for $Kf(G)$ in the class $I(n, m, \Delta, \delta)$ was derived

$$Kf(G) \geq n\left(\frac{1}{1+\Delta} + \frac{1}{\delta} + \frac{(n-3)^2}{2m-\Delta-\delta-1}\right), \tag{14}$$

where $G \neq K_n$. Equality holds if and only if either $G \cong K_{1,n-1}$, or $G \cong K_n - e$, or $G \cong K_{n-1} + e$.

Since $1 + \Delta \leq n$ from (14), follows (see [17])

$$Kf(G) \geq n\left(\frac{1}{n} + \frac{1}{\delta} + \frac{(n-3)^2}{2m-\Delta-\delta-1}\right), \tag{15}$$

with equality if and only if either $G \cong K_{1,n-1}$, or $G \cong K_n - e$, or $G \cong K_{n-1} + e$. When $G \neq K_n$, the inequality (14) is stronger than (15). In [16] the following lower bound for the Kirchhoff index in the class $I(n, m, \Delta, \Delta_2, \delta)$ was determined

$$Kf(G) \geq \frac{n}{1+\Delta} + \frac{n}{2m-\Delta-1}\left((n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\delta}\right),$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

In [54] the following inequality was proved

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{(n-1)}{2m-\Delta}\left((n-1)^2 + \left(\sqrt{\frac{\Delta_2}{\delta}} - \sqrt{\frac{\delta}{\Delta_2}}\right)^2\right),$$

with equality if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $G \in \Gamma_d$.

Although the previous two inequalities belong to the same class, they are not comparable.

In [46] (see also [1]) a lower bound for $Kf(G)$ in the class $I(n,m,\Delta,\Delta_2)$ was obtained as a special case of one more general result. It was proved that

$$Kf(G) \geq n\left(\frac{1}{1+\Delta}+\frac{1}{\Delta_2}+\frac{(n-3)^2}{2m-\Delta-\Delta_2-1}\right), \tag{16}$$

when $d_{n-2} \geq d_{n-1}+\delta-1$. Equality holds if and only if $G \cong K_{1,n-1}$. Interestingly, in [1] for the above inequality the condition $2m \leq 1+\Delta+(n-2)\Delta_2$ was put on.

In [46,83,84] lower bounds for $Kf(G)$ in the class $I(n,d_1,\ldots,d_n)$ were determined. In [83] (see also [46]) the following bound was established

$$Kf(G) \geq n\left(\frac{1}{1+\Delta}+\sum_{i=2}^{n-2}\frac{1}{d_i}+\frac{1}{d_{n-1}+\delta-1}\right), \tag{17}$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$. In [84] it was proved that

$$Kf(G) \geq -1+(n-1)\sum_{i=1}^{n}\frac{1}{d_i} = -1+(n-1)ID, \tag{18}$$

where $ID = ID(G)$ is the inverse degree of a graph (see for example [44,45]). Equality in (18) holds if and only if $G \cong K_n$, or $G \cong K_{r,n-r}$, $1 \leq r \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

Let us note that the invariant ID is also met in the literature under names general first Zagreb index and zeroth order general Randić index.

In [83] it was reported that inequalities (17) and (18) are not comparable. However, we couldn't find out an example when the lower bound (17) is better than (18).

At first glance, the inequalities (17) and (18) seem to be quite demanding, since they require knowing degrees of all vertices of a graph to compute the invariant ID. However, the invariant ID is well studied in the literature and its available lower bounds can be used to determine lower bounds for $Kf(G)$ that are even better than already mentioned in this section. Here we list some examples.

- For $k_1 = 1$, $k_2 = 0$, $p_i = d_i$, $a_i = b_i = \frac{1}{d_i}$, $i = 1,2,\ldots,n$, from (1) the inequality

$$ID = \sum_{i=1}^{n}\frac{1}{d_i} \geq \frac{n^2}{2m},$$

is obtained. From the above and (18) follows (see [54])

$$Kf(G) \geq \frac{n^2(n-1)-2m}{2m}, \tag{19}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $G \in \Gamma_d$.

Since

$$\frac{n^2(n-1)-2m}{2m} \geq \frac{n^2(n-1)-n(n-1)}{2m} = \frac{n(n-1)^2}{2m},$$

the inequality (19) is stronger than (2). This means that the lower bound (19) is better than the one determined by (2).

Since $2m \leq n\Delta$, from (19) follows [60]:

$$Kf(G) \geq \frac{n(n-1)-\Delta}{\Delta}, \tag{20}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n, or $G \in \Gamma_d$.

From the inequality

$$\frac{n(n-1)-\Delta}{\Delta} \geq \frac{(n-1)^2}{\Delta},$$

it can be concluded that the inequality (20) is stronger than (3). Hence, lower bound for $Kf(G)$ in the class $I(n,\Delta)$ obtained in(20) is better than the one determined by (3).

It is well known that for connected planar graphs hold $m \leq 3(n-2)$. Thus, from (19) we have that for connected planar graphs

$$Kf(G) \geq \frac{n^2(n-1)}{6(n-2)} - 1,$$

with equality if and only if $G \cong K_3$ or $G \cong K_4$. This inequality is stronger than (6).

Similarly, if G is a connected planar bipartite graph, then

$$Kf(G) \geq \frac{n^2(n-1)}{4(n-2)} - 1,$$

with equality if and only if $G \cong K_{2,2}$.

- For $k_1 = 2$, $k_2 = 0$, $p_i = d_i$, $a_i = b_i = \frac{1}{d_i}$, $i = 2, 3, \ldots, n$, from (1) the inequality

$$ID \geq \frac{1}{\Delta} + \frac{(n-1)^2}{2m-\Delta}, \tag{21}$$

is obtained.

Based on (18) and (21) the following lower bound for $Kf(G)$ in the class $I(n,m,\Delta)$ has been derived in [54]

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{(n-1)^3}{2m-\Delta}, \tag{22}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n, or $G \in \Gamma_d$. Since

$$\frac{n-1-\Delta}{\Delta} + \frac{(n-1)^3}{2m-\Delta} \geq n-1+\frac{n(n-1)-2m}{\Delta},$$

the bound (22) is better than the one obtained by (12) in the same class $I(n,m,\Delta)$.

Inequalities (22) and (11) are exact when $G \cong K_n$ or $G \cong K_{1,n-1}$. The inequality (22) is stronger than (11) when $G \cong P_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$, or when sequence of vertex degrees of a connected graph is of the form $D = (n-1, d_2, \ldots, d_n)$. We have performed testing on a set of connected (regular) graphs with $n \geq 4$ vertices to find out the case, if any, when the inequality (11) is stronger than (22), but we didn't find it. However, it is still an open question whether the lower bound given by (22) is the best possible in the class $I(n,m,\Delta)$.

From the inequality (22) follows that for regular graph of degree d, $1 \leq d \leq n-1$, holds

$$Kf(G) \geq \frac{n(n-1)-d}{d}, \tag{23}$$

with equality if and only if $G \cong K_n$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even, or $G \in \Gamma_d$.

The inequality (23) was proved in [60]. It is stronger than (4). Note that in the case of d-regular graphs, $1 \leq d \leq n-1$, the inequalities (12), (18), (19) and (22) reduce to (23). An open question is whether the bound (23) is the best possible in the class $I(n,d)$.

Since $ID \geq 2R_{-1}$ (see [48]) according to (18) the following inequality is obtained

$$Kf(G) \geq -1 + 2(n-1)R_{-1}, \tag{24}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $G \in \Gamma_d$. The inequality (24) determines lower bound for $Kf(G)$ in the class $I(n,R_{-1})$. When the invariant R_{-1} is replaced with its (known) lower bounds, from (24) a variety of bounds, known and new ones, for $Kf(G)$ in various classes can be obtained. Thus, for example, based on the inequality [43]

$$2R_{-1} \geq \frac{n}{n-1},$$

and (24), the inequality (5) is obtained. From the inequality [10, 72]

$$2R_{-1} \geq \frac{n}{\Delta},$$

and (24), the inequality (20) is obtained. From the inequality (see [53])

$$R_{-1} \geq \frac{n-1}{2(n-2)}\left(k - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)},$$

where k is an arbitrary real number with the property $\rho_1 \geq k \geq \rho_{n-1}$, and (24) the following is obtained

$$Kf(G) \geq n-1 + \frac{(n-1)^2}{n-2}\left(k - \frac{n}{n-1}\right)^2,$$

with equality if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$, or $k = 2$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n. In the above inequality the lower bound for $Kf(G)$ in the class $I(n,k)$ is acquired. In the special case we have

$$Kf(G) \geq n-1 + \frac{(n-1)^2}{n-2} \max\left\{\left(\rho_1 - \frac{n}{n-1}\right)^2, \left(\rho_{n-1} - \frac{n}{n-1}\right)^2\right\},$$

with equality if and only if $G \cong K_n$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even.

Let us point out on some lower bounds that can be obtained according to (24) and depend on invariants M_2, F and M_1.

From (1) follows

$$\sum_{i\sim j} d_i d_j \sum_{i\sim j} \frac{1}{d_i d_j} \geq m^2.$$

Accordingly we have that

$$R_{-1} \geq \frac{m^2}{M_2}.$$

From the above and (24) follows

$$Kf(G) \geq \frac{2(n-1)m^2}{M_2} - 1,$$

with equality if and only if $L(G)$ is regular. Thus, we obtained a lower bound for $Kf(G)$ in the class $I(n, m, M_2)$.

On the other hand, since

$$2M_2 \leq F$$

we have that

$$Kf(G) \geq \frac{4(n-1)m^2}{F} - 1$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$. This represents a lower bound for $Kf(G)$ in the class $I(n, m, F)$.

Based on the inequality (see [39])

$$F \leq (\Delta + \delta)M_1 - 2m\Delta\delta,$$

the following lower bound in the class $I(n, m, \Delta, \delta, M_1)$ can be obtained

$$Kf(G) \geq \frac{4(n-1)m^2}{(\Delta + \delta)M_1 - 2m\Delta\delta} - 1,$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

- For $k_1 = 3$, $k_2 = 0$, $p_i = d_i$, $a_i = b_i = \frac{1}{d_i}$, $i = 3, 4, \ldots, n$, from (1) the inequality

$$ID \geq \frac{1}{\Delta} + \frac{1}{\Delta_2} + \frac{(n-2)^2}{2m - \Delta - \Delta_2},$$

is obtained. From the above and (18) the following is obtained (see [54])

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{n-1}{\Delta_2} + \frac{(n-1)(n-2)^2}{2m - \Delta - \Delta_2}, \tag{25}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n, or $G \in \Gamma_d$.

The inequality (25) is stronger than (16) when $G \cong K_{\frac{n}{2},\frac{n}{2}}$, $G \cong P_n$ and $G \in \Gamma_d$. However, it is an open question whether (25) is always better than (16).

- For $k_1 = 2$, $k_2 = 1$, $p_i = d_i$, $a_i = b_i = \frac{1}{d_i}$, $i = 2, 3, \dots, n-1$, from (1) the inequality

$$ID \geq \frac{1}{\Delta} + \frac{1}{\delta} + \frac{(n-2)^2}{2m - \Delta - \delta},$$

is obtained. From the above and (18) the inequality

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{n-1}{\delta} + \frac{(n-1)(n-2)^2}{2m-\Delta-\delta}, \tag{26}$$

is obtained (see [54]). Equality holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ when n is even, or $G \in \Gamma_d$.

Inequalities (26) and (15) are not comparable. Thus, for example, for $G \cong K_{\frac{n}{2},\frac{n}{2}}$ the inequality (26) is stronger than (15), but when $G \cong K_n - e$, inequality (15) is stronger than (26).

The following lower bound for $Kf(G)$ can be obtained as a special case of one more general result reported in [85]

$$Kf(G) \geq \frac{n}{1+\Delta} + (n-2)n^{\frac{n-3}{n-2}} \left(\frac{t}{1+\Delta} \right)^{-\frac{1}{n-2}},$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Similarly, the following can be obtained from the one more general inequality proved in [18]

$$Kf(G) \geq \frac{n}{1+\Delta} + (n-2)n^{\frac{n-3}{n-2}}(1+\Delta)^{\frac{1}{n-2}} t^{-\frac{1}{n-2}} + (\Delta_2^{1/2} - \delta^{1/2})^2,$$

with equality if and only if $G \cong K_n$. This sets up a lower bound for $Kf(G)$ in the class $I(n, \Delta, \Delta_2, \delta, t)$. This inequality is stronger than the previous one.

The following double inequality which gives relationship between Kirchhoff, $Kf(G)$, and degree-Kirchhoff index, $Kf^*(G)$, was proved in [86] (see also [66])

$$\frac{n}{2m\Delta} Kf^*(G) \leq Kf(G) \leq \frac{n}{2m\delta} Kf^*(G). \tag{27}$$

Equalities hold if and only if G is regular.

Inequalities (27) can be used to determine lower and upper bounds for Kirchhoff index, $Kf(G)$, according to the bounds for degree Kirchhoff index, and vice versa. Note that obtained bounds may not be the best possible in the corresponding class. Here is one example.

Let

$$P = 1 + \sqrt{\frac{2R_{-1}}{n(n-1)}}. \tag{28}$$

In [7] (see also [2]) the following inequality for the degree Kirchhoff index was proved

$$Kf^*(G) \geq 2m \left(\frac{1}{P} + \frac{(n-2)^2}{n-P} \right),$$

with equality if and only if $G \cong K_n$. Based on this and left part of inequality (27), it follows that

$$Kf(G) \geq \frac{n}{\Delta} \left(\frac{1}{P} + \frac{(n-2)^2}{n-P} \right),$$

with equality if and only if $G \cong K_n$. This inequality, proved in [2], sets up lower bound for $Kf(G)$ in the class $I(n, \Delta, R_{-1})$. It is not known whether this inequality is the best possible in its class. Therefore, we suggest to use (27) only for regular graphs, or when there is no other way to estimate $Kf(G)$, i.e. $Kf^*(G)$.

In the sequel we provide an overview of the lower bounds for $Kf(G)$ of connected bipartite graphs.

Let $G = (V, E)$ be a connected bipartite graph $V = V_1 \cup V_2$, $V_1 \cap V_2 = \emptyset$, $|V_1| = p$, $|V_2| = q$, $p + q = n$. In [77] the authors determined the lower bound of $Kf(G)$ in the class $I(p, q)$. They proved that

$$Kf(G) \geq \frac{(p+q-1)(p^2+q^2) - pq}{pq},$$

with equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even.

In the case of connected bipartite graphs the following inequalities are valid (see for example [47] and [20])

$$\mu_1 \geq \frac{M_1}{m} \geq 2\sqrt{\frac{M_1}{n}} \geq \frac{4m}{n} \geq \frac{2m}{n-1}.$$

Now, according to (7) the following inequalities are valid:

- For $k = \frac{4m}{n}$ we have

$$Kf(G) \geq \frac{n^2(2n-3)}{4m}, \tag{29}$$

with equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n. This inequality establishes lower bound for $Kf(G)$ for connected bipartite graphs in the class $I(n, m)$.

Since $2m \leq n\Delta$, from (29) follows

$$Kf(G) \geq \frac{n(2n-3)}{2\Delta}$$

with equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n. This inequality was proved in [86] (see also [64]).

- For $k = 2\sqrt{\frac{M_1}{n}}$ we obtain

$$Kf(G) \geq \frac{n}{2}\left(\frac{1}{\sqrt{\frac{M_1}{n}}} + \frac{(n-2)^2}{m - \sqrt{\frac{M_1}{n}}}\right), \tag{30}$$

with equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even. This was proved in [85] (see also [8,47]).

- For $k = \frac{M_1}{m}$ the following is obtained

$$Kf(G) \geq n\left(\frac{m}{M_1} + \frac{m(n-2)^2}{2m^2 - M_1}\right),$$

with equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, where n is even, or $G \cong K_{1,n-1}$. This inequality, proved in [87] (see also [8, 47, 88]), sets up lower bound for $Kf(G)$ in the class $I(n, m, M_1)$ that is stronger than the bound given by (30).

Let
$$T=\frac{1}{2}\left(\Delta+\delta+\sqrt{(\Delta-\delta)^2+4\Delta}\right).$$
From one more general result, obtained in [8] for bipartite graphs, the following inequality can be obtained
$$Kf(G)\geq n\left(\frac{1}{T}+\frac{(n-2)^2}{2m-T}\right),$$
with equality if and only if $G\cong K_{1,n-1}$.

In [87] (see also [8, 88]) the following lower bound for $Kf(G)$ in $I(n,m,t,M_1)$ class for connected bipartite graphs was determined
$$Kf(G)\geq n\left(\frac{m}{M_1}+(n-2)\left(\frac{M_1}{t\,n\,m}\right)^{\frac{1}{n-2}}\right),$$
with equality if and only if $G\cong K_{\frac{n}{2},\frac{n}{2}}$ where n is even.

3. Upper bounds for the Kirchhoff index

Among the papers considering the bounds of Kirchhoff index there are far much more those dealing with lower than upper bounds. In this section we give a review of the papers considering upper bounds for the Kirchhoff index.

The following inequality that establishes upper bound for $Kf(G)$ in the class $I(n)$ was derived in [49] (see also [62])
$$Kf(G)\leq Kf(P_n)=\frac{n^3-n}{6}.$$
This is the best possible upper bound for $Kf(G)$ in the class $I(n)$.

For the graphs G_p, $2\leq p\leq\left\lfloor\frac{n}{2}\right\rfloor$, obtained by removing p edges from a complete graph K_n, in [75] the following was proved
$$Kf(G_p)\leq n-1-p+\frac{n}{n-1-p}+\frac{n(p-1)\delta}{(n-1)(n-1-p)},$$
with equality if and only if $G_p=K_n-K_{1,p}$.

Let k be an arbitrary real number so that $\mu_{n-1}\geq k$. In [68] the upper bound for $Kf(G)$ in the class $I(n,m,k)$ was determined. It reads
$$Kf(G)\leq\frac{(n+k)(n-1)-2m}{k},\tag{31}$$
with equality if and only if $k=n$ and $G\cong K_n$, or $k=1$ and $G\cong K_{1,n-1}$, or $k=\frac{n}{2}$ and $G\cong K_{\frac{n}{2},\frac{n}{2}}$, or $k=n-2$ and $G\cong K_n-e$.

As can be seen, the inequality (31) is very strong since it reaches equality in many cases. Therefore, we recommend to use (31) to evaluate upper bound for $Kf(G)$ whenever there is a good assessment of the lower bound for μ_{n-1}.

In [69] an upper bound for $Kf(G)$ in the class $I(n,m,\Delta,k)$ was reported. The authors proved that

$$Kf(G) \leq n\frac{\Delta+1+k(n-1)+n(n-2)-2m}{k(\Delta+1)}, \tag{32}$$

with equality if and only if $k=n$ and $G\cong K_n$, or when $k=1$ and $G\cong K_{1,n-1}$, or $k=n-2$ and $G\cong K_n-e$.

In [79] the following inequality was proved

$$Kf(G) \leq \binom{n-\Delta+3}{3}+(\Delta-1)\binom{n-\Delta+2}{2}+(\Delta-1)(\Delta-2), \tag{33}$$

with equality if and only if $G\cong K_n$ or $G\cong P_n$. This inequality posts an upper bound for $Kf(G)$ in the class $I(n,\Delta)$.

In [16] the following upper bound in the class $I(n,m,t,M_1)$ was determined

$$Kf(G) \leq \frac{n-1}{t}\left(\frac{4m^2-M_1-2m}{(n-1)(n-2)}\right)^{\frac{n-2}{n}}.$$

Equality holds if and only if $G\cong K_n$ or $G\cong K_{1,n-1}$.

Based on the previous and inequality $M_1\geq \frac{4m^2}{n}$ (see [20]), the following one that determines an upper bound for $Kf(G)$ in the class $I(n,m,t)$ is obtained

$$Kf(G) \leq \frac{n-1}{t}\left(\frac{2m(2m(n-1)-1)}{n(n-1)(n-2)}\right)^{\frac{n-2}{n}},$$

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

Denote with $D(n,a,b)$ a class of bipartite graphs with $n=p+q$ vertices consisting of a path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P_{n-a-b} and b independent vertices adjacent to the other pendent vertex of P_{n-a-b}. For (p,q)-bipartite graphs ($p<q$) in [77] the following upper bound for $Kf(G)$ was determined

$$Kf(G) \leq \begin{cases} \frac{1}{6}(-2p+3p^2-p^3-6pq+6p^2q+3q^2+3pq^2), & (q-p)\equiv 0(\mod 2) \\ \frac{1}{6}(-3+p+3p^2-p^3-6pq+6p^2q+3q^2+3pq^2), & (q-p)\equiv 1(\mod 2) \end{cases}$$

with equality if and only if $G\in D\left(p+q,\left\lfloor\frac{p+q+1}{2}\right\rfloor,\left\lfloor\frac{p-q+1}{2}\right\rfloor\right)$.

In the sequel we list some inequalities that can be used to obtain upper bounds for $Kf(G)$ in various classes.

In [51] the following inequalities were proved

$$Kf(G) \leq \frac{n(n-1)^2}{2m}\left(1+\frac{(\mu_1-\mu_{n-1})^2}{\mu_1\mu_{n-1}}\alpha(n-1)\right), \tag{34}$$

where

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

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

We will illustrate how (34) can be used to obtain upper bounds for $Kf(G)$ in, for example, classes $I(n, m, k, M_1)$ and $I(n, m, k)$, where k is real number with the property $\mu_{n-1} \geq k > 0$.

In [55] the following was proved

$$(\mu_1 - \mu_{n-1})^2 \leq \frac{2}{n-1}\left((n-1)(M_1 + 2m) - 4m^2\right), \tag{35}$$

with equality if and only if $G \cong K_n$. Let k be an arbitrary real number so that $\mu_{n-1} \geq k$. Then

$$\mu_1 \mu_{n-1} \geq k \frac{2m}{n-1}. \tag{36}$$

According to (34), (35) and (36) we have that

$$Kf(G) \leq \frac{n(n-1)^2}{2m}\left(1 + \frac{(n-1)(M_1 + 2m) - 4m^2}{mk}\alpha(n-1)\right), \tag{37}$$

with equality if and only if $G \cong K_n$. Thus, an upper bound for $Kf(G)$ in the class $I(n, m, k, M_1)$ is obtained. Further, since (see [9])

$$M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right),$$

from (37) we have that

$$Kf(G) \leq \frac{n(n-1)^2}{2m}\left(1 + \frac{n(n-1) - 2m}{k}\alpha(n-1)\right),$$

with equality if and only if $G \cong K_n$. Thus an upper bound for $Kf(G)$ in the class $I(n, m, k)$ is obtained.

In [51] it was proved that

$$Kf(G) \leq n\frac{(\mu_1 + \mu_{n-1})(n-1) - 2m}{\mu_1 \mu_{n-1}}, \tag{38}$$

with equality if and only if G is a complete split graph or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, for even n.

Interestingly, it is easy to obtain (31) from (38). Also, since

$$\mu_1 + \mu_{n-1} \leq n + \frac{2m}{n-1} = \frac{n(n-1) + 2m}{n-1},$$

from (36) and (38) follows

$$Kf(G) \leq \frac{n^2(n-1)^2}{2mk},$$

with equality if and only if $k = n$ and $G \cong K_n$.

Further, since

$$\mu_1 \mu_{n-1} \geq k(1 + \Delta),$$

from (38) follows

$$Kf(G) \leq \frac{n^2(n-1)}{k(1 + \Delta)},$$

with equality if and only if $k = n$ and $G \cong K_n$.

The next three inequalities may also be interesting for determining upper bounds for $Kf(G)$.

In afore mentioned paper [51] the following inequalities were also proved

$$Kf(G) \le \frac{n}{1+\Delta} + \frac{n(n-2)^2}{2m-n}\left(1 + \frac{(\mu_2 - \mu_{n-1})^2}{\mu_2\mu_{n-1}}\alpha(n-2)\right),$$

with equalities if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$, and

$$Kf(G) \le \frac{n}{1+\Delta} + n\frac{(\mu_2 + \mu_{n-1})(n-2) - (2m-n)}{\mu_2\mu_{n-1}},$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$, and

$$Kf(G) \le \frac{n(n-1)^2}{8m}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2$$

with equality if and only if $G \cong K_n$. These inequalities can be used to determine lower bounds for $Kf(G)$ in various classes (see [21] and [52]).

4. Lower bounds for the degree Kirchhoff index

In this section we present lower bounds of various classes for the degree Kirchhoff index.

Lower bound for degree Kirchhoff index $Kf^*(G)$ in the class $I(n)$ was established in [65] by the following inequality

$$Kf^*(G) \ge Kf^*(K_n) = (n-1)^3.$$

From the above, it is easy to determine lower bound for $Kf^*(G)$ in the class $I(m)$, i.e. the following is valid

$$Kf^*(G) \ge \frac{1}{8}\left(\sqrt{8m+1} - 1\right)^3,$$

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

For $k_1 = 2$, $k_2 = 1$, $p_i = \rho_i$, $a_i = b_i = \frac{1}{\rho_i}$, $i = 2, 3, \ldots, n-1$, from (1) follows

$$Kf^*(G) \ge 2m\left(\frac{1}{\rho_1} + \frac{(n-2)^2}{n-\rho_1}\right), \tag{39}$$

with equality if and only if $\rho_2 = \rho_3 = \cdots = \rho_{n-1}$.

Similarly, for $k_1 = 1$, $k_2 = 2$, $p_i = \rho_i$, $a_i = b_i = \frac{1}{\rho_i}$, $i = 1, 2, \ldots, n-2$, from (1) follows

$$Kf^*(G) \ge 2m\left(\frac{1}{\rho_{n-1}} + \frac{(n-2)^2}{n-\rho_{n-1}}\right), \tag{40}$$

with equality if and only if $\rho_1 = \rho_2 = \cdots = \rho_{n-2}$.

Now consider the function

$$f(x) = \frac{1}{x} + \frac{(n-2)^2}{n-x}.$$

This function is monotone increasing for any real x with the property $x \geq \frac{n}{n-1}$, monotone decreasing for $x \leq \frac{n}{n-1}$ and has a minimum for $x = \frac{n}{n-1}$. Thus, according to (39) and (40), we have that for any real k with the property $\rho_1 \geq k \geq \rho_{n-1}$ holds

$$Kf^*(G) \geq 2m\left(\frac{1}{k} + \frac{(n-2)^2}{n-k}\right), \tag{41}$$

with equality if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$, or $k = 2$ and $G \cong K_{1,n-1}$, or $k = 2$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ where n is even.

Since (see for example [7])

$$\rho_1 \geq P \geq \frac{\Delta+1}{\Delta} \geq \frac{n}{n-1} \geq \rho_{n-1},$$

where $P = 1 + \sqrt{\frac{2R_{-1}}{n(n-1)}}$, the followings are valid:

For $k = \frac{n}{n-1}$ from (41) we get [22] (see also [2, 38, 57, 64])

$$Kf^*(G) \geq \frac{2m(n-1)^2}{n}, \tag{42}$$

with equality if and only if $G \cong K_n$. This inequality establishes lower bound for $Kf^*(G)$ in the class $I(m, n)$.

Let us note that inequality (42) can be easily obtained in following manner

$$Kf^*(G) \geq (n-1)^3 = (n-1)(n-1)^2 \geq \frac{2m(n-1)^2}{n}.$$

This implies that the lower bound (42) is not the best possible in the class $I(n, m)$. And, really, in [61] it was proved that

$$Kf^*(G) \geq n - 1 + 2m(n-2), \tag{43}$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

The inequality (43) is stronger than (42). Hence, the lower bound (43) is better than (42) in the class $I(n, m)$.

For $k = \frac{\Delta+1}{\Delta}$ from (41) we get [22]

$$Kf^*(G) \geq 2m\left(\frac{\Delta}{\Delta+1} + \frac{(n-2)^2}{n-1-\frac{1}{\Delta}}\right), \tag{44}$$

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

In [65] the following was proved

$$Kf^*(G) \geq 2m\left(n - 2 + \frac{1}{\Delta+1}\right), \tag{45}$$

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

The inequality (45) is stronger than (44). Thus, bound (45) is better than (44) in the class $I(n, m, \Delta)$. However, the inequality (43) is stronger than (45). This follows from the inequalities (see [61])

$$2m \leq n\Delta \leq (\Delta+1)(n-1).$$

Accordingly, it is questionable whether the lower bound for $Kf^*(G)$ determined by (45) is the best possible in the class $I(n, m, \Delta)$.

Since $n \geq \Delta + 1$, from (43) follows

$$Kf^*(G) \geq \Delta + 2m(n-2), \tag{46}$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Lower bounds (45) and (46) belongs to the (same) class $I(n, m, \Delta)$. Since (45) and (46) are not comparable, the open question is what is the best lower bound for $Kf^*(G)$ in the class $I(n, m, \Delta)$.

Consider, now, d-regular graphs, $1 \leq d \leq n-1$. For these graphs hold (see Eq. (27))

$$Kf^*(G) = d^2 Kf(G).$$

From the above and inequality (23) the following is obtained

$$Kf^*(G) \geq d(n(n-1) - d),$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ when n is even, or $G \in \Gamma_d$. The question is whether the lower bound for $Kf^*(G)$ established by this inequality is the best possible for d-regular graphs in the class $I(n, d)$. Performed testings suggest that it is, but there is no explicit proof.

In [37] the following lower bound for $Kf^*(G)$ in the class $I(n, d, t)$ was obtained

$$Kf^*(G) \geq n(n-1)d^2(t \cdot n)^{-\frac{1}{n-1}},$$

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

Interestingly, from the above inequality directly follows

$$Kf(G) \geq n(n-1)(t \cdot n)^{-\frac{1}{n-1}},$$

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

For $k = P$, from (41) we obtain [7] (see also [2–4, 65])

$$Kf^*(G) \geq 2m\left(\frac{1}{P} + \frac{(n-2)^2}{n-P}\right). \tag{47}$$

Equality holds if and only if $G \cong K_n$. This inequality determines the lower bound for $Kf^*(G)$ in the class $I(n, m, R_{-1})$.

Let G be a simple connected graph different from a complete one, i.e. $G \ncong K_n$, and let β be an arbitrary real number with the property $\rho_2 \geq \beta$, $\beta \leq P$, $P + (n-2)\beta \geq n$. In [4] the following was proved as a part of one more general result

$$Kf^*(G) \geq 2m\left(\frac{1}{P} + \frac{1}{\beta} + \frac{(n-3)^2}{n-P-\beta}\right). \tag{48}$$

For $k_1 = 3$, $k_2 = 1$, $p_i = \rho_i$, $a_i = b_i = \frac{1}{\rho_i}$, $i = 3, \ldots, n-1$, and $k_1 = 2$, $k_2 = 2$, $p_i = \rho_i$, $a_i = b_i = \frac{1}{\rho_i}$, $i = 2, 3, \ldots, n-2$, from (1) the following is obtained respectively

$$Kf^*(G) \geq 2m\left(\frac{1}{\rho_1} + \frac{1}{\rho_2} + \frac{(n-3)^2}{n-\rho_1-\rho_2}\right), \tag{49}$$

and

$$Kf^*(G) \geq 2m\left(\frac{1}{\rho_1}+\frac{1}{\rho_{n-1}}+\frac{(n-3)^2}{n-\rho_1-\rho_{n-1}}\right). \tag{50}$$

Equality in (49) holds if and only if $\rho_3 = \rho_4 = \cdots = \rho_{n-1}$, and in (50) if and only if $\rho_2 = \rho_3 = \cdots = \rho_{n-2}$.

From (49), for any two real numbers r_1 and r_2 with the properties $\rho_1 \geq r_1 \geq \frac{n-\rho_2}{n-2}$ and $\rho_2 \geq r_2 \geq \frac{n-r_1}{n-2}$, holds

$$Kf^*(G) \geq 2m\left(\frac{1}{r_1}+\frac{1}{r_2}+\frac{(n-3)^2}{n-r_1-r_2}\right). \tag{51}$$

Also, from (50), for any two real numbers r_3 and r_4 with the properties $\rho_1 \geq r_3 \geq \frac{n-\rho_{n-1}}{n-2}$ and $\rho_{n-1} \geq r_4 \geq \frac{n-r_3}{n-2}$, hold

$$Kf^*(G) \geq 2m\left(\frac{1}{r_3}+\frac{1}{r_4}+\frac{(n-3)^2}{n-r_3-r_4}\right). \tag{52}$$

Equality in (51) holds if and only if $r_1 = r_2 = \frac{n}{n-1}$ and $G \cong K_n$, or $r_1 = 2$, $r_2 = 1$ and $G \cong K_{1,n-1}$, or $r_1 = 2$, $r_2 = 1$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n. Similarly, equality in (52) holds if and only if $r_3 = r_4 = \frac{n}{n-1}$ and $G \cong K_n$, or $r_3 = 2$, $r_4 = 1$ and $G \cong K_{1,n-1}$, or $r_3 = 2$, $r_4 = 1$ and $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n.

By substituting parameters r_1 and r_2 in (51), i.e. r_3 and r_4 in (52), by the specific values, a lot of known as well as some new inequalities for $Kf^*(G)$ can be obtained. Thus, for example, for $r_1 = P$, $r_2 = \frac{n-P}{n-2}$ from (51), the inequality (47) is obtained. For $r_1 = P$ and $r_2 = \beta$ from (51) the inequality (48) is obtained. For $r_3 = P$ and $r_4 = \beta$ from (52) the inequality (48) is obtained as well.

In [7] (see also [50]) a lower bound for $Kf^*(G)$ in the class $I(n, m, \prod_{i=1}^n d_i, R_{-1}, t)$ was established with the following inequality

$$Kf^*(G) \geq 2m\left(\frac{1}{P}+(n-2)\left(\frac{P\prod_{i=1}^n d_i}{2mt}\right)^{\frac{1}{n-2}}\right),$$

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

Similarly, in [22] a lower bound for $Kf^*(G)$ in the class $I(n, m, \Delta, \prod_{i=1}^n d_i, t)$ was determined. The authors proved that

$$Kf^*(G) \geq 2m\left(\frac{\Delta}{\Delta+1}+(n-2)\left(\frac{(\Delta+1)\prod_{i=1}^n d_i}{2m\Delta t}\right)^{\frac{1}{n-2}}\right),$$

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

In the sequel we list some results concerning the lower bounds of $Kf^*(G)$ for bipartite graphs.

Since for bipartite graphs hold $\rho_1 = 2$, then according to (39), i.e. for $k = 2$, and (41) we have [86] (see also [7, 64])

$$Kf^*(G) \geq m(2n-3), \tag{53}$$

with equality if and only if $G \cong K_{r,n-r}$, $1 \leq r \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Since G is connected, $m \geq n-1$ is valid. Then, from (53) follows that for any bipartite graph holds [65]:

$$Kf^*(G) \geq Kf^*(K_{1,n-1}) = (n-1)(2n-3).$$

In [7] (see also [50]) the following lower bound in the class $I(n, m, \prod_{i=1}^n d_i, t)$ for bipartite graphs was obtained

$$Kf^*(G) \geq 2m\left(\frac{1}{2} + (n-2)\left(\frac{\prod_{i=1}^n d_i}{mt}\right)^{\frac{1}{n-2}}\right),$$

with equality if and only if $G \cong K_{r,n-r}$, $1 \leq r \leq \left\lfloor \frac{n}{2} \right\rfloor$.

5. Upper bounds for the degree Kirchhoff index

The best upper bound for $Kf(G)$ in the class $I(n)$ is reached when G is a path P_n. From (27) we have that (see [64])

$$Kf^*(G) \leq \frac{2m\Delta}{n} Kf(G) \leq (n-1)^2 Kf(P_n) = \frac{1}{6}(n(n+1)(n-1)^3).$$

Since graph P_n is not a regular one, upper bound for $Kf^*(G)$ in the class $I(n)$, obtained in the above inequality, obviously is not best possible.

In [3] (see also [67]) the upper bound in the class $I(n)$ for $Kf^*(G)$ was determined. It was proved that for $n \leq 48$

$$Kf^*(G) \leq (n-1)^4,$$

and for $n \geq 49$

$$Kf^*(G) \leq \frac{1}{54}\left(n^5 + 50n^3 - 16n^2 + 165n - 52\right).$$

It was not given whether and when these bounds are achieved.

In the sequel we outline some inequalities for $Kf^*(G)$ which depend on eigenvalues ρ_1, ρ_2 and ρ_n. From the application point, these are not convenient. However, by replacing these eigenvalues with appropriate boundaries that depend on other parameters, different upper bounds for $Kf^*(G)$ in various classes can be obtained. An example follows.

In [51] following inequality was proved

$$Kf^*(G) \leq \frac{2m(n-1)^2}{n}\left(1 + \frac{(\rho_1 - \rho_{n-1})^2}{\rho_1 \rho_{n-1}} \alpha(n-1)\right). \tag{54}$$

Equality in (54) holds if and only if $G \cong K_n$.

Also, it was proved that

$$Kf^*(G) \leq 2m \frac{(n-1)(\rho_1 + \rho_{n-1}) - n}{\rho_1 \rho_{n-1}}, \tag{55}$$

with equality if and only if there is k, $1 \leq k \leq n-1$, so that $\rho_1 = \rho_2 = \cdots = \rho_k$ and $\rho_{k+1} = \rho_{k+2} = \cdots = \rho_{n-1}$.

Now, consider some consequences of the (55).

Consider the function

$$f(x) = \frac{(n-1)(x + \rho_{n-1}) - n}{x}.$$

This function is monotone increasing for every $x \neq 0$. Since $\rho_1 \leq 2$, then $f(\rho_1) \leq f(2)$, and according to (55) we have

$$Kf^*(G) \leq m\frac{(n-1)(2+\rho_{n-1})-n}{\rho_{n-1}}.$$

A function

$$g(x) = \frac{(n-1)(2+x)-n}{x}$$

is monotone decreasing for every $x \neq 0$. Let k be an arbitrary real number with the property $\rho_{n-1} \geq k > 0$. Then $g(\rho_{n-1}) \leq g(k)$, and therefore

$$Kf^*(G) \leq \frac{m(n-2+k(n-1))}{k}, \tag{56}$$

with equality if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$, or $k = 1$ and $G \cong K_{r,n-r}$, $1 \leq r \leq \left\lfloor \frac{n}{2} \right\rfloor$. Thus, an upper bound for $Kf^*(G)$ in the class $I(n,m,k)$ is obtained. The inequality (56) is analogous to (31) for upper bound of $Kf(G)$.

In a special case when G is a connected planar graph, according to (56)

$$Kf^*(G) \leq \frac{3(n-2)(n-2+k(n-1))}{k},$$

with equality if and only if $k = \frac{3}{2}$ and $G \cong K_3$, or $k = \frac{4}{3}$ and $G \cong K_4$.

Now, we will give an example how (54) can be used to determine upper bounds $Kf^*(G)$.

In [56] it was proved that

$$(\rho_1 - \rho_{n-1})^2 \leq \frac{2}{n-1}\left(2(n-1)R_{-1} - n\right). \tag{57}$$

Since, for example,

$$\rho_1\rho_{n-1} \geq k\frac{n}{n-1}, \qquad \rho_1\rho_{n-1} \geq k\frac{\Delta+1}{\Delta}, \qquad \rho_1\rho_{n-1} \geq kP,$$

from (54) and (57) following inequalities are obtained

$$\begin{aligned}
Kf^*(G) &\leq \frac{2m(n-1)^2}{n}\left(1 + \frac{2(2(n-1)R_{-1}-n)}{kn}\alpha(n-1)\right), \\
Kf^*(G) &\leq \frac{2m(n-1)^2}{n}\left(1 + \frac{2(1+\Delta)(2(n-1)R_{-1}-n)}{k\Delta(n-1)}\right), \\
Kf^*(G) &\leq \frac{2m(n-1)^2}{n}\left(1 + \frac{2(2(n-1)R_{-1}-n)}{(n-1)kP}\alpha(n-1)\right),
\end{aligned}$$

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

Now, we can obtain some other upper bounds for $Kf^*(G)$ that do not depend on R_{-1} by using upper bounds for R_{-1}, such as $R_{-1} \leq \left\lceil \frac{n}{2} \right\rceil$ (see [43]), or $R_{-1} \leq \frac{n}{2\delta}$ (see [10, 72]).

On other bounds for the Kirchhoffian indices the interested reader can refer to [14, 15, 19, 23, 26–28, 31–33, 40, 70, 73, 74, 80, 82] and the references cited therein.

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Bounds and Power Means for the General Randić and Sum–Connectivity Indices

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Abstract

We review bounds for the general Randić index, $R_\alpha = \sum_{ij\in E}(d_i d_j)^\alpha$, and use the power mean inequality to prove, for example, that $R_\alpha \geq m\lambda^{2\alpha}$ for $\alpha < 0$, where λ is the spectral radius of a graph. This enables us to strengthen various known lower and upper bounds for R_α and to generalise a non-spectral bound due to Bollobás *et al*. We also use the power mean inequality to strengthen bounds for the general sum-connectivity index, $X_\alpha = \sum_{ij\in E}(d_i + d_j)^\alpha$, and generalise a relationship between X_α and R_α.

Contents

1. Introduction

Let G be a graph with no isolated vertices with vertex set $V(G)$ where $n = |V|$, edge set $E(G)$ where $m = |E|$, degrees $\Delta = d_1 \geq ... \geq d_n = \delta \geq 1$ and average degree d. Let A denote the adjacency matrix of G, D denote the diagonal matrix of vertex degrees and $Q = A + D$ denote the signless Laplacian of G. Let λ denote the largest eigenvalue of A and ρ (often called the $Q-$index of G) denote the largest eigenvalue of Q. Let $\omega(G)$ denote the clique number of G and $\chi(G)$ denote the chromatic number of G. Define the general Randić index, R_α, and the general sum-connectivity index, X_α, as usual as:

$$R_\alpha = \sum_{ij \in E} (d_i d_j)^\alpha \text{ and } X_\alpha = \sum_{ij \in E} (d_i + d_j)^\alpha.$$

$R_{-0.5}$ is the best known and most studied topological index used by mathematical chemists. $X_{-0.5}$ and X_α were first defined and studied by Zhou and Trinajstić [24] to [26]. Gutman [10] published a recent survey of degree-based topological indices, in which he compares the performance of numerous indices in chemical applications. He notes, for example, that R_{-1} performs significantly better than $R_{-0.5}$.

Note that $R_\alpha = M_2^\alpha$ (the variable second Zagreb index), and in particular $R_1 = M_2$ and that $X_1 = M_1$ (the first Zagreb index). We will not refer to Zagreb indices again in this paper, and from here onwards M_p will refer to a generalized p-mean rather than a Zagreb index. Note also that $2X_{-1} = H(G)$, which is often called the Harmonic index.

In section 2 we introduce the power mean inequality and prove the Lemma which is the novel feature of this paper. In sections 3 and 4 we use this Lemma to derive bounds for R_α and X_α using eigenvalues and degrees respectively. We then review implications of these general bounds for R_{-1} and $R_{-0.5}$ in sections 5 and 6. We conclude with a discussion of the relationships between R_α and X_α and summarise the power means for these indices.

2. Power mean inequality

It is convenient to introduce the terminology of power means (also known as generalized means). Let $w_1, ..., w_n$ be n positive real numbers and let p be a real number. Define the sum of the p-powers as:

$$S_p(w_1, ..., w_n) = S_p(w_i) = \sum_{i=1}^{n} w_i^p$$

and the generalized p-mean, for $p \neq 0$ as:

$$M_p(w_1, ..., w_n) = M_p(w_i) = \left(\frac{1}{n} S_p(w_1, ..., w_n) \right)^{1/p}.$$

Throughout this paper we will refer to $M_p(w_i)$ as a p-power mean. Note that $p = 1$ corresponds to the arithmetic mean and $p = -1$ corresponds to the harmonic mean. We define M_0 to be the geometric mean as follows:

$$M_0(w_1, ..., w_n) = M_0(w_i) = \left(\prod_{i=1}^{n} w_i \right)^{1/n}.$$

It is important that the above definition is consistent with the following limit process:

$$M_0(w_1, ..., w_n) = \lim_{p \to 0} M_p(w_1, ..., w_n).$$

For all real $p < q$ the well known power mean inequality states that:

$$M_p(w_1, ..., w_n) \leq M_q(w_1, ..., w_n) \tag{1}$$

with equality if and only if $w_1 = ... = w_n$. There are several rigorous proofs of this inequality, including for $p = 0$, for example by Hardy *et al* [12]. Also $M_\infty(w_i) = \max(w_i)$ and $M_{-\infty} = \min(w_i)$.

We use the fact that

$$n \cdot [M_p(w_1, \ldots, w_n)]^p = S_p(w_1, \ldots, w_n) \tag{2}$$

for all $w_1, \ldots, w_n > 0$ and for all p, including the case $p = 0$.

The following lemma is used to prove many of the new bounds in this paper.

Lemma 1. *Let q be arbitrary. Assume that for the generalized q-mean*

$$L \leq M_q(w_1, ..., w_n) \leq U$$

where L and U are lower and upper bounds. Then, we have the following inequalities:

- *for $p \leq q$ and*
  - *for $p \geq 0$*
  $$S_p(w_1, ..., w_n) \leq nU^p$$
  - *for $p < 0$*
  $$S_p(w_1, ..., w_n) \geq nU^p$$
- *for $p \geq q$ and*
  - *for $p \geq 0$*
  $$nL^p \leq S_p(w_1, ..., w_n)$$
  - *for $p < 0$*
  $$nL^p \geq S_p(w_1, ..., w_n)$$

Also $\min(w_i) \leq M_q(w_i) \leq \max(w_i)$, *for all q.*

Proof. The power mean inequality (1) implies that $M_p(w_1, \ldots, w_n) \leq U$ for $p < q$ and $L \leq M_p(w_1, \ldots, w_n)$ for $p > q$.

We apply the function $x \mapsto nx^p$ to go from $M_p(w_1, \ldots, w_n)$ to $S_p(w_1, \ldots, w_n)$ as in (2). We have to reverse the direction of the above inequalities when applying this function for $p < 0$. ■

As an illustration of the use of the power mean inequality, Zhou and Trinajstić [24] proved (their Proposition 2) that:

$$X_{-0.5} \geq \frac{m\sqrt{m}}{\sqrt{X_1}}.$$

Squaring both sides and re-arranging, we see that:

$$M_1(d_i + d_j) = \frac{X_1}{m} \geq \left(\frac{m}{X_{-0.5}}\right)^2 = \left(\frac{X_{-0.5}}{m}\right)^{-2} = M_{-0.5}(d_i + d_j).$$

In other words, Proposition 2 in [24] is a special case of the power mean inequality with $w_i = (d_i + d_j)$ when $p = -0.5$ and $q = 1$.

3. Bounds for R_α and X_α using eigenvalues

Favaron *et al* [9] proved that $R_{-0.5} \geq m/\lambda$ and Runge [22] and Hofmeister [13] proved that $R_{-1} \geq m/\lambda^2$. We can generalise these results as follows.

Theorem 1. *We have the following lower and upper bounds for R_α:*

- *For $\alpha < 0$,*
$$R_\alpha \geq m\lambda^{2\alpha},$$
- *For $0 < \alpha \leq 0.5$,*
$$R_\alpha \leq m\lambda^{2\alpha},$$

Proof. Favaron *et al* [9] proved that:

$$\left(\frac{1}{m}\sum_{ij\in E}\sqrt{d_i.d_j}\right)^2 \leq \lambda^2.$$

In other words, λ^2 is an upper bound on the 0.5-power mean of the m values of $d_i \cdot d_j$ for $(i, j) \in E$. Therefore using Lemma 1 we obtain:

- For $\alpha < 0$,
$$R_\alpha = S_\alpha(d_i \cdot d_j) \geq mU^\alpha = m\lambda^{2\alpha}.$$
- For $0 < \alpha \leq 0.5$,
$$R_\alpha = S_\alpha(d_i \cdot d_j) \leq mU^\alpha = m\lambda^{2\alpha}.$$

There is equality in these bounds for R_α when $d_i \cdot d_j$ is equal for all edges in E. This is the case for regular graphs and semiregular bipartite graphs. ∎

We can derive the following corollaries from Theorem 1 which strengthen known bounds.

Bollobás and Erdos [2] proved that for $-1 \leq \alpha < 0$:

$$R_\alpha \geq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha}.$$

We can generalise and strengthen this bound as follows.

Corollary 1. *For $\alpha < 0$, R_α is bounded from below by*

$$R_\alpha \geq m(2m-n+1)^\alpha.$$

Proof. Hong [14] proved that for graphs with no isolated vertices $\lambda^2 \leq (2m-n+1)$. Therefore using Theorem 1 and that $\alpha < 0$ and that $2m \leq n(n-1)$:

$$R_\alpha \geq m\lambda^{2\alpha} \geq m(2m-n+1)^\alpha \geq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha}.$$

■

Li and Yang [17] proved that for $\alpha \leq -1$:

$$R_\alpha \geq \frac{n(n-1)^{1+2\alpha}}{2}. \tag{3}$$

We can strengthen this bound as follows.

Corollary 2. *For $\alpha \leq -1$, R_α is bounded from below by*

$$R_\alpha \geq \frac{n^{2\alpha+2}(\omega-1)^{2\alpha+1}}{2\omega^{2\alpha+1}}. \tag{4}$$

Proof. Nikiforov [21] proved that $\lambda^2 \leq 2m(\omega-1)/\omega$. Noting that $\alpha \leq -1$ we have:

$$R_\alpha \geq m\lambda^{2\alpha} \geq \frac{m(2m(\omega-1))^\alpha}{\omega^\alpha} = \frac{m^{\alpha+1}2^\alpha(\omega-1)^\alpha}{\omega^\alpha}.$$

Turan's theorem states that $m \leq n^2(\omega-1)/2\omega$. Therefore since $\alpha \leq -1$:

$$R_\alpha \geq \frac{n^{2(\alpha+1)}(\omega-1)^{\alpha+1}2^\alpha(\omega-1)^\alpha}{2^{\alpha+1}\omega^{\alpha+1}\omega^\alpha} = \frac{n^{2\alpha+2}(\omega-1)^{2\alpha+1}}{2\omega^{2\alpha+1}}.$$

We can demonstrate that (4) strengthens bound (3) as follows. We wish to show that for $\alpha \leq -1$:

$$\frac{n^{2\alpha+2}(\omega-1)^{2\alpha+1}}{2\omega^{2\alpha+1}} \geq \frac{n(n-1)^{1+2\alpha}}{2}.$$

This simplifies to:

$$(n(\omega-1))^{1+2\alpha} \geq ((n-1)\omega)^{1+2\alpha}.$$

Take the $(1+2\alpha)$ root of both sides and note that $1+2\alpha \leq -1$. Therefore:

$$n(\omega - 1) \leq (n-1)\omega$$

which is true for all graphs. ■

Lu, Liu and Tian [20] proved that for $-1 \leq \alpha < 0$:

$$R_\alpha \geq 2^{-\alpha} n^\alpha m^{1-\alpha} \lambda^{3\alpha}.$$

We can generalise this bound as follows.

Corollary 3. *For $\alpha < 0$, R_α is bounded from below by*

$$R_\alpha \geq 2^{-\alpha} n^\alpha m^{1-\alpha} \lambda^{3\alpha}.$$

Proof. Since $\alpha < 0$ and $\lambda \geq 2m/n$ we have that:

$$R_\alpha \geq m\lambda^{2\alpha} = m\lambda^{3\alpha}\lambda^{-\alpha} \geq m\lambda^{3\alpha}(2m/n)^{-\alpha} = 2^{-\alpha} n^\alpha m^{1-\alpha} \lambda^{3\alpha}.$$

■

Theorem 2. *We have the following lower and upper bounds for X_α:*

- *For $\alpha < 0$,*

$$X_\alpha \geq m\rho^\alpha,$$

- *For $0 < \alpha \leq 1$,*

$$X_\alpha \leq m\rho^\alpha.$$

Proof. Liu and Liu [19] and Elphick and Liu [8] proved that for any graph:

$$\frac{\sum_{i \in V} d_i^2}{m} = \frac{\sum_{ij \in E} d_i + d_j}{m} \leq \rho.$$

In other words, ρ is an upper bound on the 1-power mean of the m values of $d_i + d_j$ for $(i, j) \in E$. Therefore using Lemma 1 we obtain:

- For $\alpha < 0$,

$$X_\alpha = S_\alpha(d_i + d_j) \geq mU^\alpha = m\rho^\alpha.$$

- For $0 < \alpha \leq 1$,

$$X_\alpha = S_\alpha(d_i + d_j) \leq mU^\alpha = m\rho^\alpha.$$

There is equality in these bounds for X_α when $d_i + d_j$ is constant for all edges in E. This is the case, for example, for regular graphs and semiregular bipartite graphs. ■

Zhou and Trinajstić [26] proved (their Proposition 4) that for $\alpha < 0$, $X_\alpha \geq mn^\alpha$ for triangle-free graphs. We generalise this result for any clique number in the following corollary.

Corollary 4. *For $\alpha < 0$:*

$$X_\alpha \geq m \left(\frac{2n(\omega - 1)}{\omega} \right)^\alpha.$$

In particular, $H(G) = 2X_{-1} \geq \omega m/(\omega - 1)n$.

Proof. Abreu and Nikiforov [1] proved that $\rho \leq 2n(\omega - 1)/\omega$. Therefore for $\alpha < 0$:

$$X_\alpha \geq m\rho^\alpha \geq m \left(\frac{2n(\omega - 1)}{\omega} \right)^\alpha = mn^\alpha \text{ when } \omega(G) = 2.$$

■

4. Bounds for R_α and X_α using degrees

Ilić and Stevanović [15] proved that $R_\alpha \geq md^{2\alpha}$ for $\alpha \geq 0$. We reproduce and extend these inequalities in the following Theorem, using Lemma 1.

Theorem 3. *We have the following lower bound on R_α:*

- *For $\alpha \geq 0$,*

$$R_\alpha \geq md^{2\alpha}.$$

Proof. Ilić and Stevanović [15] proved that:

$$\frac{R_1}{m} = \frac{\sum_{ij \in E} d_i \cdot d_j}{m} \geq \left(\prod_{ij \in E} d_i \cdot d_j \right)^{1/m} = M_0(d_i \cdot d_j) \geq d^2.$$

Therefore d^2 is a lower bound for the 0-power mean of R_α. Hence using Lemma 1, $R_\alpha \geq md^{2\alpha}$ for $\alpha \geq 0$. ■

Bollobás and Erdös [2] proved that for $0 < \alpha \leq 1$:

$$R_\alpha \leq m \left(\frac{\sqrt{8m+1} - 1}{2} \right)^{2\alpha}.$$

We strengthen this bound in the following theorem.

Theorem 4. *For $0 < \alpha \leq 1$, R_α is bounded from above by*

$$R_\alpha \leq m(2m - n + 1)^\alpha.$$

Proof. Das and Gutman [7] proved the following bound:

$$R_1 \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)m \left(\frac{2m}{n-1} + n - 2 \right).$$

If $\delta = 1$ then clearly $R_1 \leq m(2m - n + 1)$. If $\delta > 1$ then it is straightforward to show that $R_1 \leq m(2m - n + 1)$. Therefore $R_1/m \leq 2m - n + 1$, so $(2m - n + 1)$ is an upper bound for the $1-$power mean of R_α.

Hence using Lemma 1, $R_\alpha \leq m(2m - n + 1)^\alpha$ for $0 < \alpha \leq 1$. ■

Zhou and Trinajstić [25] proved that $X_{-0.5} \leq \sqrt{nm}/2$ and also proved [26] that for $\alpha > 1$, $X_\alpha \geq 4^\alpha n^{-\alpha} m^{1+\alpha}$. We can reproduce and generalise these results as follows.

Theorem 5. *We have the following lower and upper bounds on X_α:*

- *For $\alpha \geq 1$,*
$$X_\alpha \geq m(2d)^\alpha.$$

- *For $-1 \leq \alpha < 0$,*
$$X_\alpha \leq m(2d)^\alpha.$$

Proof. Using the Cauchy-Schwartz inequality we have that $\sum_{i\in V} d_i^2 \geq 4m^2/n$. Therefore:

$$\frac{X_1}{m} = \frac{\sum_{ij\in E} d_i + d_j}{m} = \frac{\sum_{i\in V} d_i^2}{m} \geq \frac{4m^2}{mn} = 2d.$$

It is well known that $H(G) \leq n/2$ and consequently $X_{-1} = H(G)/2 \leq n/4$. Therefore:

$$\left(\frac{X_{-1}}{m}\right)^{-1} = \frac{m}{X_{-1}} \geq \frac{4m}{n} = 2d.$$

Therefore $2d$ is a lower bound for the 1-power mean of X_α and a lower bound for the -1-power mean of X_α. Hence using Lemma 1, $X_\alpha \geq m(2d)^\alpha$ for $\alpha \geq 1$ and $X_\alpha \leq m(2d)^\alpha$ for $-1 \leq \alpha < 0$. ■

Zhou and Trinajstić [24] proved (their Proposition 7) that $X_{-0.5} \leq n\sqrt{\Delta}/2\sqrt{2}$. We generalise and strengthen this result in the following corollary.

Corollary 5. *For $-1 \leq \alpha < 0$, $X_\alpha \leq n2^{\alpha-1}d^{\alpha+1}$.*

Proof. For $-1 \leq \alpha < 0$:

$$X_\alpha \leq m(2d)^\alpha = \frac{nd}{2}(2d)^\alpha = n2^{\alpha-1}d^{\alpha+1} \leq n2^{\alpha-1}\Delta^{\alpha+1}.$$

■

Theorem 6.

$$\textit{For } \alpha < 0, X_\alpha \geq m\left(\frac{m(\Delta+\delta)^2}{n\Delta\delta}\right)^\alpha \textit{ and for } 0 < \alpha \leq 1, X_\alpha \leq m\left(\frac{m(\Delta+\delta)^2}{n\Delta\delta}\right)^\alpha.$$

Proof. Ilić, Ilić and Liu [16] proved that:

$$\frac{X_1}{m} \leq \frac{m(\Delta+\delta)^2}{n\Delta\delta}.$$

Therefore $m(\Delta+\delta)^2/n\Delta\delta$ is an upper bound for the $1-$power mean of X_α. Using Lemma 1 therefore completes the proof. ■

5. Implications for R_{-1}

Cavers *et al* [4] reviewed upper and lower bounds for R_{-1} in the context of bounds for Randić energy. In particular, Shi [23] proved that:

$$R_{-1} \geq \frac{n}{2\Delta} \tag{5}$$

with equality if and only if G is regular and Li and Yang [17] proved that:

$$R_{-1} \geq \frac{n}{2(n-1)}, \tag{6}$$

with equality if and only if G is a complete graph. Liu and Gutman [18] proved that for graphs with no isolated vertex:

$$R_{-1} \geq \frac{n-1}{m} \tag{7}$$

with equality only for Star graphs. Clark and Moon [5] proved that for trees, $R_{-1} \geq 1$.

Below, in Corollary 6, we prove that:

$$R_{-1} \geq \frac{\omega}{2(\omega-1)} \text{ or equivalently } \frac{2R_{-1}}{2R_{-1}-1} \leq \omega(G), \tag{8}$$

with equality for semiregular bipartite and regular complete ω-partite graphs. (A semiregular bipartite graph is a bipartite graph for which all vertices on the same side of the bipartition have the same degree.)

Bound (8) clearly strengthens bound (6). It also demonstrates that $R_{-1} \geq 1$ not only for trees but for all triangle-free graphs. Bound (8) never outperforms bound (5) for regular graphs but it does outperform bound (5) for some irregular graphs, such as irregular complete bipartite graphs.

Corollary 6. *R_{-1} is bounded from below by*

$$R_{-1} \geq \frac{\omega}{2(\omega-1)}.$$

This is exact for semiregular bipartite and regular complete ω-partite graphs.

Proof. Letting $\alpha = -1$ we have $R_{-1} \geq m/\lambda^2$. Nikiforov [21] proved that:

$$\lambda^2 \leq \frac{2m(\omega-1)}{\omega}.$$

Therefore:

$$R_{-1} \geq \frac{m}{\lambda^2} \geq \frac{m\omega}{2m(\omega-1)} = \frac{\omega}{2(\omega-1)}.$$

■

Corollary 7. *For chemical graphs, other than K_5, $R_{-1} \geq 2/3$.*

Proof. For a chemical graph $\Delta \leq 4$. It follows from Brooks' famous theorem [3] that, excluding K_5, $\omega(G) \leq \Delta \leq 4$. Therefore:

$$R_{-1} \geq \frac{\omega}{2(\omega-1)} \geq \frac{4}{6} = \frac{2}{3}.$$

This is exact for K_4. ■

6. Implications for $R_{-0.5}$

$R_{-0.5}$ is the original topological index devised by Milan Randić in 1975 and has consequently been investigated more than any other general Randić index.

Bollobás and Erdös [2] proved that for graphs with no isolated vertex:

$$\frac{n}{2} \geq R_{-0.5} \geq \sqrt{n-1} \tag{9}$$

with equality in the lower bound only for Star graphs. In Corollary 9 we prove that:

$$R_{-0.5} \geq \frac{m}{\sqrt{2m-n+1}}. \tag{10}$$

Since connected graphs have $m \geq n-1$, it is straightforward to show that bound (10) is never worse than the well known bound (9) for connected graphs.

Hansen and Vukicević [11] proved that $\chi(G) \leq 2R_{-0.5}$. In Corollary 8 we provide a simple alternative proof of this result using Theorem 1.

Corollary 8. *Hansen and Vukicević [11] proved that $\chi(G) \leq 2R_{-0.5}$. We can use Theorem 1 to strengthen their bound as follows.*

$$2R_{-0.5} \geq \lambda + 1 \geq \chi(G).$$

Proof. As noted above $\lambda^2 \leq 2m(\omega-1)/\omega$ and it is well known that $(\omega-1)\omega \leq (\chi-1)\chi \leq 2m$ and that $\chi(G) \leq 1+\lambda$. Therefore $\lambda \leq 2m/\omega$, so:

$$\lambda(\lambda+1) \leq \frac{2m(\omega-1)}{\omega} + \frac{2m}{\omega} = 2m.$$

Hence:

$$2R_{-0.5} \geq \frac{2m}{\lambda} \geq \lambda + 1 \geq \chi(G).$$

■

Corollary 9. *Hong [14] proved that for graphs with no isolated vertices, $\lambda^2 \leq (2m-n+1)$. Therefore with $\alpha = -0.5$:*

$$R_{-0.5} \geq \frac{m}{\lambda} \geq \frac{m}{\sqrt{2m-n+1}} \geq \sqrt{n-1} \textit{ for connected graphs.}$$

Proof. Let $m = n - 1 + a$ where $a \geq 0$ because $m \geq n - 1$ for connected graphs. We are therefore seeking to prove that:

$$m^2 = (n - 1 + a)^2 \geq (n - 1)(2n - 2 + 2a - n + 1),$$

which simplifies to $a^2 \geq 0$ ■

7. Relationships between R_α and X_α

Zhou and Trinajstic [25] proved that $X_{-0.5} \leq \sqrt{mR_{-0.5}/2}$, with equality if and only if G is regular. We can generalise this relationship as follows.

Theorem 7. *For $\alpha < 0$, $X_\alpha \leq 2^\alpha \sqrt{mR_\alpha}$, with equality if and only if G is regular.*

Proof. For all edges in G:

$$0 \leq (d_i - d_j)^2 = d_i^2 + d_j^2 - 2d_i d_j = (d_i + d_j)^2 - 4d_i d_j.$$

Therefore, raising to the power of α with $\alpha < 0$ and summing over edges:

$$\sum_{ij \in E} (4d_i d_j)^\alpha \geq \sum_{ij \in E} (d_i + d_j)^{2\alpha}.$$

Then using Cauchy-Schwartz:

$$X_\alpha = \sum_{ij \in E} (d_i + d_j)^\alpha \leq \sqrt{m \sum_{ij \in E} (d_i + d_j)^{2\alpha}} \leq \sqrt{m \sum_{ij \in E} (4d_i d_j)^\alpha} = 2^\alpha \sqrt{mR_\alpha}.$$

■

8. Summary

The following tables summarise the power means we have used in this paper.

Table 1. Power means for R_α

Power mean	Lower bound	Upper bound
0.5		λ^2
0	d^2	
1		$2m - n + 1$
$\pm\infty$	$\min(d_i \cdot d_j)$	$\max(d_i \cdot d_j)$

Table 2. Power means for X_α

Power mean	Lower bound	Upper bound
1		ρ
1	$\sum d_i^2/m$	$\sum d_i^2/m$
1	$2d$	$m(\Delta+\delta)^2/n\Delta\delta$
-1	$2d$	
$\pm\infty$	$\min{(d_i+d_j)}$	$\max{(d_i+d_j)}$

There are, we expect, further useful power means for R_α and X_α to be found.

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The Reciprocal Sum–Degree Distance and Reciprocal Product–Degree Distance

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Contents

1. Introduction and Notation

Unless otherwise specified, all graphs considered in this chapter are simple, i.e., they are finite, undirected and without multiple edges or loops. Let $G = (V(G), E(G))$ denote a graph with vertex set V and edge set E. The order $n = |V(G)|$ of G is the number of its vertices, while the size $m = |E(G)|$ of G is the number of its edges.

The *degree* (valency) of a vertex $v \in V(G)$ is the number $\delta_G(v)$ (or $\delta(v)$ when no confusion can arise) of edges incident to v, and we use $\Delta(G)$ and $\underline{\Delta}(G)$ to denote the maximum and minimum degree in a graph G. The *open neighborhood* $N(v) = N_G(v)$ of a vertex in G is the set of vertices adjacent to v. Note that $\delta(v) = |N(v)|$. The *closed neighborhood* of a vertex v is defined by $N[v] = N_G[v] = N_G(v) \cup \{v\}$.

The *distance* $d(u, v) = d_G(u, v)$ between two vertices u and v in a connected graph G is the number of edges in a shortest path joining u and v. The *eccentricity* $e(v)$ of a vertex v of a connected graph G is the maximum distance from it to any other other vertex. The *diameter* $D = D(G)$ of G is the maximum eccentricity in G, or equivalently, $D = D(G)$ is the maximum distance between two vertices of G. The minimum eccentricity in G is said to be the *radius* of G and denoted by $r = r(G)$. For standard graph-theoretic notation and terminology the reader is referred to [7, 9].

A single number that can be used to characterize some property of the graph of a molecule is called a *topological index*, or *graph invariant*. Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [10]. For quite some time there has been rising interest in the field of computational chemical in topological indices. The interest in topological indices is mainly related to their use in nonempirical quantitative structure-property relationship (QSPR) and quantitative structure-activity relationships (QSAR). One of the oldest and well-studied distance-based topological index is the Wiener number $W(G)$, also termed as *Wiener index* in chemical or mathematical chemical literature, which is defined as the sum of distances over all unordered vertex pairs in G, namely,

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v). \tag{1}$$

This index was first time introduced by Wiener more than 60 years ago [59]. Initially, the Wiener index was considered as a molecular–structure descriptor used in chemical applications, but soon it attracted the interest of "pure" mathematicians [21, 22]; for details and additional references see the reviews [11, 60] and the recent papers [42, 43, 61].

To overcome the inconsistency caused by the contributions of distant pairs of vertices when compared with the contributions from close pairs to the topological indices, the sum of reciprocal values of distances between pairs of different vertices was introduced in [34, 52]. For a connected graph G, the *Harary index* is defined as

$$H = H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u, v)}. \tag{2}$$

Recently, Das et. al. [17] considered the generalized version of Harary index, namely the t-*Harary index*, which is defined as

$$H_t = H_t(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u, v) + t}, \quad t \geq 0. \tag{3}$$

For more results on Harary index, one may be referred to [18, 45, 46, 52, 64].

In 1994, Dobrynin and Kochetova [12] and Gutman [26] independently proposed a vertex-degree-weighted version of Wiener index called *sum-degree distance* or *Schultz molecular topological index*, which is defined for a connected graph G as

$$DD_+ = DD_+(G) = \sum_{\{u,v\}\subseteq V(G)} (\delta_G(u) + \delta_G(v))d_G(u,v). \tag{4}$$

This graph invariant may be regarded as weighted degree-sum version of Wiener index. One may be referred to [5, 13, 14, 35, 37, 57] and the references cited therein.

The multiplicative variant of the degree distance is put forward in [26] and called there the Schultz index of the second, but for which the name Gutman index has also sometimes been used [58] (we call it *product–degree distance*). It is defined as

$$DD_\times = DD_\times(G) = \sum_{\{u,v\}\subseteq V(G)} (\delta_G(u)\delta_G(v))d_G(u,v). \tag{5}$$

This graph invariant can be viewed as weighted degree-product version of Wiener index. The interested readers may consult [1, 24, 39, 50, 51, 62] and the references quoted therein for more details.

Noting that the sum-degree distance is a degree-weight version of the Wiener index and bearing in mind that the relation between Wiener index and Harary index, Hua et al. [30] and Alizadeh et al. [2] introduced the *reciprocal sum-degree distance* or *additively weighted Harary index* of G, which is defined is

$$RDD_+ = RDD_+(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\delta_G(u) + \delta_G(v)}{d_G(u,v)}. \tag{6}$$

Some basic mathematical properties of this index were established and its behavior under several standard graph products were investigated there. Let $\widehat{D}_G(u) = \sum_{v\in V(G)\setminus\{u\}} \frac{1}{d_G(u,v)}$, then we can rewrite Eq.(6) as

$$RDD_+(G) = \sum_{u\in V(G)} \delta_G(u)\widehat{D}_G(u),$$

which is frequently used throughout the chapter. For the research development of this graph invariant, one may be referred to [47, 53].

It is known that the intuitive idea of pairs of close atoms contributing more than the distant ones has been difficult to capture in topological indices. A possibly useful approach could be to replace the additive weighting of pairs by the multiplicative one, thus giving rise to the concept of *reciprocal product-degree distance* [2, 27]:

$$RDD_\times = RDD_\times(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\delta_G(u)\delta_G(v)}{d_G(u,v)}. \tag{7}$$

Recently, Li et al. [48] introduced a new graph invariant named the *reformulated reciprocal sum-degree distance*, which is defined as

$$RDD_+^t = RDD_+^t(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\delta_G(u) + \delta_G(v)}{d_G(u,v)+t}, t \geq 0. \tag{8}$$

W	DD_+	$DD_\times$
H	RDD_+	$RDD_\times$
H_t	RDD_+^t	$RDD_\times^t$?

In view of Eq.(3), RDD_+^t is just the additively weighted t-Harary index; while in view of Eq.(6), it is also the generalized version of the reciprocal sum-degree distance of a connected graph. In this paper, several mathematical properties of this novel graph index were studied. Let $\widehat{D}_t(G;u) = \sum_{v\in V(G)\setminus\{u\}} \frac{1}{d_G(u,v)+t}$, then we can rewrite Eq.(8) as

$$RDD_+^t(G) = \sum_{u\in V(G)} \delta_G(u)\widehat{D}_t(G;u).$$

The graph invariants, defined via Eqs. (1)–(8), can be arranged as in the Table above. From this Table it is immediately seen that one more such invariants is missing. This is the *reformulated reciprocal product–degree distance*, defined as

$$RDD_\times^t = RDD_\times^t(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\delta_G(u)\delta_G(v)}{d_G(u,v)+t}, t \geq 0. \tag{9}$$

In view of Eq.(3), $RDD_\times^t$ is just the multiplicatively weighted t-Harary index; while in view of Eq.(7), it is also the generalized version of the reciprocal product-degree distance of a connected graph.

2. The reciprocal sum-degree distance

This section is divided into several subsections, each dealing with a class of graphs.

2.1 Graphs with maximum and minimum RDD_+

Hua et al. [30] seems to be the first to prove that the maximum and minimum RDD_+ of a connected graph of order n goes to infinity with n. In fact, they proved in 2012 that for a graph G with non-isolated vertices the complete graph K_n and the path P_n respectively attains its maximum and minimum RDD_+. A little later Alizadeh et al. also showed the minimum value for this graph invariant [2]. The proof of this result is based on following two lemmas.

Lemma 2.1. *Let G be a connected graph with at least three vertices.*
(**a**) *If G is not isomorphic to K_n, then $RDD_+(G) < RDD_+(G+e)$, where $e \in E(\overline{G})$.*
(**b**) *If G has an edge e' not being a cut edge, then $RDD_+(G-e') < RDD_+(G)$.*

Proof. We first prove (a) holds. Suppose that G is not a complete graph. Then there exists a pair of vertices u and v in G such that $uv \in E(\overline{G})$. It is obvious that $d_G(x,y) \geq d_{G-uv}(x,y)$ for any pair of vertices x and y in G. Also we have $d_G(u,v) > 1 = d_{G+uv}(u,v)$. In addition, $\delta_{G+uv}(w) \geq \delta_G(w)$ for any w in G. It follows from Eq.(6) that $RDD_+(G) < RDD_+(G+e)$, as desired.

Now, we consider (b). Since the edge e' is not a cut edge, we have $G - e'$ is connected and not isomorphic to the complete graph of the same order. Thus, by (a), we have $RDD_{+}(G - e') < RDD_{+}((G - e') + e') = RDD_{+}(G)$, as claimed. ■

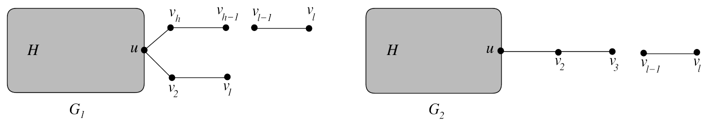

Figure 1. α_1-transformation $G_1 \Rightarrow G_2$.

Transformation 2.2. *Suppose that H is a nontrivial connected graph and u is a vertex in H. Let G_1 (resp. G_2) be a graph obtained by identifying the vertex u of H with a non-pendent vertex (resp. a pendent vertex) of the path P_l ($l \geq 3$). We call $G_1 \Rightarrow G_2$ the α_1-*transformation*, see Fig. 1.*

Lemma 2.3. *([30]) Let G_1 and G_2 be two graphs illustrated in Transformation 2.2. Then $RDD_{+}(G_2) < RDD_{+}(G_1)$.*

Proof. For each vertex x in $V(H) \setminus \{u\}$, we clearly have $\delta_{G_1}(x) = \delta_H(x) = \delta_{G_2}(x)$. Also, $\delta_{G_1}(u) = \delta_H(u) + 2$ and $\delta_{G_2}(u) = \delta_H(u) + 1$.

Without loss of generality, we label all vertices of path P_l ($l \geq 3$) as $v_1, v_2, \cdots, v_l$ and assume in G_1 that $u = v_i$ for some $2 \leq i \leq l-1$. It follows that $u = v_1$ or v_l in G_2.

For $1 \leq j \leq l$, we let $d_{ij} = d_{P_l}(v_i, v_j)$. Rearranging these d_{ij}'s and relabeling them as d'_{ij}'s such that $d'_{i1} \leq d'_{i2} \leq \cdots \leq d'_{il}$. Then $d'_{ij} \leq j-1$ for $j = 1, 2, \cdots, l$. In particular, $d'_{i1} = 0$. We complete the proof by considering two cases.

• For each vertex x in $V(H) \setminus \{u\}$, we have

$$\begin{aligned}
\widehat{D}_{G_1}(x) = & \sum_{y \in V(H)\setminus\{u,x\}} \frac{1}{d_H(x,y)} + \sum_{y \in V(P_l)} \frac{1}{d_G(x,y)} \\
= & \sum_{y \in V(H)\setminus\{u,x\}} \frac{1}{d_H(x,y)} + \sum_{1 \leq j \leq l} \frac{1}{d_H(x,u) + d_{P_l}(v_i, v_j)} \\
= & \sum_{y \in V(H)\setminus\{u,x\}} \frac{1}{d_H(x,y)} + \frac{1}{d_H(x,u)} + \sum_{\substack{1 \leq j \leq l \\ j \neq i}} \frac{1}{d_H(x,u) + d_{P_l}(v_i, v_j)} \\
= & \sum_{y \in V(H)\setminus\{u,x\}} \frac{1}{d_H(x,y)} + \frac{1}{d_H(x,u)} + \sum_{2 \leq j \leq l} \frac{1}{d_H(x,u) + d'_{ij}} \\
\geq & \sum_{y \in V(H)\setminus\{u,x\}} \frac{1}{d_H(x,y)} + \frac{1}{d_H(x,u)} + \sum_{2 \leq j \leq l} \frac{1}{d_H(x,u) + j - 1} \\
= & \widehat{D}_{G_2}(x).
\end{aligned}$$

Recall that $\delta_{G_1}(x) = \delta_H(x) = \delta_{G_2}(x)$ holds for all vertex x in $V(H) \setminus \{u\}$. Hence,

$$\sum_{x \in V(H)\setminus\{u\}} \delta_{G_1}(x)\widehat{D}_{G_1}(x) \geq \sum_{x \in V(H)\setminus\{u\}} \delta_{G_2}(x)\widehat{D}_{G_2}(x). \tag{10}$$

• For each vertex v_j in P_l, we have

$$\widehat{D}_{G_1}(v_j) = \widehat{D}_{P_l}(v_j) + \sum_{x \in V(H)\backslash\{u\}} \frac{1}{d_{P_l}(v_i, v_j) + d_H(u, x)}. \tag{11}$$

and

$$\widehat{D}_{G_2}(v_j) = \widehat{D}_{P_l}(v_j) + \sum_{x \in V(H)\backslash\{u\}} \frac{1}{d_{P_l}(v_1, v_j) + d_H(u, x)}. \tag{12}$$

For convenience, let δ'_{ij} be the degree of vertex corresponding to d'_{ij} for each $1 \leq j \leq l$. Then we have, $\delta'_{i1} = \delta_H(u) + 2$ and $\delta'_{il} = 1$. It is obvious that there must exist a positive integer j_0 in the interval $[2, l-1]$ such that $\delta'_{ij_0} = 1$.

For $1 \leq j \leq l$, we let $d_{1j} = d_{P_l}(v_1, v_j)$. It immediately follows that $d_{11} \leq d_{12} \leq \cdots \leq d_{1l}$. Clearly, $\delta_{G_2}(v_1) = \delta_H(u) + 1$ and $\delta_{G_2}(v_l) = 1$. For the above chosen j_0, we have $\delta_{G_2}(v_{j_0}) = 2$.

For $2 \leq j \leq l-1$ and $j \neq j_0$, we have $\delta'_{ij} = \delta_{G_2}(v_j) = 2$.

From the definition above it follows that $d'_{ij} \leq d_{1j}$ for any $j = 1, 2, \cdots, l$.

For simplicity, we let $f_x(j) = d'_{ij} + d_H(u, x)$ and $g_x(j) = d_{1j} + d_H(u, x)$ for each given vertex x in $V(H) \setminus \{u\}$. It follows that

$$f_x(j) \leq g_x(j), \tag{13}$$

for each x and $j = 1, 2, \cdots, l$.

Note that for each $2 \leq j \leq l$ and $j \neq i$, $\delta_{G_1}(v_j) = \delta_{G_2}(v_j) = \delta_{P_l}(v_j)$. By means of Eqs.(11) and (12), we have

$$\begin{aligned}
\sum_{j=1}^{l} \delta_{G_1}(v_j)\widehat{D}_{G_1}(v_j) =& \sum_{j=1}^{l} \delta_{G_1}(v_j)\widehat{D}_{P_l}(v_j) + \sum_{j=1}^{l} \delta'_{ij} \sum_{x \in V(H)\backslash\{u\}} \frac{1}{f_x(j)} \\
=& (\delta_H(u) + 2)\widehat{D}_{P_l}(v_i) + 1 \cdot \widehat{D}_{P_l}(v_1) + \sum_{\substack{j=2 \\ j \neq i}} \delta_{P_l}(v_j)\widehat{D}_{P_l}(v_j) \\
&+ \sum_{\substack{j=2 \\ j \neq j_0}} \delta'_{ij} \sum_{x \in V(H)\backslash\{u\}} \frac{1}{f_x(j)} + \delta'_{ij_0} \sum_{x \in V(H)\backslash\{u\}} \frac{1}{f_x(j_0)} \\
&+ \delta'_{i1} \sum_{x \in V(H)\backslash\{u\}} \frac{1}{d_H(u, x)}
\end{aligned}$$

and

$$\begin{aligned}\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_{G_2}(v_j) =&\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_{P_l}(v_j)+\sum_{j=1}^{l}\delta_{G_2}(v_j)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j)}\\ =&(\delta_H(u)+1)\widehat{D}_{P_l}(v_1)+2\cdot\widehat{D}_{P_l}(v_i)+\sum_{\substack{j=2\\ j\neq i}}\delta_{P_l}(v_j)\widehat{D}_{P_l}(v_j)\\ &+\sum_{\substack{j=2\\ j\neq j_0}}\delta_{G_2}(v_j)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j)}+\delta_{G_2}(v_{j_0})\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j_0)}\\ &+\delta_{G_2}(v_1)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_H(u,x)}.\end{aligned}$$

By above analysis and Eq.(13), we have

$$\sum_{\substack{j=2\\ j\neq j_0}}\delta'_{ij}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j)}\geq\sum_{\substack{j=2\\ j\neq j_0}}\delta_{G_2}(v_j)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j)}. \tag{14}$$

By means of Eqs.(12) and (13), we obtain

$$\begin{aligned}&\sum_{j=1}^{l}\delta_{G_1}(v_j)\widehat{D}_{G_1}(v_j)-\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_{G_2}(v_j)\\ &\geq\delta_H(u)(\widehat{D}_{P_l}(v_i)-\widehat{D}_{P_l}(v_1))+\delta'_{ij_0}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j_0)}\\ &-\delta_{G_2}(v_{j_0})\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j_0)}\\ &+(\delta_H(u)+2)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_H(u,x)}-(\delta_H(u)+1)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_H(u,x)}\\ &=\delta_H(u)(\widehat{D}_{P_l}(v_i)-\widehat{D}_{P_l}(v_1))+\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j_0)}\\ &-2\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j_0)}+\sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_H(u,x)}\\ &\geq\delta_H(u)(\widehat{D}_{P_l}(v_i)-\widehat{D}_{P_l}(v_1)).\end{aligned}$$

It is sufficient to prove that $\widehat{D}_{P_l}(v_i)>\widehat{D}_{P_l}(v_1)$ for each given $2\leq i\leq l-1$. Clearly, $\widehat{D}_{P_l}(v_1)=\sum_{k=1}^{l-1}\frac{1}{k}$. Let d'_{ij} be defined as previous. Since $0=d'_{i1}\leq d'_{i2}\leq\cdots\leq d'_{il}$ and $d'_{ij}\leq j-1$, we have $\widehat{D}_{P_l}(v_i)=\sum_{j=2}^{l}\frac{1}{d'_{ij}}\geq\sum_{j=2}^{l}\frac{1}{j-1}=\widehat{D}_{P_l}(v_1)$ for each $2\leq i\leq l-1$. Also, we have $\frac{1}{d'_{i3}}=1>\frac{1}{2}$. Hence, $\widehat{D}_{P_l}(v_i)>\widehat{D}_{P_l}(v_1)$ for each given $2\leq i\leq l-1$.

By discussion above, we have arrived at

$$\sum_{j=1}^{l}\delta_{G_1}(v_j)\widehat{D}_{G_1}(v_j)>\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_{G_2}(v_j). \tag{15}$$

Form the combination of Eqs.(10) and (15) it follows readily that $RDD_{+}(G_2) < RDD_{+}(G_1)$. ■

By means of Lemmas 2.1 and 2.3, we are able to characterize connected graphs with the maximum and minimum RDD_{+}, respectively. More precisely, we have

Theorem 2.4. *([30]) Among all nontrivial connected graphs of order n, the graphs with maximum and minimum RDD_{+} are K_n and P_n, respectively.*

Proof. The case of $n = 2$ is trivial. So in what follows we suppose that $n \geq 3$.

We first prove that K_n is maximal with respect to RDD_{+}. If G is not a complete graph, then we can repeatedly add edges into G until we obtain $G \cong K_n$. It follows from Lemma 2.1 that $RDD_{+}(G) \leq RDD_{+}(K_n)$, with equality if and only if $G \cong K_n$.

Now, let us show that P_n is minimal with respect to RDD_{+}. Suppose first that G is not isomorphic to a tree. Let $T(G)$ be a spanning tree of G. It follows from Lemma 2.1 that $RDD_{+}(T(G)) < RDD_{+}(G)$. It is sufficient to consider the case of G is a tree. If G is not isomorphic to P_n, then we can repeatedly employ α-transformation on G and we must obtain the path P_n in the end. By Lemma 2.3, each step of α_1-transformation will result in a new tree with a strictly smaller RDD_{+} than that of the previous one. Hence, $RDD_{+}(G) > RDD_{+}(P_n)$, as desired. ■

Following the approach of Ref. [28], Alizadeh et al. gave another proof of the above theorem, we encourage the interested reader to consult [2] for details.

The n-th *harmonic number* H_n is defined as the n-th partial sum of the harmonic series, $H_n = \sum_{k=1}^{n} \frac{1}{k}$. By using the asymptotic formula $H_n \approx \ln n + \gamma$ for harmonic numbers, one can obtain the asymptotic behavior of the type $(n+1)\ln n$ for the lower bound of RDD_{+}.

In [2], the authors gave an upper bound on RDD_{+} among trees with the same number of vertices and then characterize the corresponding extremal graph.

Theorem 2.5. *([2]) Among all nontrivial trees of order n, the graph with maximum RDD_{+} is the star S_n.*

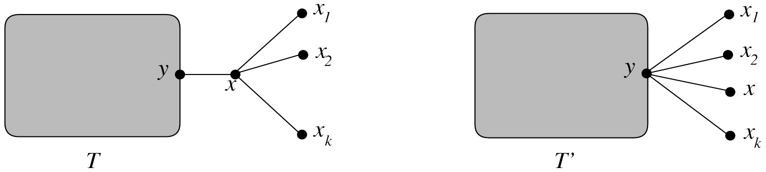

Figure 2. α_2-transformation $T \Rightarrow T'$.

Proof. Let x be a vertex of T with neighbors $x_1, x_2, \cdots, x_k, y$ such that $\delta(x_i) = 1$ for each $i = 1, 2, \cdots, k$. Let T' be the tree obtained from T by α_2-*transformation* shown in Fig. 2.

For simplicity, suppose $S_0 = \{y, x, x_1, x_2, \cdots, x_k\}$ and $S_1 = V(T) \setminus S_0$. The vertices of S_0 are not affected by α_2-*transformation*. Hence, we have

$$\begin{aligned}
RDD_+(T') - RDD_+(T) = & \sum_{v_i, v_j \in S_0} \left(\frac{\delta(v_i) + \delta(v_j)}{d_{T'}(v_i, v_j)} - \frac{\delta(v_i) + \delta(v_j)}{d_T(v_i, v_j)} \right) \\
& + \sum_{v_i \in S_0, v_j \in S_1} \left(\frac{\delta(v_i) + \delta(v_j)}{d_{T'}(v_i, v_j)} - \frac{\delta(v_i) + \delta(v_j)}{d_T(v_i, v_j)} \right) \\
& = k \left[\sum_{v_j \in S_1} \left(\frac{1}{d(y, v_j)} - \frac{1}{d(x, v_j)} \right) + \frac{1 + \delta(v_j)}{d(y, v_j) + 1} - \frac{1 + \delta(v_j)}{d(y, v_j) + 2} \right] \\
& + k \left(\frac{\delta(y) + 1}{2} + k - \delta(x) \right).
\end{aligned}$$

Since, for each vertex v_j of S_1, $d(y, v_j) < d(x, v_j)$, $RDD_+(T') - RDD_+(T) \geq k\left(\frac{\delta(y)-1}{2}\right)$, and the equality holds if and only if $\delta(y) = 1$. Applying α_2-transformation for any pair of vertices such as x and y for a finite number of times, we must get the S_n in the end. This completes the proof. ■

2.2 Graphs with given property

Recently, finding bounds for the topological indices of graphs, as well as the related problem of finding the graphs with maximum and minimum value of the respective graph invariant, attracted the attention of many researchers and many results were obtained. Indeed, over a significant class of graph, the bounds for the reciprocal sum-degree distance were obtained. In this section, we consider this problem which will be divided into several classes in the sequel.

2.2.1 Graphs with given independent and matching number

The *independent sets* is an important notion in graph theory. The problem of finding independent sets started more than two centuries ago with the eight queens puzzle, i.e., the problem of placing eight chess queens on an 8×8 chessboard such that none of them are able to capture any other using the standard chess queen's moves. However, the formal definition of independent sets was posed during the fifties. Since then, several variants of independent sets were defined and a graph invariant was associated to each variant.

Let G and H be two vertex-disjoint graphs. The *join* of graphs G and H, denoted by $G \vee H$, is defined as a graph whose vertex set is $V(G) \cup V(H)$ and edge set is $E(G) \cup E(H) \cup \{xy | x \in V(G), y \in V(H)\}$.

A vertex subset S of a graph G is called an *independent set* of G, if the subgraph induced by S is an empty graph. Then $\alpha = \max\{|S| : S \text{ is an independent set of } \}$ is said to be the *independent number* of G.

Theorem 2.6. *([30]) Let G be an n-vertex connected graph with independent number α. Then*

$$RDD_+(G) \leq n^3 - (\alpha + 1)n^2 - \left(\frac{3}{2}\alpha^2 - \frac{3}{2}\alpha - 1 \right) n + \frac{3}{2}\alpha^3 + \frac{3}{2}\alpha^2 - \alpha,$$

with equality if and only if G is isomorphic to $\alpha K_1 \vee K_{n-\alpha}$.

Proof. Let G' be a graph chosen among all n-vertex connected graphs with independent number α such that G' has the largest RDD_+. Let S be a maximal independent set in G' with $|S| = \alpha$. Since adding edges into a graph will increase its RDD_+ by Lemma 2.1, each vertex x in S is adjacent to every vertex y in $G' - S$. Moreover, the subgraph induced by vertices in $G' - S$ is a clique in G'. Consequently, it follows that $G' \cong \alpha K_1 \vee K_{n-\alpha}$. An elementary calculation gives $RDD_+(\alpha K_1 \vee K_{n-\alpha}) = (n-\alpha)(n-1)^2 + \alpha(n-\alpha)[(n-\alpha) + \frac{1}{2}(\alpha-1)] = n^3 - (\alpha+1)n^2 - (\frac{3}{2}\alpha^2 - \frac{3}{2}\alpha - 1)n + \frac{3}{2}\alpha^3 + \frac{3}{2}\alpha^2 - \alpha$, as desired. ■

The *matching number*, also called edge-independent number, $\beta(G)$ of a graph G is the maximum number of disjoint edges in G. Let $\mathscr{G}_n^\beta$ denote the class of connected graphs of order n with matching number β.

A component of a graph is said to be *odd* (resp. *even*) if it has odd (resp. even) number of vertices. Indicate the number of odd components by $o(G)$.

The following is an immediate consequence of the Tutte-Berge formula proved by Lovász and Plummer in [44].

Lemma 2.7. *Let G be a connected graph of order n. Then*

$$n - 2\beta = max\{o(G - X) - |X| : X \subset V\}.$$

Theorem 2.8. *([53]) Let G be a connected graph of order $n \geq 4$ with matching number $\beta \in [2, \lfloor \frac{n}{2} \rfloor]$. Let*

$$\sigma = \frac{23 - 4n + \sqrt{37n^2 - 121n + 109}}{21}.$$

Each of the following holds:

(a) *if $\beta = \lfloor \frac{n}{2} \rfloor$, then $RDD_+(G) \leq n(n-1)^2$, with equality if and only if $G \cong K_n$;*

(b) *if $\sigma < \beta \leq \lfloor \frac{n}{2} \rfloor - 1$, then $RDD_+(G) \leq 4\beta^3 + (2n-12)\beta^2 + (11-3n)\beta + \frac{n^2-n-4}{2}$, with equality if and only if $G \cong K_1 + (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$;*

(c) *if $\beta = \sigma$, then $RDD_+(G) \leq 4\sigma^3 + (2n-12)\sigma^2 + (11-3n)\sigma + \frac{n^2-n-4}{2} = \frac{1}{2}\sigma^3 - \frac{1}{2}\sigma^2 + \frac{n^2-3n+2}{2}\sigma$, with equality if and only if $G \cong K_\beta + \overline{K_{n-\beta}}$ or $G \cong K_1 + (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$;*

(d) *if $2 \leq \beta < \sigma$, then $RDD_+(G) \leq \frac{1}{2}\beta^3 - \frac{1}{2}\beta^2 + \frac{n^2-3n+2}{2}\beta$, with equality if and only if $G \cong K_\beta + \overline{K_{n-\beta}}$.*

Proof. Let G' be a connected graph with maximum RDD_+-value in $\mathscr{G}_n^\beta$. In view of Lemma 2.7, there exists a vertex subset $X' \subset V(G')$ such that

$$n - 2\beta = max\{o(G' - X) - |X| : X \subset V\} = o(G' - X') - |X'|.$$

For simplicity, let $|X'| = s$ and $o(G' - X') = t$. Then $n - 2\beta = t - s$.

Suppose that $s = 0$. It follows that $G' - X' = G'$, and $n - 2\beta = t \leq 1$. By our choice of G and Lemma 2.1, we obtain that $G' = K_n$, then we have $RDD_+(G') = n(n-1)^2$.

Assume in the following that $s \geq 1$, and consequently $t \geq 1$. Let $G_1^+, G_2^+, \cdots, G_t^+$ be all odd components of $G' - X'$. If $G' - X'$ has an even component, then by adding an edge in G' between a vertex of the even component and a vertex of an odd component of $G' - X'$, we obtain a graph G'', for which $n - 2\beta(G'') \geq o(G'' - X') - |X'| = o(G' - X') - |X'|$. It follows that $\beta(G'') = \beta$, and by Lemma 2.1 G'' has lager RDD_+ than that of G', a contradiction. Thus, $G' - X'$ does not have even components. Similarly, $G_1^+, G_2^+, \cdots, G_t^+$ and the subgraph induced by X' are all complete, and any vertex of $G_1^+, G_2^+, \cdots, G_t^+$ is adjacent to every vertex in X'. Let $n_i = |V(G_i^+)|$ for $i = 1, 2, \cdots, t$. Then

$$G' = K_s + (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_t}).$$

Let $\widehat{RDD_+}(G_1, G_2)$ denote the contribution to the RDD_+-value between vertices of G_1 and those of G_2, then we have

$$\begin{cases} \widehat{RDD_+}(K_{n_i}, K_{n_i}) = 2\binom{n_i}{2}(n_i + s - 1), \\ \widehat{RDD_+}(K_{n_i}, K_{n_j}) = n_i n_j (n_i + s - 1 + n_j + s - 1), \\ \widehat{RDD_+}(K_{n_i}, K_s) = s n_i (n - 1 + n_i + s - 1), \\ \widehat{RDD_+}(K_s, K_s) = 2\binom{s}{2}(n-1). \end{cases}$$

Hence, the reciprocal sum-degree distance of G' can be represented as

$$\begin{aligned} RDD_+(G') = &\sum_{i=1}^{t} \widehat{RDD_+}(K_{n_i}, K_{n_i}) + \sum_{i<j} \widehat{RDD_+}(K_{n_i}, K_{n_j}) \\ &+ \sum_{i=1}^{t} \widehat{RDD_+}(K_{n_i}, K_s) + \widehat{RDD_+}(K_s, K_s) \\ = &\sum_{i=1}^{t} n_i^3 + (2s-2)\sum_{i=1}^{t} n_i^2 + (s^2 + (n-3)s + 1)\sum_{i=1}^{t} n_i \\ &+ \sum_{i<j} n_i n_j (n_i + n_j + 2s - 2) + 2\binom{s}{2}(n-1). \end{aligned}$$

By Lagrange multiplier, we can show each of the following function

$$\begin{cases} f_1(n_1, n_2, \cdots, n_t) = n_1^3 + n_2^3 + \cdots + n_t^3, \\ f_2(n_1, n_2, \cdots, n_t) = n_1^2 + n_2^2 + \cdots + n_t^2, \\ f_3(n_1, n_2, \cdots, n_t) = n_1 + n_2 + \cdots + n_t, \\ f_4(n_1, n_2, \cdots, n_t) = \sum_{i<j} n_i n_j (n_i + n_j + 2s - 2), \end{cases}$$

attains its maximum under the conditions $n_1 + n_2 + \cdots + n_t = n - s$ and $1 \leq n_1 \leq n_2 \leq \cdots \leq n_t$ if and only if $n_1 = n_2 = \cdots = n_{t-1} = 1$ and $n_t = 2\beta - 2s + 1$.

Hence,

$$\begin{aligned} RDD_+(G') = &f_1(n_1, n_2, \cdots, n_t) + 2(s-1)f_2(n_1, n_2, \cdots, n_t) \\ &+(s^2 + (n-3) + 1)f_3(n_1, n_2, \cdots, n_t) + \frac{1}{2}f_4(n_1, n_2, \cdots, n_t), \end{aligned}$$

which attains maximum if and only if $n_1 = n_2 = \cdots = n_{t-1} = 1$ and $n_t = n - s - t + 1 = 2\beta - 2s + 1$. It follows that

$$G' = K_s + (K_{2\beta-2s+1} \cup \overline{K_{n+s-2\beta-1}}).$$

Simply calculation shows that

$$\begin{cases} \widehat{RDD_+}(K_{2\beta-2s+1}, K_{2\beta-2s+1}) = 2\binom{2\beta-2s+1}{2}(2\beta - s), \\ \widehat{RDD_+}(\overline{K_{n+s-2\beta-1}}, \overline{K_{n+s-2\beta-1}}) = \binom{n+s-2\beta-1}{2}s, \\ \widehat{RDD_+}(K_{2\beta-2s+1}, \overline{K_{n+s-2\beta-1}}) = (2\beta - 2s + 1)(n + s - 2\beta - 1)\beta, \\ \widehat{RDD_+}(K_s, K_s) = 2\binom{s}{2}(n-1). \end{cases}$$

Taking into account the contributions to RDD_+-value above, it yiels

$$\begin{aligned} RDD_+(G') =& \widehat{RDD_+}(K_{2\beta-2s+1}, K_{2\beta-2s+1}) + \widehat{RDD_+}(\overline{K_{n+s-2\beta-1}}, \overline{K_{n+s-2\beta-1}}) \\ &+ \widehat{RDD_+}(K_{2\beta-2s+1}, \overline{K_{n+s-2\beta-1}}) + \widehat{RDD_+}(K_s, K_s) \\ =& -\frac{7}{2}s^3 + \frac{4n + 24\beta - 1}{2}s^2 + \frac{n^2 - 5n - 24\beta^2 - 8n\beta + 4}{2}s \\ &+ 4\beta^3 + 2n\beta^2 + (n-1)\beta. \end{aligned}$$

Analyzing the function Φ on s

$$\begin{aligned} \Phi(s) =& -\frac{7}{2}s^3 + \frac{4n + 24\beta - 1}{2}s^2 + \frac{n^2 - 5n - 24\beta^2 - 8n\beta + 4}{2}s + 4\beta^3 \\ &+ 2n\beta^2 + (n-1)\beta. \end{aligned}$$

It follows that $s \leq \beta$, since $t - s = n - 2\beta \geq t + s - 2\beta$. By taking derivatives, we have

$$\begin{aligned} \Phi'(s) &= -\frac{21}{2}s^2 + (4n + 24\beta - 1)s + \frac{n^2 - 5n - 24\beta^2 - 8n\beta + 4}{2}, \\ \Phi''(s) &= -21s + 4n + 24\beta - 1 = 21(\beta - s) + 4n + 3\beta - 1 \geq 4n + 3\beta - 1 > 0. \end{aligned}$$

This implies that $\Phi(s)$ is a strictly convex function for $s \leq \beta$, and the maximum value of $\Phi(s)$ is attained when $s = 1$ or $s = \beta$. Let

$$\begin{aligned} \Phi(1) &= 4\beta^3 + (2n - 12)\beta^2 - (3n - 11)\beta + \frac{n^2 - n - 4}{2}, \\ \Phi(\beta) &= \frac{1}{2}\beta^3 - \frac{1}{2}\beta^2 + \frac{n^2 - 3n + 2}{2}\beta. \end{aligned}$$

After subtraction, we obtain

$$\Phi(1) - \Phi(\beta) = \frac{7}{2}\beta^3 + \frac{4n - 23}{2}\beta^2 - \frac{n^2 + 3n - 20}{2}\beta + \frac{n^2 - n - 4}{2}.$$

Now, let us consider the function Ψ on β

$$\Psi(\beta) = \frac{7}{2}\beta^3 + \frac{4n - 23}{2}\beta^2 - \frac{n^2 + 3n - 20}{2}\beta + \frac{n^2 - n - 4}{2}.$$

It follows that

$$\Psi'(\beta) = \frac{21}{2}\beta^2 + (4n - 23)\beta - \frac{n^2 + 3n - 20}{2}.$$

The quadratic equation $\Psi'(\beta) = 0$ has two distinct roots, since $37n^2 - 121n + 109 > 0$. Let σ be its positive root, namely

$$\sigma = \frac{23 - 4n + \sqrt{37n^2 - 121n + 109}}{21}.$$

If $\beta > \sigma$, and $\Psi'(\beta) > 0$, then $\Psi(\beta)$ is an increasing function, and $\Psi(\beta) > \Psi(1) = 0$ follows. This implies that $\Phi(1) > \Phi(\beta)$. If $\beta < \sigma$, then $\Phi(1) < \Phi(\beta)$. This completes the proof of Theorem 2.8. ■

2.2.2 Graphs with given chromatic number

A *coloring* of a graph G is an assignment of colors to the vertices of G such that two adjacent vertices have different colors. The minimum number of colors in a coloring of G is the *chromatic number* of G and is denoted by $\chi(G)$. The chromatic number is a very widely studied graph invariants, whose history started with the famous *four color problem*, posed by Guthrie in 1852, we encourage the interested readers to consult [8,54,55] and the work of Kempe [38] and Heawood [32] for details.

Denote by $T_{n,t}$ the *Turán graph*, a complete t-partite graph of order n with $|n_i - n_j| \leq 1$, where $n_i = 1, 2, \cdots, t$, is the number of vertices in the i-th partite set of $T_{n,t}$.

Theorem 2.9. *([30]) Let G be an n-vertex connected graph with chromatic number χ such that $n = q\chi + p$, $0 \leq p \leq \chi$. Then*

$$RDD_+(G) \leq n^3 - (3q+2)n^2 - \left(\frac{3}{2}q^2\chi + \frac{3}{2}q\chi + \frac{3}{2}q^2 + \frac{5}{2}q + 1\right)n - q(q+1)^2\chi,$$

with equality if and only if G is isomorphic to $T_{n,t}$.

Proof. Let G' be a graph chosen among all n-vertex connected graphs with chromatic number χ such that G' has the largest RDD_+. Because the addition of edges into a graph will increase its RDD_+, we must have $G' \cong \overline{K_{n_1}} \vee \overline{K_{n_2}} \vee \cdots \vee \overline{K_{n_\chi}}$, where n_i is the number of vertices in the i-th partite set.

By the definition of RDD_+, we obtain

$$\begin{aligned} RDD_+(G') =& \sum_{i=1}^{\chi} n_i(n-n_i)\left[(n-n_i) + (n_i - 1)\cdot\frac{1}{2}\right] \\ =& \sum_{i=1}^{\chi} n_i(n-n_i)\left(n - \frac{n_i}{2} - \frac{1}{2}\right) \\ =& \frac{1}{2}\sum_{i=1}^{\chi} n_i^3 + \frac{1}{2}(1-3n)\sum_{i=1}^{\chi} n_i^2 + \frac{1}{2}(2n^3 - n^2). \end{aligned}$$

Suppose that G' is not isomorphic to $T_{n,\chi}$. Then there must exist $n_j \geq n_i + 2$ for some $1 \leq i, j \leq \chi$.

Let $G'' \cong \overline{K_{n_1}} \vee \overline{K_{n_2}} \vee \cdots \vee \overline{K_{n_i+1}} \vee \cdots \vee \overline{K_{n_j-1}} \vee \cdots \vee \overline{K_{n_\chi}}$. Then

$$\begin{aligned} RDD_+(G'') - RDD_+(G') =& \frac{1}{2}[(n_j-1)^3 + (n_i+1)^3 - n_j^3 - n_i^3] \\ &+ \frac{1-3n}{2}[(n_j-1)^2 + (n_i+1)^2 - n_j^2 - n_i^2] \\ =& \frac{1}{2}(-3n_j^2 + 3n_i^2 + 3n_j + 3n_i) + \frac{1-3n}{2}(2n_i + 2 - 2n_j) \\ =& \frac{n_i + 1 - n_j}{2}(3n_j + 3n_i + 2 - 6n). \end{aligned}$$

Since G' is connected, we have $\chi \geq 2$, and then $n_i < n_j \leq n-1$. Thus, $3n_j + 3n_i + 2 - 6n < 0$. Note that $n_i + 1 - n_j < 0$, it follows that $RDD_+(G'') > RDD_+(G')$, a contradiction to our choice of G'. Hence, $G' \cong T_{n,\chi}$. Moreover, we have

$$\begin{aligned} RDD_+(T_{n,\chi}) =& p(q+1)(n-q-1)\left[(n-q-1) + q \cdot \frac{1}{2}\right] \\ &+ (\chi - p)q(n-q)\left[(n-q) + (q-1) \cdot \frac{1}{2}\right] \\ =& \sum_{i=1}^{\chi} n_i(n-n_i)\left(n - \frac{n_i}{2} - \frac{1}{2}\right) \\ =& n^3 - (3q+2)n^2 + \left(\frac{3}{2}q^2\chi + \frac{3}{2}q\chi + \frac{3}{2}q^2 + \frac{5}{2}q + 1\right)n - q(q+1)^2\chi. \end{aligned}$$

This completes the proof. ■

2.2.3 Graphs with given vertex–connectivity and edge–connectivity

The concept of connectivities are among the first notations studied in graph theory, which play an important and fundamental role in the exploration of graph properties. The connectivities also play an significant and fundamental role in graphs, especially in the notation of graph vulnerability.

We begin this section by bounding the reciprocal sum-degree distance in terms of connectivities: vertex-connectivity and edge-connectivity. The *vertex-connectivity* or simply *connectivity* is the minimum number of vertices whose deletion from a connected graph disconnects it, and the *edge-connectivity* is the minimum number of edges whose deletion from a connected graph disconnects it.

Theorem 2.10. *([30]) Let G be an n-vertex connected graph with vertex-connectivity κ. Then*

$$RDD_+(G) \leq n^3 - \frac{9}{2}n^2 + \left(2\kappa + \frac{13}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 3,$$

with equality if and only if G is isomorphic to $K_\kappa \vee (K_1 + K_{n-\kappa-1})$.

Proof. Let G' be a graph chosen among all n-vertex connected graphs with vertex-connectivity κ such that G' has the largest RDD_+. Let C be a vertex-cut in G' such that $|C| = \kappa$ and $G' - C = G_1 \cup G_2 \cup \cdots \cup G_t$ $(t \geq 2)$. It follows from Lemma 2.1 that $t = 2$, otherwise we can obtain a new graph G'' with vertex-connectivity κ by adding edges between any two components, which has a strictly larger RDD_+ than that of G', a contradiction to our choice of G'.

The same reason leads us to that both G_1 and G_2 are cliques of G', that the subgraph of G' induced by C is a clique, and that any vertex in $G_1 \cup G_2$ is adjacent to each vertex in C. Let n_i denote the order of G_i. Thus, we have $G' \cong K_\kappa \vee (K_{n_1} + K_{n_2})$.

Without loss of generality, we assume that $n_2 \geq n_1$. If $n_1 = 1$, then the result follows readily. Suppose now that $n_2 \geq n_1 \geq 2$. It follows from the definition

$$\begin{aligned}
RDD_+(G') = &\sum_{x \in V(G_1)} \delta_{G'}(x)\widehat{D}_{G'}(x) + \sum_{x \in V(G_2)} \delta_{G'}(x)\widehat{D}_{G'}(x) \\
&+ \sum_{x \in V(C)} \delta_{G'}(x)\widehat{D}_{G'}(x) \\
=& n_1(n - n_2 - 1)\left[(n - n_2 - 1) + \frac{1}{2}n_2\right] + k(n-1)^2 \\
&+ n_2(n - n_1 - 1)\left[(n - n_1 - 1) + \frac{1}{2}n_1\right] \\
=& (n^3 - 2n^2 + n) + \left(3 - \frac{5}{2}n - \frac{1}{2}k\right) n_1 n_2.
\end{aligned}$$

Let $G'' = K_\kappa \vee (K_{n_1 - 1} + K_{n_2 + 1})$. Then

$$\begin{aligned}
RDD_+(G'') - RDD_+(G') &= \left(3 - \frac{5}{2}n - \frac{1}{2}k\right)[(n_1 - 1)(n_2 + 1) - n_1 n_2] \\
&= \left(3 - \frac{5}{2}n - \frac{1}{2}k\right)(n_1 - n_2 - 1) > 0,
\end{aligned}$$

a contradiction to our choice of G'.

Thus, $G' \cong K_\kappa \vee (K_1 + K_{n-\kappa-1})$. An elementary calculation gives $RDD_+(K_\kappa \vee (K_1 + K_{n-\kappa-1})) = n^3 - \frac{9}{2}n^2 + (2\kappa + \frac{13}{2})n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 3$, as desired. ■

In the same paper, Hua et al. also showed that $K_\kappa \vee (K_1 + K_{n-\kappa-1})$ maximizes RDD_+ among all n-vertex connected graphs with edge-connectivity κ.

Theorem 2.11. *([30]) Let G be an n-vertex connected graph with edge-connectivity κ. Then*

$$RDD_+(G) \leq n^3 - \frac{9}{2}n^2 + \left(2\kappa + \frac{13}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 3,$$

with equality if and only if G is isomorphic to $K_\kappa \vee (K_1 + K_{n-\kappa-1})$.

Proof. Suppose that G' is a graph chosen among all n-vertex connected graphs with edge-connectivity κ such that G' has the maximum RDD_+. In what follows we intend to prove that $G' \cong K_\kappa \vee (K_1 + K_{n-\kappa-1})$.

Let $\{e_1, e_2, \cdots, e_\kappa\}$ be a κ-edge cut in G', and let $G' - \{e_1, e_2, \cdots, e_\kappa\} := G_1 \cup G_2$. Since adding edges into a graph will increase its RDD_+ by Lemma 2.1, both G_1 and G_2 must be complete graphs. Denote by n_i the order of G_i for $i = 1, 2$.

We claim that $n_i = 1$ or $n_i \geq \kappa \geq 2$. Suppose that $n_i \geq 2$. On one hand, G_i has $\binom{n_i}{2}$ edges, as G_i is a complete graph. On the other hand, the sum of degrees of all vertices in G_i is at least $n_i\kappa$, and thus G_i has at least $\frac{n_i\kappa-\kappa}{2}$ edges. Hence,

$$\frac{n_i(n_i-1)}{2} \geq \frac{n_i\kappa-\kappa}{2},$$

this is, $n_i^2 - (\kappa+1)n_i + \kappa \geq 0$, implying that $n_i \geq \kappa$, as claimed.

Suppose without loss of generality that $n_2 \geq n_1$. If $n_1 = 1$, $G_{\max}$ is just the graph $K_\kappa \vee (K_1 + K_{n-\kappa-1})$, as claimed.

Assume now that $n_2 \geq n_1 \geq \kappa$. In the following, we first confirm that each vertex in G' has degree at most $\kappa + 1$.

Let v be a vertex with neighbors $v_1, v_2, \cdots, v_\kappa$. Write $A = \{v_1, v_2, \cdots, v_\kappa\}$ and $B = V(G') \setminus \{v, v_1, v_2, \cdots, v_\kappa\}$. If $G[A \cup B]$, the subgraph of G' induced by $A \cup B$, is the complete graph K_{n-1}, then $G' \cong K_\kappa \vee (K_1 + K_{n-\kappa-1})$, as desired.

If $G[A \cup B]$ is not complete, then we can add an edge, say uv, between a vertex u in A and a vertex v in B and the resulting graph is denoted by G''. Clearly, the edge-connectivity of G'' is κ. But then, we have $RDD_+(G') < RDD_+(G'')$ by Lemma 2.1, a contradiction to the choice of G'.

So we may suppose that $\delta_{G'}(v) \geq \kappa + 1$ for any vertex v in G'. It follows that $n_2 \geq n_1 \geq \kappa + 1$. In fact, if $n_1 = \kappa$, then each vertex in G_1 is adjacent to at least two vertices in G_2, since each vertex in G' is of degree at most $\kappa + 1$. But then the number of edges between G_1 and G_2 is at least 2κ, a contradiction.

From [31], we know that if G is an n-vertex connected graph with edge-connectivity κ, then

$$M_1(G) \leq n^3 - 5n^2 + (2\kappa + 8)n + \kappa^2 - 3\kappa - 4,$$

with equality if and only if $G \cong_\kappa \vee (K_1 + K_{n-\kappa-1})$.

In 2012, Hua and Zhang [30] proved that for any connected graph G of order $n \geq 2$ and size $m \geq 1$, we have

$$RDD_+(G) \leq (n-1)m + \frac{M_1(G)}{2},$$

with either equality if and only if the diameter of G is at most two. Note that G' has $\binom{n_1}{2} + \binom{n_2}{2} + \kappa$ edges. Hence,

$$\begin{aligned} RDD_+(G') \leq&(n-1)\left[\binom{n_1}{2} + \binom{n_2}{2} + \kappa\right] + \frac{M_1(G')}{2} \\ \leq&(n-1)\left[\binom{n_1}{2} + \binom{n_2}{2} + \kappa\right] + \frac{n^3 - 5n^2 + (2\kappa+8)n + \kappa^2 - 3\kappa - 4}{2} \\ =&n^3 - \frac{7}{2}n^2 + \left(2\kappa + \frac{9}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 2 - (n-1)n_1n_2. \end{aligned}$$

Since $n_2 \geq n_1 \geq \kappa$ and $n_1 + n_2 = n$, we have $n_1 n_2 > \kappa(n-\kappa)$. Hence,

$$\begin{aligned} RDD_+(G') <& n^3 - \frac{7}{2}n^2 + \left(2\kappa + \frac{9}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 2 - (n-1)\kappa(n-\kappa) \\ =& n^3 - \left(\kappa + \frac{7}{2}\right)n^2 + \left(\kappa^2 + 3\kappa + \frac{9}{2}\right)n - \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 2. \end{aligned}$$

But then

$$\begin{aligned} RDD_+(K_\kappa \vee (K_1 + K_{n-\kappa-1})) - RDD_+(G') \\ >& \left[n^3 - \frac{9}{2}n^2 + \left(2\kappa + \frac{13}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 3\right] \\ &- \left[n^3 - \left(\kappa + \frac{7}{2}\right)n^2 + \left(\kappa^2 + 3\kappa + \frac{9}{2}\right)n - \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 2\right] \\ =& (\kappa-1)n^2 - (\kappa^2 + \kappa - 2)n + \kappa^2 - 1 \\ \geq& (\kappa-1)n \cdot [2(\kappa+1)] - (\kappa^2 + \kappa - 2)n + \kappa^2 - 1 \\ =& \kappa^2 n - \kappa n + \kappa^2 - 1 > 0, \end{aligned}$$

again a contradiction to our choice of G'.

From discussion above, we have completed the proof. ■

Let $f(\kappa) = n^3 - \frac{9}{2}n^2 + \left(2\kappa + \frac{13}{2}\right)n + \frac{1}{2}\kappa^2 - \frac{5}{2}\kappa - 3$. It is not difficult to see that $f(\kappa)$ is a strictly increasing function. It then follows that immediately from Theorem 2.10 and 2.11 the following sequence: for any n-vertex connected graph with vertex-connectivity (or edge-connectivity) at most κ, $f(\kappa)$ attains its maximum RDD_+ and the corresponding extremal graph is $K_\kappa \vee (K_1 + K_{n-\kappa-1})$.

2.2.4 Graphs with given pendent vertex

The results outlined in this subsection apply to arbitrary graphs with n vertices and p pendent vertices. Let K_n^p denote the graph obtained by attaching p pendent edges to a vertex of K_{n-p}.

The *Zagreb indices* have been introduced more than thirty years ago by Gutman and Trinajestić. They were originally defined as

$$M_1(G) = \sum_{u \in V(G)} (\delta_G(u))^2,$$
$$M_2(G) = \sum_{uv \in E(G)} \delta_G(u)\delta_G(v).$$

Here $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb indices. These graph invariants have rich history, the interested readers for more information on Zagreb indices can be referred to [3, 4, 31, 63, 65, 66] and therein.

We first demonstrate the validity of the following lemma.

Lemma 2.12. *([30]) Let G be an n-vertex connected graph with p pendent vertices. Then*

$$M_1(G) \leq n^3 - (3p-1)n^2 + (3p^2 + 6p + 1)n - p^3 - 3p^2 - 2p - 1,$$

with equality if and only if G is isomorphic to K_n^p.

Proof. Suppose that G' is a graph chosen among all connected graphs with n vertices and p pendent vertices such that it has the maximum first Zagreb index. Let $D(G') = \{d_1, d_2, \cdots, d_n\}$ denote the degree sequence of G'. If we label all pendent vertices of $G_{\max}$ as $v_1, v_2, \cdots, v_p$, then $G[V(G') \setminus \{v_1, v_2, \cdots, v_p\}]$ must be a clique in G', for otherwise, we can obtain a new graph with a strictly larger first Zagreb index than that of G' by adding edges into G'.

Note that the degree sequence $D(K_n^p) = \{n-1, \underbrace{n-p-1, \cdots, n-p-1}_{n-p-1}, \underbrace{1, \cdots, 1}_{p}\}$ If $G' \neq K_n^p$, then there must exist a pair (d_i, d_j) in G' with $n-p \leq d_i \leq d_j \leq n-2$. We can construct a new n-vertex and p-pendent vertex connected graph G'' by replacing the pair (d_i, d_j) in G' by the pair $(d_i - 1, d_j + 1)$. It is not difficult to check that $M_1(G') < M_1(G'')$, a contradiction to our choice of G'. Hence, G' is isomorphic to K_n^p. Simple calculation shows that $M_1(K_n^p) = n^3 - (3p-1)n^2 + (3p^2 + 6p + 1)n - p^3 - 3p^2 - 2p - 1$, as desired. ■

We now give an upper bound for the reciprocal sum-degree distance of graphs with given order and number of pendent vertices.

Theorem 2.13. *Let G be an n-vertex connected graph with p pendent vertices. Then*

$$RDD_+(G) \leq \frac{2n^3 - (5p+1)n^2 + (4p^2 + 11p + 2)n - p^3 - 4p^2 - 5p - 1}{2},$$

with equality if and only if G is isomorphic to K_n^p.

Proof. Suppose that G' is a connected graph with n vertices and p pendent vertices $v_1, v_2, \cdots, v_p$ satisfying that the induced graph by $V(G') - \{v_1, v_2, \cdots, v_p\}$ is a clique in G'. It is sufficient to consider the upper bound for RDD_+ of G' by Lemma 2.1.

It was proved by Hua et al. [30] that for any connected graph H with order n and size m, $RDD_+(H) \leq (n-1)m + \frac{M_1(H)}{2}$, and with either equality if and only if the diameter of G is at most two. Note that G' has $p + \binom{n-p}{2} = p + \frac{(n-p)(n-p-1)}{2}$ edges. It follows that

$$\begin{aligned} RDD_+(G') \leq &(n-1)m + \frac{M_1(G')}{2} \\ =&(n-1)\left[\frac{(n-p)^2 + 3p - n}{2}\right] + \frac{M_1(G')}{2} \\ \leq&(n-1)\left[\frac{(n-p)^2 + 3p - n}{2}\right] + \frac{M_1(K_n^p)}{2} \\ =&\frac{2n^3 - (5p+1)n^2 + (4p^2 + 11p + 2)n - p^3 - 4p^2 - 5p - 1}{2}. \end{aligned}$$

The first equality holds if and only if the diameter of G' is at most two and the second equality holds if and only if G' is isomorphic to K_n^p. Since K_n^p has diameter two, and therefore $RDD_+(G) \leq \frac{2n^3-(5p+1)n^2+(4p^2+11p+2)n-p^3-4p^2-5p-1}{2}$ with equality if and only if $G \cong K_n^p$. This completes the proof. ■

3. The reciprocal product–degree distance

From the fact that adding an edge to G will increase the degrees of its vertices and decrease the distances between some vertices, it follows that adding of an edge will increase the value of $RDD_{\times}$. This immediately implies that the complete graph has the largest $RDD_{\times}$ among all graphs with the same number of vertices. Hence, for any graph G on n vertices, we have $RDD_{\times}(G) \leq \frac{1}{2}n(n-1)^3$. By the analogous argument, any graph on n vertices having the smallest $RDD_{\times}$ must be tree.

3.1 General graphs with maximum and minimum $RDD_{\times}$

Deng, Krishnakumari, Venkatakrishnan and Balachandran [15] determined the minimum and maximum value of the reciprocal product-degree distance for trees. Their first lemma is based on the following transformation.

Transformation 3.1. *Let G_0 be a graph with $n_0 \geq 2$ vertices, and $P = v_1v_2v_3 \cdots v_r$ a path of length $r-1 \geq 2$. If G (resp. G^1) is the graph obtained by identifying a vertex v_0 in G_0 to v_k (resp. v_{k-1}) in P, $2 \leq k \leq \frac{r}{2}$, then $G \Rightarrow G^1$ is called the ρ_1-transformation, see Fig. 3*

Lemma 3.2. *([15]) Let G^1 be the graph obtained from G by ρ_1-transformation. Then $RDD_{\times}(G^1) < RDD_{\times}(G)$.*

Proof. Let $T = \{v_1, v_2, \cdots, v_r\}$ and let G_0 denote the subgraph of G induced by the vertex set $V(G)\backslash T$. From the definition of $RDD_{\times}(G)$, we have

$$\begin{aligned}
RDD_{\times}(G) \leq & \left[\sum_{x,y \in V(G_0)\backslash\{v_0\}} + \sum_{x,y \in T\backslash\{v_k,v_{k-1}\}} + \sum_{\substack{x \in V(G_0)\backslash\{v_0\} \\ y \in T\backslash\{v_k,v_{k-1}\}}} \right] \frac{\delta(x)\delta(y)}{d(x,y)} \\
& + \delta(v_k) \left[\sum_{x \in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{d(x,x_0)} + \sum_{x \in T\backslash\{v_k\}} \frac{\delta(x)}{d(x,v_{k-1})} \right] \\
& + \delta(v_{k-1}) \left[\sum_{x \in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{d(x,x_0)+1} + \sum_{x \in T\backslash\{v_k,v_{k-1}\}} \frac{\delta(x)}{d(x,v_{k-1})} \right].
\end{aligned}$$

After using ρ_1-transformation, the degree of v_{k-1} increases by $\delta_{G_0}(v_0)$, while the degree of the vertex v_k decreases by $\delta_{G_0}(v_0)$. During the transformation, for pairs $x, y \in V(G_0)\backslash\{v_0\}$ or $x, y \in T\backslash\{v_k, v_{k-1}\}$, the contribution $\frac{\delta(x)\delta(y)}{d(x,y)}$ does not change. Let $\alpha = \alpha(x) = \delta_{G_0}(x, v_0)$ for $x \in V(G_0) \setminus \{v_0\}$ and $H_n = \sum_{k=1}^{n} \frac{1}{k}$ be the n-th harmonic number.

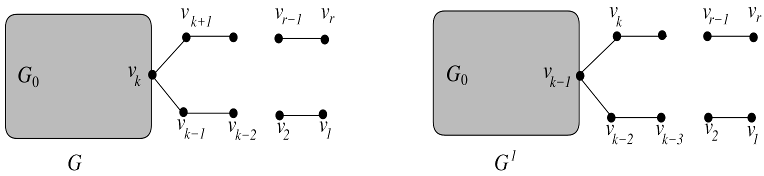

Figure 3. G^1 is obtained from G by ρ_1-transformation.

For simplicity, we distinguish the following two cases.

Case 1. $k > 2$

In the graph G, let

$$\begin{aligned} A_1 &= \sum_{\substack{x\in V(G_0)\setminus\{v_0\} \\ y\in T\setminus\{v_k,v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x,y)} \\ &= \sum_{x\in V(G_0)\setminus\{v_0\}} \delta(x)\left[\frac{1}{\alpha+k-1} + 2(H_{\alpha+k-2} - H_{\alpha+1})\right. \\ &\quad \left. 2(H_{\alpha+r-k-1} - H_\alpha) + \frac{1}{\alpha+r-k}\right]. \end{aligned}$$

$$\begin{aligned} A_2 =&\delta(v_k)\left[\sum_{x\in V(G_0)\setminus\{v_0\}} \frac{\delta(x)}{d(x,v_0)} + \sum_{x\in T\setminus\{v_k\}} \frac{\delta(x)}{d(x,v_k)}\right] \\ =&(\delta(v_0)+2)\left[\frac{1}{k-1} + 2H_{k-2} + 2H_{r-k-1} + \frac{1}{r-k} + \sum_{x\in V(G_0)\setminus\{v_0\}} \frac{\delta(x)}{\alpha}\right]. \end{aligned}$$

$$\begin{aligned} A_3 =&\delta(v_{k-1})\left[\sum_{x\in V(G_0)\setminus\{v_0\}} \frac{\delta(x)}{d(x,v_0)+1} + \sum_{x\in T\setminus\{v_{k-1},v_k\}} \frac{\delta(x)}{d(x,v_{k-1})}\right] \\ =&2\left[\frac{1}{k-2} + 2H_{k-3} + 2(H_{r-k} - H_1) + \frac{1}{r-k+1} + \sum_{x\in V(G_0)\setminus\{v_0\}} \frac{\delta(x)}{\alpha+1}\right]. \end{aligned}$$

In the graph G^1, let

$$\begin{aligned} B_1 &= \sum_{\substack{x\in V(G_0)\setminus\{v_0\} \\ y\in T\setminus\{v_k,v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x,y)} \\ &= \sum_{x\in V(G_0)\setminus\{v_0\}} \delta(x)\left[\frac{1}{\alpha+k-2} + 2(H_{\alpha+k-3} - H_\alpha)\right. \end{aligned}$$

$$2(H_{\alpha+r-k} - H_{\alpha+1}) + \frac{1}{\alpha+r-k+1}\Bigg].$$

$$\begin{aligned}
B_2 =& \delta(v_k)\left[\sum_{x\in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{d(x,v_0)+1} + \sum_{x\in T\backslash\{v_k\}} \frac{\delta(x)}{d(x,v_k)}\right] \\
=& 2\left[\frac{1}{k-1} + 2(H_{k-2} - H_1) + (\delta(v_0)+2) + 2H_{r-k-1} + \frac{1}{r-k} + \sum_{x\in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{\alpha+1}\right].
\end{aligned}$$

$$\begin{aligned}
B_3 =& \delta(v_{k-1})\left[\sum_{x\in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{d(x,v_0)} + \sum_{x\in T\backslash\{v_{k-1},v_k\}} \frac{\delta(x)}{d(x,v_{k-1})}\right] \\
=& (\delta(v_0)+2)\left[\frac{1}{k-2} + 2H_{k-3} + 2(H_{r-k} - H_1) + \frac{1}{r-k+1} + \sum_{x\in V(G_0)\backslash\{v_0\}} \frac{\delta(x)}{\alpha}\right].
\end{aligned}$$

From the above, we have

$$\begin{aligned}
RDD_\times(G) - RDD_\times(G^1) &= (A_1 + A_2 + A_3) - (B_1 + B_2 + B_3) \\
&= \sum_{x\in V(G_0)\backslash\{v_0\}} \delta(x)\Bigg[\frac{1}{\alpha+k-1} + \frac{1}{\alpha+k-2} - \frac{1}{\alpha+r-k} \\
&- \frac{1}{\alpha+r-k+1}\Bigg] \\
&+ \delta(v_0)\left[\frac{1}{k-1} + \frac{1}{k-2} - \frac{1}{r-k} - \frac{1}{r-k+1}\right] > 0.
\end{aligned}$$

The inequality holds since for $k \leq \frac{r}{2}$, we have

$$\begin{aligned}
\left[\frac{1}{\alpha+k-1} + \frac{1}{\alpha+k-2} - \frac{1}{\alpha+r-k} - \frac{1}{\alpha+r-k+1}\right] &> 0, \\
\left[\frac{1}{k-1} + \frac{1}{k-2} - \frac{1}{r-k} - \frac{1}{r-k+1}\right] &> 0.
\end{aligned}$$

Case 2. $k = 2$

In the graph G, let

$$\begin{aligned}
A_1 &= \sum_{\substack{x\in V(G_0)\backslash\{v_0\} \\ y\in T\backslash\{v_k,v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x,y)} \\
&= \sum_{x\in V(G_0)\backslash\{v_0\}} \delta(x)\left[\frac{1}{\alpha+r-2} + 2(H_{\alpha+r-3} - H_\alpha)\right].
\end{aligned}$$

$$\begin{aligned}A_2 =&\delta(v_k)\left[\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{d(x,v_0)}+\sum_{x\in T\backslash\{v_k\}}\frac{\delta(x)}{d(x,v_k)}\right]\\ =&(\delta(v_0)+2)\left[1+2H_{r-3}+\frac{1}{r-2}+\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{\alpha}\right].\end{aligned}$$

$$\begin{aligned}A_3 =&\delta(v_{k-1})\left[\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{d(x,v_0)+1}+\sum_{x\in T\backslash\{v_{k-1},v_k\}}\frac{\delta(x)}{d(x,v_{k-1})}\right]\\ =&(2H_{r-2}-1)+\frac{1}{r-1}+\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{\alpha+1}.\end{aligned}$$

In the graph G^1, let

$$\begin{aligned}B_1 &= \sum_{\substack{x\in V(G_0)\backslash\{v_0\}\\ y\in T\backslash\{v_k,v_{k-1}\}}}\frac{\delta(x)\delta(y)}{d(x,y)}\\ &= \sum_{x\in V(G_0)\backslash\{v_0\}}\delta(x)\left[\frac{1}{\alpha+r-1}+2(H_{\alpha+r-2}-H_{\alpha+1})\right].\end{aligned}$$

$$\begin{aligned}B_2 =&\delta(v_k)\left[\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{d(x,v_0)}+\sum_{x\in T\backslash\{v_k\}}\frac{\delta(x)}{d(x,v_k)}\right]\\ =&2\left[\delta(v_0)+1+2H_{r-3}+\frac{1}{r-2}+\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{\alpha+1}\right].\end{aligned}$$

$$\begin{aligned}B_3 =&\delta(v_{k-1})\left[\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{d(x,v_0)+1}+\sum_{x\in T\backslash\{v_{k-1},v_k\}}\frac{\delta(x)}{d(x,v_{k-1})}\right]\\ =&(\delta(v_0)+1)\left[(2H_{r-2}-1)+\frac{1}{r-1}+\sum_{x\in V(G_0)\backslash\{v_0\}}\frac{\delta(x)}{\alpha}\right].\end{aligned}$$

From the above, we have

$$\begin{aligned}RDD_\times(G)-RDD_\times(G^1) &= (A_1+A_2+A_3)-(B_1+B_2+B_3)\\ &= \sum_{x\in V(G_0)\backslash\{v_0\}}\delta(x)\left[\frac{2}{\alpha+1}-\frac{1}{\alpha+r-2}-\frac{1}{\alpha+r-1}\right]\end{aligned}$$

$$+ \quad \delta(v_0)\left[2-\frac{1}{r-2}-\frac{1}{r-1}\right]$$

$$+ \quad \sum_{x\in V(G_0)\setminus\{v_0\}} \delta(x)\left(\frac{1}{\alpha}-\frac{1}{\alpha+1}\right) > 0.$$

We have exhausted all the cases, so the proof is completed. ■

Repeatedly using Transformation 3.1, we can easily obtain a path from a tree. By Lemma 3.2, we have

Theorem 3.3. *([15]) Let T be a tree with $n \geq 2$ vertices, then $RDD_{\times}(P_n) \leq RDD_{\times}(T)$, with equality if and only if T is isomorphic to P_n.*

The following is an immediately consequence of Theorem 3.3. But we outline another proof for the lower bound which also was gave in [6].

Corollary 3.4. *Let G be a graph with n vertices, then $RDD_{\times}(P_n) \leq RDD_{\times}(G) \leq RDD_{\times}(K_n)$, with left (resp. right) equality if and only if T is isomorphic to P_n (resp. K_n).*

Proof. By the previous argument, we only need to consider trees on n vertices. Let T_n be such a tree, and let v be any vertex of T_n of degree at least 3 such that at least two of the components of $T_n - v$ are paths. Let those paths be of lengths s and l with $s \leq l$. We denote the tree induced by the vertices not in the above two paths by R. Let us call such a tree $T_{s,l}$. We transform $T_{s,l}$ by transplanting the end-vertex of the shorter path to the end-vertex of the longer path, obtaining a tree we denote by $T_{s-1,l+1}$. Evidently, R is not affected by such a transformation. The transformation is illustrated in Fig. 3. We proceed by comparing the contributions of various pairs of vertices to the $RDD_{\times}$-values of $T_{s,l}$ and $T_{s-1,l+1}$. We consider the following two cases.

Case 1. $s > 1$.

It is obvious that the contributions of all pairs not including the transplanted vertex and its neighbors remain unaffected by our transformation. Moreover, it is clear that the contributions involving the transplanted vertex are smaller in $T_{s-1,l+1}$ than in $T_{s,l}$ since the distances involved are greater. The only contributions that are greater in $T_{s-1,l+1}$ than in $T_{s,l}$ are those involving the former end-vertex of l-path. For a vertex x at distance d from v such contributions are $\frac{2\delta(x)}{d+l}$ and $\frac{\delta(x)}{d+l}$, respectively. Hence, the net change per vertex u of R is $\frac{\delta(x)}{d+l}$ in surplus for $T_{s-1,l+1}$. That surplus is, however, at least offset by the change in the contributions of pairs containing the new end-vertex of the shorter path. Previous contributions $\frac{2\delta(x)}{d+l}$ become $\frac{\delta(x)}{d+l}$, resulting in a net loss of $\frac{\delta(x)}{d+l}$ per vertex x at distance d from v. Since $s-1 < l$, such loss more than offsets the gain on the longer side, and hence $RDD_{\times}(T_{s-1,l+1}) \leq RDD_{\times}(T_{s,l})$.

Case 2. $s = 1$.

We still follow the same pattern discussed above. In this case, our transformation also changes the degree of v by decreasing it by 1. The only contributions that are greater in $RDD_{\times}(T_{s-1,l+1})$ than the corresponding contributions in $RDD_{\times}(T_{s,l})$ are those involving the former end-vertex on the longer side. The net surplus per vertex is again $\frac{\delta(x)}{d+l}$ per vertex x of R at distance d from v. Again, this is compensated by the loss of $\frac{\delta(x)}{d}$ per each such vertex coming from the decrease in the degree of v. It remains to consider the change in the contributions of pairs (v, y) where y is on the remaining path of length $l+1$. All such contributions in $RDD_{\times}(T_{s-1,l+1})$ are smaller than the corresponding contributions in $RDD_{\times}(T_{s,l})$ except from the last two vertices. Their combined contributions are $\frac{2(\delta(v)-1)}{l} + \frac{\delta(v)-1}{l+1}$. This quantity, however, cannot exceed the value of $\delta(v)$, representing the loss from the transplanted vertex, since $\delta(v) > \frac{2(\delta(v)-1)}{l} + \frac{\delta(v)-1}{l+1}$ for all $l \geq 2$. Again, $RDD_{\times}(T_{s-1,l+1}) \leq RDD_{\times}(T_{s,l})$. ■

We recall one more lemma from [15] as we need it in the proof of our main result.

Transformation 3.5. *Let v be a vertex of degree $p+1$ in a graph G, such that $vv_1, vv_2, \cdots, vv_p$ are pendent edges incident with v, and u is the neighbor of v distinct from $v_1, v_2, \cdots, v_p$. Denote by G^1 the graph obtained from G by removing edges $vv_1, vv_2, \cdots, vv_p$ and adding new edges $uv_1, uv_2, \cdots, uv_p$. Then we call $G \Rightarrow G^1$ the ρ_2-transformation.*

Lemma 3.6. *([15]) Let G^1 be the graph obtained from G by ρ_2-transformation. Then $RDD_{\times}(G) \leq RDD_{\times}(G^1)$, with equality if and only if G is a star with v as its center.*

Proof. Let $T = \{v, v_1, v_2, \cdots, v_p\}$ and H denote the subgraph of G induced by the vertex set $V(G) \setminus T$. From the definition of $RDD_{\times}(G)$, we have

$$\begin{aligned} RDD_{\times}(G) = & \left[\sum_{x,y \in H\setminus\{u\}} + \sum_{x,y \in T\setminus\{v\}} + \sum_{\substack{x\in H\setminus\{u\} \\ y \in T\setminus\{v\}}} \right] \frac{\delta(x)\delta(y)}{d(x,y)} \\ & + \delta(u) \left[\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + \sum_{x \in T\setminus\{v\}} \frac{\delta(x)}{d(x,u)} \right] \\ & + \delta(v) \left[\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,v)} + \sum_{x \in T\setminus\{v\}} \frac{\delta(x)}{d(x,v)} \right] + \frac{\delta(u)\delta(v)}{d(u,v)}. \end{aligned}$$

After the ρ_2-transformation, the degree of the vertex u increases by p, while the degree of the vertex v decreases by p. The distance between v_i and v_j for $i \neq j$ does not change. The distance between v_i and v increases by one, while the distance between v_i, $1 \leq i \leq p$, and other vertices decreases by one. During the transformation, for $x, y \in H \setminus \{u\}$ and $x, y \in T \setminus \{v\}$, the contribution $\sum \frac{\delta(x)\delta(y)}{d(x,y)}$ does not change.

In the graph G,

$$A_1 = \sum_{\substack{x\in H\setminus\{u\} \\ y \in T\setminus\{v\}}} \frac{\delta(x)\delta(y)}{d(x,y)} = \sum_{\substack{x\in H\setminus\{u\} \\ y \in T\setminus\{v\}}} \frac{\delta(x)}{d(x,y)}.$$

while in the graph G^1,

$$B_1 = \sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)\delta(y)}{d(x,y)} = \sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)}{d(x,y)-1}.$$

For the vertex u in the graph G,

$$\begin{aligned} A_2 =& \delta(u)\left[\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + \sum_{x\in T\setminus\{v\}} \frac{\delta(x)}{d(x,u)}\right] \\ =& \delta(u)\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + \frac{p\delta(u)}{2}. \end{aligned}$$

while in G^1, it becomes

$$\begin{aligned} B_2 =& \sum_{x\in H\setminus\{u\}} \frac{(\delta(u)+p)\delta(x)}{d(x,u)} + \sum_{x\in T\setminus\{v\}} \frac{(\delta(u)+p)\delta(x)}{d(x,u)} \\ =& \delta(u)\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + p\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + p\delta(u) + p^2. \end{aligned}$$

For the vertex v in the graph G,

$$\begin{aligned} A_3 =& \delta(v)\left[\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,v)} + \sum_{x\in T\setminus\{v\}} \frac{\delta(x)}{d(x,v)} + \frac{\delta(u)}{d(u,v)}\right] \\ =& (p+1)\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} + p(p+1) + (p+1)\delta(u) \\ =& p\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} + \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} + p^2 + p + p\delta(u) + \delta(u). \end{aligned}$$

while in G^1, it becomes

$$\begin{aligned} B_3 =& \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,v)} + \sum_{x\in T\setminus\{v\}} \frac{\delta(x)}{d(x,v)} + \frac{\delta(u)+p}{d(u,v)} \\ =& \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} + \frac{p}{2} + \delta(u) + p. \end{aligned}$$

From the above, we have

$$\begin{aligned} RDD_\times(G^1) - RDD_\times(G) &= (B_1 - A_1) + (B_2 - A_2) + (B_3 - A_3) \\ &= \left[\sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)}{d(x,y)-1} - \sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)}{d(x,y)}\right] \\ &+ \left[\delta(u)\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + p\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} + p\delta(u)\right. \end{aligned}$$

$$
\begin{aligned}
&+ \quad p^2 - \delta(u) \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)} - \frac{p\delta(u)}{2}\Bigg] \\
&+ \quad \Bigg[\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} + \frac{p}{2} + \delta(u) + p \\
&- \quad p \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} \\
&- \quad \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)+1} - p^2 - p - p\delta(u) - \delta(u)\Bigg] \\
&= \quad \sum_{\substack{x\in H\setminus\{u\}\\ y\in T-v}} \frac{\delta(x)}{(d(x,y)-1)d(x,y)} + p \sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)(d(x,u)+1)} \\
&- \quad p\frac{\delta(u)}{2} + \frac{p}{2}.
\end{aligned}
$$

Note that u has at least $\delta(u)-1$ neighbors $x \in H \setminus \{u\}$, therefore $\sum_{x\in H\setminus\{u\}} \frac{\delta(x)}{d(x,u)(d(x,u)+1)} \geq \frac{\delta(u)-1}{2}$, and consequently

$$
\begin{aligned}
RDD_\times(G^1) - RDD_\times(G) \;&\geq\; \sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)}{(d(x,y)-1)d(x,y)} + \frac{p(\delta(u)-1)}{2} - \frac{p\delta(u)}{2} + \frac{p}{2} \\
&=\; \sum_{\substack{x\in H\setminus\{u\}\\ y\in T\setminus\{v\}}} \frac{\delta(x)}{(d(x,y)-1)d(x,y)} \geq 0.
\end{aligned}
$$

The equality holds if and only if H contains only one vertex u, i.e., G is a star with v as its center. ■

For a tree T on n vertices, if T is not isomorphic to S_n, then T can be transformed into S_n by using Transformation 3.5 repeatedly. From Lemma 3.6, we have

Theorem 3.7. *([15]) Let T be a tree on n vertices, then $RDD_\times(T) \leq RDD_\times(S_n)$ with equality if and only if T is isomorphic to S_n.*

3.2 Unicyclic graphs with maximum $RDD_\times$

This section will focus on the discussion of a special class of unicyclic graphs. Let $U_{n,k}$ be the *unicyclic graph* of order $n \geq 3$ with girth $k \geq 3$ obtained from C_k by adding $n-k$ pendent vertices to a vertex of C_k.

Lemma 3.8. *([15]) Let u and v be two vertices of a graph H. We use G to denote the graph obtained from H by attaching s pendent vertices $u_1, u_2, \cdots, u_s$ and t pendent vertices $v_1, v_2, \cdots, v_t$ to u and v,* *respectively. Assume that*

$$G_1 = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$$
$$G_2 = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}.$$

Then $RDD_\times(G) < RDD_\times(G_1)$ *or* $RDD_\times(G) < RDD_\times(G_2)$.

Proof. For convenience, let $A = \{u_1, u_2, \cdots, u_s\}$, $B = \{v_1, v_2, \cdots, v_t\}$ and $d_H(u,v) = l$. From G to G_1, for any pair of vertices x, y satisfying $x, y \in H \setminus \{u,v\}$ or $x, y \in A$ or $x, y \in B$ or $x \in A$ and $y \in H \setminus \{u,v\}$, the contribution $\sum_{x,y} \frac{\delta(x)\delta(y)}{d(x,y)}$ does not change. Hence

$$\begin{aligned}
RDD_\times(G) &= \Bigg[\sum_{x,y\in H\setminus\{u,v\}} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in H\setminus\{u,v\}}}\Bigg]\frac{\delta(x)\delta(y)}{d(x,y)} \\
&+ \sum_{\substack{x\in A\\ y\in B}}\frac{\delta(x)\delta(y)}{d(x,y)} + \sum_{\substack{x\in H\setminus\{u,v\}\\ y\in B}}\frac{\delta(x)\delta(y)}{d(x,y)} \\
&+ \delta(u)\Bigg[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,u)} + \sum_{x\in A}\frac{\delta(x)}{d(x,u)} + \sum_{x\in B}\frac{\delta(x)}{d(x,u)}\Bigg] \\
&+ \delta(v)\Bigg[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,v)} + \sum_{x\in A}\frac{\delta(x)}{d(x,v)} + \sum_{x\in B}\frac{\delta(x)}{d(x,v)}\Bigg] + \frac{\delta(u)\delta(v)}{d(u,v)} \\
&= \Bigg[\sum_{x,y\in H\setminus\{u,v\}} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in H\setminus\{u,v\}}}\Bigg]\frac{\delta(x)\delta(y)}{d(x,y)} + \frac{st}{l+2} \\
&+ t\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,v)+1} + (s+\delta_H(u))\Bigg[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,v)+1} + s + \frac{t}{l+1}\Bigg] \\
&+ (t+\delta_H(v))\Bigg[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,v)} + t + \frac{s}{l+1}\Bigg] \\
&+ \frac{(s+\delta_H(u))(t+\delta_H(v))}{l}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
RDD_\times(G_1) &= \Bigg[\sum_{x,y\in H\setminus\{u,v\}} + \sum_{x,y\in A} + \sum_{x,y\in B} + \sum_{\substack{x\in A\\ y\in H\setminus\{u,v\}}}\Bigg]\frac{\delta(x)\delta(y)}{d(x,y)} + \frac{st}{2} \\
&+ t\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,u)+1} + (s+t+\delta_H(u))\Bigg[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,u)+1} + s + t\Bigg]
\end{aligned}$$

$$+ \quad \delta_H(v)\left[\sum_{x\in H\setminus\{u,v\}}\frac{\delta(x)}{d(x,v)}+\frac{t}{l+1}+\frac{s}{l+1}\right]+\frac{\delta_H(v)(s+t+\delta_H(u))}{l}.$$

Combing the previous two equalities, we get

$$\begin{aligned}
RDD_\times(G_1)-RDD_\times(G) &= \frac{stl}{2(l+2)}+t\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,v)-d(x,u)}{(d(x,u)+1)(d(x,v)+1)}\right]\\
&+ \quad t\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,v)-d(x,u)}{d(x,v)d(x,u)}\right]\\
&+ \quad 2st+t(\delta_H(u)-\delta_H(v))-\frac{2st+t(\delta_H(u))-\delta_H(v)}{l+1}\\
&- \quad \frac{st+t(\delta_H(u)-\delta_H(v))}{l}.
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
RDD_\times(G_2)-RDD_\times(G) &= \frac{stl}{2(l+2)}+s\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,u)-d(x,v)}{(d(x,u)+1)(d(x,v)+1)}\right]\\
&+ \quad s\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,u)-d(x,v)}{d(x,v)d(x,u)}\right]\\
&+ \quad 2st+s(\delta_H(v)-\delta_H(u))-\frac{2st+s(\delta_H(v)-\delta_H(u))}{l+1}\\
&- \quad \frac{st+s(\delta_H(v)-\delta_H(u))}{l}.
\end{aligned}$$

If $RDD_\times(G_1)-RDD_\times(G)>0$, then the result follows; otherwise $RDD_\times(G_1)-RDD_\times(G)\le 0$, then

$$\begin{aligned}
&\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,u)-d(x,v)}{(d(x,u)+1)(d(x,v)+1)}\right]+\sum_{x\in H\setminus\{u,v\}}\delta(x)\left[\frac{d(x,u)-d(x,v)}{d(x,v)d(x,u)}\right]\\
&\ge \frac{sl}{2(l+2)}+2s+(\delta_H(u)-\delta_H(v))-\frac{2s+(\delta_H(u)-\delta_H(v))}{l+1}\\
&-\frac{s+(\delta_H(u)-\delta_H(v))}{l}.
\end{aligned}$$

and

$$RDD_\times(G_2)-RDD_\times(G)\ge\frac{sl(s+t)}{2(l+2)}+s(s+t)\left(2-\frac{2}{l+1}-\frac{1}{l}\right)>0.$$

This completes the proof. ∎

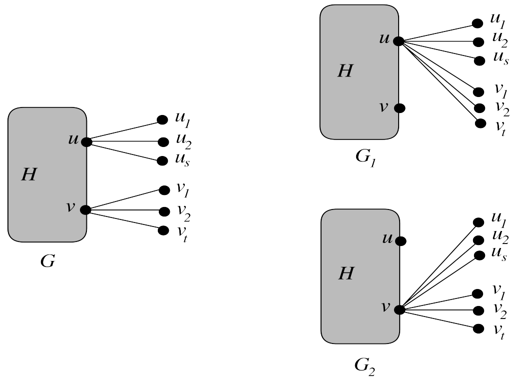

Figure 4. ρ_3-transformation $G \Rightarrow G_1$ or $G \Rightarrow G_2$.

Transformation 3.9. *Let u and v be two vertices of a connected graph H. Let G be the graph obtained from H by attaching s pendent vertices $u_1, u_2, \cdots, u_s$ and t pendent vertices $v_1, v_2, \cdots, v_t$ to u and v, respectively. Assume that $G_1 = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, $G_2 = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$. If $RDD_\times(G) < RDD_\times(G_1)$ (or $RDD_\times(G) < RDD_\times(G_2)$), then we call $G \Rightarrow G_i$ for $i = 1$ or 2 the ρ_3-transformation, see Fig 4.*

For a unicyclic graph G of order n with girth k, firstly, using Transformation 3.5 on G repeatedly, we can get a unicyclic graph from C_k by adding $n-k$ pendent vertices to the vertices of C_k, then using Transformation 3.9 repeatedly, we can get the unicyclic graph $U_{n,k}$. From Lemmas 3.6 and 3.8, we now obtain the following theorem.

Theorem 3.10. *([15]) Let G be a unicyclic graph of order n with girth k. Then $RDD_\times(G) \leq RDD_\times(U_{n,k})$ with equality if and only if G is isomorphic to $U_{n,k}$.*

Theorem 3.10 shows that $U_{n,k}$ is the unicyclic graph with the maximum $RDD_\times$ among all unicyclic graph of order n and girth k.

Theorem 3.11. *([15]) Let G be a unicyclic graph of order $n \geq 3$. Then $RDD_\times(G) \leq \frac{n(5n+1)}{4}$ with equality if and only if G is isomorphic to $U_{n,3}$.*

Theorem 3.11 shows that $U_{n,3}$ is the unique graph with maximum $RDD_\times$ among all unicyclic graph of order n.

4. Relation between RDD_+ and $RDD_\times$

We discuss in this section the relation between the reciprocal sum-degree distance and the reciprocal product-degree distance. We start with an auxiliary lemma proved by Dragomir in [16] which will be used in later proofs.

Lemma 4.1. *Let* $\overrightarrow{x} = (x_1, x_2, \cdots, x_N)$ *and* $\overrightarrow{y} = (y_1, y_2, \cdots, y_N)$ *be sequences of real numbers,* $\overrightarrow{z} = (z_1, z_2, \cdots, z_N)$ *and* $\overrightarrow{w} = (w_1, w_2, \cdots, w_N)$ *be nonnegative sequences, then*

$$\sum_{i=1}^{N} w_i \sum_{i=1}^{N} z_i x_i^2 + \sum_{i=1}^{N} z_i \sum_{i=1}^{N} w_i y_i^2 \geq 2 \sum_{i=1}^{N} z_i x_i \sum_{i=1}^{N} w_i y_i. \tag{16}$$

In particular, if z_i *and* w_i *are positive, then the equality holds in (16) if and only if* $\overrightarrow{x} = \overrightarrow{y} = \overrightarrow{k}$, *where* $\overrightarrow{k} = (k, k, \cdots, k)$ *is a constant sequence.*

Define the *inverse degree* of a graph G with no isolated vertices as

$$R(G) = \sum_{v \in V(G)} \frac{1}{\delta(v)}.$$

The inverse degree first attracted attention through conjectures of the computer program Graffiti [25]. It has been studied by several authors, see for example [19, 23].

Theorem 4.2. *Let* G *be a connected graph with* n *vertices,* m *edges, maximum degree* Δ *and minimum degree* $\underline{\Delta}$, *then*

$$\begin{aligned} 2RDD_{+}(G)RDD_{\times}(G) \leq (2m - \underline{\Delta})M_1(G) & \left[\frac{(n-1)\Delta\underline{\Delta}}{\Delta + \underline{\Delta}} \right. \\ & \left. + \frac{(n-1)(n-2)\Delta}{4} + (n-1)R(G) \right], \end{aligned} \tag{17}$$

with equality if and only if G *is isomorphic to* K_3.

Proof. Suppose that each i in Lemma 4.1 corresponds a vertex pair (v_i, v_j) such that $N = \binom{n}{2}$. Setting $z_i = w_i = \frac{1}{x_i y_i}$ and each x_i is replaced by $\frac{d(v_i,v_j)}{\delta(v_i)\delta(v_j)}$ and y_i is replaced by $\frac{d(v_i,v_j)}{\delta(v_i)+\delta(v_j)}$, then we get

$$\begin{aligned} \sum_{\{v_i,v_j\}} \frac{\delta(v_i)\delta(v_j)(\delta(v_i)+\delta(v_j))}{(d(v_i,v_j))^2} \sum_{\{v_i,v_j\}} & \left[\frac{\delta(v_i)+\delta(v_j)}{\delta(v_i)\delta(v_j)} + \frac{\delta(v_i)\delta(v_j)}{\delta(v_i)+\delta(v_j)} \right] \\ & \geq 2 \sum_{\{v_i,v_j\}} \frac{\delta(v_i)+\delta(v_j)}{d(v_i,v_j)} \sum_{\{v_i,v_j\}} \frac{\delta(v_i)\delta(v_j)}{d(v_i,v_j)}. \end{aligned} \tag{18}$$

To accomplish the proof, it is sufficient to find respectively the upper bound of

$$\zeta_1(v_i, v_j) := \sum_{\{v_i,v_j\}} \left[\frac{\delta(v_i)+\delta(v_j)}{\delta(v_i)\delta(v_j)} + \frac{\delta(v_i)\delta(v_j)}{\delta(v_i)+\delta(v_j)} \right].$$

and

$$\zeta_2(v_i, v_j) := \sum_{\{v_i.v_j\}} \frac{\delta(v_i)\delta(v_j)(\delta(v_i)+\delta(v_j))}{(d(v_i,v_j))^2}.$$

Note that $\frac{2}{\Delta} \leq \frac{1}{\delta(v_i)} + \frac{1}{\delta(v_j)} \leq \frac{2}{\underline{\Delta}}$, it immediately follows that $\frac{\delta(v_i)\,\delta(v_j)}{\delta(v_i)+\delta(v_j)} \leq \frac{\Delta}{2}$. Again since $\frac{1}{\delta(v_i)} + \frac{1}{\underline{\Delta}} \geq \frac{1}{\Delta} + \frac{1}{\underline{\Delta}}$, we have $\frac{\delta(v_i)\,\underline{\Delta}}{\delta(v_i)+\underline{\Delta}} \leq \frac{\Delta\,\underline{\Delta}}{\Delta+\underline{\Delta}}$. Suppose that v_n is the minimum degree vertex of degree $\underline{\Delta}$. Using the above results, we have

$$\begin{aligned}
\sum_{\{v_i,v_j\}} \frac{\delta(v_i)\delta(v_j)}{\delta(v_i)+\delta(v_j)} &= \sum_{\{v_i,v_n\}} \frac{\delta(v_i)\underline{\Delta}}{\delta(v_i)+\underline{\Delta}} + \sum_{\substack{\{v_i,v_j\}\\ v_j\neq v_n}} \frac{\delta(v_i)\delta(v_j)}{\delta(v_i)+\delta(v_j)} \\
&\leq \frac{(n-1)\Delta\underline{\Delta}}{\Delta+\underline{\Delta}} + \left[\frac{n(n-1)}{2} - (n-1)\right]\frac{\Delta}{2} \\
&= \frac{(n-1)\Delta\underline{\Delta}}{\Delta+\underline{\Delta}} + \frac{(n-1)(n-2)\Delta}{4}.
\end{aligned} \tag{19}$$

By simple calculations, we get

$$\begin{aligned}
\sum_{\{v_i,v_j\}} \frac{\delta(v_i)+\delta(v_j)}{\delta(v_i)\,\delta(v_j)} &= \sum_{\{v_i,v_j\}} \left[\frac{1}{\delta(v_i)} + \frac{1}{\delta(v_j)}\right] \\
&= \sum_{v_i\in V(G)}^{n} \frac{n-1}{\delta(v_i)} = (n-1)R(G).
\end{aligned} \tag{20}$$

Inequalities (19) and (20) yield

$$\begin{aligned}
\zeta_1(v_i,v_j) = &\sum_{\{v_i,v_j\}} \left[\frac{\delta(v_i)\delta(v_j)}{\delta(v_i)+\delta(v_j)} + \frac{\delta(v_i)+\delta(v_j)}{\delta(v_i)\delta(v_j)}\right] \\
\leq &\frac{(n-1)\Delta\underline{\Delta}}{\Delta+\underline{\Delta}} + \frac{(n-1)(n-2)\Delta}{4} + (n-1)R(G).
\end{aligned} \tag{21}$$

Note that $\sum_{v_i\in V(G)} \delta(v_i) = 2m$ and $d(v_i,v_j) \geq 1$, it holds that

$$\begin{aligned}
\zeta_2(v_i,v_j) &= \sum_{\{v_i,v_j\}} \frac{\delta(v_i)\delta(v_j)(\delta(v_i)+\delta(v_j))}{(d(v_i,v_j))^2} \\
&\leq \sum_{\{v_i,v_j\}} \delta(v_i)\delta(v_j)(\delta(v_i)+\delta(v_j)) \\
&= \sum_{v_i\in V(G)} \delta^2(v_i)(2m-\delta(v_i)) \\
&\leq (2m-\underline{\Delta})M_1(G).
\end{aligned} \tag{22}$$

Using the above results (21) and (22), we get the required result in (17). First part of the proof is done.

Now we assume that the equality holds in (17). From equality in (18), by Lemma 4.1, we get

$$\frac{d(v_i,v_j)}{\delta(v_i)\delta(v_j)} = \frac{d(v_i,v_k)}{\delta(v_i)\delta(v_k)} = \frac{d(v_i,v_j)}{\delta(v_i)+\delta(v_j)} = \frac{d(v_i,v_k)}{\delta(v_i)+\delta(v_k)}$$

and $d(v_i,v_j) = d(v_i,v_k)$ holds for any vertices v_i, v_j and v_k of graph G. This implies that $\delta(v_i) = \delta(v_j) = 2$ and $D(G) = 1$. Hence G is isomorphism to K_3. Conversely, one can see easily that the equality holds in (17) for K_3. ■

The following is an immediate consequence of Theorem 4.2.

Corollary 4.3. *Let G be a connected graph with n vertices, m edges, maximum degree Δ, minimum degree $\underline{\Delta}$ and p pendent vertices, then*

$$\begin{aligned}2RDD_+(G)RDD_\times(G) \leq & [(2m-\underline{\Delta})M_1(G)+(\underline{\Delta}-1)p] \\ & \left[\frac{(n-1)\Delta\underline{\Delta}}{\Delta+\underline{\Delta}}+\frac{(n-1)(n-2)\Delta}{4}+(n-1)R(G)\right],\end{aligned} \tag{23}$$

with equality if and only if G is isomorphic to K_3.

Proof. Since p is the number of pendent vertices in G, it follows that

$$\begin{aligned}\sum_{v_i\in V(G)} \delta(v_i)^3 =& p + \sum_{v_i\in V(G),\delta(v_i)\neq 1} \delta(v_i)^3 \\ \geq & p+\underline{\Delta}\sum_{v_i\in V(G),\delta(v_i)\neq 1} \delta(v_i)^2 = p+\underline{\Delta}(M_1(G)-p).\end{aligned} \tag{24}$$

Applying inequality (24) to $\zeta_2(v_i,v_j)$, it yields that

$$\begin{aligned}\zeta_2(v_i,v_j) \leq & \sum_{\{v_i,v_j\}} \delta(v_i)\delta(v_j)(\delta(v_i)+\delta(v_j)) \\ =& \sum_{v_i\in V(G)} \delta(v_i)^2(2m-\delta(v_i)) \leq (2m-\underline{\Delta})M_1(G)+(\underline{\Delta}-1)p.\end{aligned}$$

We get the required result in (23). Moreover, the equality holds in (23) if and only if G is isomorphic to K_3. ■

Lemma 4.4. (Radon's inequality) *For real numbers $p>0$, $a_1,a_2,\cdots,a_N\geq 0$ and $b_1,b_2,\cdots,b_N>0$, the following inequality holds:*

$$\sum_{l=1}^{N}\frac{a_l^{p+1}}{b_l^p} \geq \frac{\left(\sum\limits_{l=1}^{N} a_l\right)^{p+1}}{\left(\sum\limits_{l=1}^{N} b_l\right)^{p}}.$$

We now give another relation between the reciprocal sum-degree distance and reciprocal product-degree of graphs.

Theorem 4.5. *Let G be a connected graph with n vertices, m edges, maximum degree Δ and minimum degree $\underline{\Delta}$, then*

$$\frac{(RDD_+(G))^2}{RDD_\times(G)} \leq \frac{(\Delta+\underline{\Delta})^2}{\Delta\underline{\Delta}}H(G).$$

with equality if and only if G is a regular graph.

Proof. Assume that each l in Lemma 4.4 corresponds a vertex (v_i,v_j) with $N=\binom{n}{2}$ and $p=1$. Setting each a_l is replaced by $\frac{\delta(v_i)+\delta(v_j)}{d(v_i,v_j)}$ and b_l is replaced by $\frac{\delta(v_i)\delta(v_j)}{d(v_i,v_j)}$, it follows that

$$\frac{\left(\sum\limits_{\{v_i,v_j\}}\frac{\delta(v_i)+\delta(v_j)}{d(v_i,v_j)}\right)^2}{\sum\limits_{\{v_i,v_j\}}\frac{\delta(v_i)\delta(v_j)}{d(v_i,v_j)}} \leq \sum_{\{v_i,v_j\}}\frac{\left(\frac{\delta(v_i)+\delta(v_j)}{d(v_i,v_j)}\right)^2}{\frac{\delta(v_i)\delta(v_j)}{d(v_i,v_j)}},$$

which is equivalent to

$$\frac{(RDD_+(G))^2}{RDD_\times(G)} \leq \sum_{\{v_i,v_j\}} \left(\sqrt{\frac{\delta(v_i)}{\delta(v_j)}} + \sqrt{\frac{\delta(v_j)}{\delta(v_i)}}\right)^2 \frac{1}{d(v_i,v_j)}.$$

It has been proved in [20] that

$$\left(\sqrt{\frac{\delta(v_i)}{\delta(v_j)}} + \sqrt{\frac{\delta(v_j)}{\delta(v_i)}}\right)^2 \leq \frac{(\Delta + \underline{\Delta})^2}{\Delta\,\underline{\Delta}}.$$

Moreover, the equality holds if and only if G is a regular graph or G is a bipartite semiregular graph. Hence, we obtain

$$\frac{(RDD_+(G))^2}{RDD_\times(G)} \leq \sum_{\{v_i,v_j\}} \frac{(\Delta + \underline{\Delta})^2}{\Delta\underline{\Delta}} \frac{1}{d(v_i,v_j)} = \frac{(\Delta + \underline{\Delta})^2}{\Delta\underline{\Delta}} H(G).$$

The equality holds if and only if G is a regular graph. ■

We conclude this section by considering an upper bound of the difference between the reciprocal product-degree distance and reciprocal sum-degree distance.

Theorem 4.6. *Let G be a connected graph with n vertices and m edges, then*

$$\begin{aligned} RDD_\times(G) - RDD_+(G) \leq & \frac{4m^2 - (4n-6)m + n^2 - n}{4} \\ & -\frac{3}{4}M_1(G) + \frac{1}{2}M_2(G) - H(G). \end{aligned} \tag{25}$$

with equality if and only if the distance between any two non-pendent vertices in G is at most 2.

Proof. By the definition of the reciprocal product-degree distance and rciprocal sum-degree distance, we get

$$\begin{aligned} RDD_\times(G) - RDD_+(G) &= \sum_{\{v_i,v_j\}} \frac{\delta(v_i)\delta(v_j) - \delta(v_i) - \delta(v_j)}{d(v_i,v_j)} \\ &= \sum_{\{v_i,v_j\}} \frac{(\delta(v_i)-1)(\delta(v_j)-1)}{d(v_i,v_j)} - H(G) \\ &= \sum_{v_iv_j \in E(G)} (\delta(v_i)-1)(\delta(v_j)-1) \\ &+ \sum_{v_iv_j \in E(\overline{G})} \frac{(\delta(v_i)-1)(\delta(v_j)-1)}{d(v_i,v_j)} - H(G) \\ &\leq \sum_{v_iv_j \in E(G)} (\delta(v_i)-1)(\delta(v_j)-1) \end{aligned}$$

$$
\begin{aligned}
&+ \frac{1}{2} \sum_{v_i v_j \in E(\overline{G})} (\delta(v_i)-1)(\delta(v_j)-1) - H(G) \qquad (26)\\
&= \frac{1}{2} \sum_{\{v_i, v_j\}} (\delta(v_i)-1)(\delta(v_j)-1)\\
&- \frac{1}{2} \sum_{v_i v_j \in E(G)} (\delta(v_i)-1)(\delta(v_j)-1) - H(G).
\end{aligned}
$$

Simple calculations yields

$$
\begin{aligned}
\Lambda_1 :=& \sum_{\{v_i, v_j\}} (\delta(v_i)-1)(\delta(v_j)-1)\\
=&\frac{1}{2}\big[(2m-n)(2m-n+1) + 2m - M_1(G)\big]
\end{aligned}
$$

and

$$
\begin{aligned}
\Lambda_2 :=& \sum_{v_i v_j \in E(G)} (\delta(v_i)-1)(\delta(v_j)-1)\\
=&M_2(G) - M_1(G) + m.
\end{aligned}
$$

After easy manipulations, we have

$$
\begin{aligned}
RDD_\times(G) - RDD_+(G) &= \frac{1}{4}\big[(2m-n)(2m-n+1) + 2m - M_1(G)\big]\\
&+ \frac{1}{2}\big[M_2(G) - M_1(G) + m\big] - H(G).
\end{aligned}
$$

First part of the proof is done.

Now suppose that the equality holds in (25). Then the inequality in (26) must be equality, which implies that $d(v_i, v_j) = 2$ for any two vertices v_i and v_j in $\overline{G}$ with $\delta(v_i), \delta(v_j) \geq 2$. Hence the equality holds in (25) if and only if the distance between any two non-pendant vertices in G is at most 2. ■

5. The reformulated reciprocal sum–degree distance

In this section, we mainly study the mathematical properties of the reformulated reciprocal sum-degree distance under some edge-grafting transformations. Furthermore, extremal properties of the reformulated reciprocal sum-degree distance are also studied for some interesting classes of trees. For simplicity, we divide it into several subsections, each dealing with a class of graphs.

5.1 Graphs with given *k* leaves

Let $\mathscr{T}_n^k$ be the set of all n-vertex trees with k leaves. Note that there is just one tree for $k = n-1$ or 2, hence in what follows we consider $\mathscr{T}_n^k$ for $3 \leq k \leq n-2$.

In 2016, Li et al. [48] determined the graphs with maximum reformulated reciprocal sum-degree distance among the trees in $\mathscr{T}_n^k$. We begin with a significant lemma which will be used in later proofs.

Transformation 5.1. *Let G_1 be a simple graph as depicted in Fig. 5, where H_1, H_2 are two connected graphs. Let $G_2 = G_1 - \{v_l x : x \in N_{H_2}(v_l)\} + \{v_1 x : x \in N_{H_2}(v_l)\}$. We call $G_1 \Rightarrow G_2$ the θ_1-transformation.*

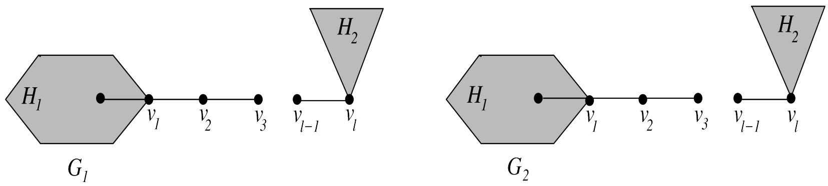

Figure 5. G_2 is obtained from G_1 by θ_1-transformation.

In particular, if G_1 is a tree, Kelmans [41] used Transformation 5.1 to prove some results on the number of spanning trees of graphs in 1976. Recently, Bollobás and Tyomkyn [9] used θ_1-transformation to count the total number of walks (resp. paths) of trees.

Theorem 5.2. *([48]) Let G_2 be the graph obtained from G_1 by Transformation 5.1, then $RDD_+^t(G_1) < RDD_+^t(G_2)$.*

Proof. For each vertex x in $V(H_1) \setminus \{v_1\}$ and for each vertex y in $V(H_2) \setminus \{v_l\}$, it is routine to check that $\delta_{G_1}(x) = \delta_{H_1}(x) = \delta_{G_2}(x)$ and $\delta_{G_1}(y) = \delta_{H_2}(y) = \delta_{G_2}(y)$. In addition, for each vertex $y \in V(H_2)$, $d_{H_2}(v_l, y) = a$ in G_1 if and only if $d_{H_2}(v_1, y) = a$ in G_2.

For convenience, we distinguish the following three cases.

• For each vertex x in $V(H_1) \setminus \{v_1\}$, we have

$$\begin{aligned}\widehat{D}_t(G_1; x) = &\sum_{y \in V(H_1)\setminus\{v_1, x\}} \frac{1}{d_{H_1}(x, y) + t} + \sum_{k=0}^{l-1} \frac{1}{d_{H_1}(x, v_1) + k + t} \\ &+ \sum_{y \in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_1}(x, v_1) + l - 1 + d_{H_2}(v_l, y) + t}.\end{aligned}$$

$$\begin{aligned}\widehat{D}_t(G_2; x) = &\sum_{y \in V(H_1)\setminus\{v_1, x\}} \frac{1}{d_{H_1}(x, y) + t} + \sum_{k=0}^{l-1} \frac{1}{d_{H_1}(x, v_1) + k + t} \\ &+ \sum_{y \in V(H_2)\setminus\{v_1\}} \frac{1}{d_{H_1}(x, v_1) + d_{H_2}(v_1, y) + t}.\end{aligned}$$

It follows that $\widehat{D}_t(G_1; x) < \widehat{D}_t(G_2; x)$. Note that, for all vertex x in $V(H_1) \setminus \{v_1\}$, we have $\delta_{G_1}(x) = \delta_{H_1}(x) = \delta_{G_2}(x)$. Hence,

$$\sum_{x \in V(H_1)\setminus\{v_1\}} \delta_{G_1}(x) \widehat{D}_t(G_1; x) < \sum_{x \in V(H_1)\setminus\{v_1\}} \delta_{G_2}(x) \widehat{D}_t(G_2; x). \tag{27}$$

• For each vertex x in $V(H_2) \setminus \{v_l\}$, we have

$$\widehat{D}_t(G_1;x) = \sum_{y\in V(H_2)\setminus\{v_l,x\}} \frac{1}{d_{H_2}(x,y)+t} + \sum_{k=0}^{l-1} \frac{1}{d_{H_2}(x,v_l)+k+t} + \sum_{y\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_l)+l-1+d_{H_1}(v_1,y)+t},$$

$$\widehat{D}_t(G_2;x) = \sum_{y\in V(H_2)\setminus\{v_l,x\}} \frac{1}{d_{H_2}(x,y)+t} + \sum_{k=0}^{l-1} \frac{1}{d_{H_2}(x,v_1)+k+t} + \sum_{y\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_1)+d_{H_1}(v_1,y)+t}.$$

It follows that $\widehat{D}_t(G_1;x) < \widehat{D}_t(G_2;x)$. Note that, for all vertex x in $V(H_2) \setminus \{v_l\}$, we have $\delta_{G_1}(x) = \delta_{H_2}(x) = \delta_{G_2}(x)$. Hence,

$$\sum_{x\in V(H_2)\setminus\{v_l\}} \delta_{G_1}(x)\widehat{D}_t(G_1;x) < \sum_{x\in V(H_2)\setminus\{v_l\}} \delta_{G_2}(x)\widehat{D}_t(G_2;x). \tag{28}$$

• For each vertex $v_j \in V(P_l) = \{v_1, v_2, \cdots, v_l\}$, we have

$$\widehat{D}_t(G_1;v_j) = \sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+j-1+t} + \widehat{D}_t(P_l;v_j) + \sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+l-j+t}. \tag{29}$$

$$\widehat{D}_t(G_2;v_j) = \sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+j-1+t} + \widehat{D}_t(P_l;v_j) + \sum_{x\in V(H_2)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_1)+j-1+t}. \tag{30}$$

Note that, for each vertex $v_j \in V(P_l) \setminus \{v_1, v_l\}$, one has $\delta_{G_1}(v_j) = \delta_{G_2}(v_j) = 2$ and it is routine to check that $\delta_{G_1}(v_1) = \delta_{H_1}(v_1) + 1$, $\delta_{G_1}(v_l) = \delta_{H_2}(v_l) + 1$, $\delta_{G_2}(v_1) = \delta_{H_1}(v_1) + \delta_{H_2}(v_1) + 1$ and $\delta_{G_2}(v_l) = 1$. From the combination of Eqs.(29) and (30), it yields

$$\begin{aligned}
\sum_{j=1}^{l} \delta_{G_1}(v_j)\widehat{D}_t(G_1;v_j) &= (\delta_{H_1}(v_1)+1)\Bigg(\sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+t} + \widehat{D}_t(P_l;v_1) \\
&+ \sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+l-1+t}\Bigg) \\
&+ (\delta_{H_2}(v_l)+1)\Bigg(\sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+t} + \widehat{D}_t(P_l;v_l)
\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+l-1+t}\Bigg) \\
&+ 2\sum_{j=2}^{l-1}\Bigg(\sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+j-1+t} + \widehat{D}_t(P_l;v_j) \\
&+ \sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+l-j+t}\Bigg),
\end{aligned}
$$

and

$$
\begin{aligned}
\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_t(G_2;v_j) &= (\delta_{H_1}(v_1)+\delta_{H_2}(v_1)+1)\Bigg(\sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+t} \\
&+ \widehat{D}_t(P_l;v_1) + \sum_{x\in V(H_2)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_1)+t}\Bigg) \\
&+ 2\sum_{j=2}^{l-1}\Bigg(\sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+j-1+t} + \widehat{D}_t(P_l;v_j) \\
&+ \sum_{x\in V(H_2)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_1)+j-1+t}\Bigg) \\
&+ \sum_{x\in V(H_2)\setminus\{v_1\}} \frac{1}{d_{H_2}(x,v_1)+l-1+t} + \widehat{D}_t(P_l;v_l) \\
&+ \sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+l-1+t},
\end{aligned}
$$

where $\widehat{D}_t(P_l;v_1) = \widehat{D}_t(P_l;v_l)$. By direct calculation, we have

$$
\begin{aligned}
&\sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_t(G_2;v_j) - \sum_{j=1}^{l}\delta_{G_1}(v_j)\widehat{D}_t(G_1;v_j) \\
&=\delta_{H_1}(v_1)\Bigg(\sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+t} - \sum_{x\in V(H_2)\setminus\{v_l\}} \frac{1}{d_{H_2}(x,v_l)+l-1+t}\Bigg) \\
&+\delta_{H_2}(v_l)\Bigg(\sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+t} - \sum_{x\in V(H_1)\setminus\{v_1\}} \frac{1}{d_{H_1}(x,v_1)+l-1+t}\Bigg) > 0,
\end{aligned}
$$

which is equivalent to

$$
\sum_{j=1}^{l}\delta_{G_1}(v_j)\widehat{D}_t(G_1;v_j) < \sum_{j=1}^{l}\delta_{G_2}(v_j)\widehat{D}_t(G_2;v_j). \tag{31}
$$

In view of (27) and (28) and (31), we have $RDD_+^t(G_1) < RDD_+^t(G_2)$. ■

Transformation 5.3. *Let G be an n-vertex connected graph as depicted in Fig. 6, where wv is a cut edge of G, H_1, H_2 are two connected subgraphs, and H_1 contains a path $P_k = w_1w_2\cdots w_k$ satisfying $|V(H_1)| \geq l+2$ and $|V(P_k)| \geq |V(P_l)|$. Let $G' = G - \{vx : x \in N_{H_2}(v)\} + \{wx : x \in N_{H_2}(v)\}$. We call $G \Rightarrow G'$ the θ_2-transformation.*

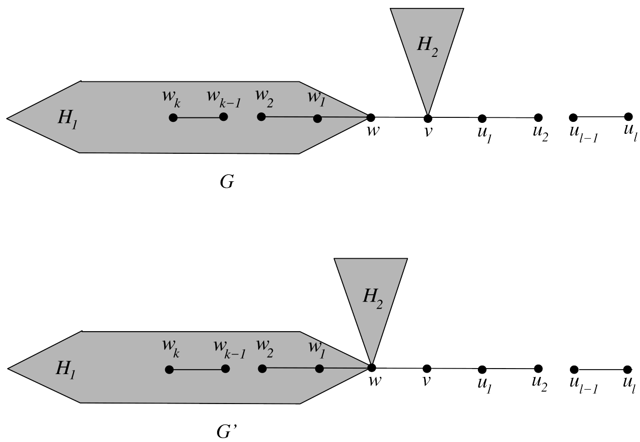

Figure 6. G' is obtained from G by θ_2-transformation.

In particular, if H_1 (resp. H_2) is a tree, Ilić [36] used Transformation 5.3 to study the Laplacian coefficients of trees; Geng et al. [29] used this transformation to study the eccentric distance sum of trees; Meng and coauthors [47] used θ_2-transformation to study the property of the reciprocal sum-degree distance of trees.

Theorem 5.4. *([48]) Let G' be the n-vertex connected graph obtained from G by Transformation 5.3 with $G' \neq G$, where G' and G are depicted in Fig. 6. Then $RDD_+^t(G) < RDD_+^t(G')$.*

Proof. Let $P_l = u_1u_2\cdots u_l$. Note that H_1 contains a path $P_k = w_1w_2\cdots w_k$ whose length is no less than that of P_l. For convenience, we distinguish the following cases.

• For all vertex $x \in V(H_1) \setminus V(P_k)$, we have

$$\begin{aligned}\widehat{D}_t(G;x) &= \sum_{y\in V(H_1)\setminus\{x,w\}} \frac{1}{d_{H_1}(x,y)+t} + \frac{1}{d_{H_1}(x,w)+t}\\ &\quad + \sum_{j=1}^{l} \frac{1}{d_{H_1}(x,w)+1+j+t} + \frac{1}{d_{H_1}(x,w)+1+t}\\ &\quad + \sum_{y\in V(H_2)} \frac{1}{d_{H_1}(x,w)+1+d_{G[V(H_2)\cup\{v\}]}(y,v)+t},\end{aligned}$$

and

$$\begin{aligned}\widehat{D}_t(G';x) &= \sum_{y\in V(H_1)\backslash\{x,w\}}\frac{1}{d_{H_1}(x,y)+t}+\frac{1}{d_{H_1}(x,w)+t}\\&+\sum_{j=1}^{l}\frac{1}{d_{H_1}(x,w)+j+1+t}+\frac{1}{d_{H_1}(x,w)+1+t}\\&+\sum_{y\in V(H_2)}\frac{1}{d_{H_1}(x,w)+1+d_{G'[V(H_2)\cup\{w\}]}(y,w)+t},\end{aligned}$$

where $d_{G[V(H_2)\cup\{v\}]}(y,v)=d_{G'[V(H_2)\cup\{w\}]}(y,w)$ for each vertex y in H_2. Hence, it is routine to check that $\widehat{D}_t(G;x)<\widehat{D}_t(G';x)$. Note that, for each vertex x in $V(H_1)\backslash V(P_k)$, one has $\delta_G(x)=\delta_{H_1}(x)=\delta_{G'}(x)$. Hence,

$$\sum_{x\in V(H_1)\backslash V(P_k)}\delta_G(x)\widehat{D}_t(G;x)<\sum_{x\in V(H_1)\backslash V(P_k)}\delta_{G'}(x)\widehat{D}_t(G';x). \tag{32}$$

• For each vertex x in $V(H_2)$, we have

$$\begin{aligned}\widehat{D}_t(G;x) &= \sum_{y\in V(H_2)\backslash\{x\}}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,y)+t}+\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+t}\\&+\sum_{j=1}^{l}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+t}+\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+t}\\&+\sum_{y\in V(H_1)\backslash\{V(P_k),w\}}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+d_{H_1}(y,w)+t}\\&+\sum_{j=1}^{k}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+d_{H_1}(w_j,w)+1+t},\end{aligned}$$

$$\begin{aligned}\widehat{D}_t(G';x) &= \sum_{y\in V(H_2)\backslash\{x\}}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,y)+t}+\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+t}\\&+\sum_{j=1}^{l}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+1+t}+\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+1+t}\\&+\sum_{y\in V(H_1)\backslash\{V(P_k),w\}}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+d_{H_1}(y,w)+t}\\&+\sum_{j=1}^{k}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+d_{H_1}(w_j,w)+t}.\end{aligned}$$

Note that $d_{H_1}(w_j,w)\le j$ for each $j\in\{1,2,\cdots,l\}$, we have

$$\widehat{D}_t(G';x)-\widehat{D}_t(G;x) \;=\; \sum_{j=1}^{l}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+1+t}$$

$$
\begin{aligned}
- & \sum_{j=1}^{l} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+t} \\
+ & \sum_{j=1}^{k} \frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+t} \\
- & \sum_{j=1}^{k} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+1+t} \\
+ & \sum_{y\in V(H_1)\setminus\{V(P_k),w\}} \left(\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+d_{H_1}(y,w)+t} \right. \\
- & \left. \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+d_{H_1}(y,w)+t} \right) > 0.
\end{aligned} \tag{33}
$$

In what follows, we shall show the above inequality holds. If $k = l$, then $|V(H_1) \setminus \{V(P_k), w\}| \geq 1$ since $|V(H_1)| \geq l+2$. Hence, $\widehat{D}_t(G';x) - \widehat{D}_t(G;x) > 0$. Otherwise, we obtain $k \geq l+1$. Combining with the condition $|V(H_1) \setminus \{V(P_k), w\}| \geq 0$, it yields that $\widehat{D}_t(G';x) - \widehat{D}_t(G;x) > 0$. In addition, for each vertex x in H_2, one has $\delta_G(x) = \delta_{H_2}(x) = \delta_{G'}(x)$. Hence,

$$
\sum_{x\in V(H_2)} \delta_G(x)\widehat{D}_t(G;x) < \sum_{x\in V(H_2)} \delta_{G'}(x)\widehat{D}_t(G';x). \tag{34}
$$

• For each vertex u_j in P_l, $1 \leq j \leq l$, we have

$$
\begin{aligned}
\widehat{D}_t(G;u_j) =& \widehat{D}_t(P_l;u_j) + \frac{1}{j+t} + \frac{1}{j+1+t} + \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+t} \\
&+ \sum_{j=1}^{k} \frac{1}{j+1+d_{H_1}(w_i,w)+t} + \sum_{x\in V(H_1)\setminus\{V(P_k),w\}} \frac{1}{j+1+d_{H_1}(x,w)+t},
\end{aligned}
$$

and

$$
\begin{aligned}
\widehat{D}_t(G';u_j) =& \widehat{D}_t(P_l;u_j) + \frac{1}{j+t} + \frac{1}{j+1+t} + \sum_{x\in V(H_2)} \frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+1+t} \\
&+ \sum_{j=1}^{k} \frac{1}{j+1+d_{H_1}(w_i,w)+t} + \sum_{x\in V(H_1)\setminus\{V(P_k),w\}} \frac{1}{j+1+d_{H_1}(x,w)+t}.
\end{aligned}
$$

Let $\Lambda_3 = \sum_{j=1}^{l} \delta_{G'}(u_j)\widehat{D}_t(G';u_j) - \sum_{j=1}^{l} \delta_G(u_j)\widehat{D}_t(G;u_j)$. It yields that

$$
\begin{aligned}
\Lambda_3 \geq & \sum_{j=1}^{l} \delta_G(u_j) \sum_{x\in V(H_2)} \frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+1+t} \\
& - \sum_{j=1}^{l} \delta_G(u_j) \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+t} \\
& = \sum_{x\in V(H_2)} \frac{-2}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+t} + \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+l+t} \\
& + \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+l+1+t}.
\end{aligned} \tag{35}
$$

• For each vertex w_j in P_k, $1 \leq j \leq k$, one has $\delta(w_j) = \delta_{G'}(w_j) = \delta_G(w_j)$. Hence,

$$
\begin{aligned}
\widehat{D}_t(G;w_j) = & \sum_{i\neq j} \frac{1}{d_{H_1}(w_i,w_j)+t} + \frac{1}{d_{H_1}(w,w_j)+t} + \frac{1}{d_{H_1}(w,w_j)+1+t} \\
& + \sum_{x\in V(H_1)\setminus\{V(P_k),w\}} \frac{1}{d_{H_1}(x,w_j)+t} + \sum_{i=1}^{l} \frac{1}{d_{H_1}(w,w_j)+1+i+t} \\
& + \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+d_{H_1}(w,w_j)+1+t},
\end{aligned}
$$

and

$$
\begin{aligned}
\widehat{D}_t(G';w_j) = & \sum_{i\neq j} \frac{1}{d_{H_1}(w_i,w_j)+t} + \frac{1}{d_{H_1}(w,w_j)+t} + \frac{1}{d_{H_1}(w,w_j)+1+t} \\
& + \sum_{x\in V(H_1)\setminus\{V(P_k),w\}} \frac{1}{d_{H_1}(x,w_j)+t} + \sum_{i=1}^{l} \frac{1}{d_{H_1}(w,w_j)+1+i+t} \\
& + \sum_{x\in V(H_2)} \frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+d_{H_1}(w,w_j)+t}.
\end{aligned}
$$

Let $\Lambda_4 = \sum_{j=1}^{k} \delta_{G'}(w_j)\widehat{D}_t(G';w_j) - \sum_{j=1}^{k} \delta_G(w_j)\widehat{D}_t(G;w_j)$. Since $d_{H_1}(w,w_j) \leq j$ for each $j \in \{1,2,\cdots,k\}$, we have

$$
\begin{aligned}
\Lambda_4 \geq & \sum_{j=1}^{k} \delta_G(w_j) \sum_{x\in V(H_2)} \frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+j+t} \\
& - \sum_{j=1}^{k} \delta_G(w_j) \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+j+1+t} \\
& \geq \sum_{x\in V(H_2)} \frac{2}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+t} - \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+k+t} \\
& - \sum_{x\in V(H_2)} \frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+k+1+t},
\end{aligned} \tag{36}
$$

where the inequality (36) follows by $\delta(w_j)\geq 2$ for $1\leq j\leq k-1$ and $d(w_k)\geq 1$.
Hence, in view of (35), (36) and $k\geq l$, we obtain

$$\begin{aligned}\Lambda_3+\Lambda_4\geq &\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+l+t}+\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+l+1+t}\\ &-\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+k+t}-\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+k+1+t}\geq 0,\end{aligned}$$

which is equivalent to

$$\sum_{j=1}^{l}\delta_G(u_j)\widehat{D}_t(G;u_j)+\sum_{j=1}^{k}\delta_G(w_j)\widehat{D}_t(G;w_j)\leq\sum_{j=1}^{l}\delta_{G'}(u_j)\widehat{D}_t(G';u_j)+\sum_{j=1}^{k}\delta_{G'}(w_j)\widehat{D}_t(G';w_j).\qquad(37)$$

• For vertices w and v. By the definition of $\widehat{D}_t(G;u)$, we have

$$\begin{aligned}\widehat{D}_t(G;w)=&\sum_{x\in V(H_1)\backslash\{w\}}\frac{1}{d_{H_1}(x,w)+t}+\frac{1}{1+t}+\sum_{j=1}^{l}\frac{1}{j+1+t}\\ &+\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+1+t}.\end{aligned}$$

$$\begin{aligned}\widehat{D}_t(G';w)=&\sum_{x\in V(H_1)\backslash\{w\}}\frac{1}{d_{H_1}(x,w)+t}+\frac{1}{1+t}+\sum_{j=1}^{l}\frac{1}{j+1+t}\\ &+\sum_{x\in V(H_2)}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+t}.\end{aligned}$$

$$\begin{aligned}\widehat{D}_t(G;v)=&\sum_{x\in V(H_1)\backslash\{w\}}\frac{1}{d_{H_1}(x,w)+1+t}+\frac{1}{1+t}+\sum_{j=1}^{l}\frac{1}{j+t}\\ &+\sum_{x\in V(H_2)}\frac{1}{d_{G[V(H_2)\cup\{v\}]}(x,v)+t}.\end{aligned}$$

$$\begin{aligned}\widehat{D}_t(G';v)=&\sum_{x\in V(H_1)\backslash\{w\}}\frac{1}{d_{H_1}(x,w)+1+t}+\frac{1}{1+t}+\sum_{j=1}^{l}\frac{1}{j+t}\\ &+\sum_{x\in V(H_2)}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+1+t}.\end{aligned}$$

For convenience, denote $m=\delta_{G[V(H_2)\cup\{v\}]}(v)$, then $\delta_{G'[V(H_2)\cup\{w\}]}(w)=m\geq 1$. Combining with the fact that $\delta_G(w)=\delta_{H_1}(w)+1$, $\delta_G(v)=m+2$, $\delta_{G'}(w)=\delta_{H_1}(w)+m+1$ and $\delta_{G'}(v)=2$, we can obtain that

$$
\begin{aligned}
&\delta_{G'}(w)\widehat{D}_t(G';w)+\delta_{G'}(v)\widehat{D}_t(G';v)-\delta_G(w)\widehat{D}_t(G;w)-\delta_G(v)\widehat{D}_t(G;v)\\
\geq& m\left(\sum_{x\in V(H_1)\backslash\{V(P_k),w\}}\frac{1}{d_{H_1}(x,w)+t}-\sum_{x\in V(H_1)\backslash\{V(P_k),w\}}\frac{1}{d_{H_1}(x,w)+1+t}\right)\\
&+(\delta_{H_1}(w)-1)\left(\sum_{x\in V(H_2)}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+t}\right.\\
&\left.-\sum_{x\in V(H_2)}\frac{1}{d_{G'[V(H_2)\cup\{w\}]}(x,w)+1+t}\right)+m\left(\frac{1}{l+1+t}-\frac{1}{k+1+t}\right),
\end{aligned}
$$

where the inequality follows by the fact $\delta_{H_1}(w,w_j)\leq j$ for each $j\in\{1,2,\cdots,k\}$. Note that $m\geq 1$ and $\delta_{H_1}(w)\geq 1$, hence

$$
\delta_G(w)\widehat{D}_t(G;w)+\delta_G(v)\widehat{D}_t(G;v)<\delta_{G'}(w)\widehat{D}_t(G';w)+\delta_{G'}(v)\widehat{D}_t(G';v). \tag{38}
$$

In view of (32), (34), (37) and (38), we obtain $RDD_+^t(G)<RDD_+^t(G')$. ∎

If taking $H_1=P_k$, $k\geq l+2$, in Theorem 5.4, we immediately obtain the following result.

Corollary 5.5. *([48]) Given a connected graph H with $v\in V(H)$, let $G_{k,l}$ be the graph obtained from H by attaching two pendent paths $P^1=vw_1w_2\cdots w_k$ and $P^2=vu_1u_2\cdots u_l$, respectively, to v of H. Set $G_{k-1,l+1}:=G_{k,l}-w_kw_{k-1}+w_ku_l$. If $k\geq l+2$, we have $RDD_+^t(G_{k,l})<RDD_+^t(G_{k-1,l+1})$.*

A *spider* is a tree with at most one vertex of degree more than 2, which is called the *hub* of the spider (if no vertex of degree more than two, then any vertex can be hub). A *leg* of spider is a path from the hub to one of its leaves.

Let $S(a_1,a_2,\cdots,a_k)$ be a spider with k legs $P^1,P^2,\cdots,P^k$ such that the length of P^i is a_i, $i=1,2,\cdots,k$, satisfying $\sum_{i=1}^k a_i=n-1$. We call $S(a_1,a_2,\cdots,a_k)$ a *balanced spider* if $|a_i-a_j|\leq 1$ for $1\leq i,j\leq k$.

Theorem 5.6. *([48]) Among $\mathscr{T}_n^k$, the balanced spider*

$$
S\left(\underbrace{\left\lfloor\frac{n-k}{k}\right\rfloor,\cdots,\left\lfloor\frac{n-k}{k}\right\rfloor}_{k-r},\underbrace{\left\lceil\frac{n-k}{k}\right\rceil,\cdots,\left\lceil\frac{n-k}{k}\right\rceil}_{r}\right)
$$

maximizes the RDD_+^t value, where $n-1\equiv r(\mod k)$.

Proof. Let T be a tree in $\mathscr{T}_n^k$ such that T has the largest RDD_+^t, then T is a spider. Otherwise, by Theorem 5.5, there exists another n-vertex tree with k leaves, say T', such that $RDD_+^t(T)<RDD_+^t(T')$, a contradiction. Denote $T:=S(a_1,a_2,\cdots,a_k)$. In order to complete the proof, it is sufficient to show that the spider is balanced, i.e., that $|a_i-a_j|\leq 1$, $1\leq i,j\leq k$. If the spider T is not balanced, then T contains two legs of length a_i and a_j such that $|a_i-a_j|\geq 2$. By Corollary 5.5, there exists another spider T'' such that $RDD_+^t(T)<RDD_+^t(T'')$, a contradiction. ∎

5.2 Graphs with given matching number

For a graph G, the *matching number* $\beta(G)$ is the cardinality of a maximum matching of G. In what follows, we are to identify the trees with the maximum RDD_+^t among all n-vertex trees with matching number β. A vertex v is *matched* if it is incident to an edge in the matching; otherwise the vertex is *unmatched.* A vertex is said to be *perfectly matched* if it is matched in all maximum matchings of G.

For convenience, let $\mathscr{T}_n^\beta$ be the set of all n-vertex trees with matching number β. Let T_n^β be the tree obtained from the star graph $S_{n-\beta+1}$ by attaching a pendent edge to each of certain $\beta - 1$ non-central vertices of $S_{n-\beta+1}$. It is easy to see that T_n^β contains an β-matching.

Theorem 5.7. *([48]) For any tree $T \in \mathscr{T}_n^\beta$ with $n \geq 2\beta$, we have*

$$\begin{aligned} RDD_+^t(T) \leq & \frac{(n+3\beta-4)+(n-\beta)^2}{t+1} + \frac{n^2-3n-\beta^2+3\beta}{t+2} \\ & + \frac{(\beta-1)(2n-\beta-4)}{t+3} + \frac{(\beta-1)(\beta-2)}{t+4} \end{aligned} \tag{39}$$

and the equality holds in (39) if and only if T is isomorphic to T_n^β.

Proof. Choose T to be a tree in $\mathscr{T}_n^\beta$ such that $RDD_+^t(T)$ is as larger as possible. Assume that there is a pendent path of length $p > 2$ attached at vertex v in T. We can consider a new tree T' that has two pendent paths attached at v with length of 2 and $p-2$. The matching number of trees T and T' is the same. Using Corollary 5.5, it follows $RDD_+^t(T) < RDD_+^t(T')$, a contradiction to the choice of T. Hence, we can assume all pendent paths have length one or two.

Let v be a vertex of degree $k+l+1$ in T. Suppose that w is a parent of v and that there s paths $vx_{11}x_{12}, vx_{21}x_{22}, \cdots, vx_{k1}x_{k2}$ and t paths $vy_1, vy_2, \cdots, vy_l$ of length attached at v. Denote by

$$\begin{aligned} T' =& T - \{vx_{i1}x_{i2} | i = 1, 2, \cdots, k\} - \{vy_j | j = 1, 2, \cdots, l\} \\ & + \{wx_{i1}x_{i2} | i = 1, 2, \cdots, k\} + \{wy_j | j = 1, 2, \cdots, l\} \end{aligned}$$

and

$$\begin{aligned} T'' =& T - \{vx_{i1}x_{i2} | i = 1, 2, \cdots, k\} - \{vy_j | j = 1, 2, \cdots, l-1\} \\ & + \{wx_{i1}x_{i2} | i = 1, 2, \cdots, k\} + \{wy_j | j = 1, 2, \cdots, l-1\}. \end{aligned}$$

In what follows, we will show that using Transformations $T \Rightarrow T'$ and $T \Rightarrow T''$ the matching number can be invariant.

First we suppose that T is not the extremal graph. If the vertex w is not perfectly matched in T, there exists a matching M of maximum cardinality, such that no edge from M is incident to w. It follows that $\beta(T') = \beta(G \setminus \{w\}) + k + 1 = \beta(G) + k + 1 = \beta(T)$. By Theorem 5.2, we can get $RDD_+^t(T) < RDD_+^t(T')$.

If the vertex w is perfectly matched in T, for each matching M of maximum cardinality, there exists an edge ww_1 from M incident to w. If $ww_1 = vw$, then we have $\beta(T') = \beta(G \setminus \{w\}) + k + 1 = \beta(G) + k + 1 = \beta(T)$. By Theorem 5.2, we can get $RDD_+^t(T) < RDD_+^t(T')$, a contradiction. If

$ww_1 \neq vw$, then $\beta(T'') = \beta(G) + k + 1$ and $RDD^t_+(T) < RDD^t_+(T'')$ by Theorem 5.2, again a contradiction.

By the previous discussion and the choice of T, we obtain that T is isomorphic to T^β_n, which is the uniqure tree with maximum RDD^t_+ in $\mathscr{T}^\beta_n$. By direct calculation, we have

$$\begin{aligned}
RDD^t_+(T^\beta_n) =&(\beta-1)\left[\frac{1}{t+1}+\frac{1}{t+2}+\frac{1}{t+3}(n-\beta-1)+\frac{1}{t+4}(\beta-2)\right]\\
&+2(\beta-1)\left[\frac{2}{t+1}+\frac{1}{t+1}(n-\beta-1)+\frac{1}{t+3}(\beta-2)\right]\\
&+(n-2\beta+1)\left[\frac{1}{t+1}+\frac{1}{t+2}(n-\beta-1)+\frac{1}{t+3}(\beta-1)\right]\\
&+(n-\beta)\left[\frac{n-\beta}{t+1}+\frac{1}{t+2}(\beta-1)\right]\\
=&\frac{(n+3\beta-4)+(n-\beta)^2}{t+1}+\frac{n^2-3n-\beta^2+3\beta}{t+2}\\
&+\frac{(\beta-1)(2n-\beta-4)}{t+3}+\frac{(\beta-1)(\beta-2)}{t+4}
\end{aligned}$$

This completes the proof. ■

5.3 Graphs with given dominating number

A subset S of $V(G)$ is called a *dominating set* of G if for every vertex $v \in V(G) \setminus S$, there exists a vertex $u \in S$ such that v is adjacent to u. A vertex in the dominating set is called a *dominating vertex*. For a dominating set S of graph G with $v \in S$, if $uv \in E(G)$ with $u \in V(G) \setminus S$, then u is said to be *dominated by* v. The *domination number* of G, denoted by $\gamma(G)$, is defined as the minimum cardinality of dominating sets of G. For convenience, let $\mathscr{D}^\gamma_n$ be the set of all n-vertex trees with domination γ.

In what follows, we are to characterize the trees with the maximum RDD^t_+ among n-vertex trees with domination number γ.

Lemma 5.8. *([48]) If $T \in \mathscr{D}^\gamma_n$ has the maximum RDD^t_+, then $\gamma(T) = \beta(T) = \gamma$.*

Proof. It was proved in [33] that $\gamma(G) \leq \beta(G)$ holds for any graph. Hence, it is sufficient to show that $\gamma(T) \geq \beta(T)$. Otherwise, by the definition of $\mathscr{D}^\gamma_n$, we have $\gamma = \gamma(T) < \beta(T)$. Assume that $S = \{v_1, v_2, \cdots, v_\gamma\}$ is a dominating set of cardinality γ. Then there must exist γ independent edges, say $v_1v'_1, v_2v'_2, \cdots, v_\gamma v'_\gamma$, in T. Let $M' = \{v_iv'_i : i = 1, 2, \cdots \gamma\}$. If M' is contained in a matching M of maximum cardinality, then there must exist another edge, say w_1w_2, which is independent of each edge $v_iv'_i$ by $\gamma(T) < \beta(T)$. Otherwise, note that $\gamma(T) < \beta(T)$, there exists an M'-augmenting path $P = u_1u_2 \cdots u_{2t+1}u_{2t+2}$ in T, where $u_{2k}t_{2k+1} = v_kv'_k$, $k = 1, 2, \cdots, t$ and $u_2 = v_1$, $u_{2t+1} = v_t$. Thus, for each pair $u_i, u_j \in S \cap V(P)$, $i < j$, we have $2 \leq j - i \leq 3$. Note that the first (resp. last) domination vertex is u_2 (resp. $u_{2\gamma+1}$), there must exist a pair $u_i, u_j \in S \cap V(P)$ satisfying $j - i = 3$. Without loss of generality, we assume that the smallest value of i for which $u_i, u_{i+3} \in S$ is i_0. Let

$$M'' = \{u_1u_2, u_3u_4, \cdots, u_{i_0-1}u_{i_0}\} \cup \{u_{i_0+3}u_{i_0+4}, u_{i_0+5}u_{i_0+6}, \cdots, u_{2t+1}u_{2t+2}\},$$

then M'' is a matching of cardinality γ, and each edge of M'' contains a vertex from S. It is easy to check that the edge $u_{i_0+1}u_{i_0+2}$ is independent of each edge from M''.

Hence, there must exist $\gamma + 1$ independent edges $v_1v_1', v_2v_2', \cdots, v_\gamma v_\gamma', w_1w_2$ in T. If w_1, w_2 are dominated by the same vertex $v_i \in S$, there would be a triangle $w_1w_2v_i$. This is impossible because of the fact that T is a tree. Therefore we claim that two vertices w_1, w_2 are dominated by two different vertices from S. Without loss of generality, assume that w_i is dominated by the vertex v_i for $i = 1, 2$. Now we construct a new tree $T' \in \mathscr{D}_n^\gamma$ by Transformation 5.1 of T on the edges v_1w_1 and v_2w_2, respectively. It follows from Theorem 5.2 that $RDD_+^t(T) < RDD_+^t(T')$, which contradicts to the choice of T. Thus we complete the proof. ■

Combing Theorem 5.7 and Lemma 5.8, the next result follows immediately.

Theorem 5.9. *([48]) For any tree $T \in \mathscr{D}_n^\gamma$, we have*

$$\begin{aligned} RDD_+^t(T) \leq & \frac{(n+3\gamma-4)+(n-\gamma)^2}{t+1} + \frac{n^2-3n-\gamma^2+3\gamma}{t+2} \\ & + \frac{(\gamma-1)(2n-\gamma-4)}{t+3} + \frac{(\gamma-1)(\gamma-2)}{t+4} \end{aligned} \tag{40}$$

and the equality holds in (40) if and only if T is isomorphic to T_n^γ.

5.4 Graphs with given bipartition

In this subsection, we investigate the property of the reformulated reciprocal sum-degree of trees by using an auxiliary transformation, which will be listed in the following.

Transformation 5.10. *([48]) Let uw be a cut edge of a bipartite graph U with $\delta(w) \geq 2$. Denote by G the graph obtained from U and the star S_{k+2} by identifying u with a pendant vertex of S_{k+2} whose center is v. Let $G[v \to w; 2]$ be the graph obtained from G by deleting all edges vz, $z \in W$ and adding all edges wz, $z \in W$, where $W = N_G(v) \setminus \{u\}$. In notation,*

$$G[v \to w; 2] = G - \{vz : z \in W\} + \{wz : z \in W\},$$

we call $G \Rightarrow G[v \to w; 2]$ the θ_3-transformation, see Fig 7.

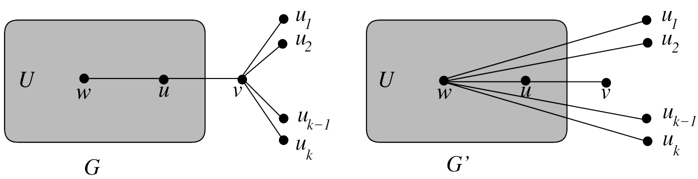

Figure 7. $G' = G[v \to w; 2]$ is obtained from G by θ_3-transformation.

In 2013, Geng et al. [29] used the θ_3-transformation to study the eccentric distance sum of trees. In the same year, Li et al. [49] used this θ_3-transformation to discuss the Laplacian permanent of trees with given bipartition. In [47], the authors explored the property of the reciprocal sum-degree distance of graphs by using the θ_3-transformation. More recently, Li et al. [48] used this Transformation as a significant tool to study the reformulated reciprocal sum-degree distance of trees.

Theorem 5.11. *([48]) Let G and $G[v \to w; 2]$ be the bipartite graphs with some labeled vertices as in Transformation 5.10. Then $RDD_+^t(G) < RDD_+^t(G[v \to w; 2])$.*

Proof. For convenience, let $G' = G[v \to w; 2]$, T_1 be the component in $G - \{wu, uv\}$ which contains u, and $A := V(U) \setminus (V(T_1) \cup \{w\})$. In what follows, we will distinguish the following four possiblities.

• For all vertex $x \in A$, by direct calculation, we have

$$\widehat{D}_t(G;x) = \sum_{y \in A\setminus\{x\}} \frac{1}{d_U(x,y)+t} + \frac{1}{d_U(x,w)+t} + \sum_{y \in V(T_1)} \frac{1}{d_G(x,y)+t} + \frac{1}{d_U(x,w)+2+t} + \frac{k}{d_U(x,w)+3+t}.$$

$$\widehat{D}_t(G';x) = \sum_{y \in A\setminus\{x\}} \frac{1}{d_U(x,y)+t} + \frac{1}{d_U(x,w)+t} + \sum_{y \in V(T_1)} \frac{1}{d_{G'}(x,y)+t} + \frac{1}{d_U(x,w)+2+t} + \frac{k}{d_U(x,w)+1+t}.$$

Note that $\sum_{y \in V(T_1)} \frac{1}{d_G(x,y)+t} = \sum_{y \in V(T_1)} \frac{1}{d_{G'}(x,y)+t}$, hence $\widehat{D}_t(G;x) < \widehat{D}_t(G';x)$. It is routine to check that for all vertex x in A, one has $\delta_G(x) = \delta_U(x) = \delta_{G'}(x)$. Hence,

$$\sum_{x \in A} \delta_G(x)\widehat{D}_t(G;x) < \sum_{x \in A} \delta_{G'}(x)\widehat{D}_t(G';x). \tag{41}$$

• For each vertex x in $V(T_1)$, it is routine to check that $\delta_G(x) = \delta_{T_1}(x) = \delta_{G'}(x)$ and $\widehat{D}_t(G;x) = \widehat{D}_t(G';x)$. Hence,

$$\sum_{x \in V(T_1)} \delta_G(x)\widehat{D}_t(G;x) = \sum_{x \in V(T_1)} \delta_{G'}(x)\widehat{D}_t(G';x). \tag{42}$$

• For each vertex $u_j \in X' = \{u_1, u_2, \cdots, u_k\}$, by direct calculation we have

$$\widehat{D}_t(G;u_j) = \sum_{x \in V(T_1)} \frac{1}{d_G(x,v)+1+t} + \frac{1}{1+t} + + \frac{k-1}{2+t} + \frac{1}{3+t} + \sum_{x \in A} \frac{1}{d_U(x,w)+3+t}.$$

$$\widehat{D}_t(G';u_j) = \sum_{x\in V(T_1)} \frac{1}{d_{G'}(x,w)+1+t} + \frac{1}{1+t} + + \frac{k-1}{2+t} + \frac{1}{3+t}$$
$$+ \sum_{x\in A} \frac{1}{d_U(x,w)+1+t}.$$

It is routine to check that $d_G(x,v) = d_{G'}(x,w)$ for any vertex $x \in V(T_1)$, hence $\widehat{D}_t(G;u_j) < \widehat{D}_t(G';u_j)$. Note that $\delta_G(u_j) = \delta_{G'}(u_j) = 1$ for any $u_j \in X'$. Hence,

$$\sum_{u_j\in X'} \delta_G(u_j)\widehat{D}_t(G;u_j) < \sum_{u_j\in X'} \delta_{G'}(u_j)\widehat{D}_t(G';u_j). \tag{43}$$

• For vertex w and v, by direct calculation we have

$$\begin{aligned}
\widehat{D}_t(G;w) =& \sum_{x\in A} \frac{1}{d_U(x,w)+t} + \sum_{x\in V(T_1)} \frac{1}{d_G(x,w)+t} + \frac{1}{2+t} + \frac{k}{3+t},\\
\widehat{D}_t(G;v) =& \sum_{x\in A} \frac{1}{d_U(x,w)+2+t} + \sum_{x\in V(T_1)} \frac{1}{d_G(x,v)+t} + \frac{1}{2+t} + \frac{k}{1+t},\\
\widehat{D}_t(G';w) =& \sum_{x\in A} \frac{1}{d_U(x,w)+t} + \sum_{x\in V(T_1)} \frac{1}{d_{G'}(x,w)+t} + \frac{1}{2+t} + \frac{k}{1+t},\\
\widehat{D}_t(G';v) =& \sum_{x\in A} \frac{1}{d_U(x,w)+2+t} + \sum_{x\in V(T_1)} \frac{1}{d_{G'}(x,v)+t} + \frac{1}{2+t} + \frac{k}{3+t}.
\end{aligned}$$

It is sufficient to show that $\Lambda_5 = \delta_{G'}(w)\widehat{D}_t(G';w) + \delta_{G'}(v)\widehat{D}_t(G';v) - \delta_G(w)\widehat{D}_t(G;w) - \delta_G(v)\widehat{D}_t(G;v) > 0$. In fact, note that $\delta_G(w) = \delta_U(w)$, $\delta_G(v) = k+1$, $\delta_{G'}(w) = \delta_U(w)+k$ and $\delta_{G'}(v) = 1$. In addition, for each vertex x in T_1, $d_G(x,w) = d_G(x,v) = d_{G'}(x,w) = d_{G'}(x,v)$, hence

$$\begin{aligned}
\Lambda_5 =& k\left(\sum_{x\in A} \frac{1}{d_U(x,w)+t} + \sum_{x\in V(T_1)} \frac{1}{d_{G'}(x,w)+t} + \frac{1}{2+t}\right)\\
&-k\left(\sum_{x\in A} \frac{1}{d_U(x,w)+2+t} + \sum_{x\in V(T_1)} \frac{1}{d_{G'}(x,v)+t} + \frac{1}{2+t}\right)\\
&+\frac{k}{1+t}(\delta_U(w)+k) - \frac{k}{3+t}\delta_U(w) + \frac{k}{3+t} - \frac{k(k+1)}{1+t}\\
>& k(\delta_U(w)-1)\left(\frac{1}{t+1} - \frac{1}{t+3}\right) > 0.
\end{aligned}$$

Hence,

$$\delta_G(w)\widehat{D}_t(G;w) + \delta_G(v)\widehat{D}_t(G;v) < \delta_{G'}(w)\widehat{D}_t(G';w) + \delta_{G'}(v)\widehat{D}_t(G';v). \tag{44}$$

Combing with (41), (42), (43)) and (44) yields $RDD_+^t(G) < RDD_+^t(G')$. ■

For a given n-vertex connected graph G satisfying its vertex set can be partitioned into two subsets V_1 and V_2, such that each edge joins a vertex in V_1 with a vertex in V_2. Suppose that V_1 has p vertices and V_2 has q vertices, where $p+q=n$. Then we say that G has a (p,q)-*bipartition*, $p \leq q$.

Let $\mathscr{T}_n^{p,q}$ the set of all n-vertex trees with a (p,q)-bipartition. In particular, S_n is an element of $\mathscr{T}_n^{1,n-1}$, and $\mathscr{T}_n^{2,n-2} = \{P_3(a,b) : a+b=n-3\}$, where $P_3(a,b)$ is obtained from P_3 by attaching a and b leaves to the endvertices of P_3, respectively.

Theorem 5.12. *([48]) Given positive integers p and q with $p \leq q$ and $p+q=n$.*

($\mathbf{a}$) If $p=2$, then we order all the numbers in $\mathscr{T}_n^{2,q}$ as follows:

$$\begin{aligned} RDD_+^t(P_3(0,n-3)) >& RDD_+^t(P_3(1,n-4)) > RDD_+^t(P_3(2,n-5)) > \cdots \\ >& RDD_+^t\left(P_3\left(\left\lfloor\frac{n-3}{2}\right\rfloor, \left\lceil\frac{n-3}{2}\right\rceil\right)\right). \end{aligned}$$

($\mathbf{b}$) If $p>2$, then for any $T \in \mathscr{T}_n^{p,q}$ we have

$$RDD_+^t(T) \leq \frac{n^2+n-2}{t+1} + \frac{(n-1)(n-2)}{t+2} + \frac{2-2n}{t+3} - 2pq\left(\frac{1}{t+1} - \frac{1}{t+3}\right).$$

The equality holds if and only if T is isomorphic to $T(p,q)$, where $T(p,q)$ is a double star with n vertices, which is obtained from an edge vw by attaching $p-1$ (resp. $q-1$) pendent edges to v (resp. w).

Proof. By direct calculation, we have

$$\begin{aligned} RDD_+^t(P_3(a-1,b+1)) -& RDD_+^t(P_3(a,b)) \\ =& \frac{2+2b-2a}{t+1} + \frac{2+2b-2a}{t+2} + \frac{2a-2b-2}{t+3} + \frac{2a-2b-2}{t+4} \\ =& (2b-2a+2)\left(\frac{1}{t+1} + \frac{1}{t+2} - \frac{1}{t+3} - \frac{1}{t+4}\right) > 0. \end{aligned}$$

This implies the proof of ($\mathbf{a}$).

For a given T in $\mathscr{T}_n^{p,q}$, by repeatedly applying Transformation 5.10 to T yields that $T(p,q)$ is the unique tree in $\mathscr{T}_n^{p,q}$ which has the maximum RDD_+^t value. By elementary calculation, we have

$$\begin{aligned} RDD_+^t(T(p,q)) =& (p-1)\left[\frac{1}{t+1} + \frac{1}{t+2}(p-1) + \frac{1}{t+3}(q-1)\right] \\ &+ p\left[\frac{p}{t+1} + \frac{1}{t+2}(q-1)\right] + q\left[\frac{q}{t+1} + \frac{1}{t+2}(p-1)\right] \\ &+ (q-1)\left[\frac{1}{t+1} + \frac{1}{t+2}(q-1) + \frac{1}{t+3}(p-1)\right] \\ =& \frac{p^2+q^2+p+q-2}{t+1} + \frac{(p+q-1)(p+q-2)}{t+2} + \frac{2(p-1)(q-1)}{t+3} \\ =& \frac{n^2+n-2}{t+1} + \frac{(n-1)(n-2)}{t+2} + \frac{2-2n}{t+3} - 2pq\left(\frac{1}{t+1} - \frac{1}{t+3}\right). \end{aligned}$$

This completes the proof of ($\mathbf{b}$). ■

6. Conclusion

In this chapter we examined various extremal problems related to the reciprocal sum-degree distance and the reciprocal product-degree distance as well as their generalized versions. We were particularly interested in the following two problems:

• finding lower and upper sharp bounds for the reciprocal sum-degree distance and the reciprocal product-degree distance and its congeners, and

• characterizing the graphs for which the reciprocal sum-degree distance (resp. the reciprocal product-degree distance) and its congeners assume extremal (minimum or maximum) values.

Researches on these extremal aspects of the theory of the reciprocal sum-degree distance and reciprocal product-degree distance started more recently. However, once the non-triviality and mathematical beauty of the problems encountered, a remarkable activity has begun, resulting in scores of papers published in mathematical and chemical journals. Almost most all relevant results were obtained in the last five years.

Our ambition was to investigate the majority of results concerned with the above stated topics, to state them in a mathematically rigorous manner, and to provide proofs thereof. We tried to be as updated as possible, which was a near-to-impossible task since new results continue to emerge almost each month. Anyway, this chapter should offer a nearly complete survey of the extremal aspects of the results on the reciprocal sum-degree and the reciprocal product-degree distance up to year 2016.

At the very end we would like to state some open problems which-in our opinion-are most interesting from a mathematical point of view. It would be interesting to explore mathematical properties and possible predictive of the reformulated reciprocal product-degree distance. Another interesting problem would be to investigate this graph invariant for various nanostructures. Since even the simplest nanostructures, the C_4 nanotubes and nanotori, arise as the Cartesian products of paths and cycles, and since the Harary-type indices do not allow for nice expressions for such structures, there is not much hope of deriving explicit formulas of the reformulated reciprocal product-degree distance. However, it might be possible to extract certain information of the asymptotic behavior of reformulated reciprocal sum-product distance.

Errors, flaws, omissions are inevitable in a text of this kind. The author will be most grateful to those who point out such weak points of their investigation, and will appreciate any criticism thereof.

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Some Bounds on the Eccentricity–Based Topological Indices of Graphs

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Abstract

The eccentricity $\varepsilon_G(v_i)$ of a vertex v in a graph G is the maximum distance from v_i to other vertices in G. As a fundamental concept in pure graph theory, the eccentricity has also been frequently used in chemical graph theory. There is a large family of eccentricity-based topological indices of (molecular) graphs, such as Zagreb eccentricity indices, eccentric connectivity index (ECI), connective eccentricity index (CEI) and average eccentricity, *etc*. In this chapter we present some upper or lower bounds on these eccentricity-based topological indices and characterize the corresponding extremal graphs at which the bounds are attained.

Contents

1. Introduction

We only consider finite, undirected, simple and connected graphs throughout this paper. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots\ldots, v_n\}$ and edge set $E(G)$. The *degree* of $v_i \in V(G)$, denoted by $\deg_G(v_i)$, is the number of vertices in G adjacent to v. For any two vertices v_i, v_j in a graph G, the distance between them, denoted by $d_G(v_i, v_j)$, is the length (i.e., the number of edges) of a shortest path connecting them in G. Other undefined notations and terminology on the graph theory can be found in [8].

For any vertex of graph G, the eccentricity $\varepsilon_G(v_i)$ is the maximum distance from v_i to other vertices of G, that is, $\varepsilon_G(v_i) = \max_{v_j \neq v_i} d_G(v_i, v_j)$. If $\varepsilon_G(v_i) = d_G(v_i, v_j)$, then v_j is an *eccentric vertex* of vertex v_i. Moreover, $rad(G) = \min_{v_i \in V(G)} \{\varepsilon_G(v_i)\}$ and $diam(G) = \max_{v_i \in V(G)} \{\varepsilon_G(v_i)\}$ are called the *radius* and the *diameter* of graph G, respectively. The *center* $C(G)$ and the *periphery* $P(G)$ of G is the set of vertices of minimum, respectively maximum, eccentricity in it, their elements are called *central*, resp. *peripheral*, vertices. In particular, two peripheral vertices v_i, v_j form a *diametrical pair* in a graph G if $d_G(v_i, v_j) = diam(G)$. The *eccentricity sequence* of a graph G is just a set of eccentricities of its vertices, that is, $\mathcal{E}(G) = \{\varepsilon_G(v_i) : v_i \in V(G)\}$. If the eccentricity $\varepsilon_G(v_i)$ appears $l_i \geq 1$ times in $\mathcal{E}(G)$, we will write $\varepsilon_G(v_i)^{(l_i)}$ in it for short. For any graph G, we denote by $\overline{G}$ the complement of G. As usual, let P_n, C_n, K_n be the path graph, cycle graph and complete graph, respectively, on n vertices.

As a special distance of graphs, the eccentricity of a vertex has some important applications in other scientific branches. In pure graph theory, there are several special eccentricity-based graphs. Any graph G with $C(G) = V(G)$ is called a self-centered graph [9]. Recently, based on the application of vertex eccentricity to location theory [10], two novel classes of graphs with specific central structure have been defined. A graph with $|C(G)| = |V(G)| - 2$, or $|P(G)| = |V(G)| - 1$, respectively, is called an *almost self-centered (ASC) graph* [7, 33], or *almost-peripheral (AP) graph* [35], respectively. An ASC (AP, resp.) graph with radius r is called an r-ASC (r-AP, resp.) graph. A graph G with $|C(G)| = |V(G)| - 2$ is called a weak almost-peripheral (WAP) graph [55].

In chemical graph theory, various graphical invariants are used for establishing correlations of chemical structures with various physical properties, chemical reactivity, or biological activity. These graphical invariants are called topological indices of (molecular) graphs in this field. There is a large family of distance-based topological indices of (molecular) graphs in chemical graph theory. They include Wiener index [16, 50] as the well-known and oldest topological index, hyper-Wiener index [32, 43], Harary index [31, 41, 56], and so on. Moreover, there are some eccentricity-based topological indices in chemical graph theory. In 2000, Gupta *et al.* [21] introduced a novel, adjacency-cum-path length based, topological descriptor named as *connective eccentricity index* (CEI) when investigating the antihypertensive activity of derivatives of N-benzylimidazole. And the connective eccentricity index of a (molecular) graph G is just

$$\xi^{ce}(G) = \sum_{v_i \in V(G)} \frac{\deg_G(v_i)}{\varepsilon_G(v_i)}.$$

Moreover, in [21], they showed that the results obtained using the connective eccentricity index were better than the corresponding values obtained using Balaban's mean square distance index [4, 5] and the accuracy of prediction was found to be about 80 percents in the active range [21]. See [1, 54, 57, 59] for recent results on the CEI of graphs. Moreover, Sharma et al. [44] introduced the *eccentric connectivity index* (ECI) for a graph G, defined below:

$$\xi^{c}(G) = \sum_{v_i \in V(G)} \deg_G(v_i)\varepsilon_G(v_i),$$

which has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [20, 44, 46]. Some mathematical and chemical properties of ECI have been reported in [2, 3, 30, 39, 40, 60, 61].

In analogy with the first and second Zagreb indices [25, 26] of graphs, D. Vukičević and A. Graovac [49] defined the first and second *Zagreb eccentricity Zagreb indices* as follows:

$$E_1(G) = \sum_{v_i \in V(G)} \varepsilon_G(v_i)^2, \qquad E_2(G) = \sum_{v_i v_j \in E(G)} \varepsilon_G(v_i)\varepsilon_G(v_j)\ .$$

Some mathematical properties of E_1 and E_2 can be found in [11, 17, 51]. And the *average eccentricity* [10] of an n-vertex graph G is defined as

$$avec(G) = \frac{1}{n} \sum_{v_i \in V(G)} \varepsilon_G(v_i)\ .$$

Very recently, the present author, Das and Maden [55] introduced a novel eccentricity-based invariant named as *non-self-centrality number* of a graph G as follows:

$$N(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} |\varepsilon_G(v_i) - \varepsilon_G(v_j)|\,,$$

which is used for measuring the non-self-centrality of all non-self-centered graphs. Some nice results on other attractive distance-based topological indices of graphs can be found in a survey paper [53] and the references therein.

In this chapter we report some upper and lower bounds on these above *eccentricity-based topological indices* (hereafter denoted by EBTI for short). In Section 2, we list some upper and lower bounds on EBTI of various sets of graphs. In Section 3, several bounds on EBTI are established in terms of other topological indices.

2. Some bounds on EBTI of graphs from various sets

In this section we propose some upper and lower bounds on EBTI of graphs from many distinct classes. And the corresponding extremal graphs are also characterized at which the upper (or lower) bounds on EBTI are attained.

2.1 Trees

As we all know, a tree is a connected acyclic graph, which can be viewed as the simplest case of connected graphs and so be a starting point when studying on some research topic in graph theory. In this subsection we focus on the upper and lower bounds on EBTI of general and special trees, respectively. First we limit our attention into the set of general trees. For $n = 2$ or 3, there is a single tree P_n of order n. Therefore we always consider a tree of order $n \geq 4$.

In the following five theorems we focus on the upper and lower bounds on EBTI of general trees of $n \geq 4$ with the corresponding extremal trees.

Theorem 2.1. ([11]) *Let T be a tree of order $n \geq 4$. Then*

(1) $E_1(S_n) \leq E_1(T) \leq E_1(P_n)$ *with the left equality holding if and only if $T \cong S_n$ and the right equality holding if and only if $T \cong P_n$;*

(2) $E_2(S_n) \leq E_2(T) \leq E_2(P_n)$ *with the left equality holding if and only if $T \cong S_n$ and right equality holding if and only if $T \cong P_n$.*

Theorem 2.2. ([29]) *Let T be a tree of order $n \geq 4$. Then*

$$avec(S_n) \leq avec(T) \leq avec(P_n)$$

with left equality holding if and only if $T \cong S_n$, right holding if and only if $T \cong P_n$.

Theorem 2.3. ([61]) *Let T be a tree of order $n \geq 4$. Then*

$$\xi^c(S_n) \leq \xi^c(T) \leq \xi^c(P_n)$$

with left equality holding if and only if $T \cong S_n$, right holding if and only if $T \cong P_n$.

Theorem 2.4. ([57,59]) *Let T be a tree of order $n \geq 4$. Then*

$$\xi^{ce}(P_n) \leq \xi^{ce}(T) \leq \xi^{ce}(S_n)$$

with left equality holding if and only if $T \cong P_n$ and right equality holding if and only if $T \cong S_n$.

Theorem 2.5. ([55]) *Let T be a tree of order $n \geq 4$. Then*

$$N(S_n) \leq N(T) \leq N(P_n)$$

with left equality holding if and only if $T \cong S_n$, right holding if and only if $T \cong P_n$.

Next we turn to the results for special trees. Before doing it, we first introduce some notations. A *dumbbell* $D_n(a, b)$ with $1 \leq a \leq b$ is a tree obtained from a path P_{n-a-b} by attaching a independent vertices to one pendant vertex of P_{n-a-b} and b independent vertices to the other pendant vertex. In particular, for an integer $d \geq 2$, a dumbbell $D_n(1, n-d)$ is a just a *broom* with diameter d and will be denoted by $B_{n,d}$ in the following. And *volcano graph* $V_{n,d}$ is a tree obtained from a path P_{d+1} by attaching $n-d-1$ pendant vertices to a central vertex (for odd d) or two adjacent central vertices (for even d) of P_d. Note that the tree $V_{n,d}$ is not unique if d is even with $d < n-2$. As two examples, $D_{10}(2, 3)$ and $B_{11,7}$ are shown in Figures 1 and 2, respectively. And $V_{10,6}$, $V_{12,7}$ are given in Figure 3.

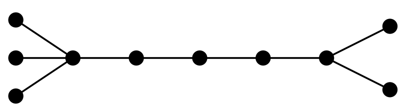

Figure 1. The tree $D_{10}(2, 3)$

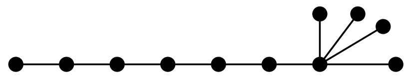

Figure 2. The tree $B_{11,7}$

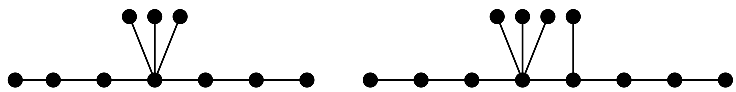

Figure 3. The tree $V_{10,6}$ (left) and a tree $V_{12,7}$ (right)

Theorem 2.6. ([51]) *Let T be a tree of order $n \geq 4$ and with diameter $d > 2$. Then*

$$E_i(V_{n,d}) \leq E_i(T) \leq E_i(D_n(a,b)) \text{ for } i = 1, 2$$

with left equality holding if and only if $T \cong V_{n,d}$, and right holding if and only if $T \cong D_n(a,b)$ with $a + b = n - d + 1$.

Theorem 2.7. ([39]) *Let T be a tree of order $n \geq 4$ and with diameter $d > 2$. Then*

$$\xi^c(V_{n,d}) \leq \xi^c(T) \leq \xi^c(B_{n,d})$$

with left equality holding if and only if $T \cong V_{n,d}$, right holding if and only if $T \cong B_{n,d}$.

Theorem 2.8. ([59]) *Let T be a tree of order $n \geq 4$ and with diameter $d > 2$. Then*

$$\xi^{ce}(D_n(a,b)) \leq \xi^{ce}(T)$$

with equality holding iff $T \cong D_n(a,b)$ with $a + b = n - d + 1$.

A *caterpillar* [27], denoted by $P^n_{k+1}(a_2, a_3, \ldots, a_k)$ with $\sum_{i=2}^{k} a_i = n - k - 1$, is a tree of order n with diameter k obtained from a path $P_{k+1} = v_1 v_2 \cdots v_{k+1}$ by attaching $a_i \geq 0$ pendant vertices to the vertex v_i for $i = 2, 3, \ldots, k$. If k is even, $a_2 + a_k + a_{\frac{k}{2}+1} = n - k - 1$ with $a_2, a_k > 0$ and $|a_2 + a_k - a_{\frac{k}{2}+1}| \leq 2$, then $P^n_{k+1}(a_2, a_3, \ldots, a_k)$ is called a *balanced caterpillar* and denoted by $BC_{n,k}$. When k is odd, the balanced caterpillar can be defined in parallel but two central vertices $v_{\frac{k+1}{2}}$ and $v_{\frac{k+3}{2}}$ in P_{k+1} with $|a_2 + a_k - a_{\frac{k+1}{2}} - a_{\frac{k+3}{2}}| \leq 2$ must be considered in the process. AS an example, some balanced caterpillar $BC_{12,7}$ is shown in Figure 4.

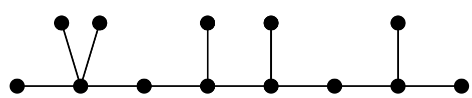

Figure 4. Some tree $BC_{12,7}$

Theorem 2.9. ([55]) *Let T be a tree of order n and with diameter d. Then*

$$N(T) \leq N(T^*)$$

with equality holding if and only if $T \cong T^*$ where T^* is isomorphic to some $BC_{n,d}$.

Next we turn to the determination of upper and lower bounds on EBTI of trees with a given matching number. And $S_{n,\beta}$ is a tree obtained from star $S_{n-\beta+1}$ by attaching a pendant edge to each $\beta - 1$ pendant vertices in $S_{n-\beta+1}$. The *Volkmann tree* [19] $VT_{n,\Delta}$ is obtained in the following way:

Starting with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. In the last level, while not all vertices need to exist, the existing vertices fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1. Some mathematical and chemical properties of Volkmann trees can be found in [36].

As two examples, the trees $S_{10,4}$ and $VT_{22,4}$ are shown in Figures 5 and 6, respectively.

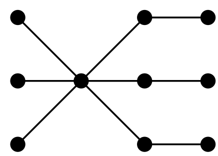

Figure 5. The tree $S_{10,4}$

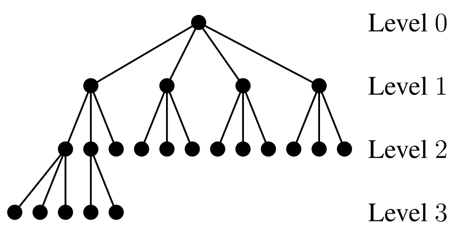

Figure 6. The tree $VT_{22,4}$

Theorem 2.10. ([51]) *Let T be a tree of order $n \geq 4$ and matching number $\beta \geq 2$. Then*

$$E_i(T) \geq E_i(S_{n,\beta}) \;\; where \;\; i = 1, 2$$

with equality holding if and only if $T \cong S_{n,\beta}$.

Theorem 2.11. ([54]) *Let T be a tree of order $n \geq 4$ and matching number $\beta \geq 2$. Then*

$$\xi^c(S_{n,\beta}) \leq \xi^c(T) \leq \xi^c(D_n(a,b))$$

with left equality holding if and only if $T \cong S_{n,\beta}$, right holding if and only if $T \cong D_n(a,b)$ with $a + b = n - 2\beta + 1$.

Theorem 2.12. ([54]) *Let T be a tree of order $n \geq 4$ and matching number $\beta \geq 2$. Then*

$$\xi^{ce}(D_n(a,b)) \leq \xi^{ce}(T) \leq \xi^{ce}(S_{n,\beta})$$

with left equality holding if and only if $T \cong D_n(a,b)$ where $a+b = n-2\beta+1$, right holding if and only if $T \cong S_{n,\beta}$.

Theorem 2.13. ([30]) *Let T be a tree of order $n \geq 4$ and with maximum degree $\Delta > 2$. Then*

$$\xi^{c}(VT_{n,\Delta}) \leq \xi^{c}(T) \leq \xi^{c}(B_{n,n-\Delta})$$

with left equality holding if and only if $T \cong VT_{n,\Delta}$, right holding if and only if $T \cong B_{n,n-\Delta}$.

Theorem 2.14. ([29]) *Let T be a tree of order $n \geq 4$ and with maximum degree $\Delta > 2$. Then*

$$avec(T) \leq avec(B_{n,n-\Delta})$$

with equality holding if and only if $T \cong B_{n,n-\Delta}$.

Theorem 2.15. ([17]) *Let T be a tree of order $n \geq 4$ and with maximum degree $\Delta > 2$. Then*

$$E_i(T) \leq E_i(B_{n,n-\Delta}) \;\; for \;\; i = 1,2$$

with equality holding if and only if $T \cong B_{n,n-\Delta}$.

2.2 General graphs

In this subsection we report some upper or lower bounds on EBTI of general graphs. Recall that an (n,m)-graph is a connected graph of order n and with m edges. In particular, an (n,n)-graph is a unicyclic graph of order n, an $(n,n+1)$-graph is a bicyclic graph with n vertices. Clearly a unicyclic graph has $n \geq 3$ vertices, and a unicyclic graph of order 3 is just a triangle C_3. And a bicyclic graph has at least 4 vertices.

Theorem 2.16. ([17]) *Let G be a unicyclic graph of order $n \geq 4$. Then*

$$E_i(G) \geq E_i(S_n^+) \;\; for \;\; i = 1,2$$

with the equality holding if and only if $G \cong S_n^+$ where and hereafter S_n^+ is a graph obtained by adding one edge to the star S_n.

Denote by $\mathcal{B}_n^*$ the set of two bicyclic graphs of order n obtained by two edges to the star S_n.

Theorem 2.17. ([17]) *Let G be a bicyclic graph of order $n \geq 4$. Then*

$$E_i(G) \geq E_i(G^*) \;\; for \;\; i = 1,2$$

with the equality holding if and only if $G^* \in \mathcal{B}_n^*$.

Theorem 2.18. ([61]) *Let G be a unicyclic graph of order n. Then*

$$\xi^c(G) \geq \xi^c(S_n^+)$$

with the equality holding if and only if $G \cong S_n^+$.

Theorem 2.19. ([61]) *Let G be a bicyclic graph of order n. Then*

$$\xi^c(G) \geq \xi^c(G^*)$$

with the equality holding if and only if $G^* \in \mathcal{B}_n^*$.

Theorem 2.20. ([59]) *Let G be a unicyclic graph of order n. Then*

$$\xi^{ce}(C_3(n-3)) \leq \xi^{ce}(G) \leq \xi^{ce}(S_n^+)$$

with left equality holding if and only if $G \cong C_3(n-3)$ where $C_3(n-3)$ is a graph obtained by attaching a pendant path of length $n-3$ to one vertex of C_3, and right holding if and only if $G \cong S_n^+$.

Let $\mathcal{DB}_n^*(a,b)$ be a set of two unicyclic graphs which are obtained from $DB_n(a,b)$ by inserting an edge between two pendant vertices adjacent to the vertex of degree $a+1$ and $b+1$, respectively.

Theorem 2.21. ([59]) *Let G be a unicyclic graph of order $n \geq 5$ and with diameter $d \geq 3$. Then*

$$\xi^{ce}(G^*) \leq \xi^{ce}(G)$$

with left equality holding if and only if $G^* \in \mathcal{DB}_n^*(a,b)$.

Moreover, the upper bounds on CEI with the corresponding extremal graphs are determined in [59] among all unicyclic graphs of order $n \geq 5$ and with diameter $d \geq 3$.

Theorem 2.22. ([54]) *Let G be a unicyclic graph of order n and with matching number $\beta \geq 2$. Then*

$$\xi^{ce}(G) \leq \xi^{ce}(F_1(n,\beta))$$

with the equality holding if and only if $G \cong F_1(n,\beta)$ where $F_1(n,\beta)$ is a graph obtained by attaching $n-2\beta+1$ pendant edges and $\beta-2$ pendant paths of length 2 to one vertex of cycle C_3.

Theorem 2.23. ([51]) *Let G be a connected graph of order $n \geq 2$ and with m edges, radius r and diameter d. Then*

(1) $nr^2 \leq E_1(G) \leq nd^2$

(2) $mr^2 \leq E_2(G) \leq md^2$

with any equality holding if and only if G is a self-centered graph.

Theorem 2.24. ([61]) *Let G be a connected graph of order $n \geq 4$. Then*

$$\xi^c(G) \geq \xi^c(S_n)$$

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

Theorem 2.25. ([61]) *Let G be a connected graph with m edges, radius r and diameter d. Then*

$$2mr \leq \xi^c(G) \leq 2md$$

with any equality holding if and only if G is a self-centered graph.

Theorem 2.26. ([55]) *Let G be a connected graph of order $n \geq 3$. Then*

$$N(G_0) \leq N(G) \leq N(P_n)$$

with the left equality holding if and only if $G \cong G_0$ where G_0 is an AP graph, and right holding if and only if $G \cong P_n$.

For a vertex v in a connected graph G, the *proximity* $\pi(v)$ is the average distance from v to all other vertices in G, that is, $\pi(v) = \frac{1}{n-1}\sum_{u \in V(G)\setminus\{v\}} d_G(u,v)$. And the *proximity* and the *remoteness* of a connected graph G are defined, respectively, as follows:

$$\pi(G) = \min_{v \in V(G)} \pi(v), \quad \rho(G) = \max_{v \in V(G)} \pi(v).$$

Let

$$f(n) = \begin{cases} \frac{3n+1}{4}\frac{n-1}{n} - \frac{n+1}{4}, & \text{if } n \text{ is odd}; \\ \\ \frac{n-1}{2} - \frac{n}{4n-4}, & \text{if } n \text{ is even}. \end{cases}$$

Theorem 2.27. ([38]) *Let G be a connected graph of order $n \geq 3$. Then*

$$avec(G) \leq \pi(G) + f(n)$$

with equality holding if and only if $G \cong P_n$.

Let $K^1_{2,a-2}$ be a connected graph obtained from $K_{2,a-2}$ with the vertices of degree $a-2$ being adjacent. And G_1 is obtained by attaching a pendant path of length $\lfloor \frac{d}{2} \rfloor$ to each vertex of degree $n-d$ in $K^1_{2,n-d-1}$. Also $K^2_{3,a-2}$ be a connected graph of order $a+1$ obtained from $K_{2,a-2}$ with the vertices of degree $a-2$ being adjacent to a new vertex. And G_2 is obtained by attaching a pendant path of length $\frac{d}{2} - 1$ to each vertex of degree $n-d$ in $K^2_{3,n-d+1}$.

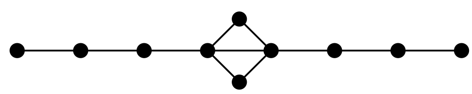

Figure 7. One example for G_1 with $n = 10$ and $d = 7$

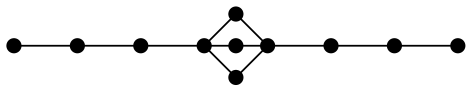

Figure 8. One example for G_2 with $n = 11$ and $d = 8$

Now we define two sets of graphs as follows.
$\Gamma_1 = \{G : G \ \ has\ diameter\ d,\ V(G) = V(G_1),\ E(G_1) \subseteq E(G)\}.$
$\Gamma_2 = \{G : G \ \ has\ diameter\ d,\ V(G) = V(G_2),\ E(G_2) \subseteq E(G)\}.$

Theorem 2.28. ([11]) *Let G be a connected graph of order n and diameter d. Then*

$$E_i(G) \geq E(G^*) \ \textit{for} \ \ i = 1, 2$$

with equality holding if and only if $G \cong G^*$ where G^* is a path P_n or belongs to Γ_1 or Γ_2.

It is interesting that the below is just a same result as the case of trees, although in it we consider the set of general graphs.

Theorem 2.29. ([40]) *Let G be a connected graph of order n and diameter d. Then*

$$\xi^c(G) \geq \xi^c(V_{n,d})$$

with equality holding if and only if $G \cong V_{n,d}$.

Moreover, some various bounds on ξ^c are obtained [60] based on the different values of m among all connected graphs of order n and with m edges diameter d.

A connected graph G is called a *cactus* if each block of G is either an edge or a cycle. Denote by C_n^k a graph obtained by inserting k independent edges into the star S_n. In the following theorem the upper bounds on ξ^{ce} is obtained among all cacti of order n and with k cycles.

Theorem 2.30. ([57]) *Let G be a cactus of order $n \geq 5$ and with k cycles. Then*

$$\xi^{ce}(G) \leq \xi^{ce}(C_n^k)$$

with equality holding if and only if $G \cong C_n^k$.

Now we end this subsection with the following two results on the upper bound on the average eccentricity in terms of independence number and clique number. Denote

$$g(n) = \begin{cases} \frac{3n^2-2n-1}{4n} + \frac{n+1}{2}, & \text{if } \ n \ \text{ is odd}\,; \\ \\ \frac{3n^2-4n-4}{4n} + \frac{n+2}{2}, & \text{if } \ n \ \text{ is even}\,. \end{cases}$$

Theorem 2.31. ([29]) *Let G be a connected graph of order $n \geq 4$. Then*

$$avec(G) \leq g(n) - \alpha(G)$$

where $\alpha(G)$ is the independence number of G. And the equality holds if and only if $G \cong P_n$ for odd n and $G \cong B_{n,n-2}$ for even n.

Theorem 2.32. ([29]) *Let G be a connected graph of order $n \geq 4$ with clique number k. Then*

$$avec(G) \leq \frac{avec(Ki_{n,k})}{k}$$

where $Ki_{n,k}$ is a kite graph obtained by attaching a pendant path of length $n-k$ to one vertex of a complete graph K_k. And the equality holds if $G \cong Ki_{n,k}$.

3. Some bounds on EBTI in terms of other topological indices

In this section we present some upper and lower bounds on EBTI in terms of other topological indices, mainly including vertex-degree-based ones, general distance-based ones.

3.1 For vertex–degree–based topological indices

For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined [25, 26] as follows:

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg_G(v)^2, \qquad M_2 = M_2(G) = \sum_{uv \in E(G)} \deg_G(u) \deg_G(v) \; .$$

Please see [52] for some recent results on Zagreb indices and [24] for a survey of vertex-degree-based topological indices of graphs.

In the following two results some upper bounds of E_i for $i = 1, 2$ are proposed, respectively, in terms of the first and the second Zagreb indices of graphs.

Theorem 3.1. ([11]) *Let G be a connected graph of order n and with m edges. Then*

$$E_1(G) \leq M_1(G) - 4mn + n^3 \; .$$

The equality holds if and only if $G \cong G_0$ where G_0 is P_4 or K_n, or an $(n-1, n-2)$-semiregular graph.

Theorem 3.2. ([11]) *Let G be a connected graph of order n and with m edges. Then*

$$E_2(G) \leq M_2(G) - nM_1(G) + mn^2 \; .$$

The equality holds if and only if $G \cong G_0$ where G_0 is P_4 or K_n, or an $(n-1, n-2)$-semiregular graph.

A connected graph G with maximum degree $\Delta(G) \leq 4$ is called a *molecular graph*. In particular, a tree T with $\Delta(T) \leq 4$ is called a *chemical tree*. Next we will list several results on the bounds on ξ^c of some specific graphs, including molecular graphs, chemical trees, and general ones, in terms of M_i for $i = 1, 2$.

Theorem 3.3. ([12]) *Let G be a connected molecular graph of order n and with diameter $d \geq 7$. Then*

$$\xi^c(G) > M_1(G) \; .$$

Theorem 3.4. ([28]) *Let G be a connected graph of order n and with diameter d such that $d \geq \max\{7, 2\Delta(G)+1\}$. Then*

$$\xi^c(G) > M_1(G).$$

Also in [28], three sufficient conditions are given for the graphs G with $\xi^c(G) \leq M_i(G)$ for $i = 1, 2$.

Theorem 3.5. ([28]) *Let G be a connected graph of order $n \geq 7$ and with minimum degree $\delta \geq \frac{n}{2} - 1$. Then*

$$\xi^c(G) \leq M_i(G) \ \text{ with } \ i = 1, 2\ .$$

Theorem 3.6. ([28]) *Let G be a connected graph of order n and with diameter $d > 3$. If $d_G(u)+d_G(v) \geq n-1$ for any edge $uv \in E(G)$, then*

$$\xi^c(G) \leq M_i(G) \ \text{ with } \ i = 1, 2.$$

Theorem 3.7. ([28]) *Let G be a connected graph of order $n \geq 3$ and with average degree $\overline{d}(G)$ and diameter d. If $\overline{d}(G) \geq d$, then*

$$\xi^c(G) \leq M_i(G) \ \text{ with } \ i = 1, 2.$$

Theorem 3.8. ([61]) *Let G be a connected graph of order $n \geq 3$ and with m edges. Then*

$$\xi^c(G) \leq 2mn - M_1(G)$$

with equality holding if and only if G is isomorphic to P_4, or K_n or a graph obtained from K_n by k independent edges with $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$.

Theorem 3.9. ([12]) *Let G be a chemical tree of order n. Then*

$$\xi^c(T) < M_1(T)$$

for $T \cong S_4, S_5$, or one of the following trees T^* and T^{**} shown in Figure 9. Otherwise, we have

$$\xi^c(T) \geq M_1(T)$$

with equality holding if and only if $T \cong S_2$, or $T \cong S_3$, or $T \cong T_0$ as shown in Figure 9.

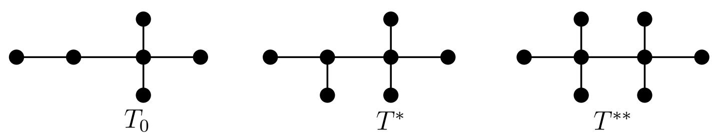

Figure 9. The trees T_0, T^* and T^{**}

For a (molecular) graph G, the *Randić index* $R(G)$ is defined [42] as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}\ .$$

In the two theorems below some bounds on the average eccentricity of graphs are given in terms of Randić index.

Theorem 3.10. ([37]) *Let G be a connected graph of order $n \geq 7$. Then*

$$R(G) + avec(G) \geq \sqrt{n-1} + 2 - \frac{1}{n}$$

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

Theorem 3.11. ([37]) *Let G be a connected graph of order $n \geq 7$. Then*

$$R(G) \cdot avec(G) \geq \begin{cases} \frac{n}{2}, & 3 \leq n \leq 13\,; \\ \\ \sqrt{n-1}(2-\frac{1}{n}), & n > 13\,. \end{cases}$$

with equality holding if and only if $G \cong K_n$ if $3 \leq n \leq 13$, and $G \cong S_n$ if $n > 13$.

3.2 For (general) distance–based topological indices

For a (molecular) graph G, as an oldest topological index, the Wiener index $W(G)$ is defined [50] as follows:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v).$$

Please see [16] for the mathematical properties and applications of the Wiener index of trees.

Theorem 3.12. ([13]) *Let T be a tree of order $n > 1$. Then $W(T) < \xi^c(T)$ for $T \cong P_k$ with $k = 2, 3, \ldots, 6$ or $D_5(2,1)$. Otherwise, we have $\xi^c(T) \leq W(T)$ with equality holding if and only if $T \cong S_4$.*

For an edge $e = uv \in E(G)$ of a graph G, we denote by $n_u(e)$ the number of vertices in G with a smaller distance to u than to v. And $n_v(e)$ can be similarly defined. As a generalization of Wiener index, Gutman [23] introduced a graph invariant, named as Szeged index, of a graph G as follows:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e).$$

Denote by $T(1,2,2)$ a tree obtained by attaching a pendant vertex to the central vertex of P_5.

Theorem 3.13. ([14]) *Let T be a tree of order $n > 1$. Then*

$$Sz(T) \geq \xi^c(T) + 3$$

if T does not belong to the following set:

$$\mathcal{G}^* = \Big\{P_2, P_3, P_4, P_5, P_6, P_7, S_4, D_5(2,1), D_6(2,1), T(1,2,2)\Big\}.$$

In the following theorem two more general results on the comparison between Sz and ξ^c are posed for the bipartite graphs.

Theorem 3.14. ([14]) *Let G be a bipartite graph of order $n > 1$. Then $Sz(G) < \xi^c(G)$ if G is isomorphic to one of the trees: P_k with $k = 2, 3, 4, 5, 6$, $D_5(2,1)$. Otherwise, we have $Sz(G) \geq \xi^c(G)$ with equality holding if and only if $G \cong C_4$ or $G \cong S_4$.*

Theorem 3.15. ([14]) *Let T be a bipartite graph of order $n > 1$. Then*

$$Sz(G) \geq \xi^c(G) + 3$$

if G does not belong to the following set $\mathcal{G}^* \bigcup \{C_4\}$ where $\mathcal{G}^*$ is just the set defined in Theorem 3.13.

In the following three theorems some comparative results are given between ξ^c and ξ^{ce} of graphs. Together with these results the corresponding extremal results are characterized which are just some special eccentricity-based graphs, such as self-centered graphs or ASC ones.

Theorem 3.16. ([55]) *Let G be a connected graph of order $n \geq 3$ with m edges and radius r, diameter d. Then*

$$\xi^{ce}(G)\, \xi^c(G) - 4m^2 \leq \frac{(d-r)^2}{2\, d\, r}\, (4m^2 - M_1(G)),$$

with the equality holding iff G is a self-centered graph.

Theorem 3.17. ([55]) *Let G be a connected graph of order $n \geq 3$ with m edges and radius r, diameter d. Then*

$$\xi^c(G) + r\, d\, \xi^{ce}(G) \leq 2m\,(r + d) + \Delta(G)(d - r)$$

with equality holding if and only if G is a self-centered graph.

Theorem 3.18. ([55]) *Let G be a connected non-self-centered graph of order n with minimum degree δ and radius r. Then*

$$\xi^c(G) - r^2\, \xi^{ce}(G) \geq 4\delta - \frac{2\delta}{r+1}$$

with equality holding if and only if G is an ASC graph with two non-central vertices having minimum degree δ.

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Sharp Bounds on the Eccentric Distance Sum of Graphs

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Contents

1. Introduction

This chapter is concerned with the so called *eccentric distance sum* (EDS) of graphs. Back in 2002, when Gupta, Singh and Madan [17] introduced the eccentric distance sum, this novel graph invariant attracts more and more researchers' attention. One gauge that such gradual rising interest on the study of EDS must be powered by some fundamental properties of the EDS parameter.

1.1 Background

In this subsection, we present the related background for introducing the concept for eccentric distance sum of graphs.

A single number that can be used to characterize some property of the graph of a molecule is called a *topological index*, or *graph invariant*. Topological index is a graph theoretic property that is preserved by isomorphism. The chemical information derived through topological index has been found usefully in chemical documentation, isomer discrimination, structure property correlations, etc; see [1].

For quite some time there has been rising interest in the field of computational chemistry in topological indices. The interest in topological indices is mainly related to their use in nonempirical quantitative structure-property relationships and quantitative structure-activity relationships.

Among various indices, the *Wiener index* has been one of the most widely used descriptors in quantitative structure activity relationships. Many recently established topological indices such as *degree distance index*, *eccentric connectivity index* and so on are used as molecular descriptors.

The *Wiener index* is defined as the sum of all distances between unordered pairs of vertices

$$W(G) = \sum_{\{u,v\}\subseteq V_G} d_G(u,v).$$

It is considered as one of the most used topological index with high correlation with many physical and chemical properties of a molecule (modeled by a graph). For the results on the Wiener index one may be referred to the survey [7] and the recently published paper [27].

The *degree distance index* $DD(G)$ was introduced by Dobrynin and Kochetova [8] and Gutman [18] as graph-theoretical descriptor for characterizing alkanes; it can be considered as a weighted version of the Wiener index

$$DD(G) = \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v))d_G(u,v),$$

where the summation goes over all pairs of vertices in G. In particular, when G is a tree on n vertices, $DD(G) = 4W(G) - n(n-1)$ (see [20, 25]).

Sharma, Goswami and Madan [37] introduced a distance–based molecular structure descriptor, *eccentric connectivity index* (ECI) defined as

$$\xi^c(G) = \sum_{v\in V_G} \varepsilon_G(v)d_G(v).$$

The index $\xi^c(G)$ was successfully used for mathematical models of biological activities of diverse nature [10,16]. For the study of its mathematical properties one may be referred to [23,24,32] and the references there in.

It is sometimes interesting to consider the sum of eccentricities of all vertices of a given graph G, which was first proposed by Dankelmann, Goddard and Swart in 2004 (see [5]). We call this quantity the *total eccentricity* of the graph G and denoted it by

$$\zeta(G) = \sum_{v \in V_G} \varepsilon_G(v).$$

Recently, a novel graph invariant, i.e., the *eccentric distance sum* (EDS), was introduced by Gupta, Singh and Madan [17]. It was defined as

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V_G} (\varepsilon_G(v) + \varepsilon_G(u)) d_G(u, v) = \sum_{v \in V_G} \varepsilon_G(v) D_G(v),$$

where $D_G(v) = \sum_{x \in V_G} d(x, v)$.

On the one hand, the eccentric distance sum offers a vast potential for structure activity/property relationships; On the other hand it can provide valuable leads for the development of safe and potent therapeutic agents of diverse nature. Comparatively, the eccentric distance sum exhibits much better correlation and lesser average errors than the Wiener index. The excellent prediction of the physical properties by the eccentric distance sum can be attributed to probable contribution of distance sum in addition to eccentricity. The physical properties are significantly responsible for the biological activity of a chemical compound. One may be referred to [17] for more details.

1.2 Some notations, terminologies and definitions

In this subsection, unless otherwise stated, we follow the traditional notations and terminologies (see, for instance, [3]). Some necessary definitions are provided.

We consider only simple connected graphs $G = (V_G, E_G)$, where V_G is the vertex set and E_G is the edge set. We call $n = |V_G|$ the *order* of G and $m = |E_G|$ the *size* of G. Let $\overline{G}$ denote the complement of G. The *distance*, $d_G(u, v)$, between two vertices u, v of G is the length of a shortest u-v path in G. The *eccentricity* $\varepsilon_G(v)$ of a vertex v is the distance between v and a furthest vertex from v. The *diameter* $\mathrm{diam}(G)$ of G is defined as the maximum of the eccentricities of vertices of G, whereas the *radius* of G is the minimum of the eccentricities of vertices of G.

Let $G = (V_G, E_G)$ be a graph. Then $G - v$, $G - uv$ denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. Denote by P_n, S_n and K_n, the path, the star, and the complete graph on n vertices, respectively.

For a vertex subset S of V_G, denoted by $G[S]$ the subgraph induced by S. Let $N_G(v)$ denote the set of vertices adjacent to v. $N_G[v] = N_G(v) \cup \{v\}$. The *degree* $d_G(v)$ of a vertex v is equal to $|N_G(v)|$. The number $\Delta(G) := \max\{d_G(v)|v \in V_G\}$ is the maximum degree of G. The number $\delta(G) := \min\{d_G(v)|v \in V_G\}$ is the minimum degree of G. We call u a *leaf* (or *pendant vertex*) of G if $d_G(u) = 1$. For convenience, let $\mathcal{G}_{n,m}$ be the class of all n-vertex connected graphs with m edges.

A *vertex cut* of a connected graph G is a set $S \subseteq V_G$ such that $G - S$ has more than one components. The *connectivity* of G, written $\kappa(G)$, is the minimum size of a vertex set S such that $G - S$ is disconnected or has only one vertex. A graph is *k-connected* if its connectivity is at least k. G is 1-connected if and only if it is connected; equivalently, $\kappa(G) = 0$ if and only if it is disconnected. Similarly, an *edge cut* of a connected graph G is a set $E' \subseteq E_G$ such that $G - E'$ has more than one components. The *edge connectivity* of G, written $\lambda(G)$, is the minimum size of an edge cut.

A subset S of V_G is called a *dominating set* of G if for every vertex $v \in V_G \setminus S$, there exists a vertex $u \in S$ such that u is adjacent to v. The *domination number* of G, denoted by $\gamma(G)$, is defined as the minimum cardinality of dominating sets of G. For a connected graph G of order n, Ore [35] obtained that $\gamma(G) \leqslant \frac{n}{2}$. And the equality case was characterized independently in [13, 39].

A subset M of E_G is called a *matching* of G if no two edges of M are adjacent in G. Let M be a matching of G. The vertex v in G is *M-saturated* if v is incident with an edge in M; otherwise, v is *M-unsaturated*. A *perfect matching* M of G means that each vertex of G is M-saturated; clearly, every perfect matching is maximum. The *matching number* of G, written as $\mu(G)$, is the cardinality of a maximum matching of G. If $\mu(G) = k$, then we also call such maximal matching as a k-matching. It is easy to prove by induction that a perfect matching of a tree is unique when it exists.

A subset S of V_G is called an *independent set* of G if no two vertices of S are adjacent in G. The *independence number* of G, denoted by $\alpha(G)$, is defined as the maximum cardinality of independent sets of G. It is known that for a bipartite graph G of order n with $\delta(G) > 0$, then $\alpha(G) + \mu(G) = n$.

A *tree* is a connected graph having no cycles. Let $P_l(a, b)$ be an n-vertex tree obtained by attaching a and b leaves to the two end-vertices of $P_l = v_1v_2 \dots v_l$, $(l \geqslant 2)$, respectively. Here, $a+b = n-l$, $a, b \geqslant 1$. A *spider* is a tree with at most one vertex of degree more than 2. Let $S(a_1, a_2, \dots, a_k)$ be a spider with k paths $P^1, P^2, \dots, P^k$ satisfying the length of P^i is a_i $(i = 1, 2, \dots, k)$, and $\sum_{i=1}^{k} a_i = n - 1$. Call $S(a_1, a_2, \dots, a_k)$ a *balanced spider* if $\mid a_i - a_j \mid \leqslant 1$ for $1 \leqslant i, j \leqslant k$.

A *bipartite graph* G is a simple graph with n vertices, whose vertex set V_G can be partitioned into two disjoint subsets V_1 and V_2 such that every edge of G joins a vertex of V_1 with a vertex of V_2. Suppose that V_1 has p vertices and V_2 has q vertices, where $p+q = n$. Then we say that G has a *(p, q)-bipartition* $(p \leqslant q)$. A bipartite graph in which every two vertices from different partition classes are adjacent is called *complete*, which is denoted by K_{n_1,n_2}, where $n_1 = |V_1|, n_2 = |V_2|$.

The *join* $G_1 \oplus G_2$ of two vertex disjoint graphs G_1 and G_2 is the graph consisting of the union $G_1 \cup G_2$, together with all edges of the type xy, where $x \in V_{G_1}$ and $y \in V_{G_2}$. For $k \geqslant 3$ vertex-disjoint graphs $G_1, G_2, \dots, G_k$, the *sequential join* $G_1 \oplus G_2 \oplus \cdots \oplus G_k$ is the graph $(G_1 \oplus G_2) \cup (G_2 \oplus G_3) \cup \cdots \cup (G_{k-1} \oplus G_k)$. The sequential join of k disjoint copies of a graph G will be denoted by $[k]G$, the union of k disjoint copies of G will be denoted by kG, while $[s]G_1 \oplus G_2 \oplus [t]G_3$ will denote the sequential join $\underbrace{G_1 \oplus G_1 \oplus \cdots \oplus G_1}_{s} \oplus G_2 \oplus \underbrace{G_3 \oplus G_3 \oplus \cdots \oplus G_3}_{t}$.

The rest of this chapter is organized as follows. In Section 2, we present some graph transformations. In Section 3, we provide several extremal graphs w.r.t. EDS among some classes of graphs including general graphs, trees, bipartite graphs, unicyclic graphs, triangle-free graphs, planar graphs and outer-planar graphs. In Section 4, we provide an overview of different bounds on EDS in terms of various invariants such that sizes, vertex degrees, (edge) connectivity, matching number, independence number, domination number, number of pendants, (p, q)-bipartition and so on. In the last section, we offer some open problems and conjectures for readers.

Further on, we need the following lemma.

Lemma 1.1 ([40]). *Let G be a connected graph of order n and $G \ncong K_n$. Then for each edge $e \notin E_G$, $\xi^d(G) > \xi^d(G+e)$.*

2. Some useful transformations

In this section, we will introduce several useful transformations as follows. We mainly study the effect of each of these transformations on the eccentric distance sum invariant.

Let T be an arbitrary tree rooted at a center vertex and let v be a vertex of degree $m+1$ ($m \geqslant 2$). Suppose that w is adjacent to v with $\varepsilon_T(v) \geqslant \varepsilon_T(w)$ and that $T_1, T_2, \ldots, T_m$ are subtrees under v with root vertices $v_1, v_2, \ldots, v_m$ such that the tree T_m is actually a path. Let $T' = T - \{vv_1, vv_2, \ldots, vv_{m-1}\} + \{wv_1, wv_2, \ldots, wv_{m-1}\}$. We say that T' is a *ρ-transformation* of T and denote it by $T' = \rho(T, v)$ (see Fig. 1).

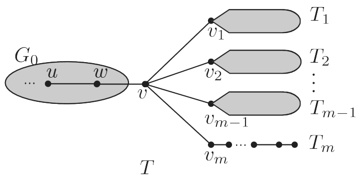

Figure 1. ρ-Transformation

Theorem 2.1 ([15]). *Let T and T' be the trees defined as above, one has $\xi^d(T) \geqslant \xi^d(T')$. The equality holds if and only if $\varepsilon_T(v) = \varepsilon_T(w)$ and $T[S]$ is one of the longest paths in T, where $S = V_{G_0} \cup V_{T_m} \cup \{v\}$.*

Theorem 2.2 ([15]). *Let T, T' be the two trees as depicted in Fig. 2. Suppose that $P = v_0v_1 \ldots v_i \ldots v_r \ldots v_d$ is one of the longest paths contained in an n-vertex tree T with $|V_{T_1}| \leqslant |V_{T_{d-1}}|$ and $r = \min\{i : |V_{T_i}| > 1, i = 2, 3, \ldots, d-1\}$; see Fig. 2. Let $T' = T - \{v_ru : u \in N_T(v_r) \setminus \{v_{r-1}, v_{r+1}\}\} + \{v_1u : u \in N_T(v_r) \setminus \{v_{r-1}, v_{r+1}\}\}$. Then we have $\xi^d(T) < \xi^d(T')$.*

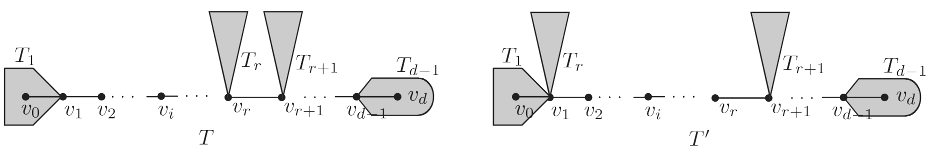

Figure 2. Trees T and T'.

By Theorem 2.2, the following theorem holds.

Theorem 2.3 ([31]). *Suppose that $P = v_0v_1 \dots v_i \dots v_r \dots v_d$ is one of the longest paths contained in an n-vertex tree T with $d_T(v_1) \leqslant d_T(v_{d-1})$ and $r = \min\{i : |V_{T_i}| \geqslant 3, i = 2, 3, \dots, d-1\}$. Let v' be an adjacent vertex of v_1 other than v_2 and $T'' = T - \{v_ru | u \in N_T(v_r) \setminus \{v_r, v_{r+1}\}\} + \{v'u | u \in N_T(v_r) \setminus \{v_r, v_{r+1}\}\}$. Then we have $\xi^d(T) < \xi^d(T'')$.*

Theorem 2.4 ([15]). *Given an n-vertex tree T with $wu, uv \in E_T$, $d_T(w) \geqslant 2$, and each member in $N_T(v) \setminus \{u\} = \{v_1, v_2, \dots, v_t\}$ is a leaf, $t \geqslant 1$. Let $T^* = T - \{vv_1, vv_2, \dots, vv_t\} + \{wv_1, wv_2, \dots, wv_t\}$; see Fig. 3. Then $\xi^d(T) > \xi^d(T^*)$.*

We call the transformation in Theorem 2.4 as **Transformation I**.

Figure 3. Trees T and T^*.

Theorem 2.5 ([40]). *Suppose $t \geqslant 1$ is an integer. Let u be a vertex of a connected graph G_0 with at least two vertices. Let G_1 be the graph obtained by identifying u and a pendant vertex of a star S_{t+2}, G_2 the graph obtained by identifying u and the center of the star S_{t+2}. Then $\xi^d(G_2) < \xi^d(G_1)$.*

We call the transformation in Theorem 2.5 as **Transformation II**.

Theorem 2.6 ([26]). *Let w be a vertex of a nontrivial connected graph G. For nonnegative integers p and q, let $G(p, q)$ denote the graph obtained from G by attaching to vertex w pendant paths $P = wv_1v_2 \dots v_p$ and $Q = wu_1u_2 \dots u_q$ of lengths p and q, respectively. Let $G(p+q, 0) = G(p, q) - wu_1 + v_pu_1$. If $\varepsilon_G(w) \geqslant p \geqslant q \geqslant 1$, then $\xi^d(G(p, q)) < \xi^d(G(p+q, 0))$.*

Theorem 2.7 ([22]). *Suppose H is a complete graph on at least $s\,(\geqslant 2)$ vertices and $v_1, \dots, v_s$ are distinct vertices of H. Let G_1 be the graph obtained from H by attaching a nontrivial connected graph H_i to v_i for $i = 1, \dots, s$, respectively. Let G_2 be the graph obtained from H by attaching all the above nontrivial connected graphs $H_1, \dots, H_s$ to a vertex, say v_1, of H. Then $\xi^d(G_1) > \xi^d(G_2)$.*

Theorem 2.8 ([22]). *Suppose H_1 and H_2 are two vertex-disjoint connected graphs of order at least 2. Take a vertex u from H_1 and a vertex v from H_2, respectively. Let G_3 be the graph obtained by connecting u and v by an edge uv and G_4 be the graph by identifying u with v and introducing a pendant edge uw (or vw) with pendant vertex w, respectively. Then $\xi^d(G_3) > \xi^d(G_4)$.*

Let T be a tree of order $n > 3$ and $e = uv$ be a non-pendant edge. Suppose that $T - e = T_1 \cup T_2$ with $u \in V_{T_1}$ and $v \in V_{T_2}$. Now we construct a new tree T_0 obtained by identifying the vertex u of T_1 with vertex v of T_2 and attaching a leaf to the $u\,(= v)$. Then we say that T_0 is obtained by running *edge-growing transformation* of T (on the edge $e = uv$), or e.g.t of T (on the edge $e = uv$) for short; see Fig. 4. By Theorem 2.8, $\xi^d(T_0) < \xi^d(T)$.

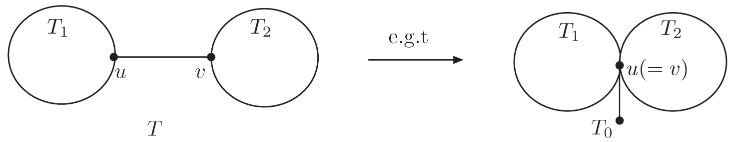

Figure 4. Two trees T and T_0.

3. Extremal graphs with respect to EDS

In this section, we survey the results on the extremal graphs w.r.t. EDS among some classes of graphs, which include general graphs, trees, bipartite graphs, unicyclic graphs, triangle-free graphs, planar graphs and outerplanar graphs.

3.1 General graphs and bipartite graphs

By Lemma 1.1, the following results follow directly.

Theorem 3.1. *Let G be a connected graph of order n. Then $\xi^d(G) \geqslant \xi^d(K_n)$ with equality if and only if $G \cong K_n$.*

Theorem 3.2 ([29]). *Let G be a bipartite graph with $V_G = (U, W)$ satisfying $|U| = n_1 \geqslant |W| = n_2$.*

(i) *If $n_1 = n_2 = 1,$ then $\xi^d(G) = 2$ and the graph is only K_2.*

(ii) *If $n_1 \geqslant 2,\ n_2 = 1$, then $\xi^d(G) = 4n_1^2 - n_1$ and the graph is only $K_{n_1,1}$.*

(iii) *If $n_2 > 1$, then $\xi^d(G) \geqslant 4n_1^2 + 4n_2^2 + 4n_1n_2 - 4n_1 - 4n_2$ with equality if and only if $G \cong K_{n_1,n_2}$.*

3.2 Trees

Yu, Feng, Illić [40] characterized the n-vertex tree with the minimal EDS. Ilić, Yu and Feng [26] proved that the path P_n is the unique extremal tree of order n having the maximal EDS. Zhang and Li [41] determined the n-vertex trees with the second-maximal, third-maximal and fourth-maximal EDS, respectively. Li et al. [30] determined the trees with the third and fourth minimal EDS among the n-vertex trees.

Let $C(a_1, a_2, \dots, a_{d-1})$ be a *caterpillar* obtained from a path $P_{d+1} = v_0v_1 \dots v_d$ by attaching a_i pendant edges to vertex $v_i, i = 1, 2, \dots, d-1$. Clearly, $C(a_1, a_2, \dots, a_{d-1})$ has diameter d and $n = d+1+\sum_{i=1}^{d-1} a_i$. For simplicity, let $C_{n,d} := C(0, \dots, 0, a_{\lfloor d/2 \rfloor}, 0, \dots, 0)$ and $C'_{n,d} := C(0, \dots, 0, a_{\lfloor d/2 \rfloor} - 1, 1, 0, \dots, 0)$, where $a_{\lfloor d/2 \rfloor} = n - d - 1$.

Let $\hat{T}_{n,i}$ be the tree obtained from $P_{n-1} = v_0v_1 \dots v_{n-2}$ by attaching a pendant vertex v_{n-1} to v_i, where $1 \leqslant i \leqslant \lfloor (n-2)/2 \rfloor$. Let $L_{n,k}$ be the n-vertex tree obtained from the star $K_{1,n-k-1}$ by attaching

k pendant edges to one of pendant vertices of $K_{1,n-k-1}$, where $k \in \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor - 1\}$. Obviously, $L_{n,1} = C_{n,3}$ and $L_{n,2} = C'_{n,3}$.

Theorem 3.3 ([26, 40]). *Let T be a tree of order n. Then $\xi^d(S_n) \leqslant \xi^d(T) \leqslant \xi^d(P_n)$. The left equality holds if and only if $T \cong S_n$, whereas the right equality holds if and only if $T \cong P_n$.*

Combining with Lemma 1.1, Theorems 3.1 and 3.3, the next corollary follows immediately.

Corollary 3.4. *Let G be a connected graph of order n. Then $\xi^d(K_n) \leqslant \xi^d(G) \leqslant \xi^d(P_n)$. The left equality holds if and only if $G \cong K_n$, and the right equality holds if and only if $G \cong P_n$.*

Theorem 3.5 ([41]). *If $n \geqslant 8$, then $\hat{T}_{n,1}, \hat{T}_{n,2}$ and $\hat{T}_{n,3}$ are the unique trees with the second-maximal, third-maximal, and fourth-maximal eccentric distance sum among the trees on n vertices.*

Theorem 3.6 ([30]). *Among trees on n vertices, $C'_{n,3}$ has the third minimal eccentric distance sum, whereas $L_{n,3}$ has the fourth minimal eccentric distance sum.*

3.3 Unicyclic graphs

Yu, Feng, Ilić [40] characterized the graphs among n-vertex unicyclic graphs with given girth having the minimal and second minimal EDS, respectively. Zhang and Li [41] characterized the extremal unicyclic graphs on $n \geqslant 8$ vertices with the maximal, second maximal and third maximal EDS, respectively.

Let $\mathscr{U}_n(k)$ be the set of n-vertex unicyclic graphs of order n with girth k and $\mathscr{U}_n$ be the set of all unicyclic graphs of order n. We denote by $H_{n,k}$ the unicyclic graph obtained from C_k by adding $n-k$ pendant vertices to a vertex of C_k. Let $H(n,k;n_1,n_2,\ldots,n_k)$ be a unicyclic graph on n vertices obtained from cycle $C_k = v_1v_2\ldots v_k$ with n_i pendant vertices attached at v_i $(i = 1, 2, \ldots, k)$. Clearly, $n-k = \sum_{i=1}^{k} n_i$. Let $H'_{n,k}(3 \leqslant k \leqslant n-2)$ be a graph obtained from cycle $C_k = v_1v_2\ldots v_k$ by attaching $n-k-1$ pendant vertices and one pendant vertex at v_1 and v_2, respectively.

Theorem 3.7 ([40]). *Let $G \in \mathscr{U}_n(k)$ be a unicyclic graph of order $n > 5$. Then*

$$\xi^d(G) \geqslant \begin{cases} -\frac{1}{8}k^4 + \frac{n-1}{4}k^3 + \frac{7-3n}{4}k^2 + (n^2 - \frac{7n}{2} + 1)k + 2n^2 - n & \text{if } k \text{ is even,} \\ -\frac{1}{8}k^4 + \frac{2n-1}{8}k^3 + \frac{13-8n}{8}k^2 + (n^2 - \frac{9n}{4} + \frac{1}{8})k + n^2 - \frac{1}{2} & \text{if } k \text{ is odd} \end{cases}$$

with equality if and only if $G \cong H_{n,k}$.

Theorem 3.8 ([40]). *Let G be a unicyclic graph of order $n > 5$. Then*

$$\xi^d(G) \geqslant 4n^2 - 9n + 1$$

with equality if and only if $G \cong H_{n,3}$.

Theorem 3.9. *Among all n-vertex $(n > 5)$ unicyclic graphs with girth k, $H'_{n,k}$ has the second minimal eccentric distance sum,*

$$\xi^d(H'_{n,k}) = \begin{cases} -\frac{1}{8}k^4 + \frac{n-1}{4}k^3 + \frac{2-3n}{4}k^2 + (n^2 - 2n - 2)k + 2n^2 + n - 2 & \text{if } k \text{ is even,} \\ 6n^2 - 11n - 15 & \text{if } k = 3, \\ -\frac{1}{8}k^4 + \frac{2n-1}{8}k^3 + \frac{3-8n}{8}k^2 + (n^2 - \frac{3}{4}n - \frac{11}{8})k + n^2 + \frac{1}{2}n - \frac{7}{4} & \text{if } k \text{ is odd and } k \geqslant 5. \end{cases}$$

Theorem 3.10 ([40]). *Let $G \in \mathscr{U}_n$ $(\neq H_{n,3})$ be a unicyclic graph on $n > 5$ vertices.*

(a) *If $n = 6$, then $\xi^d(G) \geqslant 133$ with equality if and only if $G \cong H_{6,5}$;*

(b) *If $n \geqslant 7$, then $\xi^d(G) \geqslant 6n^2 - 11n - 16$ with equality if and only if $G \cong H_{n,4}$.*

Let U_n be the graph obtained from a path $P_{n-1} = v_0v_1 \ldots v_{n-3}v_{n-2}$ and a vertex v_{n-1} by adding two edges $v_{n-1}v_{n-2}$ and $v_{n-1}v_{n-3}$. Then let $Q_n = U_n - v_{n-1}v_{n-3} + v_{n-1}v_{n-4}$ and $B_n = U_n - v_{n-1}v_{n-2} + v_{n-1}v_{n-4}$.

Theorem 3.11 ([41]). *Let G be in $\mathscr{U}_n \setminus \{U_n, Q_n, B_n\}$ with $n \geqslant 8$. Then $\xi^d(G) < \xi^d(Q_n) < \xi^d(B_n) < \xi^d(U_n)$.*

3.4 Triangle–free graphs

Li, Yu and Sun [29] determined the graphs with the smallest EDS among the n-vertex triangle-free graphs.

Lemma 3.12 ([3]). *Let G be a connected graph with $|E_G| > \frac{1}{4}|V_G|^2$. Then G contains at least one triangle.*

Lemma 3.13 ([28]). *Among $\{K_{n_1,n_2} : n_1 + n_2 = n, n_1 \geqslant 1, n_2 \geqslant 1\}$ with $n \geqslant 4$, one has $\xi^d(K_{1,n-1}) > \xi^d(K_{2,n-2}) > \cdots > \xi^d(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$.*

Theorem 3.14 ([28]). *Let G be a connected triangle-free graph of order $n \geqslant 4$. Then*

$$\xi^d(G) \geqslant 4n(n-1) - 4\lfloor n^2/4 \rfloor. \tag{1}$$

The equality holds if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. Let G be a triangle-free graph of order n with the minimum EDS. If there exists a vertex $u \in V_G$ such that $\varepsilon_G(u) = 1$, then $d_G(u) = n - 1$. Hence, we have $G \cong K_{1,n-1}$.

In what follows, we consider that the eccentricity of each vertex in V_G is greater than one. It is easy to see that, for each vertex x of G, one has $d_G(x) \leqslant n - 2$. Hence, for $x \in V_G$, we have $\varepsilon_G(x) \geqslant 2$ and

$$D_G(x) = \sum_{u \in N_G(x)} d_G(u,x) + \sum_{u \in V_G \setminus N_G[x]} d_G(u,x) \geqslant d_G(x) + 2(n-1-d_G(x)) = 2n - 2 - d_G(x) \tag{2}$$

where the inequality in (2) follows from the fact that the distance between x and the vertex which is not adjacent to x is at least two. Together with the definition of the EDS, we have

$$\begin{aligned}
\xi^d(G) &= \sum_{x \in V_G} \varepsilon_G(x) D_G(x) \\
&\geqslant \sum_{x \in V_G} 2(2n - 2 - d_G(x)) \qquad (3) \\
&= 4n(n-1) - 4|E_G| \\
&\geqslant 4n(n-1) - 4\lfloor n^2/4 \rfloor, \qquad (4)
\end{aligned}$$

where the inequality (3) follows by (2) and the inequality (4) follows by Lemma 3.12.

Hence, we have $\xi^d(G) \geqslant 4n(n-1) - 4\lfloor n^2/4 \rfloor$ with equality if and only if $\varepsilon_G(x) = 2$ for each vertex x in V_G and $|E_G| = \lfloor n^2/4 \rfloor$. In order to complete the proof, it suffices to identify all the n-vertex triangle-free graphs with $\varepsilon_G(x) = 2$ for each $x \in V_G$ and $|E_G| = \lfloor n^2/4 \rfloor$ attaining the minimum EDS value $4n(n-1) - 4\lfloor n^2/4 \rfloor$.

According to Turán Theorem, $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ is the unique triangle-free graph with n vertices and $\lfloor n^2/4 \rfloor$ edges. So G attains the minimum EDS value $4n(n-1) - 4\lfloor n^2/4 \rfloor$ if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

From our proof, we obtain that $G \cong K_{1,n-1}$ if there exists a vertex u in V_G such that $\varepsilon(u) = 1$ and $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ if $\varepsilon(u) > 1$ for all u in V_G. Hence, by Lemma 3.13, we obtain that $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ is the unique n-vertex triangle-free graph which makes the equality in (1) hold, as desired. ■

3.5 (Outerplanar) planar graphs

Li and Wu [28] determined the graph with the smallest EDS among the (outerplanar) planar graphs. Recall that $\mathcal{G}_{n,m}$ is the class of all connected n-vertex graphs with m edges.

Lemma 3.15 ([28]). *Let G_1, G_2 be in $\mathcal{G}_{n,m}$ with $\Delta(G_1) = n-1$ and $\Delta(G_2) < n-1$. Then $\xi^d(G_1) < \xi^d(G_2)$.*

Theorem 3.16 ([28]). *Let G be a planar graph on n $(n \geqslant 6)$ vertices, then $\xi^d(G) \geqslant 4n^2 - 18n + 26$ with equality if and only if $G \cong K_2 \oplus P_{n-2}$.*

Proof. Choose G, a planar graph of order n, such that its EDS is as small as possible. Since the EDS decreases by adding edges to the graph preserving that the resultant graph is still planar, G must be a maximal planar graph, which means that there are $3n-6$ edges in G.

We claim that G has at most two vertices of degree $n-1$, otherwise as $|E_G| = 3|V_G| - 6$, we have $G \cong K_3 \oplus (n-3)K_1$, which implies that G is not a planar graph, a contradiction. By Lemma 3.15, G must have at least one vertex with degree $n-1$. Hence, we proceed by distinguishing the following two cases.

Case 1. G contains just one vertex of degree $n-1$, say w.

By the definition of the EDS, one has

$$\begin{aligned}
\xi^d(G) &= \varepsilon_G(w) D_G(w) + \sum_{v \in V_G \setminus \{w\}} \varepsilon_G(v) D_G(v) \\
&\geqslant n - 1 + \sum_{v \in V_G \setminus \{w\}} 2(2n - 2 - d_G(v)) \\
&= 4(n-1)^2 + 3(n-1) - 4m \\
&= 4n^2 - 17n + 25.
\end{aligned}$$

Case 2. G has exactly two vertices, say w_1, w_2, of degree $n-1$.

By the definition of the EDS, one has

$$\begin{aligned}
\xi^d(G) &= \varepsilon_G(w_1)D_G(w_1) + \varepsilon_G(w_2)D_G(w_2) + \sum_{v\in V_G\setminus\{w_1,w_2\}} \varepsilon_G(v)D_G(v) \\
&\geqslant 2(n-1) + \sum_{v\in V_G\setminus\{w_1,w_2\}} 2(2n-2-d_G(v)) \\
&= 4(n-1)(n-2) + 6(n-1) - 4m \\
&= 4n^2 - 18n + 26.
\end{aligned}$$

It is easy to check that $4n^2-18n+26 < 4n^2-17n+25$. Hence, $\xi^d(G) \geqslant 4n^2-18n+26$ with equality if and only if $G \cong K_2 \oplus P_{n-2}$. ■

Theorem 3.17 ([28]). *Let G be an outerplanar graph on* n $(n \geqslant 6)$ *vertices, then* $\xi^d(G) \geqslant 4n^2-13n+13$ *with equality if and only if* $G \cong K_1 \oplus P_{n-1}$.

4. Relationship between the EDS invariant and some other graph invariants

In this section we establish the relationship between the EDS invariant and some other graph invariants, such as the number of edges, degree sequence, (edge) connectivity, matching number, independence number, domination number, diameter, number of pendants, (p,q)-bipartition and so on.

4.1 Bounds on EDS involving the number of edges

Li and Wu [29] characterized the n-vertex connected graphs of size m having the minimum EDS.

For any integer m with $n-1 \leqslant m \leqslant \frac{n(n-1)}{2}-1$, there must exist some $k \in \{1,2,\ldots,n-2\}$ such that $nk-\frac{k(k+1)}{2} \leqslant m \leqslant n(k+1)-\frac{(k+1)(k+2)}{2}-1$. For convenience, assume $nk-\frac{k(k+1)}{2} \leqslant m \leqslant n(k+1)-\frac{(k+1)(k+2)}{2}-1$ for some $k \in \{1,2,\ldots,n-2\}$. Then let

$$\mathcal{G}_{n,m}^k = \left\{G \in \mathcal{G}_{n,m} | G = H \oplus K_k, |V_H| = n-k, |E_H| = m - nk + \frac{k^2}{2} + \frac{k}{2}\right\}$$

be the set of graphs each of which contains exactly k vertices of degree $n-1$.

Theorem 4.1 ([28]). *Let G be a graph in* $\mathcal{G}_{n,m}$ *with* $nk-\frac{k(k+1)}{2} \leqslant m \leqslant n(k+1)-\frac{(k+1)(k+2)}{2}-1$ *for some* $k \in \{1,2,\ldots,n-2\}$. *Then* $\xi^d(G) \geqslant 4n^2-4n-kn+k-4m$ *with equality if and only if G is in* $\mathcal{G}_{n,m}^k$.

Proof. Let G be a graph with the minimal EDS in $\mathcal{G}_{n,m}$, where $nk-\frac{k(k+1)}{2} \leqslant m \leqslant n(k+1)-\frac{(k+1)(k+2)}{2}-1$ for some fixed $k \in \{1,2,\ldots,n-2\}$. By Lemma 3.15, G contains at least one vertex of degree $n-1$. We are to show that the graph G contains at most k vertices of degree $n-1$. Suppose that G contains at least $k+1$ vertices of degree $n-1$. For convenience, let $A = \{u \in V_G | d_G(u) = n-1\}$. Then $|A| \geqslant k+1$

and it is easy to see that for $u \in V_G \setminus A$, one has $d_G(u) \geqslant k+1$. Therefore, by Handshaking lemma, we have

$$\begin{aligned} m &= \frac{1}{2}\sum_{u\in V_G} d_G(u) = \frac{1}{2}\left(\sum_{u\in A} d_G(u) + \sum_{u\in V_G\setminus A} d_G(u)\right) \\ &\geqslant \frac{1}{2}[|A|(n-1)+(n-|A|)(k+1)] \\ &\geqslant \frac{1}{2}n(k+1)+\frac{1}{2}(k+1)(n-k-2) \qquad (5) \\ &= n(k+1)-\frac{(k+1)(k+2)}{2} \\ &> n(k+1)-\frac{(k+1)(k+2)}{2}-1, \end{aligned}$$

a contradiction to the assumption that $m \leqslant n(k+1) - \frac{(k+1)(k+2)}{2} - 1$, where the inequality in (5) follows by $|A| \geqslant k+1$.

Now suppose that G is a graph in $\mathcal{G}_{n,m}$ with t vertices of degree $n-1$, where $1 \leqslant t \leqslant k$. Hence, $|A| = t$. Based on the structure of G, we have $\varepsilon_G(v) = 1, D_G(v) = n-1$ for any $v \in A$; $\varepsilon_G(v) = 2, D_G(v) = 2n-2-d_G(v)$ for any $v \in V_G \setminus A$. By the definition of the EDS, we have

$$\begin{aligned} \xi^d(G) &= \sum_{v\in A}\varepsilon_G(v)D_G(v) + \sum_{v\in V_G\setminus A}\varepsilon_G(v)D_G(v) \\ &= t(n-1) + \sum_{v\in V_G\setminus A} 2(2n-2-d_G(v)) \\ &= t(n-1)+4(n-t)(n-1) - \sum_{v\in V_G\setminus A} 2d_{G_1}(v) \\ &= 4n^2-4n-t(n-1)-4m. \end{aligned}$$

Obviously, we can view $\xi^d(G) = 4n^2 - 4n - t(n-1) - 4m$ as a real decreasing function in t with $1 \leqslant t \leqslant k$. Then G attains the minimum value on $\xi^d(G)$ only when $t = k$. In this case, G has exactly k vertices of degree $n-1$. Hence, $G \in \mathcal{G}^k_{n,m}$.

This completes the proof. ■

Now we characterize the extremal graphs obtained the minimum EDS with respect to trees, unicyclic graphs, bicyclic graphs and tricyclic graphs, respectively. The following corollaries follow directly by Theorem 4.1.

Corollary 4.2 ([28,40]). *If G is a tree in $\mathcal{G}_{n,n-1}$, then $\xi^d(G) \geqslant 4n^2 - 9n + 5$ with equality if and only if $G \cong K_{1,n-1}$.*

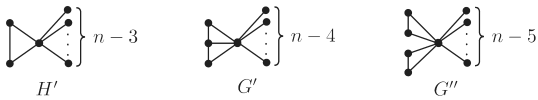

Figure 5. Graphs H', G' and G''.

Corollary 4.3 ([28, 40]). *If G is a unicyclic graph in $\mathcal{G}_{n,n}$, then $\xi^d(G) \geqslant 4n^2 - 9n + 1$ with equality if and only if $G \cong H'$, where H' is depicted in Fig. 5.*

Corollary 4.4 ([28]). *If G is a bicyclic graph in $\mathcal{G}_{n,n+1}$, then $\xi^d(G) \geqslant 4n^2 - 9n - 3$ with equality if and only if $G \in \{G', G''\}$, where G', G'' are depicted in Fig. 5.*

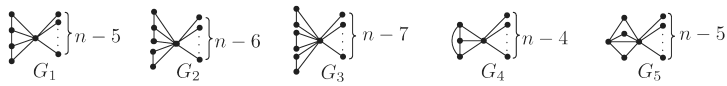

Figure 6. Tricyclic graphs G_1, G_2, G_3, G_4, G_5 with the minimum EDS.

Corollary 4.5 ([28]). *If G is a tricyclic graph in $\mathcal{G}_{n,n+2}$, then $\xi^d(G) \geqslant 4n^2 - 9n - 7$ with equality if and only if $G \in \{G_1, G_2, G_3, G_4, G_5\}$, where G_1, G_2, G_3, G_4, G_5 are depicted in Fig. 6.*

4.2 Bounds on EDS involving the vertex degrees

Let $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ denote the non-increasing sequence of vertex degrees. Recall that the largest and the smallest vertex degrees are denoted, respectively, as $\Delta = d_1$ and $\delta = d_n$. Hua, Zhang and Xu [22] gave the upper bound for EDS of connected graphs in terms of degree sequence. Mukungunugwa and Mukwembi [33] determined the asymptotic upper bounds for EDS of graphs according to its order and minimum degree. Miao et al. [31] determined the trees having the maximum EDS among the n-vertex trees with maximum degree Δ. For convenience, let $\mathscr{T}^{n,\Delta}$ be the set of all n-vertex trees with the maximum degree Δ.

Note that $d_G(u, v) \leqslant \varepsilon_G(v) \leqslant n - d_G(v)$ for any vertex $u, v \in V_G$. Thus,

Theorem 4.6 ([22]). *Let G be a connected graph on $n \geqslant 2$ vertices with degree sequence $(d_1, d_2, \ldots, d_n)$. Then*

$$\xi^d(G) \leqslant (n-1) \sum_{i=1}^{n} (n - d_i)^2$$

with equality if and only if $d_1 = d_2 = \cdots = d_n = n - 1$, that is, $G \cong K_n$.

From Theorem 4.6, the following consequence follows immediately.

Corollary 4.7 ([22]). *Let G be a connected graph on $n \geqslant 2$ vertices with minimum degree δ. Then*

$$\xi^d(G) \leqslant n(n-1)(n-\delta)^2$$

with equality if and only if $\delta = n-1$, that is, $G \cong K_n$.

Theorem 4.8 ([33]). *Let G be a connected graph of order n and minimum degree $\delta \geqslant 2$. Then*

$$\xi^d(G) \leqslant \frac{3 \cdot 5^2}{2^5 \cdot (\delta+1)^2} n^4 + O(n^3).$$

Moreover, for a fixed δ, this bound is asymptotically sharp.

Theorem 4.9 ([31]). *Among $\mathscr{T}^{n,\Delta}$ $(3 \leqslant \Delta \leqslant n-2)$, $S(a_1, 1, \ldots, 1)$ maximizes the EDS where $a_1 = n - \Delta$.*

4.3 Bounds on EDS involving the (edge) connectivity

Hua, Zhang and Xu [22] characterized the graphs with the minimum EDS among all the graphs on n vertices with edge-connectivity λ. Ilić, Yu and Feng [26] established the sharp lower bound on the EDS among all connected graphs on n vertices with a given connectivity. Li and Wu [28] considered the sharp upper bound on the EDS of graphs with even connectivity. Li, Wu and Sun [29] identified all the extremal graphs having the minimal EDS in the class of all connected n-vertex bipartite graphs with a given connectivity.

Theorem 4.10 ([22]). *Let G be a graph on n vertices with edge-connectivity λ. Then*

$$\xi^d(G) \geqslant 2n^2 - \lambda n + 2n - 3\lambda - 4$$

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

Theorem 4.11 ([26]). *Let G be a connected graph of order n with connectivity κ. Then*

$$\xi^d(G) \geqslant 2n^2 - \kappa n + 2n - 3\kappa - 4$$

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

Let G_n^k be a graph of order n obtained from a cycle C_n by adding edges between vertices with distance no more than $k/2$ on this n-vertex cycle, where k is even. For example, graphs G_8^4 and G_8^6 are depicted in Fig. 7.

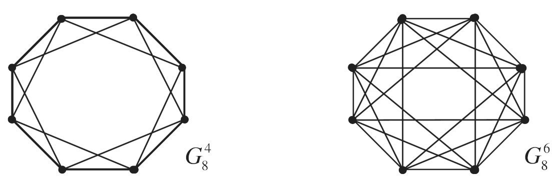

Figure 7. Graphs G_8^4 and G_8^6.

Theorem 4.12 ([28]). *Let G be a k-connected graph on n vertices with $n \geqslant k+1$. If k is even, then*

$$\xi^d(G) \leqslant n\left(n+\frac{k}{2}-1\right)\left\lfloor\frac{n+k-2}{k}\right\rfloor^2-\frac{kn}{2}\left\lfloor\frac{n+k-2}{k}\right\rfloor^3.$$

Moreover, the bound is best possible when the graph is G_n^k.

Proof. Choose any vertex $v \in V_G$ and let ε be the eccentricity of v. Let $V_i = \{x : d_G(v,x) = i\}$ and put $a_i = |V_i|$ for $i \in \{0,1,2,\ldots,\varepsilon\}$. We can see that $a_i \geqslant k$ for every $i = 1,2,\ldots,\varepsilon-1$. As we have

$$D_G(v) = 1a_1 + 2a_2 + \cdots + \varepsilon a_\varepsilon,$$

we need to maximize the last sum under the constraints

$$a_1 + a_2 + \cdots + a_\varepsilon = n-1, \qquad a_1, a_2, \ldots, a_{\varepsilon-1} \geqslant k,\ a_\varepsilon \geqslant 1.$$

Thus, we have

$$\begin{aligned} D_G(v) = 1a_1 + 2a_2 + \cdots + \varepsilon a_\varepsilon &\leqslant (1+2+\cdots+\varepsilon-1)k + \varepsilon(n-1-k(\varepsilon-1)) \qquad (6)\\ &= (n+\frac{k}{2}-1)\varepsilon - \frac{k}{2}\varepsilon^2, \end{aligned}$$

where the equality in (6) holds if and only if $a_1 = a_2 = \cdots = a_{\varepsilon-1} = k, a_\varepsilon = n-1-k(\varepsilon-1) \geqslant 1$.

From the above discussion, we obtain

$$\begin{aligned} \xi^d(G) &= \sum_{x\in V_G} \varepsilon_G(x) D_G(x) \\ &\leqslant \sum_{x\in V_G} \varepsilon\left[(n+\frac{k}{2}-1)\varepsilon - \frac{k}{2}\varepsilon^2\right] \qquad (7)\\ &= n(n+\frac{k}{2}-1)\varepsilon^2 - \frac{kn}{2}\varepsilon^3, \end{aligned}$$

where the inequality of (7) follows by (6).

Let $f = n(n+\frac{k}{2}-1)x^2 - \frac{kn}{2}x^3$ be a real function in x. By a direct derivation on f, we have

$$f'(x) = nx\left[2(n+\frac{k}{2}-1) - \frac{3k}{2}x\right].$$

It is easy to see that f is decreasing when $x \leqslant 0$ or $x \geqslant \frac{4n+2k-4}{3k}$ and increasing when $0 \leqslant x \leqslant \frac{4n+2k-4}{3k}$. As $1 \leqslant \varepsilon \leqslant \frac{n+k-2}{k}$ and $\frac{4n+2k-4}{3k} > \frac{n+k-2}{k}$, we have

$$\xi^d(G) \leqslant n(n+\frac{k}{2}-1)\left\lfloor\frac{n+k-2}{k}\right\rfloor^2 - \frac{kn}{2}\left\lfloor\frac{n+k-2}{k}\right\rfloor^3, \qquad (8)$$

where the equality of (8) holds if and only if $a_1 = a_2 = \cdots = a_{\varepsilon-1} = k, \varepsilon = \lfloor\frac{n+k-2}{k}\rfloor$ for each vertex of G, that is, $G \cong G_n^k$. ■

Next, we consider the extremal bipartite graphs with a given vertex connectivity. We define a bipartite graph $O_s \vee_1 (K_{n_1,n_2} \cup K_{m_1,m_2})$, where $\cup$ is the union of two graphs, O_s $(s \geqslant 1)$ is an empty graph of order s and $\vee_1$ is a graph operation that joins all the vertices in O_s to the vertices belonging to the partitions of cardinality n_1 in K_{n_1,n_2} and m_1 in K_{m_1,m_2}, respectively. In the rest of this subsection, K_1 may be regarded as $K_{1,0}$.

Lemma 4.13 ([29]). *If $3p < 7q + 6s + 1$ and $p \geqslant s$, then $\xi^d(O_s \vee_1 (K_1 \cup K_{p,q})) > \xi^d(O_s \vee_1 (K_1 \cup K_{p+1,q-1}))$.*

Lemma 4.14 ([29]). *If $p \geqslant q \geqslant 1$, then $\xi^d(O_s \vee_1 (K_1 \cup K_{q,p})) \geqslant \xi^d(O_s \vee_1 (K_1 \cup K_{p,q}))$ with equality if and only if $p = q$.*

Lemma 4.15 ([29]). *If $3p > 7q + 6s + 11$ and $p \geqslant s$, $q \geqslant 1$, then $\xi^d(O_s \vee_1 (K_1 \cup K_{p,q})) > \xi^d(O_s \vee_1 (K_1 \cup K_{p-1,q+1}))$.*

Lemma 4.16 ([29]). *If $2 \leqslant s \leqslant \lfloor \frac{n-12}{8} \rfloor$, then $\xi^d(K_{s,n-s}) > \xi^d(O_s \vee_1 (K_1 \cup K_{n-s-2,1}))$.*

For convenience, let $\mathscr{C}_n^s$ be the class of connected n-vertex bipartite graphs with connectivity s.

Lemma 4.17 ([29]). *If $G \in \mathscr{C}_n^s$ and U is a vertex-cut of order s in G such that $G - U$ has two nontrivial components, then G cannot be the graph with the minimal EDS among $\mathscr{C}_n^s$.*

Theorem 4.18 ([29]). *Let G be in $\mathscr{C}_n^s$ with vertex-cut U satisfying $|U| = s$ and having the minimal EDS.*

(i) *If all the components of $G - U$ are singletons and $\frac{n-12}{8} \leqslant s \leqslant \lfloor \frac{n}{2} \rfloor$, then $G \cong K_{s,n-s}$.*

(ii) *If $G - U$ contains a non-trivial component, then $G \cong O_s \vee_1 (K_1 \cup K_{p,q})$ for some p and q, where $p + q = n - s - 1$. In particular,*

  (a) *$2 \leqslant s < \frac{n-12}{8}$ and $p < \frac{7n-s-6}{10}$, one has $G \cong G_1^*$;*

  (b) *$2 \leqslant s < \frac{n-12}{8}$ and $\frac{7n-s-6}{10} \leqslant p \leqslant \frac{7n-s+4}{10}$, one has $G \cong G_1^*$ or G_2^* if $10 | (7n - s - 6)$ and $G \cong G_2^*$ if $10 \nmid (7n - s - 6)$;*

  (c) *For $2 \leqslant s < \frac{n-12}{8}$ and $p > \frac{7n-s+4}{10}$, one has $G \cong G_2^*$;*

  (d) *For $\frac{n-12}{8} \leqslant s < \lfloor \frac{n}{2} \rfloor$, one has $G \cong G_1^*$ or G_2^*,*

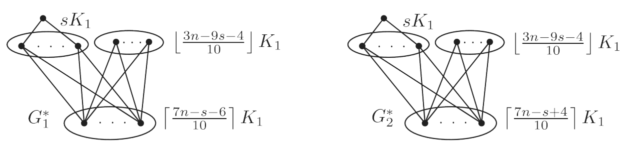

Figure 8. Graphs G_1^*, G_2^* used in Theorem 4.18.

where G_1^* and G_2^* are depicted in Fig. 8.

4.4 Bounds involving the matching number

Ilić, Yu and Feng [26] determined the graphs with the minimum EDS with given matching number. Li et al. [30] characterized the trees with the minimum and second minimum EDS among all the n-vertex trees with given matching number. Miao et al. [31] determined the trees having the maximum EDS among the n-vertex trees with given matching number. Li, Wu and Sun [29] characterized the sharp lower bound on the EDS in the class of all connected bipartite graphs with given matching number.

We denote by $T_{n,\mu}$ the tree obtained from the star graph $S_{n-\mu+1}$ by attaching a pendant edge to each of certain $\mu - 1$ non-central vertices of $S_{n-\mu+1}$. It is easy to see that $T_{n,\mu}$ contains a μ-matching. If $n = 2\mu$, then it has a perfect matching. We denote by $T'_{2\mu,\mu}$ the tree obtained from $T_{2\mu-2,\mu-1}$ by attaching a P_3 to a vertex of degree 2 in $T_{2\mu-2,\mu-1}$. Graphs $T_{n,\mu}$ and $T'_{2\mu,\mu}$ are depicted in Fig. 9.

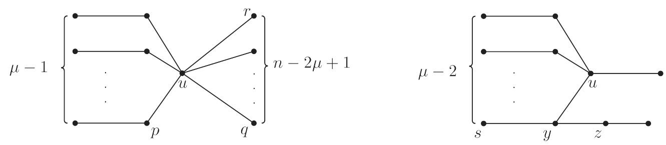

Figure 9. Graphs $T_{n,\mu}$ and $T'_{2\mu,\mu}$ with some vertices labeled.

Theorem 4.19 ([26]). *Let G be a connected graph of order n with matching number μ, $2 \leqslant \mu \leqslant \lfloor \frac{n}{2} \rfloor$. Let $b = \frac{1}{20}(9 + 5n + \sqrt{(9+5n)^2 + 40(1-5n)})$.*

- (i) *If $\mu = \lfloor \frac{n}{2} \rfloor$, then $\xi^d(G) \geqslant n(n-1)$ with equality if and only if $G \cong K_n$;*
- (ii) *If $b < \mu \leqslant \lfloor \frac{n}{2} \rfloor - 1$, then $\xi^d(G) \geqslant 4n^2 - 9n - 8\mu^2 + 12\mu + 1$ with equality if and only if $G \cong K_1 \oplus (K_{2\mu-1} \cup \overline{K}_{n-2\mu})$;*
- (iii) *If $\mu = b$, then $\xi^d(G) \geqslant 4n^2 - 9n - 8\mu^2 + 12\mu + 1 = 4n^2 - 5n\mu - 4n + 2\mu^2 + 3\mu$ with equality if and only if $G \cong K_1 \oplus (K_{2\mu-1} \cup \overline{K}_{n-2\mu})$, or $G \cong K_\mu \oplus \overline{K}_{n-\mu}$;*
- (iv) *If $2 \leqslant \mu < b$, then $\xi^d(G) \geqslant 4n^2 - 5n\mu - 4n + 2\mu^2 + 3\mu$ with equality if and only if $G \cong K_\mu \oplus \overline{K}_{n-\mu}$.*

Lemma 4.20 ([19]). *Let T be a tree with n $(n > 2)$ vertices and with a perfect matching. Then T has at least two pendant vertices such that they are adjacent to vertices of degree 2, respectively.*

Lemma 4.21 ([19]). *Let T be an n-vertex tree with a μ-matching, and $n = 2\mu + 1$. Then T has a pendant vertex which is adjacent to a vertex of degree 2.*

Lemma 4.22 ([4, 19]). *Let T be an n-vertex tree with a μ-matching where $n > 2\mu$. Then there is a μ-matching M and a pendant vertex v such that M does not saturate v.*

Theorem 4.23 ([30]). *Let $T \in \mathscr{T}_{2\mu,\mu}$. Then $\xi^d(T) \geqslant 43\mu^2 - 72\mu + 34$. The equality holds if and only if $T \cong T_{2\mu,\mu}$, where $T_{2\mu,\mu}$ is depicted in Fig. 9.*

Theorem 4.24 ([30]). *Let T be the tree in $\mathscr{T}_{2\mu,\mu} \setminus \{T_{2\mu,\mu}\}$. Then $\xi^d(T) \geqslant 55\mu^2 - 66\mu - 52$. The equality holds if and only if $T \cong T'_{2\mu,\mu}$, where $T'_{2\mu,\mu}$ is depicted in Fig. 9.*

Theorem 4.25 ([30]). *Let T be an n-vertex ($n \geqslant 2\mu$) tree with a μ-matching. Then*

$$\xi^d(T) \geqslant 6n^2 + \mu^2 + 9\mu n - 22n - 28\mu + 34$$

and the equality holds if and only if $T \cong T_{n,\mu}$, where $T_{n,\mu}$ is depicted in Fig. 9.

Theorem 4.26 ([30]). *Let T be the tree in $\mathscr{T}_{n,\mu} \setminus \{T_{n,\mu}\}$ ($n > 2\mu \geqslant 6$). Then*

$$\xi^d(T) \geqslant 6n^2 + \mu^2 + 9\mu n - 13n - 26\mu - 9$$

and the equality holds if and only if $T \cong T'_{n,\mu}$, where $T'_{n,\mu} = T_{n,\mu} - uq + pq$ and $T_{n,\mu}$ is depicted in Fig. 9.

Theorem 4.27 ([31]). *Among all the trees of order n with matching number μ, the tree $P_l(a,b)$ has the maximum EDS, where $l = 2\mu - 1$ and $0 \leqslant b - a \leqslant 1$.*

Let $\mathscr{A}_n^\mu$ be the class of all connected bipartite graphs of order n with matching number μ.

Theorem 4.28 ([29]). *Let $G = (U, W) \in \mathscr{A}_n^\mu$.*

(i) *If $\mu = 1$, then $\xi^d(G) = \xi^d(K_{1,n-1}) = 4n^2 - 9n + 5$;*
(ii) *If $\mu \geqslant 2$, then $\xi^d(G) \geqslant 4n^2 + 4\mu^2 - 4n\mu - 4n$ with equality if and only if $G \cong K_{\mu,n-\mu}$.*

4.5 Bounds on EDS involving the independence number

Ilić, Yu and Feng [26] characterized the graphs having the minimum EDS of order n with the independence number α. Miao et al. [31] determined the trees having the maximum and minimum EDS among the n-vertex trees with independence number α.

Theorem 4.29 ([26]). *Let G be a connected graph of order n with independence number α. Then*

$$\xi^d(G) \geqslant n^2 + (\alpha - 1)n + 2\alpha^2 - 3\alpha$$

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

Theorem 4.30 ([31]). *Among all the trees of order n and with independence number α, the tree $T_{n,n-\alpha}$ has the minimum EDS.*

Theorem 4.31 ([31]). *Among all trees of order n and with independence number α, the tree $P_l(a,b)$ has the maximum EDS, where $l = 2(n-\alpha) - 1$ and $0 \leqslant b - a \leqslant 1$.*

Combining with Theorems 4.30 and 4.31, we have the following corollary.

Corollary 4.32. *Let G be a connected graph of order n with independence number α. Then*

$$\xi^d(\overline{K}_\alpha \oplus K_{n-\alpha}) \leqslant \xi^d(G) \leqslant \xi^d(P_l(a,b)).$$

The left equality attains if and only if $G \cong \overline{K}_\alpha \oplus K_{n-\alpha}$, and the right equality attains if and only if $G \cong P_l(a,b)$.

4.6 Bounds on EDS involving the domination number

Geng, Li and Zhang [15] characterized the tree among n-vertex trees with domination number γ having the minimum EDS and they also determined the graph among n-vertex trees with domination number γ satisfying $n = k\gamma$ having the maximum EDS, $k = 2, n/3, n/2$. Miao et al. [31] characterized the tree having the maximum EDS among n-vertex trees with domination number $\gamma = 3$.

For convenience, let $\mathcal{T}_{n,\gamma}$ be the set of all n-vertex trees with domination number γ.

Lemma 4.33 ([15]). *If $T' \in \mathcal{T}_{n,\gamma}$ has the minimum EDS, then we have $\gamma(T') = \beta(T') = \gamma$.*

Combining Theorem 4.25 and Lemma 4.33, the following is obvious.

Theorem 4.34 ([15]). *For any tree $T \in \mathcal{T}_{n,\gamma}$, we have $\xi^d(T) \geqslant 6n^2 + \gamma^2 + 9\gamma n - 22n - 28\gamma + 34$. The equality holds if and only if $T \cong T_{n,\gamma}$.*

Lemma 4.35 ([11]). *Let T be a tree of order n. Then $W(S_n) \leqslant W(T) \leqslant W(P_n)$. The left equality holds if and only if $T \cong S_n$, and the right equality holds if and only if $T \cong P_n$.*

The *corona* of two graphs G_1 and G_2, introduced in [14], is a new graph $G_1 \circ G_2$ obtained from one copy of G_1 and $|V_{G_1}|$ copies of G_2 such that the i^{th} vertex of G_1 is adjacent to every vertex in the i^{th} copy of G_2. As an example, the corona $G \circ K_1$ is a graph obtained from attaching a leaf to each vertex of G. In particular, for a positive integer p, we denote by $G^{(p)}$ the graph obtained by attaching p leaves to every vertex of G. Note that $G^{(p)}$ has $(p+1)n$ vertices and $G \circ K_1 = G^{(1)}$.

Lemma 4.36 ([15]). *Let T be a tree of order n and $T^{(m)}$ be the graph as defined above. Then $\xi^d(S_n^{(m)}) \leqslant \xi^d(T^{(m)}) \leqslant \xi^d(P_n^{(m)})$. The left equality holds if and only if $T \cong S_n$, and the right equality holds if and only if $T \cong P_n$.*

Lemma 4.37 ([13, 39]). *If $n = 2\gamma$, then a tree T belongs to $\mathcal{T}_{n,\gamma}$ if and only if there exists a tree H of order γ such that $T = H \circ K_1$.*

Theorem 4.38 ([15]). *Among all the trees in $\mathcal{T}_{n,\frac{n}{2}}$, the tree $P_{\frac{n}{2}} \circ K_1$ has the maximum EDS.*

Proof. By Lemma 4.37, any tree in $\mathcal{T}_{n,\frac{n}{2}}$ must be of the form $H \circ K_1$ where H is a tree of order $\frac{n}{2} = \gamma$. Taking $m = 1$ in Lemma 4.36 implies the result immediately. ■

Theorem 4.39 ([15]). *Among all the trees in $\mathcal{T}_{n,\lceil\frac{n}{3}\rceil}$ with $n > 4$, the tree P_n has the maximum EDS.*

Lemma 4.40 ([15]). $\xi^d(P_l(1, n-l-1)) < \xi^d(P_l(2, n-l-2)) < \cdots < \xi^d(P_l(\lfloor\frac{n-l}{2}\rfloor, \lceil\frac{n-l}{2}\rceil))$.

Theorem 4.41 ([15]). *Among all the trees in $\mathcal{T}_{n,2}$ with $n \geqslant 4$, the tree $P_4(\lfloor\frac{n-4}{2}\rfloor, \lceil\frac{n-4}{2}\rceil)$ has the maximum EDS.*

Proof. In view of Theorem 4.39, the result holds for $n = 4, 5, 6$. So in what follows, we only consider the case for $n \geqslant 7$. Assume that $T_1 \in \mathcal{T}_{n,2}$ has the maximum EDS and $S = \{w_1, w_2\}$ is a dominating set of T_1. Now we show the following two claims:

Claim 1. w_1 *is not adjacent to* w_2 .

Proof of Claim 1. If not, then T_1 must be of the form $P_2(a,b)$ with $a+b=n-2$ and $a \leqslant b$. By Lemma 4.40, we have $b-a \leqslant 1$. That is to say, $T_1 \cong P_2(\lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil)$. Note that $\frac{n-2}{2} \geqslant \frac{5}{2} > 2$. After running the converse of e.g.t. on the edge w_1w_2 of T_1, we obtain a new tree $T_2 \cong P_3(\lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil - 1)$ which still belongs to $\mathcal{T}_{n,2}$. By Theorem 2.8, we have $\xi^d(T_2) > \xi^d(T_1)$, which contradicts the choice of T_1. ■

Claim 2. $d_{T_1}(w_1,w_2) = 3$.

Proof of Claim 2. From Claim 1, we have $d_{T_1}(w_1,w_2) \geqslant 2$. If $d_{T_1}(w_1,w_2) \geqslant 4$, then there exists at least one vertex x on the shortest path between w_1 and w_2 such that x can not be dominated by the two vertices w_1 and w_2. This contradicts the fact that $T_1 \in \mathcal{T}_{n,2}$. Then we get $2 \leqslant d_{T_1}(w_1,w_2) \leqslant 3$. If $d_{T_1}(w_1,w_2) = 2$, then we find that $T_1 \cong P_3(\lfloor\frac{n-3}{2}\rfloor, \lceil\frac{n-3}{2}\rceil)$ by Lemma 4.40. Assume that the common neighbor of w_1 and w_2 is w_0. Note that $\frac{n-3}{2} \geqslant 2 > 1$. By running the converse of e.g.t. on the edge w_0w_1 or w_0w_2, in view of Theorem 2.8, we get a new tree of the form $P_4(a,b)$ with $a+b=n-4$, which is still in $\mathcal{T}_{n,2}$ but has a larger EDS. This is impossible because of the maximality of $\xi^d(T_1)$, as desired. ■

By Claims 1 and 2, T_1 must be of the form $P_4(a,b)$ with $a+b=n-4$. By Lemma 4.40, this theorem follows immediately. ■

Theorem 4.42 ([31]). *Among* $\mathcal{T}_{n,3}$ *with* $n \geqslant 10$, $P_7(\lfloor\frac{n-7}{2}\rfloor, \lceil\frac{n-7}{2}\rceil)$ *maximizes the EDS.*

4.7 Bounds on EDS involving the diameter

Let $\mathscr{T}_n^d$ be the set of all n-vertex trees of diameter d. Yu, Feng and Illić [40] that $C_{n,d}$ is unique tree in $\mathscr{T}_n^d$ with the minimum EDS. As a consequence, they determined the n-vertex trees with minimum and second minimum EDS. Li et al. [30] characterized the extremal trees with the second minimum EDS among the n-vertex trees of a given diameter. Li and Wu [28] characterized the n-vertex graphs with diameter d having minimum EDS. Li, Wu and Sun [29] considered the same problem in the class of all the connected bipartite graphs of odd diameter d.

Given a positive integer t, let $C_d(t)$ be the tree obtained from $C_{n-t,d}$ and S_{t+1} by identifying a pendant vertex, say u, in the neighborhood of $v_{\lfloor d/2\rfloor}$ with the center of the star S_{t+1}.

Theorem 4.43 ([40]). *Among trees on* n *vertices and diameter* d, *caterpillar* $C_{n,d}$ *has the minimal eccentric distance sum*[1],

$$\xi^d(C_{n,d}) = \begin{cases} -\frac{7}{96}d^4 + (\frac{n}{3} - \frac{17}{24})d^3 + (\frac{n}{4} + \frac{7}{24})d^2 + (n^2 - \frac{23}{6}n + \frac{23}{6})d + 2n^2 - 5n + 3, & \text{if } d \text{ is even;} \\ -\frac{7}{96}d^4 + (\frac{n}{3} - \frac{5}{6})d^3 + (\frac{3n}{8} + \frac{11}{48})d^2 + (n^2 - \frac{29}{6}n + \frac{29}{6})d + 3n^2 - \frac{55}{8}n + \frac{123}{32}, & \text{if } d \text{ is odd.} \end{cases}$$

Theorem 4.44 ([30]). $C'_{n,d}$ $(d \geqslant 3)$ *has the second minimal eccentric distance sum in* $\mathscr{T}_n^d$,

$$\xi^d(C'_{n,d}) = \begin{cases} -\frac{7}{96}d^4 + (\frac{n}{3} - \frac{17}{24})d^3 + (\frac{n}{4} - \frac{11}{24})d^2 + (n^2 - \frac{17}{6}n - \frac{2}{3})d + 2n^2 - 4, & \text{if } d \text{ is even;} \\ -\frac{7}{96}d^4 + (\frac{n}{3} - \frac{5}{6})d^3 + (\frac{3n}{8} - \frac{37}{48})d^2 + (n^2 - \frac{23}{6}n - \frac{1}{6})d + 3n^2 - \frac{31}{8}n - \frac{69}{32}, & \text{if } d \text{ is odd.} \end{cases}$$

[1]The value of $\xi^d(C_{n,d})$ in [40] is not correct. Here, we give the correct version.

Next, we characterize the n-vertex graphs with diameter d having the minimum EDS. Clearly, K_n (resp. P_n) is the unique graph of diameter 1 (resp. $n-1$). Hence, we consider in what follows that $2 \leqslant d \leqslant n-2$. In particular, if d is odd, let

$$\mathscr{G}_n^d := \{G_{n,d} | G_{n,d} = [(d-1)/2]K_1 \oplus K_{n_1+1} \oplus K_{n_2+1} \oplus [(d-1)/2]K_1, n_1 \geqslant 0, n_2 \geqslant 0, n_1+n_2 = n-d-1\}.$$

A *bug* Bug_{p,q_1,q_2} is a graph obtained from a complete graph K_p by deleting an edge uv and attaching paths P_{q_1} and P_{q_2} at u and v, respectively. It is obvious that the number of vertices of Bug_{p,q_1,q_2} is $p+q_1+q_2-2$. For example, $Bug_{6,3,3}$ is depicted in Fig. 10.

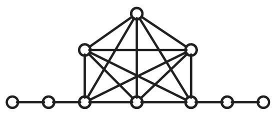

Figure 10. $Bug_{6,3,3}$.

Theorem 4.45 ([28]). *Let G be an n-vertex graph of diameter d with the minimal EDS, $2 \leqslant d \leqslant n-2$. Then $G \cong Bug_{n-d+2,\frac{d}{2},\frac{d}{2}}$ if d is even, and G is in $\mathscr{G}_n^d$ otherwise.*

Proof. Choose G among the n-vertex graphs with diameter d such that its EDS is as small as possible. Let x_0 be a vertex of G with the maximal eccentricity d, then there exists a vertex x_d such that $d_G(x_0, x_d) = d$. For convenience, let $P := x_0x_1 \dots x_d$ be a path of length d in G connecting x_0 and x_d. Denote by L_i the set of vertices at distance i from x_0 for $i \in \{0, 1, \dots, d\}$. It is routine to check that $L_0 \cup L_1 \cup \cdots \cup L_d$ is the vertex partition of V_G. We proceed by considering the following two facts. By Lemma 1.1, the first fact is obvious.

Fact 1. *$G[L_i]$ (resp. $G[L_{j-1} \cup L_j]$) induces a complete graph for $i = 0, 1, \dots, d$ (resp. $j = 1, 2, \dots, d$).*

Fact 2. *Consider the vertex partition $V_G = L_0 \cup L_1 \cup \cdots \cup L_d$ of G.*

(i) *For even d, if $d = 2$, then $|L_0| = |L_2| = 1$ and $|L_1| = n-2$; if $d \geqslant 4$, then $|L_0| = |L_1| = \cdots = |L_{\frac{d}{2}-1}| = |L_{\frac{d}{2}+1}| = \cdots = |L_{d-1}| = |L_d| = 1$, $|L_{\frac{d}{2}}| = n-d$.*

(ii) *For odd d, one has $|L_0| = |L_1| = \cdots = |L_{\frac{d-3}{2}}| = |L_{\frac{d+3}{2}}| = \cdots = |L_{d-1}| = |L_d| = 1$, and $|L_{\frac{d-1}{2}}| + |L_{\frac{d+1}{2}}| = n-d+1$.*

Proof of Fact 2. (i) It is routine to check that $|L_0| = |L_d| = 1$. Hence, if $d = 2$, then $|L_1| = n-2$. In what follows we only show that $|L_1| = 1$ for diameter $d \geqslant 4$ holds.

In fact, if $|L_1| \geqslant 2$, then choose $u \in L_1 \setminus \{x_1\}$ and let $G' = G - ux_0 + \{ux : x \in L_3\}$. Then, $L_0 \cup (L_1 \setminus \{u\}) \cup (L_2 \cup \{u\}) \cup L_3 \cup \cdots \cup L_d$ is the vertex partition of $V_{G'}$. By Fact 1 and the choice of G, we know that $G'[L_i]$ for $i \in \{0, 1, \dots d\}$ and $G'[L_{i-1} \cup L_i]$ for $i \in \{1, 2, \dots, d\}$ induce a complete subgraph.

By the structure of G and G', we obtain that $\varepsilon_G(u) = d-1, \varepsilon_{G'}(u) = d-2$, and $\varepsilon_G(x) = \varepsilon_{G'}(x)$ for all $x \in V_G \setminus \{u\}$. And we have

$$\begin{array}{rcll} D_G(x_0) & = & D_{G'}(x_0) - 1, & D_G(u) = D_{G'}(u) - 1 + \sum\limits_{i=3}^{d} |L_i|, \\ D_G(x) & = & D_{G'}(x), & \text{for each } x \in (L_1 \setminus \{u\}) \cup L_2, \\ D_G(x) & = & D_{G'}(x) + 1, & \text{for each } x \in L_3 \cup \ldots \cup L_d. \end{array}$$

Hence, by the definition of the EDS, we have

$$\begin{aligned} \xi^d(G) - \xi^d(G') &= \sum_{x \in V_G} \varepsilon_G(x) D_G(x) - \sum_{x \in V_{G'}} \varepsilon_{G'}(x) D_{G'}(x) \\ &= \varepsilon_G(x_0)(D_G(x_0) - D_{G'}(x_0)) + \sum_{x \in L_1 \setminus \{u\} \cup L_2} \varepsilon_G(x)(D_G(x) - D_{G'}(x)) \\ &\quad + \varepsilon_G(u) D_G(u) - \varepsilon_{G'}(u) D_{G'}(u) + \sum_{x \in L_3 \cup \cdots \cup L_d} \varepsilon_G(x)(D_G(x) - D_{G'}(x)) \\ &> -d + 0 + (d-2)\left(-1 + \sum_{i=3}^{d} |L_i|\right) + \sum_{x \in L_3 \cup \cdots \cup L_d} \varepsilon_G(x) \qquad (9) \\ &= (d-2)\left(\sum_{i=3}^{d} |L_i| - 1\right) + \sum_{x \in L_3 \cup \cdots \cup L_{d-1}} \varepsilon_G(x) > 0\,, \qquad (10) \end{aligned}$$

where the inequality in (9) follows by $\varepsilon_G(u) = d-1 > \varepsilon_{G'}(u) = d-2$, whereas the inequality in (10) holds by $d \geqslant 4, |L_i| \geqslant 1$ for $i \in \{3, 4, \ldots, d\}$ and $\varepsilon_G(x) \geqslant 2$ for any $x \in L_3 \cup \cdots \cup L_d$. Hence, $\xi^d(G) > \xi^d(G')$, a contradiction. Therefore, $|L_1| = 1$. By a similar discussion, we may also show that $|L_2| = \cdots = |L_{\frac{d}{2}-1}| = |L_{\frac{d}{2}+1}| = \cdots = |L_{d-1}| = 1$, we omit the procedure here. As $|L_0| = |L_1| = \cdots = |L_{\frac{d}{2}-1}| = |L_{\frac{d}{2}+1}| = \cdots = |L_{d-1}| = |L_d| = 1$, it is easy to see that $|L_{\frac{d}{2}}| = n - d$.

(ii) This is proved by an argument analogous to that used in (i), which is omitted here. Hence, $G \in \mathscr{G}_n^d$. ■

Now we come back to show our results.

If d is even, by Facts 1 and 2(i), we know that G is just the bug $Bug_{n-d+2, \frac{d}{2}, \frac{d}{2}}$, as desired. If d is odd, by Facts 1 and 2(ii), the graph G is in the set $\mathscr{G}_n^d$. In what follows, we shall show that each graph in $\mathscr{G}_n^d$ attains the minimum EDS by proving $\xi^d(G_1) = \xi^d(G_2)$ for any graphs G_1, G_2 in $\mathscr{G}_n^d$.

Let G_1 and G_2 be graphs in $\mathscr{G}_n^d$, where $G_1 = [\frac{d-1}{2}]K_1 \oplus K_{n_1+1} \oplus K_{n_2+1} \oplus [\frac{d-1}{2}]K_1$ and $G_2 = [\frac{d-1}{2}]K_1 \oplus K_{n_3+1} \oplus K_1 \oplus [\frac{d-1}{2}]K_1$, satisfying $n_1 > 0, n_2 > 0, n_3 > 0$. It is easy to see that $n_3 = n_1 + n_2 = n - d - 1$. Let $\{x_0\} \cup \{x_1\} \cup \cdots \cup \{x_{\frac{d-3}{2}}\} \cup L_{\frac{d-1}{2}} \cup L_{\frac{d+1}{2}} \cup \{x_{\frac{d+3}{2}}\} \cup \cdots \cup \{x_d\}$ be the vertex partition of V_{G_1} as previously discussed. Then G_2 can be obtained from G_1 by the following graph transformation:

$$G_2 = G_1 - \{ux_{\frac{d+3}{2}} : u \in L_{\frac{d+1}{2}} \setminus \{x_{\frac{d+1}{2}}\}\} + \{ux_{\frac{d-3}{2}} : u \in L_{\frac{d+1}{2}} \setminus \{x_{\frac{d+1}{2}}\}\}.$$

Then $\{x_0\} \cup \{x_1\} \cup \cdots \cup \{x_{\frac{d-3}{2}}\} \cup (L_{\frac{d-1}{2}} \cup (L_{\frac{d+1}{2}} \setminus \{x_{\frac{d+1}{2}}\})) \cup \{x_{\frac{d+1}{2}}\} \cup \{x_{\frac{d+3}{2}}\} \cup \cdots \cup \{x_d\}$ is the vertex partition of V_{G_2}. Compared the structure of G_1 with G_2, one has $\varepsilon_{G_1}(x) = \varepsilon_{G_2}(x)$, for each $x \in V_{G_1}$.

Furthermore,

$$D_{G_1}(x) = D_{G_2}(x) + n_2, \text{ for each } x \in \{x_0\} \cup \cdots \cup \{x_{\frac{d-3}{2}}\},$$
$$D_{G_1}(x) = D_{G_2}(x) - n_2, \text{ for each } x \in \{x_{\frac{d+3}{2}}\} \cup \cdots \cup \{x_d\},$$

which depends on the equation $n_1 + n_2 = n_3$. By direct calculation, one has $D_{G_1}(x) = n + \frac{d^2-2d-3}{4}$, $D_{G_2}(x) = n + \frac{d^2-2d-3}{4}$ for each $x \in L_{\frac{d-1}{2}} \cup L_{\frac{d-1}{2}}$. Thus, $D_{G_1}(x) = D_{G_2}(x)$ for each $x \in L_{\frac{d-1}{2}} \cup L_{\frac{d+1}{2}}$.

By the definition of the EDS, one has

$$\begin{aligned}
\xi^d(G_1) - \xi^d(G_2) &= \sum_{x \in L_0 \cup \cdots \cup L_{\frac{d-3}{2}}} (\varepsilon_{G_1}(x) D_{G_1}(x) - \varepsilon_{G_2}(x) D_{G_2}(x)) + \sum_{x \in L_{\frac{d+3}{2}} \cup \cdots \cup L_d} (\varepsilon_{G_1}(x) D_{G_1}(x) \\
&\quad - \varepsilon_{G_2}(x) D_{G_2}(x)) + \sum_{x \in L_{\frac{d-1}{2}}} \varepsilon_{G_1}(x) D_{G_1}(x) + \sum_{x \in L_{\frac{d+1}{2}}} \varepsilon_{G_1}(x) D_{G_1}(x) \\
&\quad - \sum_{x \in L_{\frac{d-1}{2}}} \varepsilon_{G_2}(x) D_{G_2}(x) - \sum_{x \in L_{\frac{d+1}{2}}} \varepsilon_{G_2}(x) D_{G_2}(x) \\
&= \left(\sum_{x \in L_0 \cup \ldots \cup L_{\frac{d-3}{2}}} \varepsilon_{G_1}(x) \cdot n_2 + \sum_{x \in L_{\frac{d+3}{2}} \cup \cdots \cup L_d} \varepsilon_{G_1}(x) \cdot (-n_2) \right) \\
&\quad + \frac{d+1}{2} \cdot \left(n + \frac{d^2 - 2d - 3}{4} \right) \cdot ((n_1+1) + (n_2+1) - (n_3+1) - 1) = 0\,.
\end{aligned}$$

Hence, $\xi^d(G_1) = \xi^d(G_2)$, which means that every graph in $\mathscr{G}_n^d$ attains the minimum EDS for odd d, as desired.

This completes the proof. ■

Let $\mathscr{B}_n^d$ be the class of all connected bipartite graphs of order n with diameter d. Now we consider the graphs in $\mathscr{B}_n^d$ having the minimum EDS for odd d. For each member in $\mathscr{B}_n^d$, assume that $P = v_0 v_1 \ldots v_d$ is one of its longest paths. Then for any $G = (V_G, E_G)$ in $\mathscr{B}_n^d$, there is a partition $V_0, V_1, \ldots, V_d$ of V_G such that $|V_0| = 1$ with $d(v_0, v) = i$ for each vertex $v \in V_i$ $(i = 0, 1, 2, \ldots, d)$. We call V_i a *block* of V_G. Two blocks V_i, V_j of V_G are adjacent if $|i - j| = 1$.

Lemma 4.46 ([36]). *For any graph $G \in \mathscr{B}_n^d$ with the above partition of V_G, $G[V_i]$ induces an empty graph (i.e., containing no edge) for each $i \in \{0, 1, \ldots, d\}$.*

Given integers n, d with $3 \leqslant d \leqslant n - 1$, define a path-complete bipartite graph as follows:

$$G(n,d) = \left[\frac{d-1}{2}\right] K_1 \oplus \overline{K}_{n_1} \oplus \overline{K}_{n_2} \oplus \left[\frac{d-1}{2}\right] K_1,$$

where $n_1 = \lfloor \frac{n-d+1}{2} \rfloor$ and $n_2 = \lceil \frac{n-d+1}{2} \rceil$.

Theorem 4.47 ([29]). *Let G be the graph in $\mathscr{B}_n^d$ with the minimum EDS for odd $d \geqslant 3$. Then $G \cong G(n,d)$, where $G(n,d)$ is defined as above.*

4.8 Bounds on EDS involving the number of pendant vertices

Let $\mathscr{T}_n^k$ be the set of all n-vertex trees with k leaves. Geng, Li and Zhang [15] determined the trees with the minimum and the maximum EDS among the n-vertex trees each of which contains k leaves. Hua, Zhang and Xu [22] characterized the graph with k pendant edges having the minimum EDS. Note that there is just one tree for $k = n-1$ or 2, hence in what follows we consider $3 \leqslant k \leqslant n-2$.

Theorem 4.48 ([15]). *Among $\mathscr{T}_n^k$, the balanced spider* $S(\underbrace{\lceil \frac{n-1}{k} \rceil, \ldots, \lceil \frac{n-1}{k} \rceil}_{r}, \underbrace{\lfloor \frac{n-1}{k} \rfloor, \ldots, \lfloor \frac{n-1}{k} \rfloor}_{k-r})$ *minimizes the EDS, where $n-1 \equiv r \pmod{k}$.*

Theorem 4.49 ([15]). *Let T be an n-vertex tree with k leaves, then $\xi^d(T) \leqslant \xi^d(P_{n-k}(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil))$ with equality if and only if $T \cong P_{n-k}(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)$.*

Proof. Let T^* be the n-vertex tree with k leaves which has the maximal EDS, then T^* is of the form $P_{n-k}(a,b)$, where $a+b=k$. Otherwise, by Theorem 2.2 there exists another n-vertex tree with k leaves, say $\hat{T}$, such that $\xi^d(T^*) < \xi^d(\hat{T})$, a contradiction. By Lemma 4.40, among $\{P_{n-k}(a,b) : a+b = k,\ a,b \geqslant 1\}$, only $P_{n-k}(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)$ has the largest EDS. This completes the proof. ■

For $1 \leqslant k \leqslant n-1$ ($k \neq n-2$), we let K_n^k be the graph obtained by attaching k pendant edges to a vertex of complete graph K_{n-k}. For the sake of consistency, if $k=0$, we let $K_n^0 = K_n$.

Theorem 4.50 ([22]). *Let G be a connected graph on n vertices with k cut edges. Then*

$$\xi^d(G) \geqslant 2n^2 + (4k-3)n - 2k^2 - 6k + 1$$

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

Theorem 4.51 ([22]). *Let G be a connected graph on n vertices with k pendant edges. Then*

$$\xi^d(G) \geqslant 2n^2 + (4k-3)n - 2k^2 - 6k + 1$$

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

4.9 Bounds on EDS involving the (*p*, *q*)-bipartition

Let $\mathscr{T}_n^{p,q}$ be the set of all n-vertex trees, each of which has a (p,q)-bipartition $(p+q=n)$. Geng, Li and Zhang [15] determined the trees with the first, second and third minimum EDS in $\mathscr{T}_n^{p,q}$. Note that $\mathscr{T}_n^{1,n-1}$ contains just S_n, whereas $\mathscr{T}_n^{2,n-2} = \{P_3(a,b),\ a+b = n-3\}$.

By Lemmas 4.40 and Theorem 2.8, we have $\xi^d(P_3(0,n-3)) < \xi^d(P_3(1,n-4)) < \xi^d(P_3(2,n-5)) < \xi^d(P_3(3,n-6)) < \ldots < \xi^d(P_3(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil))$. Hence in what follows we consider $p \geqslant 3$.

Note that, in Theorem 2.4, if T is in $\mathscr{T}_n^{p,q}$, it is easy to see that T^* is also in $\mathscr{T}_n^{p,q}$. Furthermore, $\mathrm{diam}(T^*) \leqslant \mathrm{diam}(T)$. Applying Transformation I repeatedly yields the following theorem.

Theorem 4.52 ([15]). *The tree $T(p,q)$ is the unique tree in $\mathscr{T}_n^{p,q}$ which has the minimum EDS, where $T(p,q)$ is depicted in Fig. 11.*

Next, we determine the unique tree with the second minimum EDS in $\mathscr{T}_n^{p,q}$. Let $\mathscr{A} = \{T_s : 1 \leqslant s \leqslant \frac{p-1}{2}\} \bigcup \{T'_t : 1 \leqslant t \leqslant \frac{q-1}{2}\}$, where T_s and T'_t are depicted in Fig. 11.

Theorem 4.53 ([15]). *Among $\mathscr{T}_n^{p,q}$, T_1 is the unique tree with the second minimum EDS for $3 \leqslant p \leqslant q$.*

Proof. Choose $T \in \mathscr{T}_n^{p,q} \setminus \{T(p,q)\}$ such that its EDS is as small as possible. Note that Transformation Ⅱ strictly decreases the EDS of trees. It is easy to see that applying Transformation Ⅱ once to T, the resultant graph is just $T(p,q)$. Together with the definition of $\mathscr{A}$ we know the tree among $\mathscr{T}_n^{p,q}$ with the second minimal EDS must be in $\mathscr{A}$.

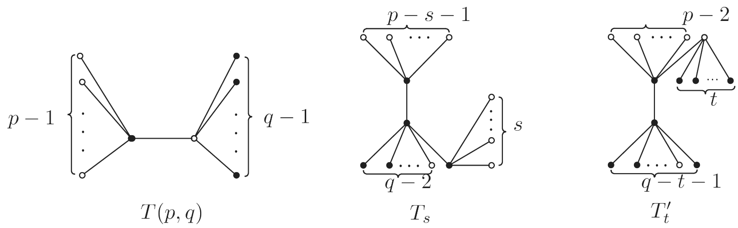

Figure 11. Trees $T(p,q), T_s$ and T'_t

By the definition of EDS, we have

$$\begin{aligned}\xi^d(T_s) =&4(p-s-1)(1+2(p-s-1)+3(q-1)+4s)+3(p-s+2(q-1)+3s)\\ &+2(q+2(p-1))+3(q-2)(1+2(q-1)+3(p-1))+3(s+1+2(q-1)\\ &+3(p-s-1))+4s(1+2s+3(q-1)+4(p-s-1))\\ =&6n^2+9np-7p^2-22n-4p+16ps-16s^2-16s+18=f(s).\end{aligned}$$

By direct verification, it follows $f'(s) = 16p - 32s - 16 = 16(p-1-2s) \geqslant 0$, which implies $f(s)$ is an increasing function in s with $1 \leqslant s \leqslant \frac{p-1}{2}$. Hence, we have

$$\xi^d(T_1) < \xi^d(T_2) < \cdots < \xi^d(T_{\lfloor \frac{p-1}{2} \rfloor}). \tag{11}$$

Similarly, we have

$$\begin{aligned}\xi^d(T'_t) =&4(q-t-1)(1+2(q-t-1)+3(p-1)+4t)+3(q-t+2(p-1)+3t)\\ &+2(p+2(q-1))+3(p-2)(1+2(p-1)+3(q-1))+3(t+1+2(p-1)\\ &+3(q-t-1))+4t(1+2t+3(p-1)+4(q-t-1))\\ =&6n^2+9nq-7q^2-22n-4q+16qt-16t^2-16t+18=g(t).\end{aligned}$$

By direct verification, it follows $g'(t) = 16q - 32t - 16 = 16(q-1-2t) \geqslant 0$, which implies $g(t)$ is an increasing function in t with $1 \leqslant t \leqslant \frac{q-1}{2}$. Hence,

$$\xi^d(T'_1) < \xi^d(T'_2) < \cdots < \xi^d(T'_{\lfloor \frac{q-1}{2} \rfloor}). \tag{12}$$

In order to characterize the tree with second minimal EDS in $\mathscr{A}$, in view of (11) and (12) it suffices to compare the EDS of T_1 with that of T_1'. On the one hand, if $p = q$ we have $T_1 \cong T_1'$, our result holds in this case. On the other hand, if $p < q$, by direct computing we have

$$\xi^d(T_1) = 6n^2 + 9np - 7p^2 - 22n + 12p - 14, \quad \xi^d(T_1') = 6n^2 + 9nq - 7q^2 - 22n + 12q - 14.$$

This gives that $\xi^d(T_1) - \xi^d(T_1') = 2(n+6)(p-q) < 0$, i.e., $\xi^d(T_1) < \xi^d(T_1')$, as desired. ■

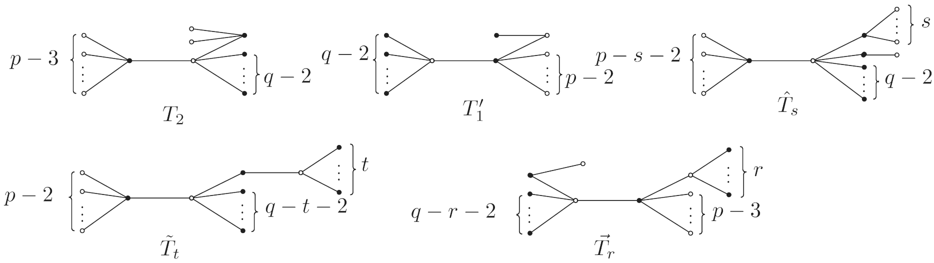

Figure 12. Trees $T_2, T_1', \hat{T}_s, \tilde{T}_t$ and $\vec{T}_r$.

Finally, we determine the tree with the third minimum EDS in $\mathscr{T}_n^{p,q}$. Let $\mathscr{B} = \{T_2,\ T_1'\} \bigcup \{\hat{T}_s :\ 1 \leqslant s \leqslant p-3\} \bigcup \{\tilde{T}_t :\ 1 \leqslant t \leqslant p-3\} \bigcup \{\vec{T}_r :\ 1 \leqslant r \leqslant q-3\}$, where $T_2,\ T_1', \hat{T}_s,\ \tilde{T}_t$ and $\vec{T}_r$ are depicted in Fig. 12.

Theorem 4.54 ([15]). *Among $\mathscr{T}_n^{p,q}$ with $4 \leqslant p < q$.*

(i) *If $n > p - 3 + \sqrt{p^2 + 9p - 23}$, then T_2 is the unique tree with the third minimum EDS;*

(ii) *If $n < p - 3 + \sqrt{p^2 + 9p - 23}$, then T_1' is the unique tree with the third minimum EDS.*

4.10 Bounds involving other graph invariants

Hua, Xu and Wen [21] obtained the sharp lower bound on the EDS of n-vertex cacti. The sharp lower bounds for EDS of connected graphs in terms of Wiener index and Harary index are established in [22]. Ilić et al., [26] established various lower and upper bounds for EDS in terms of other graph invariants including the Wiener index, the degree distance, eccentric connectivity index, chromatic number and clique number.

A *cactus* is a connected graph, each of whose blocks is either a cycle or an edge. It is obvious that if a cactus has no cycles, then it is just a tree, and if a cactus has exactly one cycle, then it is just a unicyclic graph. Let $Cat_{n,k}$ be the cactus obtained by introducing k independent edges among pendant vertices of S_n.

Theorem 4.55 ([21]). *Let G be a cactus with $n \geqslant 4$ and $k \geqslant 0$ cycles. Then $\xi^d(G) \geqslant 4n^2 - 9n - 4k + 5$ with equality if and only if $G \cong Cat_{n,k}$.*

Theorem 4.56 ([22]). *Let G be a connected graph on $n \geqslant 2$ vertices. Then*

$$\xi^d(G) \geqslant \frac{4}{n(n-1)}(W(G))^2$$

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

Recall that the *Harary index* [6,12,42] is defined as $H(G) = \sum_{u,v \in V_G} \frac{1}{d_G(u,v)}$. By the definition of $H(G)$, we have $W(G) \geqslant H(G)$, with equality if and only if $G \cong K_n$. Combining the fact and Theorem 4.56, the next corollary follows directly.

Corollary 4.57 ([22]). *Let G be a connected graph on $n \geqslant 2$ vertices. Then*

$$\xi^d(G) \geqslant \frac{4}{n(n-1)}(H(G))^2$$

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

Using simple inequality $r(G) \leqslant \varepsilon_G(v) \leqslant d(G)$ and $\sum_{v \in V_G} D_G(v) = 2W(G)$, Illić, Yu and Feng [26] obtained the following result.

Theorem 4.58 ([26]). *Let G be a connected graph with radius $r(G)$ and diameter $d(G)$. Then*

$$2W(G) \cdot r(G) \leqslant \xi^d(G) \leqslant 2W(G) \cdot d(G)$$

with equality if and only if G is a self-centered graph.

Let $K_n - ke$ be the graph formed by deleting k $(k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor)$ independent edges from the complete graph K_n. It is easily seen that $\varepsilon_G(v) \leqslant n - d_G(v)$.

Theorem 4.59 ([26]). *Let G be a connected graph on $n \geqslant 3$ vertices. Then*

$$\xi^d(G) \leqslant 2n \cdot W(G) - DD(G)$$

with equality if and only if $G \cong K_n - ke$ for $k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$ or $G \cong P_4$.

Note that the relation $D_G(v) \geqslant d_G(v)$ and the equality holds if and only if $\varepsilon_G(v) = 1$ and $d_G(v) = n - 1$. Hence, the next result follows.

Theorem 4.60 ([26]). *Let G be a connected graph on $n \geqslant 3$ vertices. Then $\xi^c(G) \geqslant \xi^d(K_n)$ with equality if and only if $G \cong K_n$.*

Let $T_{n,k}$ be the Turán graph which is a complete k-partite graph on n vertices whose partite sets differ in size by at most one. The famous graph appears in many extremal graph theory problems [2,34,38].

Theorem 4.61 ([26]). *Let G be a connected graph of order n with chromatic number χ. Assume that $n = \chi s + r$ with $0 \leqslant r < \chi$. Then*

$$\xi^d(G) \geqslant 2(n^2 + (n + r - \chi)s - n)$$

with equality if and only if $G \cong T_{n,\chi}$.

The *clique number* of a graph G is the size of a maximal complete subgraph of G and it is denoted as $\omega(G)$. The *kite* $K(n,k)$ is obtained from a complete K_k and a path P_{n-k+1}, by joining one of the end vertices of P_{n-k+1} to one vertex of K_k (see Fig. 13). An asymptotically sharp upper bound for the eccentric connectivity index is derived independently in [9, 32], with the extremal graph $K(n, \lfloor n/3 \rfloor)$. Furthermore, it is shown that the eccentric connectivity index grows no faster than a cubic polynomial in the number of vertices. Motivated by these facts, Yu, Feng and Illić [26] characterized the n-vertex graph with clique number having the maximum EDS.

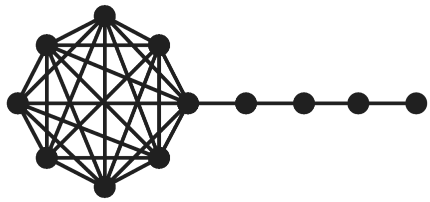

Figure 13. The Kite $K(12, 8)$.

Theorem 4.62 ([26]). *Let G be a connected graph of order n with clique number ω. Then*

$$\xi^d(G) \leqslant \xi^d(K(n,\omega))$$

with equality if and only if $G \cong K(n,\omega)$.

5. Conclusion

We conclude with several open problems and conjectures.

Problem 5.1. *How to determine the sharp upper bound on EDS of several graphs including bipartite graphs, triangle-free graphs, planar graphs and outerplanar graphs?*

Problem 5.2. *How to determine the graph with maximal EDS among n-vertex graphs with a given edge-connectivity?*

Problem 5.3 ([28]). *Let G be a k-connected graph on n vertices with $n \geqslant k+1$. If k is odd, how to determine the sharp upper bound on the EDS of G?*

Problem 5.4 ([29]). *How to determine the graph with minimum EDS among n-vertex bipartite graphs with a given even diameter?*

Problem 5.5 ([29]). *How to determine the graph with minimum EDS among n-vertex bipartite graphs with a given radius?*

Problem 5.6 ([29]). *How to determine the graph with minimum EDS among n-vertex bipartite graphs with a given edge-connectivity?*

Problem 5.7. *How to determine the tree with the minimum EDS in $\mathscr{T}_n^{p,q}$?*

Problem 5.8. *Let G be a connected triangle-free graph on $n \geqslant 5$ vertices. If $\bar{G}$ is connected, how to determine the sharp upper bound on the Nordhaus–Gaddum type relations for the EDS of G?*

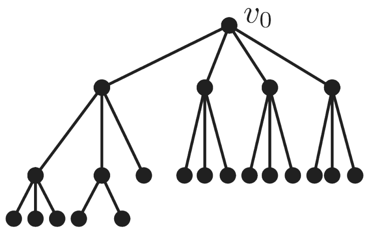

Figure 14. Trees T^* with $n = 22$ and $\Delta = 4$.

Conjecture 5.9 ([31])**.** *Among $\mathscr{T}^{n,\Delta}$, T^* minimizes the EDS, where T^* is a Volkmann tree. When $n = 22$, $\Delta = 4$, T^* is depicted in Fig. 14.*

Conjecture 5.10 ([31])**.** *Among $\mathcal{T}_{n,\gamma}$ with $4 \leqslant \gamma \leqslant \frac{n}{3}$, $P_\alpha(\lfloor\frac{n-\alpha}{2}\rfloor, \lceil\frac{n-\alpha}{2}\rceil)$ maximizes the EDS, where $\alpha = 3(\gamma - 1) + 1$.*

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Extremal Properties of Hexagonal Systems

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Contents

1. Introduction

Our main concern are hexagonal systems, natural graph representations of benzenoid hydrocarbons which are of great importance in organic chemistry. For the definition of hexagonal systems and details of their theory we refer to [13]. We denote by $\mathcal{HS}_h$ the set of hexagonal systems with h hexagons. The hexagons of a hexagonal system can be classified according to the number and position of edges shared with the adjacent hexagons. Figure 1 shows the 12 different types of hexagons that can occur in a hexagonal system.

When going along the perimeter of a hexagonal system, then certain features may be encountered, called [13] fissure, bay, cove, and fjord (see Figure 1). These, respectively, correspond to vertex degree sequences

$$(2,3,2) \quad , \quad (2,3,3,2) \quad , \quad (2,3,3,3,2) \quad , \quad (2,3,3,3,3,2) \tag{1}$$

The number of fissures, bays, coves, and fjords of a hexagonal system H are denoted by $f = f(H), B = B(H), C = C(H)$, and $F = F(H)$, respectively. The parameter

$$r = r(H) = f + B + C + F$$

was introduced in [20], and is called the number of inlets of H.

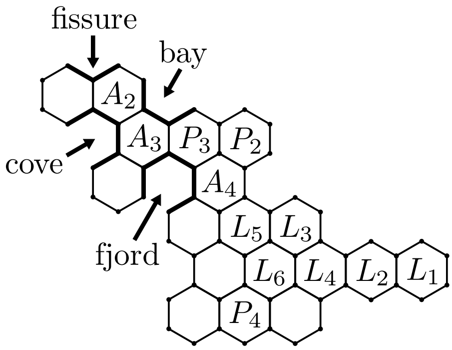


Figure 1. Types of hexagons in a hexagonal system. Some structural features on the perimeter.

Lemma 1.1. *[20] Let H be a hexagonal system with n vertices, h hexagons, r inlets and m_{ij} edges between vertices of degree i and degree j. Then*

$$m_{22} = n - 2h - r + 2 \tag{2}$$

$$m_{23} = 2r \tag{3}$$

$$m_{33} = 3h - r - 3\,. \tag{4}$$

Proof. Relation (3) follows directly from the definition of an inlet, namely an inlet corresponds to a sequence of vertices on the perimeter, of which the first and the last are 2-vertices and all other are 3-vertices. From the fact that the number of 3-vertices in H is

$$n_3 = 2(h-1)$$

it follows

$$m_{23} + 2\,m_{33} = 3\,n_3 = 6\,h - 6$$

which combined with (3) results in (4). In hexagonal systems, $m_{22} + m_{23} + m_{33}$ is just the total number of edges, m, known to conform to the relation

$$m = n + h - 1\,.$$

Substituting the relations (3) and (4) into

$$m_{22} + m_{23} + m_{33} = n + h - 1$$

one readily obtains (2). ■

Another quantity much studied in the theory of hexagonal systems [13] is the number of bay regions $b = b(H)$ defined as

$$b = B + 2C + 3F.$$

It is easy to recognize that b counts the number of edges on the perimeter, connecting two vertices of degree 3. These two quantities are related as follows :

Lemma 1.2. *[2] Let H be a hexagonal system with h hexagons, r inlets, b number of bay regions and n_i internal vertices. Then*

$$r = 2(h-1) - (b + n_i) \tag{5}$$

Proof. It is well-known [13] that

$$m_{23} = 4h - 4 - 2b - 2n_i.$$

From (3) we know that $m_{23} = 2r$ which yields (5). ■

The number of bay regions b and the number of inlets r are two parameters related in a simple manner to the structure of a hexagonal system, which play a significant role in theory of vertex-degree-based topological indices (molecular descriptors). Recall that a vertex-degree-based topological index, denoted by TI, is defined from a set of nonnegative real numbers $\{\varphi_{ij}\}$, where $1 \le i \le j \le n-1$, as

$$TI(G) = \sum_{1 \le i \le j \le n-1} m_{ij}\varphi_{ij} \tag{6}$$

where G is a graph (i.e. undirected graph) with n vertices and $m_{ij} = m_{ij}(G)$ the number of ij-edges, i.e. the number of edges in G with end vertices of degree i and j ([10], [14], [15], [17], [24]). When $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ we obtain the Randić index ([28]), one of the most widely used in applications to physical and chemical properties ([7], [18], [19], [29]). Due to the success of the Randić index many other topological indices appeared in the mathematical-chemistry literature, which are particular cases of the formula given in (6). For instance, the second Zagreb index is obtained by setting $\varphi_{ij} = ij$ [11], in the atom-bond connectivity index $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [8], in the geometric-arithmetic index $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [30], in the sum-connectivity index $\varphi_{ij} = \frac{1}{\sqrt{i+j}}$ [32], in the augmented Zagreb index $\varphi_{ij} = \frac{(ij)^3}{(i+j-2)^3}$ [9] and in the harmonic index $\varphi_{ij} = \frac{2}{i+j}$ [31], just to mention the most important ones.

Since any hexagonal system has only vertices of degree 2 and 3, the general expression for its vertex-degree-based topological index reads

$$TI(H) = m_{22}\varphi_{22} + m_{23}\varphi_{23} + m_{33}\varphi_{33}. \tag{7}$$

From the relations (2), (3),(4) and the well-known relation [13]

$$n = 4h + 2 - n_i$$

we deduce from (7) that for every $S, U \in \mathcal{HS}_h$

$$TI(S) - TI(U) = q[r(S) - r(U)] + \varphi_{22}[n_i(U) - n_i(S)] \tag{8}$$

where

$$q = 2\varphi_{23} - \varphi_{22} - \varphi_{33}. \tag{9}$$

By (5) we can also express the variation of TI in terms of the number of bay regions

$$TI(S) - TI(U) = q[b(U) - b(S)] + (q + \varphi_{22})[n_i(U) - n_i(S)] \tag{10}$$

It becomes clear from the expressions (8) and (10) that the extremal values of TI depend on the extremal values of r, b and n_i.

Our main interest in this chapter is to find extremal values of the parameters r and b over significant classes of hexagonal systems, such as catacondensed hexagonal systems, pericondensed hexagonal systems, or convex hexagonal systems, and then use relations (8) and (10) to deduce extremal values of a vertex-degree-based topological index TI over such classes.

2. Extremal values of *r* and *b* over catacondensed hexagonal systems

Recall that W is a catacondensed hexagonal system if $n_i(W) = 0$, or equivalently, if W only has A_2, A_3, L_1 and L_2 hexagons. We denote by $a_2(W), a_3(W), l_1(W)$ and $l_2(W)$ the number of A_2, A_3, L_1 and L_2 hexagons the hexagonal system W has, respectively. If it's clear from the context we just write a_2, a_3, l_1 and l_2. We will denote by $\mathcal{CHS}_h$ the set of catacondensed hexagonal systems with h hexagons.

Lemma 2.1. *[26] Let $W \in \mathcal{CHS}_h$. Then*

$$\begin{aligned} m_{22} &= a_2 + 3a_3 + 6 \\ m_{23} &= 4(h-1) - 2a_2 - 6a_3 \\ m_{33} &= h - 1 + 3a_3 + a_2 \end{aligned}$$

Proof. The following relations are well-known [12]

$$\begin{aligned} m_{22} &= a_2 + 3a_3 + 6 \\ m_{23} &= 4l_1 + 4l_2 + 2a_2 - 2a_3 - 4 \\ m_{33} &= l_1 + l_2 + 2a_2 + 4a_3 - 1 \end{aligned} \tag{11}$$

Since

$$\begin{gathered} l_1 = a_3 + 2 \\ h = l_1 + l_2 + a_2 + a_3 \end{gathered} \tag{12}$$

we deduce

$$\begin{aligned} l_2 &= h - l_1 - a_2 - a_3 \\ &= h - (a_3 + 2) - a_2 - a_3 \\ &= h - 2a_3 - a_2 - 2 \end{aligned}$$

Now substituting the expressions

$$\begin{aligned} l_1 &= a_3 + 2 \\ l_2 &= h - 2a_3 - a_2 - 2 \end{aligned}$$

in (11) gives the result. ∎

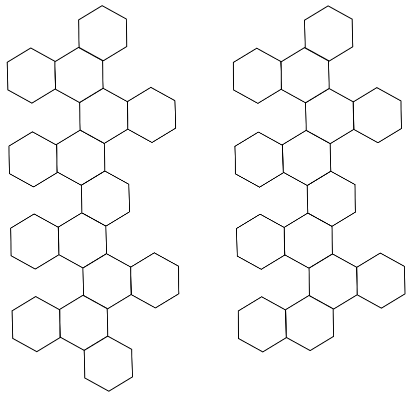


Figure 2. Catacondensed hexagonal system E_h when h is even (on the left) and when h is odd (on the right).

Lemma 2.2. *[26] Let $h \geq 3$ and $W \in \mathcal{CHS}_h$. Then*

$$0 \leq a_3(W) \leq \left\lfloor \frac{1}{2}(h-2) \right\rfloor$$

Moreover, equality on the left is attained in hexagonal chains and the equality on the right is attained in E_h (See Figure 2).

Proof. From the relations given in (12) we deduce

$$a_3 = \frac{1}{2}(h - (a_2 + l_2 + 2)) \tag{13}$$

If h is even then it follows from (13)

$$a_3 \leq \frac{1}{2}(h-2)$$

since $a_2 + l_2 \geq 0$. If h is odd then again by (13) $a_2 + l_2 \geq 1$, since $a_2 + l_2 = 0$ implies that a_3 is not an integer, a contradiction. Hence

$$a_3 \leq \frac{1}{2}(h-3)$$

The equality on the left is clear for hexagonal chains. On the other hand, note that $a_2(E_h) = 0 = l_2(E_h)$ if h is even, $a_2(E_h) = 1$ and $l_2(E_h) = 0$ if h is odd. It follows from (13) that

$$a_3(E_h) = \begin{cases} \frac{1}{2}(h-2) & \text{if } h \text{ is even} \\ \frac{1}{2}(h-3) & \text{if } h \text{ is odd} \end{cases}$$

■

Consider the subset $\mathcal{CHS}_{h,p}$ of $\mathcal{CHS}_h$ defined by

$$\mathcal{CHS}_{h,p} = \{W \in \mathcal{CHS}_h : a_3(W) = p\}$$

Lemma 2.3. *[26] Let $h \geq 3$ and $0 \leq p \leq \left\lfloor \frac{1}{2}(h-2) \right\rfloor$. If $W \in \mathcal{CHS}_{h,p}$ then*

$$0 \leq a_2(W) \leq h - 2(p+1).$$

Proof. From relations (12) and the fact that $l_2 \geq 0$ we deduce

$$a_2 = h - 2p - l_2 - 2 \leq h - 2(p+1).$$

■

Now we can find the minimal value of r over $\mathcal{CHS}_h$.

Theorem 2.4. *[21] Let $h \geq 3$ and $W \in \mathcal{CHS}_h$. Then*

$$\left\lceil \frac{h}{2} + 1 \right\rceil \leq r(W) \leq 2(h-1).$$

Proof. For the upper bound we use (5) and the fact that $n_i(W) = 0$ to deduce

$$r(W) = 2(h-1) - b(W) \leq 2(h-1)$$

since $b \geq 0$. For the lower bound by Lemmas 2.1, 2.3 and 2.2:

$$\begin{aligned} m_{23}(W) &= 4(h-1) - 2a_2 - 6a_3 \\ &\geq 4(h-1) - 2(h - 2(a_3+1)) - 6a_3 \\ &= 2h - 2a_3 \geq 2h - 2\left(\left\lfloor \frac{1}{2}(h-2) \right\rfloor\right) \\ &= 2\left\lceil \frac{h}{2} + 1 \right\rceil. \end{aligned}$$

It follows from (3) that $r(W) \geq \left\lceil \frac{h}{2} + 1 \right\rceil$. ■

Note that $r(E_h) = \left\lceil \frac{h}{2} + 1 \right\rceil$ and $r(L_h) = 2(h-1)$ (see Figure 3). Hence Theorem 2.4 states that E_h and L_h have the minimal and maximal number of inlets, respectively, among all catacondensed hexagonal systems with h hexagons.

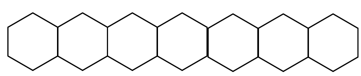


Figure 3. Linear hexagonal system L_h.

The extremal values of b over $\mathcal{CHS}_h$ can be easily deduced from Theorem 2.4.

Theorem 2.5. *Let $h \geq 3$ and $W \in \mathcal{CHS}_h$. Then*

$$0 \leq b(W) \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil.$$

Proof. By (5) and the fact that $n_i(W) = 0$ we deduce

$$b(W) = 2(h-1) - r(W)$$

It follows from Theorem 2.4 that

$$0 \leq b(W) \leq 2(h-1) - \left\lceil \frac{h}{2} + 1 \right\rceil = \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil.$$

■

Since $b(E_h) = \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil$ and $b(L_h) = 0$, Theorem 2.5 states that E_h and L_h have maximal and minimal number of regions, respectively, among all catacondensed hexagonal systems with h hexagons.

From Theorems 2.4 or 2.5 we can easily deduce the extremal values of a vertex-degree-based topological index TI over $\mathcal{CHS}_h$. Recall that q is given by formula (9).

Theorem 2.6. *Let TI be a vertex-degree topological index of the form (7). Then*

1. *If $q = 0$ then TI is constant over $\mathcal{CHS}_h$;*
2. *If $q > 0$ then L_h (resp. E_h) attains the maximal (resp. minimal) value of TI over $\mathcal{CHS}_h$;*
3. *If $q < 0$ then E_h (resp. L_h) attains the maximal (resp. minimal) value of TI over $\mathcal{CHS}_h$.*

Proof. From (8)

$$TI(S) - TI(U) = q\left[r(S) - r(U)\right],$$

for all $S, U \in \mathcal{CHS}_h$. The result follows from Theorem 2.4. ■

The results of Theorem 2.6 were obtained in [23] using linearizing and unbranching operations in catacondensed hexagonal systems.

3. Convex hexagonal systems with maximal number of internal vertices

We already know by Harary-Harborth's paper [16] that the spiral hexagonal system S_h (see Figure 4) has the maximal value of internal vertices, among all hexagonal systems with h hexagons. More precisely,

$$n_i(H) \leq 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil = n_i(S_h) \tag{14}$$

for every $H \in \mathcal{HS}_h$.

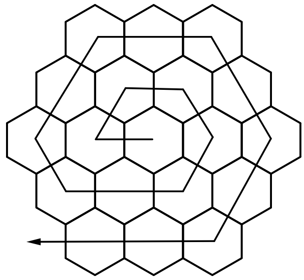


Figure 4. Spiral hexagonal system S_h

Looking at the expression (10), the following question arises naturally: are there convex hexagonal systems $W \in \mathcal{HS}_h$ such that

$$n_i(W) = 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil? \tag{15}$$

When this occurs then we have the following result.

Theorem 3.1. *[25] Let W be a convex hexagonal system with h hexagons which satisfies (15). If $-\varphi_{22} \le q \le 0$ then W has minimal TI-value among all hexagonal systems with h hexagons.*

Proof. It follows from (10) that for every $S \in \mathcal{HS}_h$

$$TI(S) - TI(W) = q\left[-b(S)\right] + \left[\varphi_{22} + q\right]\left[\left(2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil\right) - n_i(S)\right]$$

In particular if $-\varphi_{22} \le q \le 0$, then $TI(S) - TI(W) \ge 0$ by (15) and (14). ■

Remark 3.2. *As we can see in Table 1, all topological indices listed in the introduction except the atom-bond-connectivity index satisfy the condition $-\varphi_{22} \le q \le 0$. So for all these indices, the minimal TI-value is attained in W.*

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{2}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-.0168	-.0404	-.0333	-.0138	-3.3906	.0404
φ_{22}	4	.5	1	.5	.5	8	0.70

Table 1. Values of q and φ_{22} for well-known VDB topological indices.

Note that in general the spiral hexagonal system S_h satisfies

$$b(S_h) = 0 \qquad or \qquad b(S_h) = 1.$$

When $h = 3k^2 - 3k + 1$, where k is a positive integer, then $W = S_h$ is convex and satisfies (15). Are there other values of h possible? We will now determine necessary and sufficient conditions for the existence of convex hexagonal systems with maximal number of internal vertices. A convex hexagonal system can be expressed as

$$H(a_1, a_2, a_3, a_4, a_5, a_6)$$

for positive integers $a_1, a_2, a_3, a_4, a_5, a_6$ (see Figure 5).

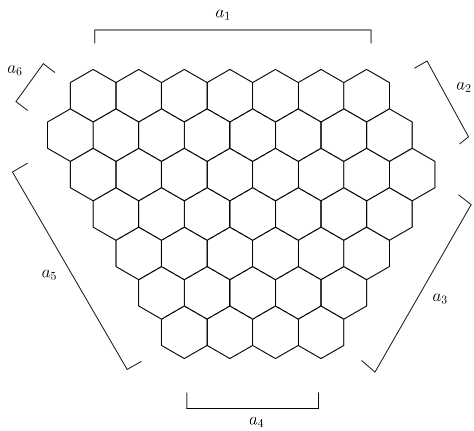


Figure 5. The general form of a convex hexagonal system.

However, these parameters are not all mutually independent. From the fact that the sides 1 and 4 are parallel, it follows that condition (17) must be obeyed. In a fully analogous manner we arrive also at (16) and (18):

$$a_1 + a_2 = a_4 + a_5 \tag{16}$$

$$a_2 + a_3 = a_5 + a_6 \tag{17}$$

$$a_3 + a_4 = a_6 + a_1 \tag{18}$$

Of these relations only two are linearly independent, e.g., (16) and (17), and then the values of a_5 and a_6 can be expressed in terms of a_1, a_2, a_3, a_4 :

$$a_5 = a_1 + a_2 - a_4 \tag{19}$$

$$a_6 = a_3 + a_4 - a_1 \tag{20}$$

We thus arrive at the following:

Theorem 3.3. *[2] Let $H = H(a_1, a_2, a_3, a_4, a_5, a_6)$ be a convex hexagonal system (see Figure 5). Four parameters among $a_1, a_2, a_3, a_4, a_5, a_6$ fully determine H. Of these four parameters only two can correspond to opposite sides of H. In particular, the structure of H is fully determined by a_1, a_2, a_3, a_4.*

From Figure 5 one may get the impression that the shape of any convex hexagonal system has six sides. Some noteworthy special cases need to be pointed out. These are depicted in Figure 6.

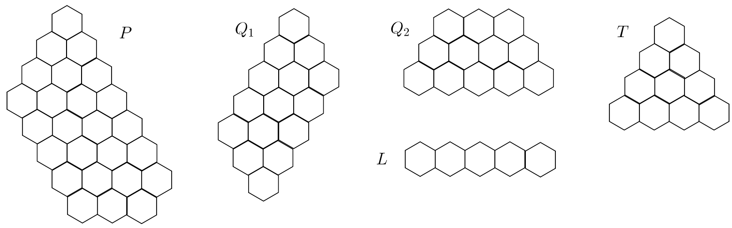


Figure 6. Special cases of convex hexagonal systems $H = H(a_1, a_2, a_3, a_4, a_5, a_6)$, when some of the parameters a_i are equal to unity. Pentagon-shaped P ($a_1 = 1, a_2, a_3, a_4, a_6 > 1$), quadrangle-shaped Q_1 ($a_2 = a_5 = 1$, $a_1 = a_4$, $a_3 = a_6$) and Q_2 ($a_2 = a_5 = 1$, $a_2 = a_6$), triangle-shaped T ($a_1 = a_3 = a_5 = 1$, $a_2 = a_4 = a_6$), and linear L ($a_2 = a_3 = a_5 = a_6 = 1$, $a_1 = a_4$).

In view of Theorem 3.3 we may ask how the basic structural parameters of a convex hexagonal system are determined by the parameters a_1, a_2, a_3, a_4. A partial answer to this question is given in Theorem 3.4.

Theorem 3.4. *[2] Let $H = H(a_1, a_2, a_3, a_4, a_5, a_6)$ be a convex hexagonal system (see Figure 5). Let $r(H), h(H)$, and $n_i(H)$ be the number of inlets, hexagons, and internal vertices of H. Then*

$$\begin{aligned} r(H) &= a_1 + 2a_2 + 2a_3 + a_4 - 6 && (21) \\ h(H) &= a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 \\ &\quad -\frac{1}{2}a_1(a_1+1) - \frac{1}{2}a_4(a_4+1) + 1 && (22) \\ n_i(H) &= 2(a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4) \\ &\quad -a_1(a_1+2) - a_4(a_4+2) - 4(a_2+a_3) + 6. && (23) \end{aligned}$$

Proof. Eq. (21) follows from the fact that the i-th side of H has $a_i - 1$ inlets. Therefore

$$r(H) = a_1 + a_2 + a_3 + a_4 + a_5 + a_6 - 6.$$

Eq. (21) is then obtained by taking into the relations (19) and (20).

Eq. (22) is deduced by counting the hexagons in the auxiliary hexagonal system depicted in Figure 7 and subtracting the number of shaded hexagons. By taking into account that a triangle-shaped hexagonal system (T in Figure 6) of size $\frac{k(k-1)}{2}$ hexagons, and using the relations (19) and (20), after a lengthy calculation we arrive at Eq. (22).

Eq. (23) is deduced in an analogous manner as Eq. (22), bearing in mind that a triangle-shaped hexagonal of size k has $(k-1)^2$ internal vertices. ∎

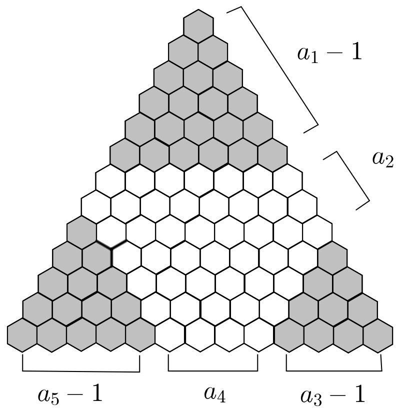


Figure 7. An auxiliary triangle-shaped hexagonal system used in the proof of Theorem 3.4.

Now we give a characterization of convex hexagonal systems with maximal number of internal vertices.

Theorem 3.5. *[25] Let h be a positive integer. The following conditions are equivalent:*

1. *There exists a hexagonal system W with h hexagons satisfying (15);*

2. *There exist a set of positive integers a_1, a_2, a_3, a_4 which are solution of the system of equations*

$$\left.\begin{aligned} h &= a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 \\ &\quad - \tfrac{1}{2}a_1(a_1+1) - \tfrac{1}{2}a_4(a_4+1) + 1 \\ \left\lceil \sqrt{12h-3} \right\rceil &= a_1 + 2a_2 + 2a_3 + a_4 - 3 \end{aligned}\right\} \tag{24}$$

Proof. 1. $\Rightarrow$ 2. Assume that W is a convex hexagonal system with h hexagons, satisfying (15). Let $a_1, a_2, a_3, a_4, a_5, a_6$ be positive integers such that $W = H(a_1, a_2, a_3, a_4, a_5, a_6)$.

We know from Theorem 3.4 that

$$\begin{aligned} h &= a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 - a_2 - a_3 \\ &\quad - \frac{1}{2}a_1(a_1+1) - \frac{1}{2}a_4(a_4+1) + 1 \\ n_i(W) &= 2(a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4) - a_1(a_1+2) \\ &\quad - a_4(a_4+2) - 4(a_2+a_3) + 6\,. \end{aligned} \tag{25}$$

Substituting these expressions of h and $n_i(W)$ back into (15) yields

$$\left\lceil \sqrt{12h-3} \right\rceil = a_1 + 2a_2 + 2a_3 + a_4 - 3\,.$$

2. $\Rightarrow$ 1. Conversely, if the set of positive integers a_1, a_2, a_3, a_4 is a solution of the system of equations (24), consider the convex hexagonal system $Z = H(a_1, a_2, a_3, a_4, a_5, a_6)$, where a_5 and a_6 are given by (19) and (20). Again by Theorem 3.4, we have expressions for h and $n_i(Z)$ as in (25). Consequently,

$$2h + 1 - n_i(Z) = a_1 + 2a_2 + 2a_3 + a_4 - 3 = \left\lceil \sqrt{12h-3} \right\rceil .$$

Solving for $n_i(Z)$ in this relation, we deduce that

$$n_i(Z) = 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil .$$

■

We now show that not for every positive integer h there is a solution for the system of equations (24). This is a consequence of our next result.

Theorem 3.6. *[25] Let h be a positive integer. If the set of positive integers $\{a_1, a_2, a_3, a_4\}$ is a solution of the system of equations (24), then there exists a solution to the Diophantine equation*

$$21x^2 + 3y^2 + z^2 = 28H \tag{26}$$

where $H = \left\lceil \sqrt{12h-3} \right\rceil^2 - (12h-3)$.

Proof. Substituting

$$a_2 = \frac{1}{2}\left\lceil \sqrt{12h-3} \right\rceil - a_3 - \frac{1}{2}a_4 - \frac{1}{2}a_1 + \frac{3}{2} \tag{27}$$

in the first equation of (24) we deduce that

$$\begin{aligned} h &= \frac{3}{2}a_3 + \frac{3}{2}a_4 - \frac{1}{2}\left\lceil \sqrt{12h-3} \right\rceil - \frac{1}{2}a_1^2 - a_3^2 - a_4^2 + \frac{1}{2}a_1 a_3 + \frac{1}{2}a_1 a_4 - \frac{3}{2}a_3 a_4 \\ &+ \frac{1}{2}a_3\left\lceil \sqrt{12h-3} \right\rceil + \frac{1}{2}a_4\left\lceil \sqrt{12h-3} \right\rceil - \frac{1}{2} \end{aligned}$$

and solving for a_4 in this equation it follows that

$$a_4 = \frac{1}{4}a_1 - \frac{3}{4}a_3 + \frac{1}{4}\left\lceil \sqrt{12h-3} \right\rceil + \frac{3}{4} \pm \frac{1}{4}\sqrt{P(a_1, a_3)} \tag{28}$$

where

$$\begin{aligned} P(a_1, a_3) &= -7a_1^2 + 2a_1 a_3 + 2a_1\left\lceil \sqrt{12h-3} \right\rceil + 6a_1 - 7a_3^2 + 2a_3\left\lceil \sqrt{12h-3} \right\rceil + \\ &\quad 6a_3 + \left\lceil \sqrt{12h-3} \right\rceil^2 - 2\left\lceil \sqrt{12h-3} \right\rceil - 16h + 1 . \end{aligned}$$

Since $\sqrt{P(a_1, a_3)} \in \mathbb{Z}$, we may assume that $P(a_1, a_3) = x^2$ for some $x \in \mathbb{N}$. Solving for a_1 we get

$$a_1 = \frac{1}{7}a_3 + \frac{1}{7}\left\lceil \sqrt{12h-3} \right\rceil + \frac{3}{7} \pm \frac{1}{7}\sqrt{Q(a_3)} \tag{29}$$

where

$$\begin{aligned} Q(a_3) &= -7x^2 - 48a_3^2 + 16a_3\left\lceil \sqrt{12h-3} \right\rceil + 48a_3 + 8\left\lceil \sqrt{12h-3} \right\rceil^2 \\ &- 8\left\lceil \sqrt{12h-3} \right\rceil - 112h + 16 . \end{aligned}$$

Since $\sqrt{Q\left(a_3\right)} \in \mathbb{Z}$, there exists an integer $y \in \mathbb{N}$ such that $Q\left(a_3\right) = y^2$. Now we solve for a_3 to obtain

$$a_3 = \frac{1}{6}\left\lceil \sqrt{12h-3} \right\rceil + \frac{1}{2} \pm \frac{1}{12}\sqrt{R} \tag{30}$$

where

$$R = -21x^2 - 3y^2 + 28\left(\left\lceil \sqrt{12h-3} \right\rceil^2 - (12h-3)\right). \tag{31}$$

Similarly $\sqrt{R} \in \mathbb{Z}$ and so $R = z^2$ for $z \in \mathbb{N}$. Hence

$$z^2 = -21x^2 - 3y^2 + 28\left(\left\lceil \sqrt{12h-3} \right\rceil^2 - (12h-3)\right)$$

and we are done. ■

Theorem 3.6 gives a method to find values of h for which there are no convex hexagonal systems which satisfy (15).

Example 3.7. *Let h be a positive integer and H as in the hypothesis of Theorem 3.6. If $28H - 21x^2 - 3y^2$ is not the square of an integer for every $(x, y) \in \mathbb{N} \times \mathbb{N}$ satisfying*

$$0 \leq x \leq \sqrt{\frac{28H}{21}} \qquad \text{and} \qquad 0 \leq y \leq \sqrt{\frac{28H - 21x^2}{3}} \tag{32}$$

then there are no convex hexagonal systems with h hexagons satisfying (15). Using a computer is easy to check that the first values of h are the following:

$$\begin{array}{cccccccccc} 121 & 163 & 211 & 235 & 265 & 292 & 325 & 355 & 391 & 424 \\ 463 & 499 & 541 & 580 & 625 & 667 & 706 & 715 & 760 & 802 \\ 811 & 859 & 904 & 913 & 955 & 964 & 1012 & 1021 & 1066 & 1075 \\ 1126 & 1135 & 1183 & 1192 & 1246 & 1255 & 1306 & 1315 & 1372 & 1381 \end{array} \tag{33}$$

On the other hand, for those values of h where the Diophantine equation (26) has a solution, we were able to find convex hexagonal systems with maximal number of vertices, using the proof of Theorem 3.6 as follows: starting from a solution x, y, z of (26), we compute R, a_3, a_1, a_4 and a_2, in this order, from relations (31), (30), (29), (28), and (27), respectively. Then a_5 and a_6 are computed using equations (19) and (20). It turns out that $W = H\left(a_1, a_2, a_3, a_4, a_5, a_6\right)$ is a convex hexagonal system satisfying (15). For instance,

$$\begin{array}{ccc} h = 120 & h = 5306 & h = 10000 \\ H\left(7,6,8,6,7,7\right) & H\left(39,43,42,47,35,50\right) & H\left(63,60,54,59,64,50\right) \end{array}$$

Now we return to the study of vertex-degree-based topological indices of hexagonal systems. If the system of equations (24) has a solution for a positive integer h, then there exists a convex hexagonal system W such that (15) holds, which implies by Theorem 3.1 that W has a minimal TI-value when $-\varphi_{22} \leq q \leq 0$. So a question arises naturally: if (24) has no solution for certain h, which is the minimal TI-value in the set of all hexagonal systems with h hexagons?

Theorem 3.8. *[25] Let h be a positive integer and assume that the system of equations (24) has no solution. If $\frac{-\varphi_{22}}{2} \leq q \leq 0$, then the spiral hexagonal system S_h has minimal TI-value over the set of all hexagonal systems with h hexagons.*

Proof. Since (24) has no solution, $b(S_h) = 1$. Let S be a hexagonal system with h hexagons. From (10)

$$TI(S) - TI(S_h) = q\,[1 - b(S)] + [\varphi_{22} + q]\,[n_i(S_h) - n_i(S)]\,. \tag{34}$$

We consider two cases. If $b(S) = 0$, then $n_i(S_h) - n_i(S) \geq 1$ since (24) has no solution. Consequently from (34) and the fact that $\frac{-\varphi_{22}}{2} \leq q \leq 0$ we deduce

$$\begin{aligned} TI(S) - TI(S_h) &= q + [\varphi_{22} + q]\,[n_i(S_h) - n_i(S)] \\ &\geq q + [\varphi_{22} + q] = 2q + \varphi_{22} \geq 0\,. \end{aligned}$$

Otherwise $b(S) \geq 1$ which implies $1 - b(S) \leq 0$. Since $n_i\,(S_h) - n_i\,(S) \geq 0$ by (14) then again by (34) and $\frac{-\varphi_{22}}{2} \leq q \leq 0$ it follows that

$$TI\,(S) - TI(S_h) = q\,[1 - b(S)] + [\varphi_{22} + q]\,[n_i(S_h) - n_i(S)] \geq 0\,.$$

Thus S_h has minimal TI-value among all hexagonal systems with h hexagons. ∎

Example 3.9. *For every value of h given in Example 3.7 (33), the spiral hexagonal system S_h has minimal TI-value over $\mathcal{HS}_h$.*

Remark 3.10. *We can easily see that all topological indices listed in the introduction except the atom-bond-connectivity index satisfy the condition $\frac{-\varphi_{22}}{2} \leq q \leq 0$ (see Table 1).*

4. Extremal values of *b* over hexagonal systems

For every positive integer h we can easily construct convex hexagonal systems with h hexagons (for instance, the linear hexagonal chain L_h). These have obviously minimal number of bay regions in $\mathcal{HS}_h$. So we now consider the problem of maximal number of bay regions in $\mathcal{HS}_h$.

Recall that every hexagonal system with $h \geq 2$ hexagons is obtained from a hexagonal system with $h - 1$ hexagons by adding a hexagon of type L_1 (one-contact addition), or P_2 (two-contact addition), or L_3 (three-contact addition), or P_4 (four-contact addition) or L_5 (five-contact-addition) (see [13]). In particular, every hexagonal system has one of the mentioned hexagons: L_1, P_2, L_3, P_4 and L_5. The proof of our next result is based on this observation.

Another well-known relation [13] we will use frequently from now on is

$$m_{22}\,(H) = b\,(H) + 6. \tag{35}$$

Theorem 4.1. *[4] [6] Let $H \in \mathcal{HS}_h$ with $h \geq 2$. Then*

$$b(H) \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Proof. The proof is by induction on h. It is easy to check the result for $h = 2, 3, 4$. Let $h \geq 5$ and assume that the result is true for any hexagonal system with less than h hexagons. Let H be a hexagonal system with h hexagons. We consider several cases:

1. H contains a L_3, P_4 or L_5 hexagon, or a P_2 hexagon of the form depicted in Figure 8. In this case we will show that there exists a (sub)hexagonal system H_1 with $h-1$ hexagons such that $b(H) \leq b(H_1) + 1$. If this is so then by induction we easily obtain

$$b(H) \leq b(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-1) - \frac{7}{2} \right\rceil + 1 \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Note that in each case, splitting H into the dark shadowed (sub)hexagonal system H_1 of $h-1$ hexagons and the corresponding hexagon L_3, P_4, L_5 or P_2, we obtain at least five new 2-2-edges. Hence

$$m_{22}(H) \leq m_{22}(H_1) + 6 - 5 = m_{22}(H_1) + 1,$$

and from relation (35) we deduce

$$b(H) \leq b(H_1) + 1.$$

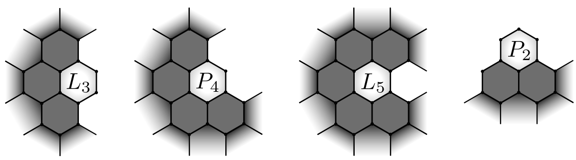


Figure 8. Hexagonal systems used in the proof of Theorem 4.1, case 1.

2. H contains a P_2 hexagon of the form depicted in Figure 9. In this case we will show that there exist (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$. Then by induction

$$b(H) \leq b(H_1) + b(H_2) + 3 \leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 3 \leq \left\lceil \frac{3}{2}h - \frac{7}{2} \right\rceil .$$

Splitting H into the two hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

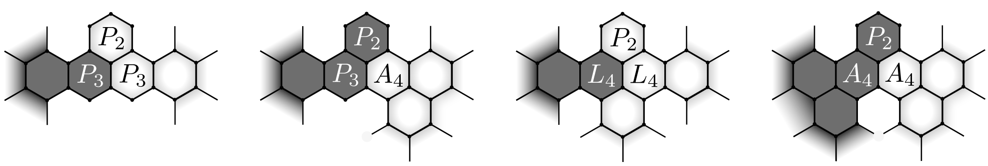


Figure 9. Hexagonal systems used in the proof of Theorem 4.1, case 2.

3. H contains a L_1 hexagon and the hexagon adjacent to it is not A_3. In this case we show that there exist two (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$ and the result follows as in part 2 of this theorem.

   Let X be the hexagon adjacent to the L_1 hexagon in H. Then X must be L_2, A_2, P_3 or L_4 (see Figure 10). In each case, we split H into the two hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, obtaining at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

   or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

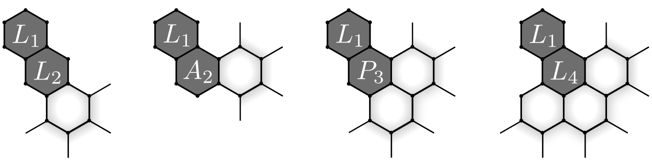


Figure 10. Hexagonal systems used in the proof of Theorem 4.1, case 3.

4. H contains a A_3 hexagon and X is one of the hexagons next to it which is not A_3 nor L_1. Then we will show that there exist (sub)systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$ and $b(H) \leq b(H_1) + b(H_2) + 3$ The result would follow as in part 2 of this theorem.

   Clearly X must be a L_2, L_4, A_2 or P_3 hexagon (see Figure 11). In each case, we split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system, obtaining at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

   or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

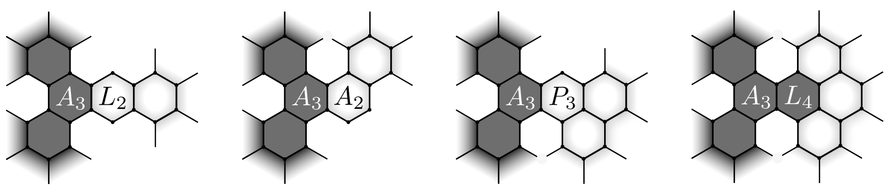


Figure 11. Hexagonal systems used in the proof of Theorem 4.1, case 4.

5. Finally, all hexagons in H are L_1 or A_3. Then H is a catacondensed hexagonal system and the result follows by Theorem 2.5. ■

5. Extremal values of r over hexagonal systems

We first find the hexagonal system with maximal number of inlets.

Lemma 5.1. *[2] Let H be a hexagonal system with h hexagons and r inlets, then $r \leq 2(h-1)$.*

Proof. By (5)

$$r = 2(h-1) - (b + n_i) \leq 2(h-1)$$

since $b + n_i \geq 0$. ■

Note that $r(L_h) = 2(h-1)$, where L_h is the linear hexagonal chain with h hexagons (see Figure 3). Hence Lemma 5.1 states that the linear hexagonal chain has the maximal number of inlets among all hexagonal systems with h hexagons.

Now we can determine extremal values of a vertex-degree-based topological index TI over $\mathcal{HS}_h$.

Theorem 5.2. *Let TI be a vertex-degree topological index of the form (7) and q as in formula (9). Then*

1. *If $q = 0$ then the catacondensed hexagonal systems (resp. spiral hexagonal systems) have maximal (resp. minimal) TI-value over $\mathcal{HS}_h$;*
2. *If $q > 0$ then the linear hexagonal chain has maximal TI-value over $\mathcal{HS}_h$;*
3. *If $q \leq -\varphi_{22}$ then the linear hexagonal chain has minimal TI-value over $\mathcal{HS}_h$.*

Proof. Let H be a hexagonal system with h hexagons.

1. Assume that $q = 0$ and let S_h be the spiral hexagonal system with h hexagons. Then by (8) and (14)

$$TI(S_h) - TI(H) = \varphi_{22}[n_i(H) - n_i(S_h)] \leq 0.$$

Consequently S_h has minimal TI-value. If V is a catacondensed hexagonal system then $n_i(V) = 0$ which implies

$$TI(V) - TI(H) = \varphi_{22}[n_i(H)] \geq 0$$

and so V has maximal TI-value.

2. Suppose that $q > 0$. We know from Lemma 5.1 that $r(H) \leq r(L_h) = 2(h-1)$. Since $n_i(L_h) = 0$ and $n_i(H) \geq 0$ it follows from (10) that

$$\begin{aligned} TI(L_h) - TI(H) &= q[b(H) - b(L_h)] + (q + \varphi_{22})[n_i(H) - n_i(L_h)] \\ &= q[b(H)] + (q + \varphi_{22})[n_i(H)] \geq 0 \end{aligned}$$

Thus L_h has maximal TI-value.

3. Suppose that $q \leq -\varphi_{22}$. From (10) we deduce

$$\begin{aligned} TI(L_h) - TI(H) &= q[b(H) - b(L_h)] + (q + \varphi_{22})[n_i(H) - n_i(L_h)] \\ &= q[b(H)] + (q + \varphi_{22})[n_i(H)] \leq 0. \end{aligned}$$

Thus L_h has minimal TI value. ■

Next we determine the minimal value of r over $\mathcal{HS}_h$. For each $H \in \mathcal{HS}_h$, consider the set $\mathcal{A}(H)$ of all hexagonal systems with $h+1$ hexagons that contains H:

$$\mathcal{A}(H) = \{H' \in \mathcal{HS}_{h+1} \,:\, H \subset H'\}.$$

Definition 5.3. *Let $H \in \mathcal{HS}_h$. We say that H is an inlet-increasing hexagonal system if $r(H) < r(H')$ for every $H' \in \mathcal{A}(H)$.*

The hexagonal system H_1 in Figure 12 is inlet-increasing since $\mathcal{A}(H_1) = \{H_1', H_2''\}$, $r(H_1) = 3$ and $r(H_1') = r(H_1'') = 4$. On the other hand, the hexagonal system H_2 in the same figure is not inlet-increasing since $H_2' \in \mathcal{A}(H_2)$ and $r(H_2) > r(H_2')$.

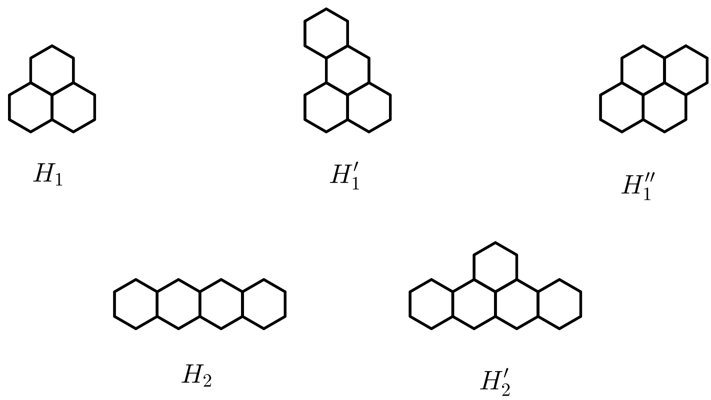


Figure 12. Inlet-increasing and not inlet-increasing hexagonal systems.

Let $a(H)$ be the number of adjacent inlets of H (i.e. pair of inlets that have a common vertex of degree 2) introduced in [22]. Next we describe the inlets of an inlet-increasing hexagonal system.

Proposition 5.4. *[5] Let H be an inlet-increasing hexagonal system. Then H has no fjords and $a(H) =$ 0.*

Proof. Let H be an inlet-increasing hexagonal system with h hexagons and r inlets.

1. Suppose H has a fjord formed by the perimetral path $a, x_1, x_2, x_3, x_4,\ x_5, x_6, b$ with degree sequence $(d_a, 2, 3, 3, 3, 3, 2, d_b)$ where d_a and d_b are the degrees of the vertices a and b respectively. Adding the edge x_1x_6 we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = d_b = 2$, or $r(H') = r - 1$ if $d_a \neq d_b$ or $r(H') = r - 2$ if $d_a = d_b = 3$ (see Figure 13). Since H is inlet-increasing we get a contradiction.

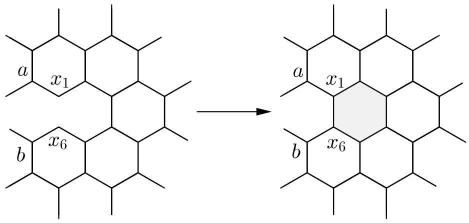


Figure 13. Figure used in the proof of Proposition 5.4 part 1.

2. Suppose $a(H) > 0$. Since H has no fjords, we have to consider the following cases:

   Case 1: H has two adjacent fissures with a common vertex u. Then H has a perimetral path a, x_1, x_2, u, y_1, y_2 with degree sequence $(d_a, 2, 3, 2, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 14). This contradicts the fact that H is inlet-increasing.

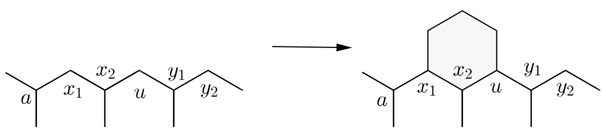


Figure 14. Figure used in the proof of Proposition 5.4 part 2, Case 1.

   Case 2: A fissure and a bay of H are adjacent with a common vertex u. Then H has a perimetral path $a, x_1, x_2, u, y_1, y_2, y_3$ with degree sequence $(d_a, 2, 3, 2, 3, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 15). This contradicts the fact that H is inlet-increasing.

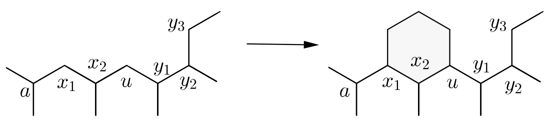


Figure 15. Figure used in the proof of Proposition 5.4 part 2, Case 2.

Case 3: A fissure and a cove of H are adjacent with a common vertex u. Then H has a perimetral path $a, x_1, x_2, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 2, 3, 3, 3, 2)$. Adding a hexagon with edges x_1x_2 and x_2u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 16). This contradicts the fact that H is inlet-increasing.

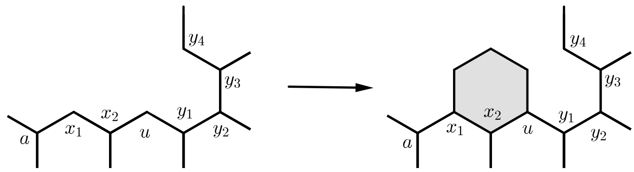


Figure 16. Figure used in the proof of Proposition 5.4 part 2, Case 3.

Case 4: H has two adjacent bays with a common vertex u. Then H has a perimetral path $a, x_1, x_2, x_3, u, y_1, y_2, y_3$ with degree sequence $(d_a, 2, 3, 3, 2, 3, 3, 2)$. Adding a hexagon with edges x_1x_2, x_2x_3 and x_3u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 16). This contradicts the fact that H is inlet-increasing.

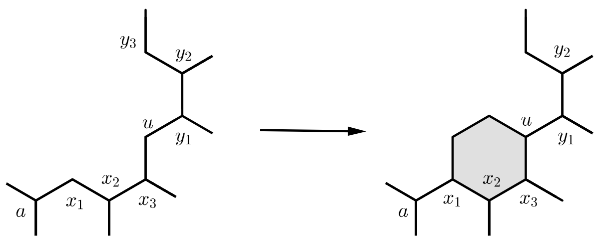


Figure 17. Figure used in the proof of Proposition 5.4 part 2, Case 4.

Case 5: A bay and a cove of H are adjacent with a common vertex u. Then H has a perimetral path $a, x_1, x_2, x_3, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 3, 2, 3, 3, 3, 2)$. Adding a hexagon with edges x_1x_2, x_2x_3 and x_3u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 18). This contradicts the fact that H is inlet-increasing.

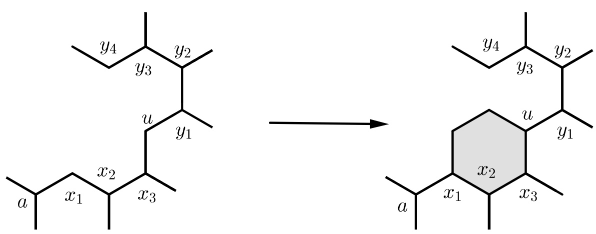


Figure 18. Figure used in the proof of Proposition 5.4 part 2, Case 5.

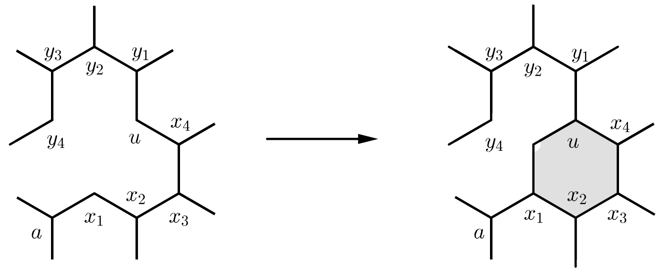


Figure 19. Figure used in the proof of Proposition 5.4 part 2, Case 6.

Case 6: H has two adjacent coves with a common vertex u. Then H has a perimetral path $a, x_1, x_2, x_3, x_4, u, y_1, y_2, y_3, y_4$ with degree sequence $(d_a, 2, 3, 3, 3, 2, 3, 3, 3, 2)$. Adding a hexagon with edges x_1x_2, x_2x_3, x_3x_4 and x_4u we obtain a new hexagonal system $H' \in \mathcal{A}(H)$ with $r(H') = r$ if $d_a = 2$ or $r(H') = r - 1$ if $d_a = 3$ (see Figure 19). This contradicts the fact that H is inlet-increasing. ■

Proposition 5.5. *[5] Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Then there exists a convex hexagonal system H' that contains H such that*

$$r' = r(H') \leq 2r \tag{36}$$

$$h' = h(H') = h + r' - r \tag{37}$$

Proof. By Proposition 5.4, the inlets of the maximal hexagonal system H are fissures, bays and coves and there are no adjacent inlets. We construct a new hexagonal system H' in the following way:

To each bay in H, with perimetral path a, x_1, x_2, x_3, x_4, b and degree sequence $(2, 2, 3, 3, 2, 2)$ we add a hexagon with edges x_1x_2, x_2x_3, x_3x_4 (see Figure 20).

To each cove in H, with perimetral path $a, x_1, x_2, x_3, x_4, x_5, b$ and degree sequence $(2, 2, 3, 3, 3, 2, 2)$ we add a hexagon with edges $x_1x_2, x_2x_3, x_3x_4, x_4x_5$ (see Figure 20).

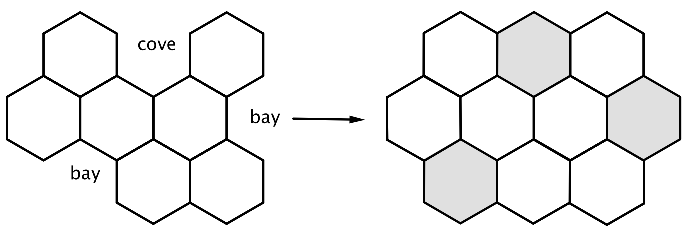


Figure 20. A inlet-increasing hexagonal system and its corresponding convex hexagonal system.

Note that the obtained hexagonal system H' has no bay regions so it is a convex hexagonal system. Moreover, for each bay and each cove we add one hexagon and obtain two fissures in H', then

$$\begin{aligned} r' &= f(H) + 2B(H) + 2C(H) = r + B(H) + C(H) \leq 2r \\ h' &= h + B(H) + C(H) = h + r + B(H) + C(H) - r = h + r' - r \end{aligned}$$

■

Next we find the lower bound on the number of inlets for the inlet-increasing hexagonal systems.

Proposition 5.6. *[5] Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Then*

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil$$

Proof. Let H be an inlet-increasing hexagonal system with h hexagons and r inlets. Let $H' = H'(a_1, a_2, a_3, a_4)$ be a convex hexagonal system obtained from H as described in Proposition 5.5. We use the method of Lagrange multipliers to find the maximal value of the function $h'(a_1, a_2, a_3, a_4)$, determined by equation (22), imposing the condition (21).

The maximal value of the function $h'(a_1, a_2, a_3, a_4)$ is attained for

$$a_1 = a_2 = a_3 = a_4 = \frac{r'}{6} + 1$$

and

$$h'_{\text{max}} = 3\left(\frac{r'}{6} + 1\right)\left(\frac{r'}{6}\right) + 1.$$

Using relations (36) and (37) in Proposition 5.5 we obtain:

$$\begin{aligned} h &= h' - r' + r \leq h'_{\text{max}} - r' + r \\ &= 3\left(\frac{r'}{6} + 1\right)\left(\frac{r'}{6}\right) + 1 - r' + r = \frac{r'}{12}\left(r' - 6\right) + 1 + r \\ &\leq \frac{r^2}{3} + 1 \end{aligned}$$

which implies

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil.$$

■

In order to extend Proposition 5.6 for general hexagonal systems we need the following lemma.

Lemma 5.7. *Let $H \subset H_1 \subset H_2 \subset \cdots \subset H_i \subset \cdots$ be a sequence of hexagonal systems such that $H \in \mathcal{HS}_h$, $H_i \in \mathcal{HS}_{h_i}$ for all $i = 1, 2, 3 \ldots$ and $h < h_1 < h_2 < \cdots < h_i < \cdots$. Then*

$$\lim_{i \to \infty} r(H_i) = +\infty.$$

Proof. Let $H \in \mathcal{HS}_h$ with n_2^* (resp. n_3^*) external vertices of degree 2 (resp. 3) . It is well known [13] that

$$\begin{aligned} n_2^* &= 2h + 4 - n_i \\ n_3^* &= 2h - 2 - n_i \end{aligned}$$

where n_i is the number of internal vertices. It follows that

$$\begin{aligned} n_2^* &\geq \left\lceil \sqrt{12h-3} \right\rceil + 3 \\ n_3^* &\geq \left\lceil \sqrt{12h-3} \right\rceil - 3 \end{aligned}$$

since $n_i \leq 2h + 1 - \lceil \sqrt{12h-3} \rceil$ by (14). Hence the number of external vertices of degree 2 and 3 in the perimeter of a hexagonal system approaches infinity as h approaches infinity. Since there are at most four consecutive vertices of degree 2 in the perimeter, the number of inlets $r = 2m_{23}$ (see (3)), also approaches infinity. ■

Theorem 5.8. *[5] Let H be a hexagonal system with h hexagons and r inlets. Then*

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil .$$

Proof. If H is an inlet-increasing hexagonal system, by Proposition 5.6 we are done. Otherwise we will show that there exists an inlet-increasing hexagonal system $H_s \in \mathcal{HS}_{h+s}$ such that $r = r(H) \geq r(H_s)$.

In fact, if H is not inlet-increasing there exists $H_1 \in \mathcal{A}(H)$ such that $r \geq r(H_1)$. If H_1 is not inlet-increasing there exists $H_2 \in \mathcal{A}(H_1)$ such that $r \geq r(H_1) \geq r(H_2)$.

Continuing this process we construct a sequence

$$H = H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_i \subset \cdots$$

such that $H_i \in \mathcal{A}(H_{i-1})$ and

$$r = r(H) \geq r(H_1) \geq r(H_2) \geq \cdots \geq r(H_i) \geq \cdots$$

Note that the sequence $\{r(H_i)\}_i$ is bounded by r. Consequently by Lemma 5.7, the sequence is finite. In other words, there exists $H_s \in \mathcal{A}(H_{s-1})$ such that H_s is inlet-increasing and $r = r(H) \geq r(H_1) \geq \cdots \geq r(H_s)$. Hence, by Proposition 5.6

$$r = r(H) \geq r(H_s) \geq \sqrt{3(h+s-1)} \geq \sqrt{3(h-1)}$$

which implies

$$r \geq \left\lceil \sqrt{3(h-1)} \right\rceil .$$

■

Let $S_{h'}$ be the spiral hexagonal system with h' hexagons. The number of internal vertices $n_i' = n_i\left(S_{h'}\right)$, the number of bay regions $b' = \left(S_{h'}\right)$ and the number of inlets $r' = r\left(S_{h'}\right)$ satisfy the following relations:

$$
\begin{aligned}
n_i' &= n_i'(S_{h'}) = 2h' + 1 + \left\lceil \sqrt{12h' - 3} \right\rceil && (38)\\
b' &= b'(S_{h'}) \in \{0, 1\} && (39)\\
r' &= r'(S_{h'}) = \left\lceil \sqrt{12h' - 3} \right\rceil - 3 - b' && (40)
\end{aligned}
$$

Now we introduce a parametrization of the spiral hexagonal system $S_{h'}$ that will be useful in the sequel. Let $h' \geq 7$ and k be the greatest integer such that $3k(k-1)+1 \leq h' < 3k(k+1)+1$. Since $0 \leq h' - 3k(k-1) - 1 < 6k$, let

$$
\begin{aligned}
q' &= \left\lfloor \frac{h' - 3k(k-1) - 1}{k} \right\rfloor\\
l' &= h' - 3k(k-1) - 1 - q'k.
\end{aligned}
$$

Then h' has a unique representation of the form

$$h' = h'(k, q', l') = 3k(k-1) + 1 + q'k + l' \tag{41}$$

where $k = 2, 3, \ldots$, $q' \in \{0, 1, 2, 3, 4, 5\}$ and $l' = 0, 1, \ldots, k-1$. From the construction of $S_{h'}$ we conclude that k is the number of complete loops in $S_{h'}$, q' is the side of the spiral to which belongs the last hexagon in $S_{h'}$ and l' is the number of the last hexagon in the side q. In Figure 21 the spiral system $S_{h'}$ for every value of $h' = h'(2, q', l')$ are depicted.

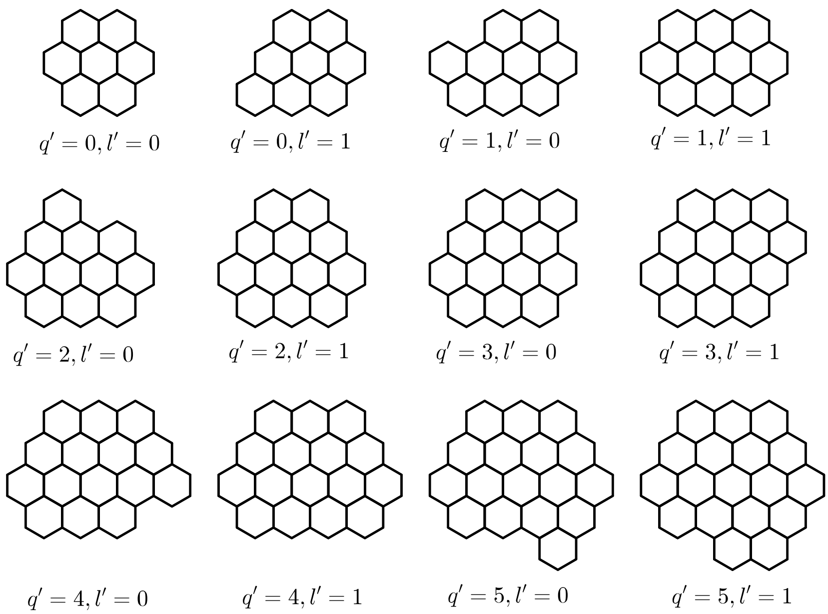


Figure 21. Spiral systems $S_{h'}$ for every value of $h' = h'(2, q', l')$.

Next we obtain the number of bay regions, the number of inlets and the number of hexagons in the perimeter of $S_{h'}$ in terms of the introduced parameters k, q' and l'.

Proposition 5.9. *[5] Let $h' = h'(k, q', l')$ of the form (41) and h'_e be the number of hexagons in the perimeter of $S_{h'}$. Then*

$$\begin{aligned} b' &= b'(S_{h'}) = \begin{cases} 0 & \textit{if} \quad l' = 0, \quad q' = 0 \\ 0 & \textit{if} \quad l' = k-1, \quad q' < 5 \\ 1 & \textit{otherwise} \end{cases} \\ r' &= r'(S_{h'}) = \begin{cases} 6k-6 & \textit{if} \quad l' = 0, \quad q' = 0 \\ 6k-5+q' & \textit{if} \quad l' = k-1, \quad q' < 5 \\ 6k-6+q' & \textit{otherwise} \end{cases} \\ h'_e &= h'_e(S_{h'}) = \begin{cases} 6k-6 & \textit{if} \quad l = 0, \quad q' = 0 \\ 6k-5+q' & \textit{otherwise} \end{cases} \end{aligned}$$

Proof. Since

$$12h'^2 - 36k + 12q'k + 12l' + 9$$

we have:
If $q' = 0$ and $l' = 0$ then $12h'^2$. Consequently, $\lceil\sqrt{12h'-3}\rceil = 6k-3$.
If $q' = 0$ and $0 < l' \leq k-1$ we have

$$\begin{aligned} &12h'^2, \\ 12h'^2 - 24k - 3 &< (6k-2)^2. \end{aligned}$$

Consequently, $\lceil\sqrt{12h'-3}\rceil = 6k-3$.
If $0 < q' \leq 5$ and $0 \leq l' \leq k-1$ we have

$$\begin{aligned} 12h'^2 - 36k + 12q'k + 9 = (6k-3+q'^2 + 9 - (3-q'^2 &> (6k-3+q'^2, \\ 12h'^2 - 36k + 12q'k + 12k - 3 &< (6k-2+q'^2. \end{aligned}$$

Consequently, $\lceil\sqrt{12h'-3}\rceil = 6k-2+q'$.
It follows that

$$\left\lceil\sqrt{12h'-3}\right\rceil = \begin{cases} 6k-3 & \text{if} \quad l' = 0, q' = 0 \\ 6k-2+q' & \text{otherwise} \end{cases} \tag{42}$$

Note that $b' = b(S_{h'}) = 0$ if and only if $n_i(S_{h'+1}) = n_i(S_{h'}) + 1$. From (38) this fact occurs if and only if

$$\left\lceil\sqrt{12h'-3}\right\rceil + 1 = \left\lceil\sqrt{12(h'+1)-3}\right\rceil.$$

From (42) we obtain the expression for b' in terms of k and q'. From (40) and the fact that $h'_e = r' + b'$ we obtain the expressions for r' and h'_e in terms of k and q'. ■

Theorem 5.10. *[5] For any $h \geq 4$ there exists a hexagonal system B_h such that $r(B_h) = \left\lceil\sqrt{3(h-1)}\right\rceil$.*

Proof. Let $h \geq 4$ and k be the greatest integer such that $3(k-1)^2+1 \leq h < 3k^2+1$. Since $0 \leq h-3(k-1)^2-1 < 3(2k-1)$, let

$$\begin{aligned} q &= \left\lfloor \frac{h-3(k-1)^2-1}{2k-1} \right\rfloor \\ l &= h-3(k-1)^2-1-q(2k-1). \end{aligned}$$

Then h has a unique representation of the form

$$h = h(k,q,l) = 3(k-1)^2+1+q(2k-1)+l \tag{43}$$

where $k = 3, 4, \ldots$, $q \in \{0,1,2\}$ and $l = 0, 1, \ldots, 2k-2$.

In order to construct a system B_h with minimal number of inlets for each $h \geq 4$, we take the spiral system $S_{h'}$, with an appropriate value of $h' = h'(k,q',l')$ of the form (41), and remove alternately $\lfloor h'_e/2 \rfloor$ hexagons from the perimeter of $S_{h'}$, starting from the last hexagon and moving in opposite direction with respect to the construction of the spiral systems described in Figure 4. Consider the following cases:

- $h = h(k,0,0) = 3(k-1)^2+1$.

  Let $h' = h'(k,0,0) = 3k(k-1)+1$. By Proposition 5.9, $h'_e = r' = 6k-6$ and $S_{h'}$ has no bay regions. Note that when we remove from $S_{h'}$ each one of the $3k-3$ hexagons, we reduce by one the number of inlets of $S_{h'}$. Note that

$$\begin{aligned} h'(k,0,0) - \left\lfloor \frac{h_e}{2} \right\rfloor &= 3(k-1)^2+1 = h(k,0,0) \\ r &= \frac{r'}{2} = 3(k-1) \end{aligned}$$

- $h = h(k,q,l)$ where $(q,l) \neq (0,0)$, $q \in \{0,1,2\}$ and $l = 0, \ldots k-2$.

  Let $h' = h'(k,q',l')$ where $q' = 2q$ and $l' = l$. By Proposition 5.9, $h'_e = 6k-5+2q$ and $S_{h'}$ has one bay region next to the last hexagon in $S_{h'}$. When we remove the last hexagon in $S_{h'}$, the number of inlets does not change, while when we remove each one of the remained $\left\lfloor \frac{h'_e}{2} \right\rfloor - 1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Note that

$$\begin{aligned} h'(k,q',l') - \left\lfloor \frac{h_e}{2} \right\rfloor &= 3k(k-1)+2qk+l-[3(k-1)+q] \\ &= 3(k-1)^2+1+q(2k-1)+l = h\,(k,q,l) \\ r &= r' - \left(\left\lfloor \frac{h_e}{2} \right\rfloor - 1 \right) = 6k-6+2q+1-[3(k-1)+q] \\ &= 3k-2+q \end{aligned}$$

- $h = h(k,q,l)$ where $q \in \{0,1,2\}$ and $l = k-1, \ldots 2k-3$.

  Let $h' = h'(k,q',l')$ where $q' = 2q+1$ and $l' = l-k+1$. By Proposition 5.9, $h'_e = 6k-4+2q$ and $S_{h'}$ has one bay region next to the last hexagon in $S_{h'}$. When we remove the last hexagon in

$S_{h'}$ the number of inlets does not change, while when we remove each one of the remained $\frac{h_e}{2}-1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Note that

$$\begin{aligned} h'(k,q',l') - \frac{h_e}{2} &= 3k(k-1)+1+(2q+1)k+l-k+1-[3k-2+q] \\ &= 3(k-1)^2+1+q(2k-1)+l = h(k,q,l) \\ r &= r' - \left(\frac{h_e}{2}-1\right) = 6k-6+(2q+1)+1-[3k-2+q] \\ &= 3k-2+q \end{aligned}$$

- $h = h(k,q,l)$ where $q \in \{0,1,2\}$ and $l = 2k-2$.

  Let $h' = h'(k,q',l')$ where $q' = 2q+1$ and $l' = k-1$. By Proposition 5.9, $h'_e = 6k-4+2q$. Note that

$$\begin{aligned} h'(k,q',l') - \frac{h_e}{2} &= 3k(k-1)+1+(2q+1)k+k-1-[3k-2+q] \\ &= 3(k-1)^2+1+q(2k-1)+l = h(k,q,l) \end{aligned}$$

  If $q' = 2q+1 = 5$ then $S_{h'}$ has one bay region next to the last hexagon in $S_{h'}$. When we remove the last hexagon in $S_{h'}$ the number of inlets does not change, while when we remove each one of the remained $\frac{h_e}{2}-1$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Then

$$\begin{aligned} r &= r' - \left(\frac{h_e}{2}-1\right) = 6k-6+2q+1+1-[3k-2+q] \\ &= 3k-2+q \end{aligned}$$

  If $q' = 2q+1 < 5$ then $S_{h'}$ has no bay regions. When we remove each one of the $\frac{h_e}{2}$ hexagons, the number of inlets of $S_{h'}$ reduces by one. Then

$$\begin{aligned} r &= r' - \frac{h_e}{2} = 6k-5+2q+1-[3k-2+q] \\ &= 3k-2+q \end{aligned}$$

  In both cases we obtain $r = 3k-2+q$.

For each value of $h = h(k,q,l)$ we constructed a hexagonal system B_h such that $r = r(B_h) = 3k-3$ if $(q,l) = (0,0)$ and $r = r(B_h) = 3k-2+q$ otherwise. In Figure 22 the hexagonal systems B_h for every value of $h = h(2,q,l)$ are depicted. Now we show that $r = \left\lceil \sqrt{3(h-1)} \right\rceil$.

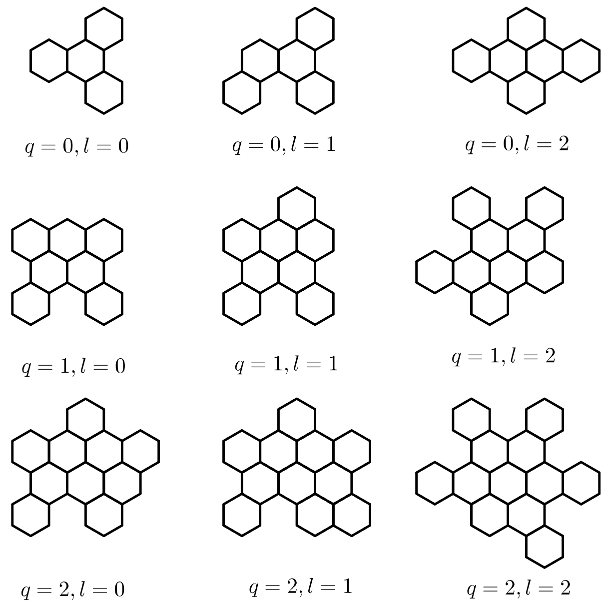


Figure 22. Hexagonal systems B_h for every value of $h = h(2, q, l)$.

If $(q, l) = (0, 0)$ we have $3(h-1) = 9(k-1)^2$ and $\sqrt{3(h-1)} = 3(k-1) = r$.
If $(q, l) \neq (0, 0)$, since $l \leq 2k-2$ and $q \in \{0, 1, 2\}$ we have

$$\begin{aligned} 3(h-1) &= 9(k-1)^2 + 3q(2k-1) + 3l \leq 9k^2 - 6k(2-q) + 3 - 3q \\ &= (3k-2+q)^2 + 3 - (2-q)^2 - 3q < (3k-2+q)^2 . \end{aligned}$$

On the other hand, if $q = 0$ then $l > 0$ and

$$3(h-1) = 9(k-1)^2 + 3l > 9(k-1)^2.$$

If $q \neq 0$ then $l \geq 0$ and

$$\begin{aligned} 3(h-1) &= 9(k-1)^2 + 3q(2k-1) + 3l \geq 9k^2 - 6k(3-q) + 9 - 3q \\ &= (3k-3+q)^2 + 9 - (3-q)^2 - 3q > (3k-3+q)^2 . \end{aligned}$$

It means that if $(q, l) \neq (0, 0)$ then

$$(3k-3+q)^2 < 3(h-1) < (3k-2+q)^2.$$

We conclude that

$$\left\lceil \sqrt{3(h-1)} \right\rceil = 3k - 2 + q = r.$$

■

Note that the hexagonal system B_h, when $h = h\,(p-1, 0, 0)$ where p isan even integer such that $p \geq 4$, coincide with the systems $B_{p,p-2}$ obtained in [3].

From Theorems 5.8 and 5.10 we obtain the following result.

Corollary 5.1. *[5] The system B_h is a hexagonal system with minimal number of inlets in $\mathcal{HS}_h$ for every value of $h \geq 4$.*

6. Extremal values of r and b over pericondensed hexagonal systems

Recall that H is a pericondensed hexagonal system if $n_i(H) \geq 1$. We will denote by $\mathcal{PHS}_h$ the set of pericondensed hexagonal systems with h hexagons. We first determine the extremal values of r over $\mathcal{PHS}_h$.

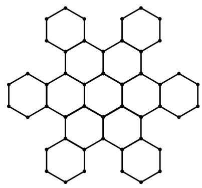


Figure 23. Hexagonal system B_h with minimal number of inlets over $\mathcal{HS}_h$.

It was shown in Section 5 that the hexagonal system B_h (see Figure 23) has $\left\lceil \sqrt{3(h-1)} \right\rceil$ inlets and this is the minimal number of inlets among all hexagonal systems in $\mathcal{HS}_h$. Since B_h is a pericondensed hexagonal system, then B_h attains the minimal number of inlets in $\mathcal{PHS}_h$.

We need the following result to find the hexagonal system with maximal number of inlets in $\mathcal{PHS}_h$.

Lemma 6.1. *Let $H \in \mathcal{HS}_h$ and $h \geq 4$. If $n_i(H) = 1$ then $b(H) \geq 1$.*

Proof. If $n_i(H) = 1$ then H has a subhexagonal system of the form depicted in Figure 31 (a), where no hexagon can be adjacent to the fissures. Since $h \geq 4$, there must be an hexagon adjacent to any of the edges that are not part of the fissures, and this hexagon will transform one of the fissures into a bay. Hence, $b(H) \geq 1$. ∎

We now show that the pericondensed hexagonal system M_h depicted in Figure 24 has the maximal number of inlets in $\mathcal{PHS}_h$.

Theorem 6.2. *Let $h \geq 4$. Then for all $P \in \mathcal{PHS}_h$*

$$\left\lceil \sqrt{3(h-1)} \right\rceil = r(B_h) \leq r(P) \leq r(M_h) = 2(h-2).$$

Proof. We only have to prove the upper bound. Let $P \in \mathcal{PHS}_h$ and assume that $n_i(P) \geq 2$. Then $b(P) + n_i(P) \geq 2$ and so by (5)

$$\begin{aligned} r(P) &= 2(h-1) - (b(P) + n_i(P)) \\ &\leq 2(h-1) - 2 = 2(h-2) \end{aligned}$$

If $n_i(P) = 1$ then $b(P) \geq 1$ by Lemma 6.1. Hence $b(P) + n_i(P) \geq 2$ and again $r(P) \leq 2(h-2)$. Finally, it is easy to show that $r(M_h) = 2(h-2)$. ∎

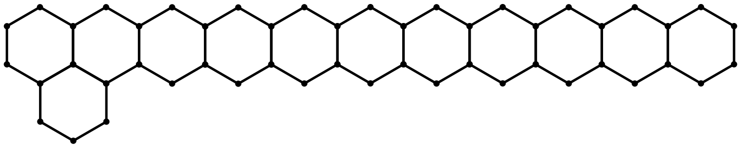


Figure 24. Hexagonal systems M_h with maximal number of inlets over $\mathcal{PHS}_h$.

Now we look at the bounds for b over $\mathcal{PHS}_h$. For every positive integer h we can easily construct convex pericondensed hexagonal systems as we can see in Figure 25. These have obviously minimal number of bay regions in $\mathcal{PHS}_h$.

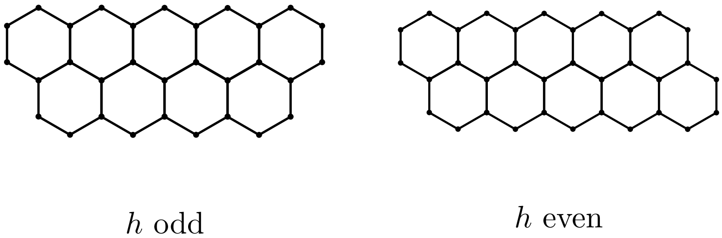


Figure 25. Convex pericondensed hexagonal systems.

So now we are interested in finding the maximal number of bay regions among all hexagonal systems in $\mathcal{PHS}_h$. As in the proof of Theorem 4.1, we use the fact that every hexagonal system has a hexagon of the form L_1, P_2, L_3, P_4 or L_5.

Theorem 6.3. *[6] Let $H \in \mathcal{PHS}_h$ with $h \geq 4$. Then*

$$b(H) \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil .$$

Proof. The proof is by induction on h. It is easy to check the result for $h = 4, 5, 6$. Let $h \geq 7$ and assume that the result is true for any pericondensed hexagonal system with less than h hexagons. Let H be a pericondensed hexagonal system with h hexagons. First assume that $n_i(H) \geq 5$.

1. H contains a L_3, P_4 or L_5 hexagon, or a P_2 hexagon of the form depicted in Figure 8. Then by part 1 of the proof of Theorem 4.1, there exists a (sub)hexagonal system H_1 with $h-1$ hexagons such that $b(H) \leq b(H_1)+1$. Moreover, since $n_i(H) \geq 5$, $H_1 \in \mathcal{PHS}_{h-1}$. Hence by induction we deduce
$$b(H) \leq b(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-1) - \frac{11}{2} \right\rceil + 1 \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil .$$
2. H satisfies any of the cases 2, 3 or 4 in the proof of Theorem 4.1. Then there exist two (sub)hexagonal systems H_1 and H_2 of H, with $h_1 \geq 2$ and $h_2 \geq 2$ hexagons respectively, such that $h = h_1 + h_2$

and $b(H) \leq b(H_1) + b(H_2) + 3$. Since $n_i(H) \geq 5$, one of the two hexagonal systems is pericondensed, say H_1. Then by induction we deduce

$$b(H) \leq b(H_1) + b(H_2) + 3 \leq \left\lceil \frac{3}{2}h_1 - \frac{11}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 3 \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil .$$

The only possibility left is case 5 in Theorem 4.1, but this cannot occur since $H \in \mathcal{PHS}_h$. So we only have to consider when $1 \leq n_i(H) \leq 4$.

If $n_i(H) = 4$ then the proof works the same as in the case $n_i(H) \geq 5$ except when there is a L_5 hexagon. Note that in the splitting of H in that case, none of the (sub)hexagonal systems is pericondensed. However, if $n_i(H) = 4$ then we can split H (see Figure 26) into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system with at least four hexagons. In this case, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed (with exactly one internal vertex), the results follow as in part 2 of this theorem. Note that if H_1 has exactly three hexagons, then one of these hexagons is a P_2 hexagon and the results follows as in part 1 of this theorem.

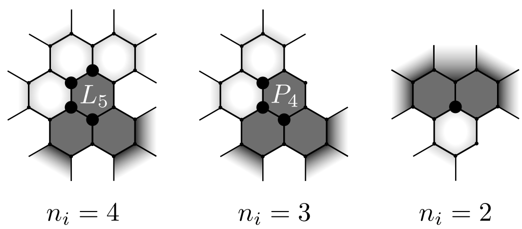


Figure 26. Pericondensed hexagonal systems with $n_i \in \{2, 3, 4\}$.

If $n_i(H) = 3$ then H does not contain a L_5 hexagon. Again, the proof works as in the case $n_i(H) \geq 5$ except when H contains a P_4 hexagon. However, since $n_i(H) = 3$ we can split H into the two (sub)hexagonal systems H_1 and H_2 (see Figure 26), where H_1 is the dark shadowed (sub)hexagonal system with at least four hexagons. In this case, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed (with exactly one internal vertex), the results follow as in part 2 of this theorem. Note that if H_1 has exactly three hexagons, then one of these hexagons is a P_2 hexagon and the results follows as in part 1 of this theorem.

If $n_i(H) = 2$, H is of the form depicted in Figure 26. Note that one internal vertex is highlighted and the other one belongs to the dark shadowed (sub)hexagonal system. We split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system. If H_2 has two or more hexagons, we obtain at least three new 2-2-edges in H_1 and H_2. Hence

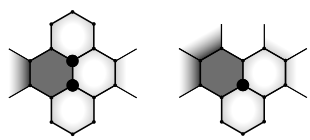
$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed, the results follow as in part 2 of this theorem.

On the other hand, if H_2 consists of only one hexagon then the system H has the form (a) or the form (b) depicted in Figure 27. Note that in case (b) one internal vertex is highlighted and the other one belongs to the dark shadowed (sub)hexagonal system. In each case, we split system H into the two (sub)hexagonal systems H_1 and H_2, where H_1 is the dark shadowed (sub)hexagonal system.



(a) (b)

Figure 27. Pericondensed hexagonal systems with $n_i = 2$ when H_2 consists of only one hexagon.

In case (a) we obtain at least five new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 5,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 1.$$

Since neither H_1 nor H_2 are pericondensed, by Theorem 4.1 we deduce

$$\begin{aligned} b(H) &\leq b(H_1) + b(H_2) + 1 \leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 1 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

In case (b) we obtain at least three new 2-2-edges in H_1 and H_2. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) - 3,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 3.$$

Since H_1 is pericondensed, the results follow as in part 2 of this theorem.

Finally, if $n_i(H) = 1$, we split H into three (sub) hexagonal system H_1, H_2 and H_3 of H as depicted in Figure 28, where $h = h_1 + h_2 + h_3$. If $h_2 = h_3 = 1$ then

$$m_{22}(H) \leq m_{22}(H_1) + 6 + 6 - 4 - 4 - 3 = m_{22}(H_1) + 1,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + 1.$$

From Theorem 4.1

$$\begin{aligned} b\,(H) &\leq b\,(H_1) + 1 \leq \left\lceil \frac{3}{2}(h-2) - \frac{7}{2} \right\rceil + 1 \\ &\leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

If $h_2 > 1$ and $h_3 = 1$ then

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) + 6 - 4 - 3 - 3 = m_{22}(H_1) + m_{22}(H_2) - 4,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 2.$$

From Theorem 4.1 and the fact that $h = h_1 + h_2 + 1$ we obtain

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + 2 \leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + 2 \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil .$$

Now, if $h_2 > 1$ and $h_3 > 1$ we obtain at least nine new 2-2-edges. Hence

$$m_{22}(H) \leq m_{22}(H_1) + m_{22}(H_2) + m_{22}(H_3) - 9,$$

or equivalently,

$$b\,(H) \leq b\,(H_1) + b\,(H_2) + b\,(H_3) + 3.$$

It follows from Theorem 4.1 and the fact that $h = h_1 + h_2 + h_3$ that

$$\begin{aligned} b\,(H) &\leq b\,(H_1) + b\,(H_2) + b\,(H_3) + 3 \\ &\leq \left\lceil \frac{3}{2}h_1 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_2 - \frac{7}{2} \right\rceil + \left\lceil \frac{3}{2}h_3 - \frac{7}{2} \right\rceil + 3 \leq \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil . \end{aligned}$$

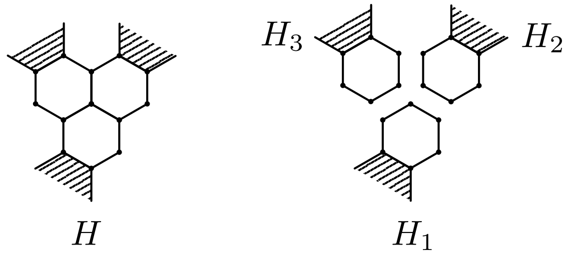


Figure 28. Split of pericondensed (sub)hexagonal system H with $n_i = 1$.

■

Example 6.4. *The hexagonal system F_h depicted in Figure 29 has maximal value of b over the set of pericondensed hexagonal systems with h hexagons.*

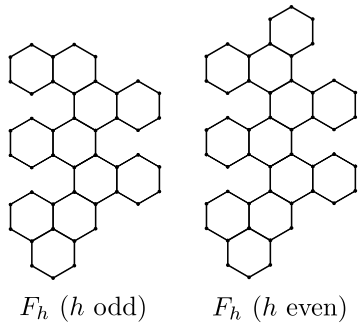


Figure 29. Hexagonal system with maximal value of b over $\mathcal{PHS}_h$.

Next we discuss the extremal value problem of TI over $\mathcal{PHS}_h$. Recall that the spiral hexagonal system S_h has maximal number of internal vertices

$$n_i(S_h) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil$$

among all hexagonal systems in $\mathcal{HS}_h$. In Section 3 we characterized the values of h for which there exists a convex hexagonal system W with maximal number of internal vertices, i.e.

$$n_i(W) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil . \tag{44}$$

Note that $W \in \mathcal{PHS}_h$. Hence we deduce from Theorems 3.1 and 3.8:

Theorem 6.5. *[6] Let TI be a vertex-degree-based topological index of the form (7).*

1. *If there exists a convex hexagonal system W with h hexagons satisfying (44) and $-\varphi_{22} \leq q < 0$ then W has minimal TI-value among all hexagonal systems in $\mathcal{PHS}_h$.*
2. *If there is no convex hexagonal system with h hexagons satisfying (44) and $\frac{-\varphi_{22}}{2} \leq q < 0$, then the spiral S_h has minimal TI-value over $\mathcal{PHS}_h$.*

Now based on Theorems 6.2 and 6.3 we find the maximal value of TI over $\mathcal{PHS}_h$.

Theorem 6.6. *[6] Let TI be a vertex-degree-based topological index of the form (7). If $-\varphi_{22} \leq q < 0$ then F_h (see Figure 29) has maximal TI -value over $\mathcal{PHS}_h$.*

Proof. Let $P \in \mathcal{PHS}_h$. Then $n_i(P) \geq 1$. It follows from (10) and Theorem 6.3 that

$$\begin{aligned} TI(F_h) - TI(P) &= q\left[b(P) - b(F_h)\right] + (q + \varphi_{22})\left[n_i(P) - n_i(F_h)\right] \\ &= q\left[b(P) - \left\lceil \frac{3}{2}h - \frac{11}{2} \right\rceil\right] + (q + \varphi_{22})\left[n_i(P) - 1\right] \geq 0. \end{aligned}$$

Consequently, $TI(F_h) \geq TI(P)$ for all $P \in \mathcal{PHS}_h$. ∎

Remark 6.7. *The condition* $\frac{-\varphi_{22}}{2} \leq q < 0$ *holds for most of the well-known topological indices, as we can see in Table 1. Consequently, for all these indices the extremal values of* TI *over* $\mathcal{PHS}_h$ *are determined for all* h*, by Theorems 6.5 and 6.6.*

In the case of the Atom-Bond-Connectivity index $q > 0$.

Theorem 6.8. *[6] Let* TI *be a vertex-degree-based topological index of the form (7). If* $q > 0$ *then* M_h *has maximal* TI*-value among all hexagonal systems in* $\mathcal{PHS}_h$*.*

Proof. Let $P \in \mathcal{PHS}_h$. Then $n_i(P) \geq 1$. By (8) and Theorem 6.2

$$\begin{aligned} TI(M_h) - TI(P) &= q\left[r(M_h) - r(P)\right] + \varphi_{22}\left[n_i(P) - n_i(M_h)\right] \\ &= q\left[2(h-2) - r(P)\right] + \varphi_{22}\left[n_i(P) - 1\right] \geq 0. \end{aligned}$$

Hence $TI(M_h) \geq TI(P)$ for all $P \in \mathcal{PHS}_h$. ■

7. Hexagonal systems with equal number of vertices

Let Λ_n denote the set of hexagonal systems with exactly n vertices. We will find in this section the hexagonal systems with maximal number of inlets in Λ_n and then, we will apply this result in the study of extremal values of vertex-degree-based topological indices. Figure 30 shows several hexagonal systems belonging to Λ_{42}.

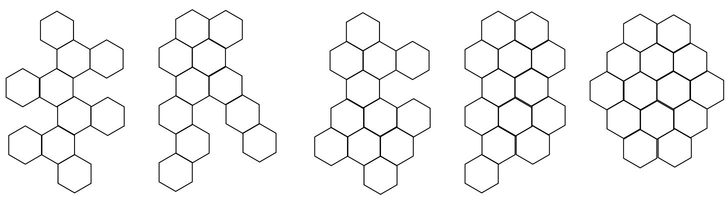


Figure 30. Hexagonal systems in Λ_{42}.

Note that the number of hexagons in hexagonal systems belonging to Λ_n is variable. In fact, if $H \in \Lambda_n$ then it follows from [16] that

$$\left\lceil \frac{1}{4}(n-2) \right\rceil \leq h(H) \leq n + 1 - \left\lceil \frac{1}{2}\left(n + \sqrt{6n}\right) \right\rceil \tag{45}$$

where $h(H)$ denotes the number of hexagons H has. Since n is fixed then for each value $h(H)$ in the interval defined by (45), the number of internal vertices $n_i(H)$ is also determined via the relation

$$n = 4h(H) + 2 - n_i(H) \tag{46}$$

Example 7.1. *Consider the set* Λ_{42}*. Then by (45), if* $H \in \Lambda_{42}$ *then*

$$10 \leq h(H) \leq 14$$

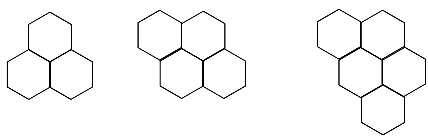
Hence we can classify the hexagonal systems in Λ_{42} *depending on the number of hexagons as:*

$h = 10$	$h = 11$	$h = 12$	$h = 13$	$h = 14$
$n_i = 0$	$n_i = 4$	$n_i = 8$	$n_i = 12$	$n_i = 16$

Recall that $\mathcal{HS}_h$ is the set of hexagonal systems with h hexagons.

Lemma 7.2. *Let* $H \in \mathcal{HS}_h$ *and* $h \geq 4$*. Assume that* H *has an internal vertex* v_0 *such that no adjacent vertex of* v_0 *is internal. Then* H *is not a convex hexagonal system.*

Proof. By hypothesis, H has a subhexagonal system of the form depicted in Figure 31 (a), where no hexagon can be adjacent to the fissures indicated by heavy lines. Since $h \geq 4$, there must be an hexagon adjacent to any of the edges that are not part of the fissures, and this hexagon will transform one of the fissures into a bay. Hence, $b(H) \geq 1$ and H is not a convex hexagonal system. ■



(a) (b) (c)

Figure 31. Hexagonal systems with 1,2 and 3 internal vertices, respectively.

Lemma 7.3. *Let* $H \in \mathcal{HS}_h$*. In each of the following conditions* H *is not a convex hexagonal system:*

1. *If* $h \geq 4$ *and* $n_i(H) = 1$;
2. *If* $h \geq 5$ *and* $n_i(H) = 2$;
3. *If* $h \geq 6$ *and* $n_i(H) = 3$.

Proof. 1. This is an immediate consequence of Lemma 7.2.

2. We may assume that the two internal vertices are adjacent, otherwise we apply Lemma 7.2 and the result follows. Then H has a subhexagonal system of the form shown in Figure 31 (b), where no hexagons are adjacent to the fissures indicated in heavy lines. Since $h \geq 5$, there must be an hexagon adjacent to an edge that is not part of the fissures, and this hexagon will transform one of the fissures into a bay. Hence, $b(H) \geq 1$.

3. Again by Lemma 7.2 we may assume that H has a subhexagonal system of the form shown in Figure 31 (c), and a similar argument as above shows that $b(H) \geq 1$. ■

Next we find the hexagonal system with maximal number of inlets in $\mathcal{HS}_h$ with a fixed number of internal vertices. Recall that M_h, N_h and Q_h are the hexagonal systems depicted in Figure 32.

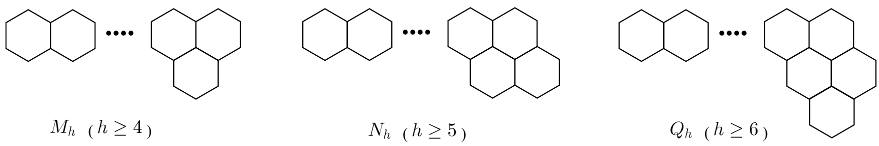


Figure 32. Hexagonal systems with maximal number of inlets in $\mathcal{HS}_h$.

Proposition 7.4. *Let $H \in \mathcal{HS}_h$. Then:*

1. *If $n_i(H) = 1$ then*

$$r(H) \leq r(M_h) = \begin{cases} 3 & \text{if } h = 3 \\ 2h-4 & \text{if } h \geq 4 \end{cases};$$

2. *If $n_i(H) = 2$ then*

$$r(H) \leq r(N_h) = \begin{cases} 4 & \text{if } h = 4 \\ 2h-5 & \text{if } h \geq 5 \end{cases};$$

3. *If $n_i(H) = 3$ then*

$$r(H) \leq r(Q_h) = \begin{cases} 5 & \text{if } h = 5 \\ 2h-6 & \text{if } h \geq 6 \end{cases}$$

Proof. 1. If $n_i(H) = 1$ then clearly $h \geq 3$. If $h = 3$ then $H = M_3$ is the unique hexagonal system in $H \in \mathcal{HS}_3$ such that $n_i(H) = 1$ and so the result follows. Assume that $h \geq 4$. Then by Lemma 7.3 part 1., H is not a convex hexagonal system. Hence $b(H) \geq 1$ and from (5) we deduce

$$r(H) = 2h - 3 - b(H) \leq 2h - 4$$

2. If $n_i(H) = 2$ then $h \geq 4$. If $h = 4$ then $H = N_4$ and we are done. Otherwise, $h \geq 5$ and so by Lemma 7.3 part 2., $b(H) \geq 1$. Then using (5) we get

$$r(H) = 2h - 4 - b(H) \leq 2h - 5$$

3. If $n_i(H) = 3$ then $h \geq 5$. If $h = 5$ then $H = Q_5$ and we are done. Otherwise, $h \geq 6$ and so by Lemma 7.3 part 3., $b(H) \geq 1$. It follows from (5) that

$$r(H) = 2h - 5 - b(H) \leq 2h - 6$$

■

Now we can find the hexagonal system with maximal number of inlets in Λ_n, the set of hexagonal systems with n vertices. Recall that L_h is the linear hexagonal chain with h hexagons.

Theorem 7.5. *[1] Let $H \in \Lambda_n$. Then:*

1. *If $n \equiv 0\,(mod4)$ then $r(H) \leq \frac{n-10}{2} = r\left(N_{\frac{n}{4}}\right)$;*
2. *If $n \equiv 1\,(mod4)$ then $r(H) \leq \frac{n-9}{2} = r\left(M_{\frac{n-1}{4}}\right)$;*
3. *If $n \equiv 2\,(mod4)$ then $r(H) \leq \frac{n-6}{2} = r\left(L_{\frac{n-2}{4}}\right)$;*
4. *If $n \equiv 3\,(mod4)$ then $r(H) \leq \frac{n-11}{2} = r\left(Q_{\frac{n+1}{4}}\right)$.*

Proof. We know by (45) that

$$\left\lceil \frac{1}{4}(n-2) \right\rceil \leq h(H) \leq n+1-\left\lceil \frac{1}{2}\left(n+\sqrt{6n}\right) \right\rceil$$

1. If $n \equiv 0\,(mod4)$ then $\left\lceil \frac{1}{4}(n-2) \right\rceil = \frac{n}{4}$. Consider first the case that $h(H) = \frac{n}{4}$. Then by (46)

$$n = 4h(H) + 2 - n_i(H) = 4\frac{n}{4} + 2 - n_i(H) = n + 2 - n_i(H)$$

which implies $n_i(H) = 2$. Now we can apply Proposition 7.4 part 2., to conclude that $r(H) \leq r\left(N_{\frac{n}{4}}\right)$ and we are done. So assume now that $h(H) \geq \frac{n}{4} + 1$. Then by (5)

$$\begin{aligned} r(H) &= n - 2h(H) - b(H) - 4 \leq n - 2\left(\frac{n}{4}+1\right) - b(H) - 4 \\ &= \frac{1}{2}n - b(H) - 6 \leq \frac{n-12}{2} \leq \frac{n-10}{2} = r\left(N_{\frac{n}{4}}\right) \end{aligned}$$

2. If $n \equiv 1\,(mod4)$ then $\left\lceil \frac{1}{4}(n-2) \right\rceil = \frac{n-1}{4}$. If $h(H) = \frac{n-1}{4}$ then by (46)

$$n = 4h(H) + 2 - n_i(H) = 4\frac{n-1}{4} + 2 - n_i(H) = n + 1 - n_i(H)$$

and so $n_i(H) = 1$. By Proposition 7.4 part 1., $r(H) \leq r\left(M_{\frac{n-1}{4}}\right)$. If $h(H) \geq \frac{n-1}{4} + 1$. Then by (5)

$$\begin{aligned} r(H) &= n - 2h(H) - b(H) - 4 \leq n - 2\left(\frac{n-1}{4}+1\right) - b(H) - 4 \\ &= \frac{1}{2}n - b(H) - \frac{11}{2} \leq \frac{n-11}{2} \leq \frac{n-9}{2} = r\left(M_{\frac{n-1}{4}}\right) \end{aligned}$$

3. If $n \equiv 2\,(mod4)$ then $\left\lceil \frac{1}{4}(n-2) \right\rceil = \frac{n-2}{4}$. Since $h(H) \geq \frac{n-2}{4}$ then by (46)

$$\begin{aligned} r(H) &= n - 2h(H) - b(H) - 4 \leq n - 2\left(\frac{n-2}{4}\right) - b(H) - 4 \\ &= \frac{1}{2}n - b(H) - 3 \leq \frac{n-6}{2} = r\left(L_{\frac{n-2}{4}}\right) \end{aligned}$$

4. If $n \equiv 3\,(mod4)$ then $\left\lceil \frac{1}{4}(n-2) \right\rceil = \frac{n+1}{4}$. If $h(H) = \frac{n+1}{4}$ then by (46)

$$n = 4h(H) + 2 - n_i(H) = 4\frac{n+1}{4} + 2 - n_i(H) = n + 3 - n_i(H)$$

which implies that $n_i(H) = 3$. Now by Proposition 7.4 part 3., $r(H) \leq r\left(Q_{\frac{n+1}{4}}\right)$. In the case that $h(H) \geq \frac{n+1}{4} + 1$ then by (46)

$$\begin{aligned} r(H) &= n - 2h(H) - b(H) - 4 \leq n - 2\left(\frac{n+1}{4} + 1\right) - b(H) - 4 \\ &= \frac{1}{2}n - b - \frac{13}{2} \leq \frac{n-13}{2} \leq \frac{n-11}{2} = r\left(Q_{\frac{n+1}{4}}\right) \end{aligned}$$

■

Let TI be a vertex-degree-based topological index induced by the real nonnegative numbers $\{\varphi_{ij}\}$. From (2), (3), (4) and (7) we deduce that if $H \in \Lambda_n$ then

$$TI(H) = \varphi_{22}n + [3\varphi_{33} - 2\varphi_{22}]h + [2\varphi_{23} - \varphi_{22} - \varphi_{33}]r + [2\varphi_{22} - 3\varphi_{33}]. \tag{47}$$

If $H, U \in \Lambda_n$ then clearly

$$TI(H) - TI(U) = [3\varphi_{33} - 2\varphi_{22}](h(H) - h(U)) + [2\varphi_{23} - \varphi_{22} - \varphi_{33}](r(H) - r(U)) \tag{48}$$

From now on we set $p = 3\varphi_{33} - 2\varphi_{22}$ and $q = 2\varphi_{23} - \varphi_{22} - \varphi_{33}$.

Theorem 7.6. *[1] Let TI be a topological index of the form (7) induced by the nonnegative real numbers $\{\varphi_{22}, \varphi_{23}, \varphi_{33}\}$. Assume that H_0 is a hexagonal system with maximal number of inlets in Λ_n. Then:*

1. *If $p \leq 0$ and $q \geq 0$ then TI reaches its maximal value in H_0;*
2. *If $p \geq 0$ and $q \leq 0$ then TI reaches its minimal value in H_0.*

Proof. Let $U \in \Lambda_n$. Then by (48)

$$TI(H_0) - TI(U) = p(h(H_0) - h(U)) + q(r(H_0) - r(U)) \tag{49}$$

By hypothesis $r(H_0) - r(U) \geq 0$. By (45) and Theorem 7.5,

$$h(U) \geq \left\lceil \frac{1}{4}(n-2) \right\rceil = h(H_0)$$

Hence by (49), if $p \leq 0$ and $q \geq 0$ then

$$TI(H_0) - TI(U) \geq 0$$

and if $p \geq 0$ and $q \leq 0$ then

$$TI(H_0) - TI(U) \leq 0$$

In other words, if $p \leq 0$ and $q \geq 0$ then $TI(H_0) \geq TI(U)$ for all $U \in \Lambda_n$, which implies that TI reaches its maximal value in H_0. Similarly, if $p \geq 0$ and $q \leq 0$ then $TI(H_0) \leq TI(U)$ for all $U \in \Lambda_n$, and so TI reaches its minimal value in H_0. ■

Example 7.7. *The following table contains the values of p and q for several well-known topological indices:*

$$\begin{array}{c||cccccc} & ij & \frac{1}{\sqrt{ij}} & \frac{2\sqrt{ij}}{i+j} & \frac{2}{i+j} & \frac{1}{\sqrt{i+j}} & \frac{(ij)^3}{(i+j-2)^3} \\ \hline q & \text{-1} & \text{-.0168} & \text{-.0404} & \text{-.0333} & \text{-.0138} & \text{-3.3906} \\ \hline p & 19 & 0 & 1 & 0 & 0.22 & 18.17 \end{array} \tag{50}$$

Hence, by Theorems 7.5 and 7.6 we can deduce the minimal value of each TI over Λ_n, for every n. More precisely, the minimal value of every TI that appears in Table (50) over Λ_n is as follows:

$$\begin{array}{cccc} n \equiv 0\,(mod4) & n \equiv 1\,(mod4) & n \equiv 2\,(mod4) & n \equiv 3\,(mod4) \\ \downarrow & \downarrow & \downarrow & \downarrow \\ N_{\frac{n}{4}} & M_{\frac{n-1}{4}} & L_{\frac{n-2}{4}} & Q_{\frac{n+1}{4}} \end{array}$$

If H is a hexagonal system with n vertices, then from the relations (5), (46) and (47) we deduce

$$\begin{aligned} TI\,(H) &= [2\varphi_{23} - \varphi_{33}]\,n + [5\varphi_{33} - 4\varphi_{23}]\,h\,(H) + [-2\varphi_{23} + \varphi_{22} + \varphi_{33}]\,b\,(H) \\ &\quad + [6\varphi_{22} + \varphi_{33} - 8\varphi_{23}]\,. \end{aligned}$$

Consequently, for hexagonal systems $W, Z \in \Lambda_n$

$$\begin{aligned} TI\,(W) - TI\,(Z) &= [5\varphi_{33} - 4\varphi_{23}]\,[h\,(W) - h\,(Z)] + \\ &\quad [-2\varphi_{23} + \varphi_{22} + \varphi_{33}]\,[b\,(W) - b\,(Z)] \end{aligned} \tag{51}$$

Set $t = 5\varphi_{33} - 4\varphi_{23}$ and keep the notation for q introduced earlier. Then

$$TI\,(W) - TI\,(Z) = t\,[h\,(W) - h\,(Z)] - q\,[b\,(W) - b\,(Z)] \tag{52}$$

As we can see this expression only depends on the number of hexagons and the number of bay regions. We know from (45) that the maximal value possible of hexagons in a system with n vertices is $n + 1 - \left\lceil \frac{1}{2}\left(n + \sqrt{6n}\right)\right\rceil$, and this occurs precisely in the spirals S_n.

Theorem 7.8. *[1] Let h such that S_h is convex and $n = 2h + 1 + \left\lceil \sqrt{12h - 3} \right\rceil$. Then*

1. *If $u \geq 0$ and $q \geq 0$ then S_h has the maximal TI-value over Λ_n;*
2. *If $u \leq 0$ and $q \leq 0$ then S_h has the minimal TI-value over Λ_n.*

Proof. Since $n_i\,(S_h) = 2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil$ then

$$n\,(S_h) = 4h + 2 - \left(2h + 1 - \left\lceil \sqrt{12h - 3} \right\rceil\right) = 2h + 1 + \left\lceil \sqrt{12h - 3} \right\rceil$$

and so S_h has n vertices. Also we know by hypothesis that $b\,(S_h) = 0$. On the other hand, $n = 2h + 1 + \left\lceil \sqrt{12h - 3} \right\rceil$ implies $h = n + 1 - \left\lceil \frac{1}{2}\left(n + \sqrt{6n}\right)\right\rceil$. Hence by (52) and (45) it follows that for any hexagonal system $H \in \Lambda_n$

$$\begin{aligned} TI\,(H) - TI\,(S_h) &= t\,[h\,(H) - h\,(S_h)] - q\,[b\,(H) - b\,(S_h)] \\ &= t\left[h\,(H) - \left(n + 1 - \left\lceil \frac{1}{2}\left(n + \sqrt{6n}\right)\right\rceil\right)\right] - q\,[b\,(H)] \\ &\quad \begin{cases} \leq 0 & \text{if } t \geq 0 \text{ and } q \geq 0 \\ \geq 0 & \text{if } t \leq 0 \text{ and } q \leq 0 \end{cases}. \end{aligned}$$

■

Example 7.9. *Consider the atom-bond connectivity index defined by the numbers* $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$*. Then* $t \cong 0.505$ *and* $q \cong 0.04$*. Hence by part 1. of Theorem 7.8 we can determine its maximal value for those* h *such that* S_h *is convex.*

8. Hexagonal systems with equal number of edges

From now on we will denote by Γ_m the set of hexagonal systems with m edges. The main idea in this section consists in constructing hexagonal systems with maximal number of inlets in Γ_m which have simultaneously minimal number of hexagons. Figure 33 shows several hexagonal systems belonging to Γ_{51}.

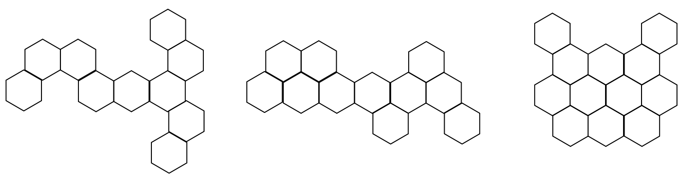


Figure 33. Hexagonal systems with equal number of edges

We note that the number of hexagons in the hexagonal systems of Γ_{51} is variable. In general, given a positive integer m, the variation of the number of hexagons in Γ_m is completely determined by Harary and Harborth [16]: if $H \in \Gamma_m$ then

$$\left\lceil \frac{1}{5}(m-1) \right\rceil \leq h(H) \leq m - \left\lceil \frac{1}{3}\left(2m-2+\sqrt{4m+1}\right) \right\rceil . \tag{53}$$

Example 8.1. *Consider the set* Γ_{51}*. Then by (45), if* $H \in \Gamma_{51}$ *then*

$$10 \leq h(H) \leq 12$$

Hence we can classify the hexagonal systems in Γ_{51} *depending on the number of hexagons as:*

$$\left| \begin{array}{c} h=10 \\ n_i=0 \end{array} \right| \begin{array}{c} h=11 \\ n_i=5 \end{array} \left| \begin{array}{c} h=12 \\ n_i=10 \end{array} \right|$$

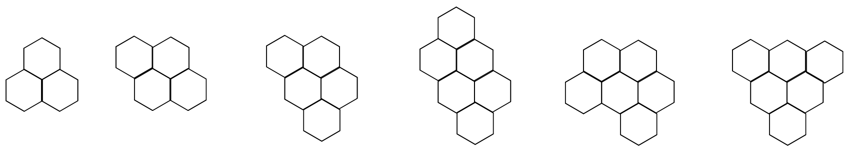
We have to extend Proposition 7.4 to hexagonal systems with four internal vertices.

Lemma 8.2. *Let* H *be a hexagonal system such that* $n_i(H) = 4$*. Then* H *must contain a subhexagonal system of the form given in Figure 34, where no hexagons are adjacent to the fissures.*

Proof. If the four internal vertices are connected then H must have a subhexagonal system of type (d), (e) or (f) in Figure 34. Clearly, no hexagons are adjacent to the fissures, otherwise $n_i(H) \geq 5$. If the four internal vertices are not connected then the possibilities that H has subhexagonal systems are as shown in the columns of the following table:

type (a)	1	0	2	4
type (b)	0	2	1	0
type (c)	1	0	0	0

In any case, no hexagons are adjacent to the fissures, otherwise $n_i(H) \geq 5$. ■



(a) (b) (c) (d) (e) (f)

Figure 34. Hexagonal systems with 1,2,3 and 4 internal vertices, respectively.

Let us define the hexagonal system R_h as in Figure 35.

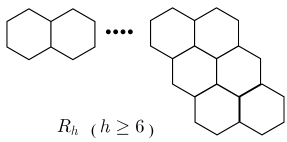


Figure 35. Hexagonal systems with maximal number of inlets.

Proposition 8.3. *Let H be a hexagonal system with h hexagons. If $n_i(H) = 4$ then*

$$r(H) \leq r(R_h) = \begin{cases} 6 & \text{if } h = 6 \\ 2h - 7 & \text{if } h \geq 7 \end{cases}.$$

Proof. If $h = 6$ then H is one of the hexagonal systems (d), (e) and (f) in Figure 34. In any case it is clear that $r(H) \leq r(R_6)$. So let us assume that $h \geq 7$. By Lemma 8.2, H has a subhexagonal system as in Figure 34, where no hexagons are adjacent to the fissures. Since $h \geq 7$ there must exist hexagons adjacent to a (2-2)-edge, and these hexagons will transform one of the fissures into a bay, cove or fjord. Consequently, $b(H) \geq 1$. Then by (5)

$$r(H) = 2h(H) - b(H) - 6 \leq 2h - 7.$$

■

Next we find a hexagonal system with maximal number of inlets in the set of hexagonal systems with equal number of edges. Recall that for $H \in \Gamma_m$ the following relation holds [13]

$$m(H) = 5h(H) + 1 - n_i(H). \tag{54}$$

We then deduce from (5) and (54) that

$$r(H) = m(H) - 3 - 3h(H) - b(H). \tag{55}$$

Theorem 8.4. *[27] Let $H \in \Gamma_m$. Then*

$$r(H) \leq \begin{cases} r\left(M_{\frac{m}{5}}\right) & \textit{if} \;\; m \equiv 0\,(\textit{mod}\,5) \\ r\left(L_{\frac{m-1}{5}}\right) & \textit{if} \;\; m \equiv 1\,(\textit{mod}\,5) \\ r\left(R_{\frac{m+3}{5}}\right) & \textit{if} \;\; m \equiv 2\,(\textit{mod}\,5) \\ r\left(Q_{\frac{m+2}{5}}\right) & \textit{if} \;\; m \equiv 3\,(\textit{mod}\,5) \\ r\left(N_{\frac{m+1}{5}}\right) & \textit{if} \;\; m \equiv 4\,(\textit{mod}\,5) \end{cases}$$

Proof. Recall that $h(H) \geq \left\lceil \frac{1}{5}(m-1) \right\rceil$ (see (53)).

(a) Assume that $m \equiv 0\,(\text{mod}\,5)$. Then $\left\lceil \frac{1}{5}(m-1) \right\rceil = \frac{m}{5}$. If $h(H) = \frac{m}{5}$ then by (54)

$$m = 5\left(\frac{m}{5}\right) + 1 - n_i(H)$$

which implies that $n_i(H) = 1$. Then $r(H) \leq r\left(M_{\frac{m}{5}}\right)$ by part 1 of Proposition 7.4. Otherwise $h(H) \geq \frac{m}{5} + 1$ and so by (55) and the fact that $b(H) \geq 0$

$$\begin{aligned} r(H) &= m - 3 - 3h(H) - b(H) \leq m - 3 - 3\left(\frac{m}{5} + 1\right) \\ &= \frac{2m-30}{5} \leq \frac{2m-20}{5} = r\left(M_{\frac{m}{5}}\right). \end{aligned}$$

(b) Assume that $m \equiv 1\,(\text{mod}\,5)$. Then $\left\lceil \frac{1}{5}(m-1) \right\rceil = \frac{m-1}{5}$. It follows from (55)

$$\begin{aligned} r(H) &= m - 3 - 3h(H) - b(H) \leq m - 3 - 3\left(\frac{m-1}{5}\right) \\ &= \frac{2m-12}{5} = r\left(L_{\frac{m-1}{5}}\right). \end{aligned}$$

(c) Assume that $m \equiv 2\,(\text{mod}\,5)$. Then $\left\lceil \frac{1}{5}(m-1) \right\rceil = \frac{m+3}{5}$. If $h(H) = \frac{m+3}{5}$ then by (54)

$$m = 5\left(\frac{m+3}{5}\right) + 1 - n_i(H)$$

which implies that $n_i(H) = 4$. It follows from Proposition 8.3 that $r(H) \leq r\left(R_{\frac{m+3}{5}}\right)$. Otherwise $h(H) \geq \frac{m+3}{5} + 1$ and then by (55)

$$\begin{aligned} r(H) &= m - 3 - 3h(H) - b(H) \leq m - 3 - 3\left(\frac{m+3}{5} + 1\right) \\ &= \frac{2m-39}{5} \leq \frac{2m-29}{5} = r\left(R_{\frac{m+3}{5}}\right). \end{aligned}$$

(d) Assume that $m \equiv 3 \,(\mathrm{mod}\ 5)$. Then $\left\lceil \frac{1}{5}(m-1) \right\rceil = \frac{m+2}{5}$. If $h(H) = \frac{m+2}{5}$ then by (54)

$$m = 5\left(\frac{m+2}{5}\right) + 1 - n_i(H)$$

which implies $n_i(H) = 3$. It follows from Proposition 7.4 that $r(H) \leq r\left(Q_{\frac{m+2}{5}}\right)$. Otherwise $h(H) \geq \frac{m+2}{5} + 1$ and then by (55)

$$\begin{aligned} r(H) &= m - 3 - 3h(H) - b(H) \leq m - 3 - 3\left(\frac{m+2}{5} + 1\right) \\ &= \frac{2m-36}{5} \leq \frac{2m-26}{5} = r\left(Q_{\frac{m+2}{5}}\right). \end{aligned}$$

(e) Assume that $m \equiv 4 \,(\mathrm{mod}\ 5)$. Then $\left\lceil \frac{1}{5}(m-1) \right\rceil = \frac{m+1}{5}$. If $h(H) = \frac{m+1}{5}$ then by (54)

$$m = 5\left(\frac{m+1}{5}\right) + 1 - n_i(H)$$

which implies $n_i(H) = 2$. It follows from Proposition 7.4 that $r(H) \leq r\left(N_{\frac{m+1}{5}}\right)$. Otherwise $h(H) \geq \frac{m+1}{5} + 1$ and then by (55)

$$\begin{aligned} r(H) &= m - 3 - 3h(H) - b(H) \leq m - 3 - 3\left(\frac{m+1}{5} + 1\right) \\ &= \frac{2m-33}{5} \leq \frac{2m-23}{5} = r\left(N_{\frac{m+1}{5}}\right). \end{aligned}$$

■

Let TI be a vertex-degree-based topological index defined by the nonnegative real numbers $\{\varphi_{ij}\}$. By (2), (3), (4) and the well-known fact [13]

$$n = m - h + 1$$

we deduce from (7)

$$TI(H) = \varphi_{22}m + 3(\varphi_{33} - \varphi_{22})h + (2\varphi_{23} - \varphi_{22} - \varphi_{33})r + 3(\varphi_{22} - \varphi_{33}). \tag{56}$$

In particular, if $H, U \in \Gamma_m$ then

$$\begin{aligned} TI(H) - TI(U) = 3(\varphi_{33} - \varphi_{22})(h(H) - h(U)) \\ + (2\varphi_{23} - \varphi_{22} - \varphi_{33})(r(H) - r(U)). \end{aligned} \tag{57}$$

Define $q = 2\varphi_{23} - \varphi_{22} - \varphi_{33}$ and $s = \varphi_{33} - \varphi_{22}$.

Theorem 8.5. *[27] Let TI be a vertex-degree-based topological index defined by the nonnegative real numbers $\{\varphi_{22}, \varphi_{23}, \varphi_{33}\}$. Assume that $q \geq 0$ and $s \leq 0$ (resp. $q \leq 0$ and $s \geq 0$). Then the maximal (resp. minimal) TI-value over Γ_m is attained in:*

1. $M_{\frac{m}{5}}$ *if* $m \equiv 0\,(\textit{mod}\,5)$;

2. $L_{\frac{m-1}{5}}$ *if* $m \equiv 1\,(\textit{mod}\,5)$;

3. $R_{\frac{m+3}{5}}$ *if* $m \equiv 2\,(\textit{mod}\,5)$;

4. $Q_{\frac{m+2}{5}}$ *if* $m \equiv 3\,(\textit{mod}\,5)$;

5. $N_{\frac{m+1}{5}}$ *if* $m \equiv 4\,(\textit{mod}\,5)$.

Proof. Let $H \in \Gamma_m$. Note that by (53)

$$h(H) \geq \left\lceil \frac{1}{5}(m-1) \right\rceil = \begin{cases} h\left(M_{\frac{m}{5}}\right) & \text{if} \quad m \equiv 0\,(\text{mod}\,5) \\ h\left(L_{\frac{m-1}{5}}\right) & \text{if} \quad m \equiv 1\,(\text{mod}\,5) \\ h\left(R_{\frac{m+3}{5}}\right) & \text{if} \quad m \equiv 2\,(\text{mod}\,5) \\ h\left(Q_{\frac{m+2}{5}}\right) & \text{if} \quad m \equiv 3\,(\text{mod}\,5) \\ h\left(N_{\frac{m+1}{5}}\right) & \text{if} \quad m \equiv 4\,(\text{mod}\,5) \end{cases}$$

Hence by Theorem 8.4 the hexagonal systems $M_{\frac{m}{5}}, L_{\frac{m-1}{5}}, R_{\frac{m+3}{5}}, Q_{\frac{m+2}{5}}$ and $N_{\frac{m+1}{5}}$ have simultaneously maximal number of inlets and minimal number of hexagons over the set of hexagonal systems with m edges. Hence the result follows from (57) and the signs of q and s. ■

Example 8.6. *The following table contains the values of q and s for several well-known topological indices:*

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{2}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-.0168	-.0404	-.0333	-.0138	-3.390	0.040
s	5	-.1667	0	-.1667	-0.091	3.390	-0.040

(58)

Hence by Theorem 8.5, in the case of the second Zagreb index, geometric-arithmetic index and the augmented Zagreb index we can determine the minimal value of TI, and for the atom-bond-connectivity index we can determine the maximal value of TI.

Susbstituting (55) in (56) we obtain a new expression for TI

$$TI(H) = (2\varphi_{23} - \varphi_{33})\,m + 6(\varphi_{33} - \varphi_{23})\,h + (\varphi_{22} - 2\varphi_{23} + \varphi_{33})\,b + 6(\varphi_{22} - \varphi_{23})$$

and so for every $H, U \in \Gamma_m$

$$TI(H) - TI(U) = u\,(h(H) - h(U)) - q\,(b(H) - b(U)) \tag{59}$$

where $u = 6(\varphi_{33} - \varphi_{23})$ and q as before. We will now use this expression to find extremal values of TI over the set of hexagonal systems with m edges. Recall that a hexagonal system H with m edges satisfies (53)

$$h(H) \leq m - \left\lceil \frac{1}{3}\left(2m - 2 + \sqrt{4m+1}\right) \right\rceil .$$

Theorem 8.7. *[27]Let h such that the spiral S_h is convex and $m = 3h + \left\lceil \sqrt{12h-3} \right\rceil$. Then*

1. *If $u \geq 0$ and $q \geq 0$ then S_h has the maximal TI-value over Γ_m;*

2. *If $u \leq 0$ and $q \leq 0$ then S_h has the minimal TI-value over Γ_m.*

Proof. Since $n_i(S_h) = 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil$ then

$$m(S_h) = 5h + 1 - \left(2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil\right) = 3h + \left\lceil \sqrt{12h-3} \right\rceil = m$$

and so S_h has m edges. Also we know by hypothesis that $b(S_h) = 0$. On the other hand, $m = 3h + \left\lceil \sqrt{12h-3} \right\rceil$ implies $h = m - \left\lceil \frac{1}{3}\left(2m - 2 + \sqrt{4m+1}\right) \right\rceil$. Hence by (59) and (53) it follows that for any hexagonal system $H \in \Gamma_m$

$$\begin{aligned} TI(H) - TI(S_h) &= u(h(H) - h) - qb(H) \\ & \begin{cases} \leq 0 & \text{if } u \geq 0 \text{ and } q \geq 0 \\ \geq 0 & \text{if } u \leq 0 \text{ and } q \leq 0 \end{cases}. \end{aligned}$$

■

Remark 8.8. *Note that in general the spiral hexagonal system S_h satisfies*

$$b(S_h) = 0 \qquad or \qquad b(S_h) = 1.$$

In Section 5 there is a precise description of the (infinite) values of h for which S_h is convex. For instance, if $h = 3k^2 - 3k + 1$ for any positive integer k then S_h is convex. So the hypothesis of Theorem 8.7 holds for a large number of values of h.

Example 8.9. *The following table contains the values of q and u for several well-known topological indices:*

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{2}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$	$\sqrt{\frac{i+j-2}{ij}}$
q	-1	-.0168	-.0404	-.0333	-.0138	-3.390	0.040
u	18	-.449	0.121	-0.4	-0.233	20. 344	-0.242

(60)

It follows from Theorem 8.7 that the Randić index, the harmonic index and the sum-connectivity index have minimal TI values in the spiral S_h.

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On Degree–Based Indices of Dendrimers

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Abstract

The Narumi-Katayama index of a graph G, denoted by $NK(G)$, is equal to the product of degrees of vertices of G. In this chapter, we report our recent results on computing an important degree-based topological index, which is called Narumi-Katayama index, for dendrimers. Also, we gather some of our results about the Narumi-Katayama index of some graph compositions which using them, the Narumi-Katayama index of many chemical graphs can be computed. Next, we demonstrate some applications to chemically relevant graphs and show how the Narumi-Katayama index can be used as a measure of graph irregularity.

Contents

1. Introduction

Several hundreds of topological invariants of molecular graphs have been defined and employed in the QSAR/QSPR research during the last couple of decades [13]. One of the simplest, defined as the product of degrees of all vertices, was introduced by Narumi and Katayama in 1984 and named, accordingly, the "simple topological index" [12]. In the subsequent papers the more informative name "Narumi–Katayama index" was introduced and became established, so we use it in the present chapter. In the beginning, the index attracted only a moderate attention [4,6], but recently a number of papers appeared studying its various mathematical properties (such as the extremal graphs and values [5]) and its values over special classes of graphs [14]. Further, it also spawned various generalizations such as the degree product polynomial considered recently by Klein and Rosenfeld [10, 11]. This chapter aims to further contribute to the better understanding of the Narumi-Katayama index by investigating its behavior under several binary operations on graphs. The results in this chapter are mainly taken from [7,8]. We start by defining the terms.

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds [15]. For a given graph G we denote its vertex set by $V(G)$ and its edge set by $E(G)$. The number of vertices is denoted by n. If we consider several graphs, $G_1, \ldots, G_k$, the quantities pertaining to a given graph are denoted by the corresponding subscript. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of neighbors of v in G. When the graph G is clear from the context, we omit the subscript.

The **Narumi–Katayama index** of a graph G is defined as the product of degrees of all its vertices,

$$NK(G) = \prod_{i=1}^{n} d_G(v_i).$$

It is clear from the definition that we can restrict our attention to connected graphs, since for a graph with several connected components its Narumi–Katayama index is equal to the product of the indices of components. (This restriction also takes care of graphs with isolated vertices, among which the index cannot discriminate.)

Let $U = \{u_1, u_2, \ldots, u_k\}$ be a subset of $V(G)$. We define the **truncated Narumi–Katayama index** (with respect to U) as

$$NK^{(U)}(G) = \prod_{v \in V(G)-U} d_G(v).$$

In the case when U is the empty set, we obtain $NK^{(\emptyset)}(G) = NK(G)$. Note that here the vertices of U are not deleted from $V(G)$, and the degrees of vertices not in U are not affected. The truncated Narumi–Katayama index will enable us to express some of our results in a more compact form.

2. Composite graphs

Many interesting classes of graphs arise from simpler graphs *via* binary operations sometimes known as graph products. (We refer the reader to a monograph by Imrich and Klavžar [9] for a comprehensive introduction.) Our aim here is to study how the Narumi–Katayama indices of such graphs can be expressed in terms of Narumi–Katayama indices of operands and some auxiliary invariants. We start by three simple operations on the union of two graphs.

2.1 Splice, link and gate

Let G_1 and G_2 are two graphs with disjoint vertex sets. For given vertices $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$ the **splice** of G_1 and G_2 by vertices v_1 and v_2, $(G_1 \cdot G_2)(v_1, v)$, is defined by identifying the vertices v_1 and v_2 in the union of G_1 and G_2. Similarly, the **link** of G_1 and G_2 by vertices v_1 and v_2 is defined as the graph $(G_1 \sim G_2)(v_1, v_2)$ obtained by joining v_1 and v_2 by an edge in the union of these graphs. We shorten the notation to $G_1 \cdot G_2$ and $G_1 \sim G_2$ when the vertices v_1, v_2 are clear from the context. (These two operations also appear in the literature under different names; we follow here the terminology introduced in [2].)

The **gate** $(G_1||G_2)(u_1, v_1; u_2, v_2)$ is obtained from G_1 and G_2 by identifying the edges u_1v_1 of G_1 and u_2v_2 of G_2 so that u_1 is identified with u_2 and v_1 with v_2. We denote the end-vertices of the identified edge in $G_1||G_2$ by u_{12} and v_{12}.

Obviously, the only vertices whose degrees are affected by the above operations are u_i and v_i, for $i = 1, 2$. If we denote by v_{12} the vertex of $G_1 \cdot G_2$ obtained by identifying v_1 and v_2, we have the following expressions.

$$d_{G_1 \cdot G_2}(v_{12}) = d_{G_1}(v_1) + d_{G_2}(v_2);$$

$$d_{G_1 \sim G_2}(v_1) = d_{G_1}(v_1) + 1;$$

$$d_{G_1 \sim G_2}(v_2) = d_{G_2}(v_2) + 1;$$

$$d_{G_1||G_2}(u_{12}) = d_{G_1}(u_1) + d_{G_2}(u_2) - 1;$$

$$d_{G_1||G_2}(v_{12}) = d_{G_1}(v_1) + d_{G_2}(v_2) - 1.$$

The following results are direct consequences of the above observations.

Proposition 1

$$NK(G_1 \cdot G_2) = NK(G_1)NK(G_2)\frac{d_{G_1}(v_1) + d_{G_2}(v_2)}{d_{G_1}(v_1)d_{G_2}(v_2)};$$

$$NK(G_1 \sim G_2) = NK(G_1)NK(G_2)\frac{(d_{G_1}(v_1) + 1)(d_{G_2}(v_2) + 1)}{d_{G_1}(v_1)d_{G_2}(v_2)};$$

$$NK(G_1||G_2) = NK(G_1)NK(G_2)\frac{(d_{G_1}(u_1) + d_{G_2}(u_2) - 1)(d_{G_1}(v_1) + d_{G_2}(v_2) - 1)}{d_{G_1}(u_1)d_{G_2}(u_2)d_{G_1}(v_1)d_{G_2}(v_2)}.$$

■

An alternative way of writing the second result is

$$NK(G_1 \sim G_2) = NK(G_1)NK(G_2) + NK(G_1 \cdot G_2) + NK^{(V(G_1)-v_1)}(G_1)NK^{(V(G_2)-v_2)}(G_2).$$

The results for splice can be in a straightforward way generalized to more than two operands. If we have graphs $G_1, \ldots, G_k$ and $v_i \in V(G_i)$ for each $i = 1, \ldots, k$, then their splice in vertices v_i is obtained by identifying all k vertices v_i.

Corollary 2

$$NK(G_1 \cdot G_2 \cdot \ldots \cdot G_k) = \frac{\sum_{i=1}^{k} d_{G_i}(v_i)}{\prod_{i=1}^{k} d_{G_i}(v_i)} \prod_{i=1}^{k} NK(G_i).$$

■

If we have k copies of the same graph G and splice them at the same vertex v, we obtain $G^{\cdot k}$, the k-th **splice-power** of G. The above result then simplifies to

$$NK(G^{\cdot k}) = \frac{k\,[NK(G)]^k}{d_G(v)^{k-1}}.$$

By considering links of more than two graphs we arrive at the next class of composite graphs considered here, the chain (or bridge) graphs.

2.2 Chains and necklaces

Let G_i, $1 \le i \le k$, be some graphs and $v_i \in V(G_i)$. A **chain graph** denoted by $G = G(G_1, \ldots, G_k, v_1, \ldots, v_k)$ is obtained from the union of the graphs G_i, $i = 1, \ldots, k$, by adding the edges $v_i v_{i+1}$ $1 \le i \le k-1$, see Fig. 1. Then $|V(G)| = \sum_{i=1}^{k} |V(G_i)|$ and $|E(G)| = (k-1) + \sum_{i=1}^{k} |E(G_i)|$. By adding the edge $v_k v_1$ to a chain graph we obtain the corresponding **necklace** $G_0 = G_0(G_1, \ldots, G_k, v_1, \ldots, v_k)$.

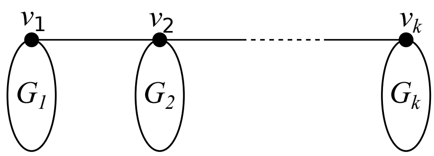

Figure 1. The chain graph $G = G(G_1, \ldots, G_k, v_1, \ldots, v_k)$.

One can see that $G(G_1, G_2, v_1, v_2) \cong (G_1 \sim G_2)(v_1, v_2)$.

It is worth noting that the above specified classes of chain graphs and necklaces embrace, as special cases, all trees (among which are the molecular graphs of alkanes) and all unicyclic graphs (among which are the molecular graphs of monocycloalkanes). Also the molecular graphs of many polymers and dendrimers are chain graphs. Further, when all G_i are equal to G and all v_i are equal, we have the rooted products of P_k and G and of C_k and G.

It is clear that the root vertices are the only ones whose degrees are affected by the chain and necklace construction. Hence,

$$d_G(u) = \begin{cases} d_{G_i}(u) & \text{if } u \in V(G_i) \text{ and } u \neq v_i \\ d_{G_i}(v_i) + 1 & \text{if } u = v_i,\ i = 1, k \\ d_{G_i}(v_i) + 2 & \text{if } u = v_i,\ 2 \le i \le k-1 \end{cases}.$$

$$d_{G_0}(u) = \begin{cases} d_{G_i}(u) & \text{if } u \in V(G_i) \text{ and } u \neq v_i \\ d_{G_i}(v_i) + 2 & \text{if } u = v_i,\ 1 \le i \le k \end{cases}.$$

Theorem 3

$$\begin{aligned} NK(G(G_1,\ldots,G_k,v_1,\ldots,v_k)) &= (d_{G_1}(v_1)+1)(d_{G_k}(v_k)+1)\prod_{i=2}^{k-1}(d_{G_1}(v_i)+2) \\ &\times \prod_{i=1}^{n} NK^{(V(G_i)-v_i)}(G_i). \end{aligned}$$

■

Theorem 4

$$NK(G_0(G_1,\ldots,G_k,v_1,\ldots,v_k)) = \prod_{i=1}^{k}(d_{G_1}(v_i)+2)\prod_{i=1}^{n} NK^{(V(G_i)-v_i)}(G_i).$$

■

In both cases the proof follows immediately by using the definition of the truncated NK index, and we omit the details.

2.3 Join

The **join** (sometimes also called the **sum**) of two graphs G_1 and G_2 is obtained by taking their union and adding all possible edges between $V(G_1)$ and $V(G_2)$. We denote it by $G_1 \nabla G_2$. When one of the graphs is K_1, the join of K_1 and G is called the **suspension** of G. The degree of a vertex of G in its suspension increases by one, while the degree of the vertex of K_1 is equal to $|V(G)| = n$. Hence the Narumi–Katayama index of $K_1 \nabla G$ is given by

$$NK(K_1\nabla G) = n\prod_{i=1}^{n}(d_G(v_i)+1).$$

The product on the right-hand side of the above formula can be expressed in terms of truncated Narumi–Katayama indices with respects to all subsets of $V(G)$. The result follows by expanding the product into a sum of 2^n terms and noting that the products of degrees of each of 2^n subsets of $V(G)$ appear exactly once in the sum.

Proposition 5

$$NK(K_1\nabla G) = n\sum_{U\subseteq V(G)} NK^{(U)}(G).$$

■

The above result can be straightforwardly generalized to the case when one of the components of a join is the set of m independent vertices, i.e., the complement $\overline{K}_m$ of the complete graph K_m.

Proposition 6

$$NK(\overline{K}_m\nabla G) = n^m\left(\sum_{U\subseteq V(G)} NK^{(U)}(G)m^{n-|U|}\right).$$

■

A closer look on the above formula should reveal that all effects of the independence of vertices of $\overline{K}_m$ are concentrated in the n^m term. Hence, the contribution of vertices of one component in a join of two graphs depends only on the number of vertices in the other component, and not on its internal structure. From this observation we can deduce the formula for the general case.

Proposition 7 Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, respectively. Then

$$NK(G_1 \nabla G_2) = \left(\sum_{U_1 \subseteq V(G_1)} NK^{(U_1)}(G_1) n_2^{n_1 - |U_1|} \right) \left(\sum_{U_2 \subseteq V(G_2)} NK^{(U_2)}(G_2) n_1^{n_2 - |U_2|} \right).$$

■

The results of this subsection could be further generalized to joins of more than two graphs, but we leave that to the interested reader. Instead, we use them to derive formulas for the Narumi–Katayama index of a corona of two graphs.

2.4 Corona

The **corona** of two graphs G and H is the graph obtained by taking $|V(G)|$ copies of H and connecting each vertex in the i-th copy of H to the vertex v_i of G. It is usually denoted by $G \circ H$. (We have used G and H instead of G_1 and G_2 in order to stress the fact that the components enter their corona in an asymmetric way.) Hence, a corona is a collection of n suspensions of H on a scaffold provided by G. This is reflected in the formula for its Narumi–Katayama index.

Proposition 8 Let G and H be two graphs with n and m vertices, respectively. Then

$$NK(G \circ H) = \left(\sum_{U \subseteq V(G)} NK^{(U)}(G) m^{n - |U|} \right) \left(\sum_{W \subseteq V(H)} NK^{(W)}(H) \right)^n .$$

■

2.5 Composition

The **composition** of two graphs G and H is the graph with vertex set $V(G) \times V(H)$, and the vertex $u = (u_1, v_1)$ is adjacent to the vertex $v = (u_2, v_2)$ whenever either $u_1u_2 \in E(G)$ or $u_1 = u_2$ and $v_1v_2 \in E(H)$. This graph operation is denoted by $G[H]$. So the degree of the vertex (u, v) in $G[H]$ is $d_{G[H]}(u, v) = d_H(v) + nd_G(u)$, where n is the number of vertices of G. The composition of two graphs is also known as **graph substitution**, a name that bears witness to the fact that $G[H]$ can be obtained from G by substituting a copy of H, labeled H_w, for every vertex w in $V(G)$ and then joining all vertices of H_w with all vertices of $H_{w'}$ if and only if $ww' \in E(G)$, and there are no edges between vertices in H_u and $H_{u'}$ otherwise. Now by the above approach, one can see the Narumi-Katayama index of the composition of two graphs as follows:

Proposition 9 Let G and H be two graphs with n and m vertices, respectively. Then

$$NK(G[H]) = \prod_{u \in V(G)} \sum_{U \subseteq V(H)} NK^{(U)}(H) \, (nd_G(u))^{m - |U|}.$$

■

2.6 Cartesian product

The **Cartesian product** $G_1 \Box G_2$ of graphs G_1 and G_2 is a graph such that $V(G_1 \Box G_2) = V(G_1) \times V(G_2)$, and any two vertices (u_1, v_1) and (u_2, v_2) are adjacent in $G_1 \Box G_2$ if and only if either ($u_1 = u_2$ and v_1 is adjacent with v_2), or ($v_1 = v_2$ and u_1 is adjacent with u_2). It is easy to see that $d_{G_1 \Box G_2}(u, v) = d_{G_1}(u) + d_{G_2}(v)$. According to the previous subsections, we can write the Narumi-Katayama index of the Cartesian product of two graphs G_1 and G_2 with n and m vertices, respectively, by

$$\prod_{u \in V(G_1)} \sum_{U \subseteq V(G_2)} NK^{(U)}(G_2) \left(d_{G_1}(u)\right)^{m-|U|}$$

or

$$\prod_{v \in V(G_2)} \sum_{W \subseteq V(G_1)} NK^{(W)}(G_1) \left(d_{G_2}(v)\right)^{n-|W|}.$$

So to preserve the symmetric of the formula for the Narumi-Katayama index of Cartesian product of two graphs, we have the next proposition.

Proposition 10 Let G_1 and G_2 be two graphs with n and m vertices, respectively. Then

$$\begin{aligned} NK(G_1 \Box G_2) &= \frac{1}{2} \prod_{u \in V(G_1)} \sum_{U \subseteq V(G_2)} NK^{(U)}(G_2) \left(d_{G_1}(u)\right)^{m-|U|} \\ &+ \frac{1}{2} \prod_{v \in V(G_2)} \sum_{W \subseteq V(G_1)} NK^{(W)}(G_1) \left(d_{G_2}(v)\right)^{n-|W|}. \end{aligned}$$

■

3. Applications and concluding remarks

3.1 Spiro and polyphenyl hexagonal chains

A **(poly)spiro compound** is a polycyclic organic compound whose rings are connected by one atom. The rings may be of various lengths. The connecting atom, most often a carbon, is also called the **spiroatom**. Their graphs appear in the mathematical literature as **cactus graphs**; if a polyspiro compound is unbranched, the corresponding graph is also known as cactus chain [3]. If all cycles (rings) are of the same length, we say that the chain is uniform. An example of a uniform (hexagonal) spiro chain of length 6 is shown in Fig. 2.

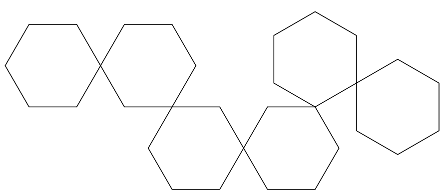

Figure 2. A hexagonal spiro chain of length 6.

Let a hexagonal chain of length h be denoted by H_h. From the first claim of Proposition 1 we obtain the recurrence for $NK(H_h)$,

$$NK(H_{h+1}) = NK(H_h)NK(H_1).$$

This, together with the obvious initial condition $NK(H_1) = 2^6 = 64$, yields the following result.

Corollary 11

$$NK(H_h) = 64^h.$$

■

The same reasoning remains valid also when the cycles are not all of the same length. In general, if G_h is a cactus graph with h blocks in which every cut-vertex is shared by exactly two cycles, then

$$NK(G_h) = 2^{|V(G_h)|},$$

regardless of the structure of G_h.

A class of polycyclic compounds in which two or more benzene rings are connected by a cut edge is known as polyphenyl compounds. Their graphs are called polyphenyl hexagonal chains. An example is shown in Fig. 3. We denote such a chain with h hexagons by PP_h.

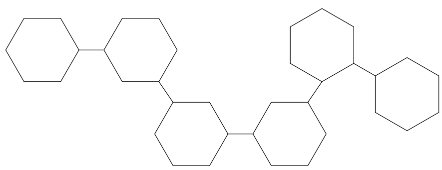

Figure 3. A polyphenyl hexagonal chain of length 6.

By using the second claim of Proposition 1 we immediately obtain

$$NK(PP_h) = \left(\frac{9}{4}\right)^{h-1} NK(H_h),$$

leading to the explicit expression $NK(PP_h) = \frac{4}{9}144^h$.

3.2 Catacondensed benzenoids

It is clear that the graph of any catacondensed benzenoid can be constructed by starting from a single hexagon and adding one hexagon at a time by the gate operation. If we denote a catacondensed benzenoid with h hexagons by B_h, we obtain a recurrence for $NK(B_h)$ in the form

$$NK(B_{h+1}) = \left(\frac{9}{16}\right) NK(B_h)NK(B_1),$$

resulting in the explicit formula $NK(B_h) = \left(\frac{9}{16}\right)^{h-1} NK(B_1)^h = \frac{16}{9}36^h$. (See also [14].)

3.3 Phenylenes and their hexagonal squeezes

The last class of object we consider here are phenylenes and their hexagonal squeezes as defined in [14]. It is obvious that any phenylene can be constructed starting from a single hexagon and adding one hexagon at a time by iterating the two-step construction shown in Fig. 4. Hence, we first

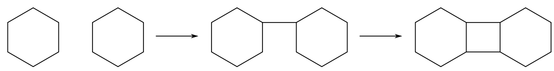

Figure 4. Two-step construction of a phenylene.

link a hexagon to the already constructed graph, and then add an edge. We will need the following lemma that describes the effect of adding an edge to G.

Lemma 12 Let G be a connected graph and $u, v \in V(G)$ two non-adjacent vertices of G. Then

$$NK(G+uv) = NK(G)\frac{(d(u)+1)(d(v)+1)}{d(u)d(v)}.$$

■

By combining Lemma 12 with the second claim of Proposition 1 we obtain a recurrence for the Narumi-Katayama indices of phenylenes and their hexagonal squeezes. It leads to explicit formulas that confirm the relationships between them established in reference [14].

3.4 Dendrimers

The goal of this section is computing the truncated NK index of an infinite class of dendrimers. To do this, we use from Theorem 2. The truncated NK index for other classes of dendrimers, can be computed similarly.

Consider the graph G_1 shown in Fig. 5.

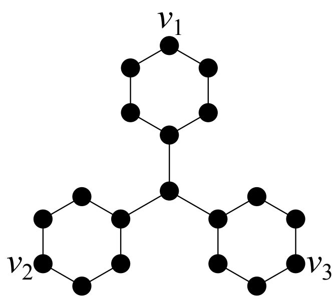

Figure 5. The graph of dendrimer G_n for $n = 1$.

It is easy to see that

$$NK(G_1) = 2^{15}3^4,$$

$$NK^{(v_1)}(G_1) = NK^{(v_2)}(G_1) = NK^{(v_3)}(G_1) = NK^{(v)}(G_1) = 2^{14}3^4,$$

and so, for $1 \leq i, j \leq 3$, $i \neq j$,

$$NK^{(v,v)}(G_1) = NK^{(v_i,v_j)}(G_1) = 2^{13}3^4.$$

Now consider the graph $G_n = (G_{n-1} \sim H_1)(v_1, u_1)$, shown in Fig. 2 (for $n = 1$) and Fig. 3, respectively. It is easy to see that $H_i \cong G_1$, $(1 \leq i \leq n-1)$ and

$$\begin{aligned}
G_n &= (G_{n-1} \sim H_1)(v_1, u_1)\\
G_{n-1} &= (G_{n-2} \sim H_2)(v_2, u_2)\\
&\vdots\\
G_{n-i} &= (G_{n-i-1} \sim H_{i+1})(v_{i+1}, u_{i+1})\\
&\vdots\\
G_2 &= (G_1 \sim H_{n-1})(v_{n-1}, u_{n-1})
\end{aligned}$$

Then by using Theorem 3, we have the following relations:

$$\begin{aligned}
NK(G_n) &= NK^{(v_1)}(G_{n-1})\ NK^{(u_1)}(H_1) \times 3^2\\
NK^{(v_1)}(G_{n-1}) &= NK^{(v_2)}(G_{n-2})\ NK^{(v_1,u_2)}(H_2) \times 3^2\\
&\vdots\\
NK^{(v_i)}(G_{n-i}) &= NK^{(v_{i+1})}(G_{n-i-1})\ NK^{(v_i,u_{i+1})}(H_{i+1}) \times 3^2\\
&\vdots\\
NK^{(v_{n-2})}(G_2) &= NK^{(v_{n-1})}(G_1)\ NK^{(v_{n-2},u_{n-1})}(H_{n-1}) \times 3^2
\end{aligned}$$

Production of two sides of these relations yields

$$NK(G_n) = NK^{(v_{n-1})}(G_1)\ NK^{(u_1)}(H_1) \prod_{i=2}^{n-1} NK^{(v_{i-1},u_i)}(H_i) \times 3^{2(n-1)}$$

and it is easy to obtain

$$\begin{aligned}
NK(G_n) &= (NK^{(v_1)}(G_1)\,)^2\ \ (NK^{(v_1,v_2)}(G_1)\,)^{n-2} \times 3^{2(n-1)}\\
&= 2^{13n+2}3^{6n-2}.
\end{aligned}$$

In other words we arrived at the following:

Theorem 13 Consider the graph $G_n = (G_{n-1} \sim H_1)(v_1, u_1)$, $(2 \leq n)$, shown in Fig. 6. Then,

$$NK(G_n) = 2^{13n+2}3^{6n-2}.$$

Corollary 14 Consider the dendrimer D, shown in Fig. 7. Then,

$$NK(D) = 2^{13n+2}3^{6n-2},$$

where n is the number of repetition of the fragment G_1.

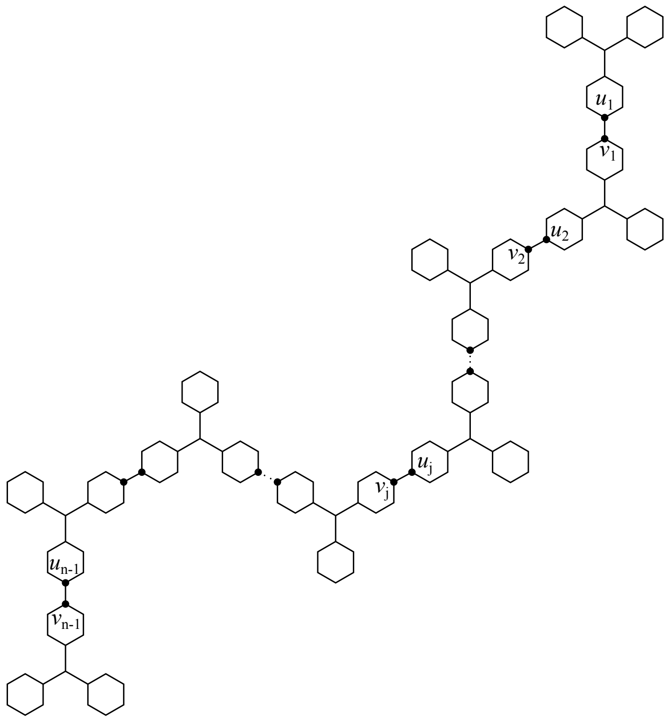

Figure 6. The graph G_n and the labeling of its vertices.

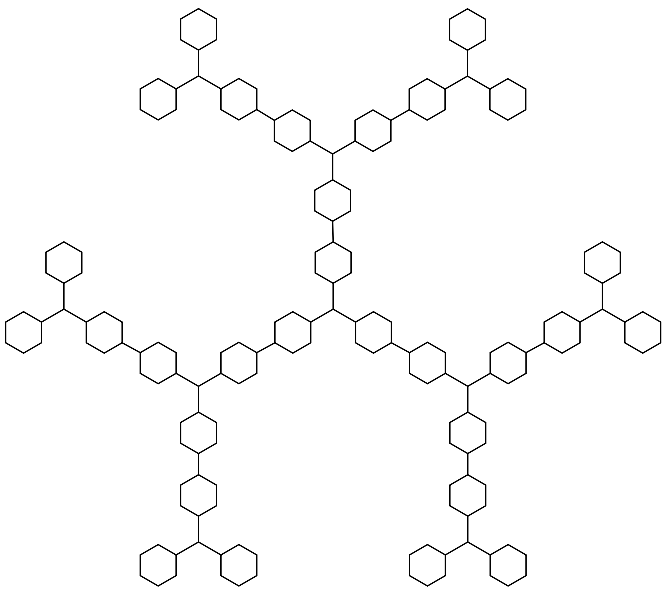

Figure 7. The graph of the dendrimer D.

3.5 Graph irregularity

Regularity of a graph is a binary property - a graph is either regular or not. However, while all regular graphs (of a given order and size) are equally regular, the non-regular graphs of the same order and size are not all equally far from being regular. There are several proposed measures of non-regularity of a graph. Most of them are based on measuring local discrepancies, i.e., quotients or differences of degrees of adjacent vertices. An example is the invariant, first introduced and studied by Albertson [1] and called irregularity. The **irregularity** of a graph G is defined as

$$irr(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)| \, .$$

(The same quantity is sometimes called also the **third Zagreb index**.) Further examples are the arithmetic-geometric index and other indices based on combinations of various means of degrees of adjacent vertices.

Let G be a graph on n vertices and m edges. It is clear from the Arithmetic–Geometric Mean inequality that the Narumi-Katayama index of a graph cannot exceed the n-th power of the average degree of the graph $\left(\frac{2m}{n}\right)^n$. Furthermore, the bound is attained if and only if G is regular. Hence, it is to be expected that a greater variability of degrees of vertices of G will be reflected in a smaller value of its Narumi-Katayama index. This indeed seems to be the case. In Fig. 8 we show the scatter-plot of $irr(G)$ *vs.* $NK(G)$ for all trees (left) and all unicyclic graphs (right) on 8 vertices.

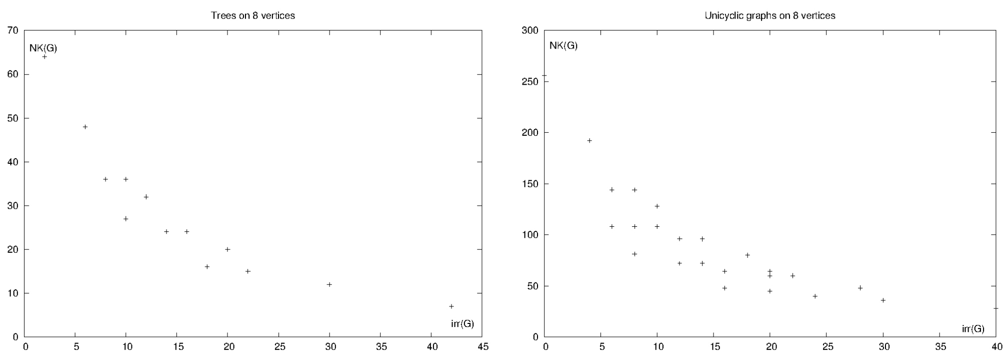

Figure 8. The Narumi-Katayama index vs. irregularity for trees (left) and unicyclic graphs (right) on 8 vertices.

Although the exact nature of the relationship remains unexplored and the trend becomes less pronounced for denser graphs, it is clear that the Narumi-Katayama index can serve as a useful global measure of the graph irregularity.

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