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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. 19, completed in January 2017.

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New Trends in Majorization Techniques for Bounding Topological Indices

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1. Introduction

The appeal of the research on molecular descriptors in Mathematical Chemistry stems, in no small measure, from the wide variety of approaches to the subject and their fruitful interactions. In the paragraphs that follow we will focus on one of those viewpoints, the majorization technique, with some support from the theory of electric networks.

Majorization allows to find upper and lower bounds for many descriptors through the identification of maximal and minimal tuples in some subsets of the n-dimensional real space, endowed with a partial order, and the monotonicity of the descriptors when thought of as Schur-convex functions defined on those suitable subspaces.

On the other hand, the theory of electric networks provides a number of sum rules for the effective resistances, such as Foster's theorems, and also a monotonicity notion, Rayleigh's monotonicity principle. These electric ideas are applicable not only to the resistive descriptors, such as the Kirchhoff index and its relatives, but also to other descriptors defined in terms only of the degrees of the vertices, such as the ABC and AZI indices. In these cases, the majorization is performed on the effective resistances, not on the degrees of the vertices or on the eigenvalues of the graph.

In general, proofs are omitted for the sake of brevity, although these can be found in the references provided. A final section on numerical results compares in some specific instances our results obtained with majorization and those found in the literature.

2. Notations and preliminaries

In this Section we present the notations and some basic facts used in the sequel. For the sake of clarity, we have split the section in three subsections addressing the main topics of majorization, graphs and effective resistance in electric networks.

2.1 Majorization order and Schur convex functions

This section concerns some reminds about the notions of majorization and its extension known as p-majorization. The main references are the classical book [104], the technical report [26] and the recent paper [13].

Let $\mathcal{D} = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq ... \geq x_n\}$ and denote by $[x_1^{\alpha_1}, x_2^{\alpha_1}, \cdots, x_p^{\alpha_p}]$ a vector in $\mathbb{R}^n$ with α_i components equal to x_i, where $\sum_{i=1}^{p} \alpha_i = n$. If $\alpha_i = 1$ we use x_i instead of $x_i^{\alpha_i}$ for convenience, while x_i^0 means that the component x_i is not present.

Let $\mathbf{e}^{\mathbf{j}}$, $j = 1, ...n$, be the fundamental vectors of $\mathbb{R}^n$, $\mathbf{s}^{\mathbf{j}} = [1^j, 0^{n-j}]$, with $j = 1, 2, \cdots, n$ and $\mathbf{v}^{\mathbf{j}} = [0^j, 1^{n-j}]$, with $j = 0, \cdots, n$

The Hadamard product of two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ is defined as follows:

$$\mathbf{x} \circ \mathbf{y} = [x_1 y_1, x_2 y_2, ..., x_n y_n]^T ,$$

Denoting by $\langle \cdot, \cdot \rangle$ the inner product in $\mathbb{R}^n$, the following properties hold:

i) $\langle \mathbf{x} \circ \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{y} \circ \mathbf{z} \rangle$

ii) $\langle \mathbf{s}^{\mathbf{h}}, \mathbf{v}^{\mathbf{k}} \rangle = h - \min\{h, k\}$

iii) $\mathbf{s}^{\mathbf{k}} \circ \mathbf{s}^{\mathbf{j}} = \mathbf{s}^{\mathbf{h}}$, $h = \min\{k, j\}$

iv) $\mathbf{v}^{\mathbf{k}} \circ \mathbf{s}^{\mathbf{j}} = \mathbf{s}^{\mathbf{j}} - \mathbf{s}^{\mathbf{h}} = \mathbf{v}^{\mathbf{h}} - \mathbf{v}^{\mathbf{j}}$, $h = \min\{k, j\}$

Definition 1. *Fix* $\mathbf{p} > \mathbf{0}$. *Given two vectors* $\mathbf{y}$, $\mathbf{z} \in \mathcal{D}$, *the* p*-majorization order* $\mathbf{y} \trianglelefteq_p \mathbf{z}$ *means:*

$$\left\langle \mathbf{p} \circ \mathbf{y}, \mathbf{s}^{\mathbf{k}} \right\rangle \leq \left\langle \mathbf{p} \circ \mathbf{z}, \mathbf{s}^{\mathbf{k}} \right\rangle, \; k = 1, ..., (n-1)$$

and

$$\langle \mathbf{p} \circ \mathbf{y}, \mathbf{s}^{\mathbf{n}} \rangle = \langle \mathbf{p} \circ \mathbf{z}, \mathbf{s}^{\mathbf{n}} \rangle .$$

For $\mathbf{p} = \mathbf{s}^{\mathbf{n}}$, p-majorization reduces to the usual majorization. Thus in the sequel all our results entail as particular cases the results known for classical majorization. In this case we will use the notation $\mathbf{y} \trianglelefteq \mathbf{z}$.

The class of functions which preserve the p-majorization order are known as p-Schur-convex functions (see [26]). Let ρ be a permutation of $\{1, \cdots n\}$ and $\mathbf{x}^\rho$ be the vector obtained exchanging the components of $\mathbf{x}$ according to ρ.

Definition 2. *Given a fixed vector of positive components* $\mathbf{p}$, *a function* $\phi(\cdot, \mathbf{p}) : \mathbb{R}^n \longrightarrow \mathbb{R}$, *is said to be* p*-Schur-convex if*

$$\phi(\mathbf{x}, \mathbf{p}) = \phi(\mathbf{x}^\rho, \mathbf{p}^\rho) \textit{ for all } \rho \tag{1}$$

$$\phi(\mathbf{x}, \mathbf{p}) \leq \phi(\mathbf{y}, \mathbf{p}) \textit{ whenever } \mathbf{x}, \mathbf{y} \in D \textit{ and } \mathbf{x} \trianglelefteq_p \mathbf{y}. \tag{2}$$

If in addition, $\phi(\mathbf{x}) < \phi(\mathbf{y})$ *for* $\mathbf{x} \trianglelefteq_p \mathbf{y}$ *but* $\mathbf{x}$ *is not a permutation of* $\mathbf{y}$, ϕ *is said to be* p*-strictly Schur-convex. A function* ϕ *is (strictly)* p*-Schur-concave if* $-\phi$ *is (strictly)* p*- Schur-convex.*

Note that for $\mathbf{p} = \mathbf{s^n}$, we recover the classical notion of Schur-convex and strictly Schur-convex functions.

Next result gives an important characterization of differentiable p-Schur-convex functions.

Theorem 3. *(see [26]) Let $\mathbf{p} > \mathbf{0}$ be fixed and $\phi : \mathbb{R}^n \longrightarrow \mathbb{R}$ be a differentiable function satisfying (1). Then the function ϕ is p-Schur-convex if and only if for all $\mathbf{x}$,*

$$(x_i - x_j)\left(\frac{1}{p_i}\frac{\partial \phi(\mathbf{x};\mathbf{p})}{\partial x_i} - \frac{1}{p_j}\frac{\partial \phi(\mathbf{x};\mathbf{p})}{\partial x_j}\right) \geq 0 \qquad \textit{for all i,j=1,...,n.} \tag{3}$$

Another useful criterion to prove the p-Schur-convexity is given by the following proposition.

Proposition 4. *Let $I \subset \mathbb{R}$ be an interval and let $\phi(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^n p_i g(x_i)$, where $g : I \to \mathbb{R}$. If g is (strictly) convex on I , then ϕ is (strictly) p-Schur-convex on $I^n = \underbrace{I \times \cdots \times I}_{n-times}$.*

The above results can be restated, letting $\mathbf{p} = \mathbf{s^n}$, to prove the Schur-convexity of a function.

2.2 Graph theory

Let us now recall some basic concepts from graph theory (for more details we refer the reader to [16] and [137]).

Let $G = (V, E)$ be a simple, connected and undirected graph, where $V = \{v_1, ..., v_n\}$ is the set of vertices and $E \subseteq V \times V$ the set of edges. We consider graphs with fixed order $|V| = n$ and fixed size $|E| = m$, the cardinality of the sets V and E respectively. An undirected graph is a graph in which $(v_i, v_j) \in E$ whenever $(v_j, v_i) \in E$.When two vertices share a link, they are called adjacent. The degree d_i of a vertex v_i $(i = 1, ..., n)$ is the number of edges incident with it. A walk is a sequence of adjacent vertices $v_1, v_2, ..., v_l$. A $v_i - v_j$ path is a walk connecting v_i and v_j in which all vertices are distinct. A shortest path joining vertices v_i and v_j is called a $v_i - v_j$ geodesic. The distance $dist\,(v_i, v_j)$ between two vertices v_i and v_j is the length of the $v_i - v_j$ geodesic. A graph is connected if for each pair of vertices v_i and v_j there is a path connecting v_i and v_j. A graph is bipartite if V can be divided into two separate sets V_1 and V_2 such that every node in V_1 and V_2 is not connected to each other. By simple graph we refer to an unweighted, undirected graph contatining no-self-loops or multiple edges. Moreover, a weight w_{ij} is possibly associated to each edge, in this case we will have a weighted (or valued) graph.

In the sequel we consider a particular class of graph, so-called c-cyclic graphs, where c is the cyclomatic number of the graph G and it is given by $c = |E| - n + 1$. It corresponds to the number of independent cycles in G (see [16]). In particular, graphs with cyclomatic number $c = 0$ are trees and graphs with cyclomatic number $c = 1$ are unicyclic graphs.

Let $\pi = (d_1, d_2, .., d_n)$ denote the degree sequence of G arranged in non increasing order $d_1 \geq d_2 \geq \cdots \geq d_n$, where d_i is the degree of the vertex v_i. We recall that the sequences of integers which are degree sequences of a simple graph were characterized by Erdős and Gallai ([50]). It is well known that $\sum_{i=1}^n d_i = 2m$. Also, if G is a tree, i.e. a connected graph without cycles, then $m = n - 1$.

If π is a fixed degree sequence and $\mathbf{x} \in \mathbb{R}^m$ the vector whose components are $d_i^\alpha + d_j^\alpha$, $\alpha \neq 0$, $(v_i, v_j) \in E$, extending the result proved in [99], it is possible to show that

$$\sum_{i=1}^{m} x_i = \sum_{(v_i,v_j)\in E} \left(d_i^\alpha + d_j^\alpha\right) = \sum_{i=1}^{n} d_i^{\alpha+1} \tag{4}$$

and thus $\sum_{i=1}^{m} x_i$ is a constant.

Associated with a graph there are certain types of matrices which have important properties related to their eigenvalues. Let $A(G)$ be the *adjacency matrix* of G , i.e. the non-negative $n-$square matrix representing the adjacency relationships between vertices of G: the off-diagonal elements a_{ij} of A are equal to 1 if vertices u and v are adjacent and 0 otherwise. Let $D(G)$ be the diagonal matrix of vertex degrees. The matrix $L(G) = D(G) - A(G)$ is called the *Laplacian matrix* of G, while $\mathcal{L}(G) = D(G)^{-1/2} L(G) D(G)^{-1/2}$ is known as the *normalized Laplacian*.

Let $\lambda_1(L) \geq \lambda_2(L) \geq ... \geq \lambda_n(L)$ be the set of (real) eigenvalues of $L(G)$ and $\lambda_1(\mathcal{L}) \geq \lambda_2(\mathcal{L}) \geq ... \geq \lambda_n(\mathcal{L})$ be the (real) eigenvalues of $\mathcal{L}(G)$. Given a connected graph G of order $n \geq 2$,the following properties of the spectra of $L(G)$ and $\mathcal{L}(G)$ hold:

$$\sum_{i=1}^{n} \lambda_i(L) = \mathrm{tr}(L(G)) = 2m; \;\; \lambda_1(L) \geq 1 + d_1 \geq \frac{2m}{n}; \;\; \lambda_n(L) = 0, \; \lambda_{n-1}(L) > 0;$$

$$\sum_{i=1}^{n} \lambda_i(\mathcal{L}) = \mathrm{tr}(\mathcal{L}(G)) = n; \;\; \sum_{i=1}^{n} \lambda_i^2(\mathcal{L}) = \mathrm{tr}(\mathcal{L}^2(G)) = n + 2 \sum_{(v_i,v_j)\in E} \frac{1}{d_i d_j}; \;\; \lambda_n(\mathcal{L}) = 0.$$

Furthermore $\frac{n}{n-1} \leq \lambda_1(\mathcal{L}) \leq 2$ and the left inequality is attained if and only if G is a complete graph, while the right inequality holds when G is a bipartite graph.

Note that the condition $\lambda_{n-1}(L) > 0$ characterizes the connected graphs.
Finally, we cite the *transition matrix* $P = D^{-1}A$ which arises in the simple random walk on G. This is the process that jumps from a vertex v_i to any adjacent vertex v_j with equal transition probabilities $\frac{1}{d_i}$. In other words, this process is the Markov chain with transition matrix P and its real eigenvalues are $1 = \lambda_1(P) > \lambda_2(P) \geq \cdots \geq \lambda_n(P) \geq -1$. For a bipartite graph, the spectrum of P is symmetric and, in particular, $\lambda_n(P) = -1$.

For any square matrix M of order n let $\mu(M) = \frac{\mathrm{tr}(M)}{n}$ and $\sigma^2(M) = \frac{\mathrm{tr}(M^2)}{n} - \left(\frac{\mathrm{tr}(M)}{n}\right)^2$. If M admits real eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$, the inequalities below hold ([138]):

$$\mu(M) - \sigma(M)\sqrt{\frac{i-1}{n-i+1}} \leq \lambda_i \leq \mu(M) + \sigma(M)\sqrt{\frac{i-1}{n-i+1}}, \; i = 1, \cdots, n. \tag{5}$$

and, in particular, more binding inequalities hold for the smallest and largest eigenvalues:

$$\lambda_1 \geq \mu(M) + \frac{\sigma(M)}{\sqrt{n-1}}, \quad \lambda_n \leq \mu(M) - \frac{\sigma(M)}{\sqrt{n-1}} \tag{6}$$

In the case of the normalized Laplacian we get

$$\sigma^2(\mathcal{L}(G)) = \left(\frac{2}{n}\right) \sum_{(v_i,v_j)\in E} \frac{1}{d_i d_j},$$

and inequality (6) yields

$$\lambda_1(\mathcal{L}) \geq 1 + \sqrt{\frac{2}{n(n-1)} \sum_{(v_i,v_j)\in E} \frac{1}{d_i d_j}} \tag{7}$$

Notice that for every connected graph of order n we have

$$1 > \sigma(\mathcal{L}(G)) \geq \frac{1}{\sqrt{n-1}},$$

and the right inequality is attained for the complete graph $G = K_n$.

2.3 Effective resistance in general electric networks

We can view any connected graph $G(V, E)$ with n vertices and m edges as an electric network, where to each edge $(i, j) \in E$ of the graph is associate a resistance r_{ij} ($r_{ij} = 1$ in case of simple graphs), and this viewpoint enables us to apply a number of results taken from the theory of electric networks. This will be expanded below, but for the time being, if we denote by R_{ij} the effective resistance between the vertices i and j found using Ohm's law, we will use these results:

1) Foster's first formula (see [56])

$$\sum_{(i,j)\in E} R_{ij} = n - 1 \tag{8}$$

2)

$$\frac{2}{n} \leq R_{ij} \leq 1.$$

The inequality on the left hand side of 2) follows taking $d_i = d_j = n - 1$ in the general bound proved in [118]

$$1 \geq R_{ij} \geq \frac{d_i + d_j - 2}{d_i d_j - 1} \geq \frac{2}{n}, \tag{9}$$

where $(i, j) \in E$. The inequality on the right hand side follows noting that the effective resistance R_{ij} between two adjacent vertices i and j is equal to one if there is only one path connecting them, otherwise it is strictly less than one.

It is worth mentioning that (9) holds when $(i, j) \in E$, otherwise if $(i, j) \notin E$ we have:

$$R_{ij} \geq \frac{1}{d_i} + \frac{1}{d_j}. \tag{10}$$

In addition to the electrical formulas (8) and (9) used previously, Foster's second law, given in [57], is also fundamental:

$$\sum_{i<j;v} \frac{R_{ij}}{d_v} = n - 2, \tag{11}$$

where the summation is taken over all adjacent edges (i, v) and (v, j) and where d_v is the degree of the common vertex v.

We recall also the monotonicity law (see [47], p. 67), which states that if in a given network the resistance of an individual resistor is decreased then the effective resistance between any two nodes of

the network can only decrease. Thus, when we add an edge to a graph, since the resistance between the nodes where the edge is added decreases from infinity to 1, the effective resistance between any two nodes of the new graph is bounded above by the effective resistance between those same nodes in the original graph.
For a general electric network, assuming $k \leq r_{ij} \leq K$, the previous relations 1) and 2) generalize as follows

1') Generalized Foster's first formula:
$$\sum_{(i,j)\in E} \frac{R_{ij}}{r_{ij}} = n-1$$

2')
$$\frac{2k}{n} \leq R_{ij} \leq K$$

Relation 2') can be obtained via electric arguments as we will show below. Indeed, we can prove a more general result that extends the lower bound (9).

Proposition 5. *If* $(i,j) \in E$ *then*

$$R_{ij} \geq \frac{k(d_i + d_j - 2)}{d_i d_j - 1}. \tag{12}$$

Corollary 6. *If* $d_i \leq d$ *for all* $i \in V$ *then*

$$R_{ij} \geq \frac{2k}{d+1} \tag{13}$$

for all $(i,j) \in E$.

For the detailed proofs of Proposition 5 and Corollary 6 we refer the reader to [9]. Note that the bound (13) holds in particular if the graph is d-regular. Finally, since $d_i \leq n-1$ for all $i \in V$, it follows that
$$R_{ij} \geq \frac{2k}{n}, \text{ for all } (i,j) \in E.$$

3. Majorization techniques

Optimization problems involving Schur-convex or Schur-concave functions have received much attention in the literature providing some useful applications in different fields: for example they became a convenient tool to localize eigenvalues of a real spectrum matrix ([14], [127]) or more generally to obtain bounds for an arbitrary order statistic distribution ([19]). More recently some issues related to the structural properties of graphs, characterized in terms of their topological invariants, have been explored solving suitable optimization problems via majorization techniques ([12], [63]) In this section we present our general methodology based on the majorization order and Schur-convexity, already introduced in Section 1.2.1, that provides a unified approach to recover many well-known bounds of some graph topological indices, which can be expressed as Schur-convex functions, as well as to obtain better ones. Furthermore, applying the majorization technique, we will show how better estimate the subset on which the topological indices are defined.

3.1 A class of constrained optimization problems

Fix positive real numbers a and p. Let

$$\Sigma_a(\mathbf{p}) = \mathcal{D} \cap \{\mathbf{x} \in \mathbb{R}^n_+ : \langle \mathbf{x}, \mathbf{p} \rangle = a\}.$$

We set, in particular $\Sigma_a(\mathbf{s^n}) = \Sigma_a$.

To undestand the manner in which the majorization technique works for bounding topological indices, let $F(\mathbf{x}, \mathbf{p})$ be any topological index which is a p-Schur-convex (p-Schur-concave) function and consider the following constrained optimization problem

$$\begin{cases} \max \ (\min) F(\mathbf{x}, \mathbf{p}) \\ \text{subject to } \mathbf{x} \in S \end{cases} \tag{P}$$

where S is a closed subset of $\Sigma_a(\mathbf{p})$.

By the order preserving property of p-Schur-convex (p-Schur-concave) functions, the solution of the non linear constrained nonlinear optimization problem (P) can be obtained in a straightforward way.

To this aim, let us recall that given a subset S of $\Sigma_a(\mathbf{p})$, a vector $\mathbf{x}^{*p}(S) \in S$ is said to be maximal for S with respect to the p-majorization order if $\mathbf{x} \trianglelefteq_p \mathbf{x}^{*p}(S)$ for each $\mathbf{x} \in S$. Analogously, a vector $\mathbf{x}_{*p}(S) \in S$ is said to be minimal for S with respect to the p-majorization order if $\mathbf{x}_{*p}(S) \trianglelefteq_p \mathbf{x}$ for each $\mathbf{x} \in S$.

The maximal and the minimal elements of a subset S of Σ_a with respect to the majorization order will be denote by $\mathbf{x}^*(S)$ and $\mathbf{x}_*(S)$, respectively.

Now, if the set S admits maximal vector $\mathbf{x}^{*p}(S)$ and minimal vector $\mathbf{x}_{*p}(S)$ with respect to the p-majorization order, the maximum and the minimum are attained at $\mathbf{x}^{*p}(S)$ and $\mathbf{x}_{*p}(S)$ respectively; the opposite holds if ϕ is a p-Schur-concave function. This allows us to solve problem (P) in a more direct way, avoiding the extensive numerical computations performed through the standard approach of Karush-Kuhn-Tucker method.

Indeed, if F is a p-Schur-convex function, we get

$$F(\mathbf{x}_{*\mathbf{p}}(S), \mathbf{p}) \leq F(\mathbf{x}, \mathbf{p}) \leq F(\mathbf{x}^{*\mathbf{p}}(S), \mathbf{p}), \forall \mathbf{x} \in S.$$

Analogously, if if F is a p-Schur-concave function:

$$F(\mathbf{x}^{*\mathbf{p}}(S), \mathbf{p}) \leq F(\mathbf{x}, \mathbf{p}) \leq F(\mathbf{x}_{*\mathbf{p}}(S), \mathbf{p}), \forall \mathbf{x} \in S.$$

We note that tighter bounds for the elements of the subsets S, will imply sharper bounds for the p-Schur-convex (p-Schur-concave) functions representing the topological indices, as shown in the following proposition:

Proposition 7. *Let us consider two sets $S^{''}$ and S', with $S^{''} \subseteq S'$, which admit maximal and minimal elements with respect to the majorization order. If F is a p-strictly Schur-convex function, then*

$$F(\mathbf{x}^{*\mathbf{p}}(S''), \mathbf{p}) \leq F(\mathbf{x}^{*\mathbf{p}}(S'), \mathbf{p})$$
$$F(\mathbf{x}_{*\mathbf{p}}(S'), \mathbf{p}) \leq F(\mathbf{x}_{*\mathbf{p}}(S''), \mathbf{p})$$

and the equality holds if and only if $\mathbf{x}^{*\mathbf{p}}(S'') = \mathbf{x}^{*\mathbf{p}}(S')$ and $\mathbf{x}_{*\mathbf{p}}(S'') = \mathbf{x}_{*\mathbf{p}}(S')$.

In a straitghforward way the result for a p-Schur-concave function can be derived.

Now, it is worth pointing out that, in virtue of the above proposition, the more accurate is the estimate of the set S, the tighter is the bound of the index.

It is evident that all the considerations above hold if we consider the problem (P) for $\mathbf{p} = \mathbf{s^n}$ and $S \subseteq \Sigma_a$.

In the following section we will evaluate the maximal and minimal elements of particular subsets of $\Sigma_a(\mathbf{p})$ given by

$$S_a(\mathbf{p}) = \Sigma_a(\mathbf{p}) \cap \{\mathbf{x} \in \mathbb{R}^n : M_i \geq x_i \geq m_i,\ i = 1, ...n\}, \tag{14}$$

where $\mathbf{m} = [m_1, m_2, ..., m_n]^T$ and $\mathbf{M} = [M_1, M_2, ..., M_n]^T$ are two assigned vectors arranged in non-increasing order with $0 \leq m_i \leq M_i$, for all $i = 1, ...n$, and a is a positive real number such that $\langle \mathbf{m}, \mathbf{p} \rangle \leq a \leq \langle \mathbf{M}, \mathbf{p} \rangle$. However, it may happen that the bounds on the variable x_i, $i = 1, \cdots, n$ are not directly available. In such cases, we will show how majorization technique could efficiently provide the required bounds.

3.2 Extremal elements with respect to the majorization order

Given a positive real number a, let us consider the sets $\Sigma_a(\mathbf{p})$ and Σ_a. By direct calculations we can easily show that the maximal and the minimal elements of $\Sigma_a(\mathbf{p})$ with respect to the p-majorization order are respectively:

$$\mathbf{x}^{*p}(\Sigma_a(\mathbf{p})) = \frac{a}{p_1}\mathbf{e}^1 \qquad \text{and} \qquad \mathbf{x}_{*p}(\Sigma_a(\mathbf{p})) = \left(\frac{a}{\sum_{i=1}^n p_i}\right)\mathbf{s^n} = \left[\left(\frac{a}{\sum_{i=1}^n p_i}\right)^n\right]$$

(see [26] and [9]), while the maximal and the minimal elements of the set Σ_a with respect to the majorization order are

$$\mathbf{x}^*(\Sigma_a) = a\mathbf{e}^1 = [a, 0^{n-1}], \quad \text{and} \quad \mathbf{x}_*(\Sigma_a) = \frac{a}{n}\mathbf{s^n} = \left[\left(\frac{a}{n}\right)^n\right]$$

(see [104]).

In this section we extend the previous result finding the maximal and the minimal elements, with respect to the p-majorization order, of the set $S_a(\mathbf{p})$.

The existence of maximal and minimal elements of $S_a(\mathbf{p})$ with respect to the p-majorization are ensured by the compactness of the set $S_a(\mathbf{p})$ and by the closure of the upper and lower level sets:

$$U(\mathbf{x}) = \{\mathbf{z} \in S_a(\mathbf{p}) : \mathbf{x} \trianglelefteq_{\mathbf{p}} \mathbf{z}\},\ L(\mathbf{x}) = \{\mathbf{z} \in S_a(\mathbf{p}) : \mathbf{z} \trianglelefteq_{\mathbf{p}} \mathbf{x}\}.$$

3.2.1 Maximal elements

We start computing the maximal element of the set $S_a(\mathbf{p})$. For the reader's convenience the proof will be included.

Theorem 8. *([9]) Let $k \geq 0$ be the smallest integer such that*

$$\left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle + \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^k} \right\rangle \leq a < \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s}^{k+1} \right\rangle + \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^{k+1}} \right\rangle, \tag{15}$$

and $\theta = \dfrac{a - \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^{k+1}} \right\rangle}{p_{k+1}}$. Then

$$\mathbf{x}^{*p}(S_a(\mathbf{p})) = \mathbf{M} \circ \mathbf{s^k} + \theta \mathbf{e}^{k+1} + \mathbf{m} \circ \mathbf{v^{k+1}}. \tag{16}$$

Proof. First of all we verify that $\mathbf{x}^{*p}(S_a) \in S_a(\mathbf{p})$.

It easy to see that $\langle p \circ \mathbf{x}^{*p}(S_a(\mathbf{p})), \mathbf{s^n} \rangle = a$ and that $m_i \leq [\mathbf{x^{*p}}(S_a)]_i \leq M_i$ for $i \neq k+1$. To prove that $m_{k+1} \leq \mathbf{x}^{*p}_{k+1}(S_a(\mathbf{p})) \leq M_{k+1}$, notice that from (15)

$$p_{k+1} m_{k+1} \leq a - \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^{k+1}} \right\rangle = \theta p_{k+1} < p_{k+1} M_{k+1}.$$

Now we show that $\mathbf{x} \trianglelefteq_p \mathbf{x}^{*p}(S_a(\mathbf{p}))$ for all $\mathbf{x} \in S_a(\mathbf{p})$. By property i) it follows

$$\left\langle \mathbf{p} \circ \mathbf{x}^*_p(S_a(\mathbf{p})), \mathbf{s^j} \right\rangle = \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \circ \mathbf{s^j} \right\rangle + \theta p_{k+1} \left\langle \mathbf{e^{k+1}}, \mathbf{s^j} \right\rangle + \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^{k+1}} \circ \mathbf{s^j} \right\rangle, \; j = 1, ...(n-1)$$

and by iii) and iv)

$$\left\langle \mathbf{p} \circ \mathbf{x}^*_p(S_a(\mathbf{p})), \mathbf{s^j} \right\rangle = \begin{cases} \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^j} \right\rangle & 1 \leq j \leq k \\ \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle + \theta p_{k+1} + \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{s^j} - \mathbf{s^{k+1}} \right\rangle & (k+1) \leq j \leq (n-1) \end{cases}.$$

Thus, given a vector $\mathbf{x} \in S_a(\mathbf{p})$, for $1 \leq j \leq k$ we obtain

$$\left\langle \mathbf{p} \circ \mathbf{x}, \mathbf{s^j} \right\rangle \leq \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^j} \right\rangle = \left\langle \mathbf{p} \circ \mathbf{x}^*(S_a(\mathbf{p})), \mathbf{s^j} \right\rangle,$$

while for $(k+1) \leq j \leq (n-1)$, by iii),

$$\begin{aligned} \langle \mathbf{p} \circ \mathbf{x}, \mathbf{s^j} \rangle &= \langle \mathbf{p} \circ \mathbf{x}, \mathbf{s^n} \rangle - \left\langle \mathbf{p} \circ \mathbf{x}, \mathbf{v^j} \right\rangle \\ &\leq a - \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^j} \right\rangle \\ &= \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle + \theta p_{k+1} + \langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^{k+1}} \rangle - \langle \mathbf{p} \circ \mathbf{m}, \mathbf{v^J} \rangle = \\ &= \left\langle \mathbf{p} \circ \mathbf{M}, \mathbf{s^k} \right\rangle + \theta p_{k+1} + \left\langle \mathbf{p} \circ \mathbf{m}, \mathbf{s^j} - \mathbf{s^{k+1}} \right\rangle = \\ &= \left\langle \mathbf{p} \circ \mathbf{x^{*p}}(\mathbf{S_a}(\mathbf{p})), \mathbf{s^j} \right\rangle \end{aligned}$$

and the result follows. $\square$

For the particular case $\mathbf{p} = \mathbf{s^n}$, letting $S_a(\mathbf{p}) = S_a$, we get the following

Corollary 9. *([13]) Let $k \geq 0$ be the smallest integer such that*

$$\left\langle \mathbf{M}, \mathbf{s^k} \right\rangle + \left\langle \mathbf{m}, \mathbf{v^k} \right\rangle \leq a < \left\langle \mathbf{M}, \mathbf{s}^{k+1} \right\rangle + \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle, \tag{17}$$

and $\theta = a - \left\langle \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle$. Then

$$\mathbf{x}^*(S_a) = \mathbf{M} \circ \mathbf{s^k} + \theta \mathbf{e}^{k+1} + \mathbf{m} \circ \mathbf{v^{k+1}} = [M_1, M_2, \cdots, M_k, \theta, m_{k+2}, \cdots m_n]. \tag{18}$$

Remark 10.

In the following list we recall the maximal elements of particular subsets of $S_a(\mathbf{p})$ and S_a useful in forthcoming Sections. We denote by $\lfloor x \rfloor$ the integer part of the real number x.

I. $S_a^1(\mathbf{p}) = \Sigma_a(\mathbf{p}) \cap \{\mathbf{x} \in \mathbb{R}^n : M \geq x_1 \geq x_2 \geq \cdots \geq x_n \geq m\}$
where $0 \leq m \leq \dfrac{a}{\sum_{i=1}^n p_i} \leq M$. Then

$$\mathbf{x}^{*p}(S_a^1(\mathbf{p})) = M\mathbf{s^k} + \theta \mathbf{e^{k+1}} + m\mathbf{v^{k+1}},$$

where k is the first integer such that

$$M \sum_{i=1}^{k} p_i + m \sum_{i=k+1}^{n} p_i \leq a < M \sum_{i=1}^{k+1} p_i + m \sum_{i=k+2}^{n} p_i$$

and $\theta = \dfrac{a - M \sum_{i=1}^k p_i - m \sum_{i=k+2}^n p_i}{p_{k+1}}$ (see [9]).
When $\mathbf{p} = \mathbf{s^n}$ we obtain $k = \left\lfloor \dfrac{a - nm}{M - m} \right\rfloor$ and $\theta = a - Mk - m\,(n - k - 1)$. In particular when $m = 0$ we have $\mathbf{x}^*(S_a^1) = M\mathbf{s^k} + \theta \mathbf{e^{k+1}}$, where $k = \left\lfloor \dfrac{a}{M} \right\rfloor$ and $\theta = a - Mk$ (see [104] and [13]).

II. $S_a^2 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \geq \alpha, i = 1, ...h\}$
where $1 \leq h \leq n$ and $0 < \alpha \leq a/h$. Then

$$\mathbf{x}^*(S_a^2) = (a - h\alpha)\,\mathbf{e}^1 + \alpha \mathbf{s^h}.$$

(see [14])

III. $S_a^{[h]} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_1 \geq x_1 \geq ... \geq x_h \geq m_1, M_2 \geq x_{h+1} \geq ... \geq x_n \geq m_2\}$
where $1 \leq h \leq n$, $0 \leq m_2 \leq m_1,\ 0 \leq M_2 \leq M_1,\ m_i < M_i, i = 1, 2$ and $hm_1 + (n-h)m_2 \leq a \leq hM_1 + (n-h)M_2$.
Let $a^* = hM_1 + (n-h)m_2$ and

$$k = \begin{cases} \left\lfloor \dfrac{a - h(m_1 - m_2) - nm_2}{M_1 - m_1} \right\rfloor & \text{if} \quad a < a^* \\[2ex] \left\lfloor \dfrac{a - h(M_1 - M_2) - nm_2}{M_2 - m_2} \right\rfloor & \text{if} \quad a \geq a^* \end{cases}.$$

Then

$$\mathbf{x}^*(S_a^{[h]}) = \begin{cases} \left[M_1^k, \theta, m_1^{h-k-1}, m_2^{n-h}\right] & \text{if} \quad a < a^* \\ \\ \left[M_1^h, M_2^{k-h}, \theta, m_2^{n-k-1}\right] & \text{if} \quad a \geq a^* \end{cases},$$

where $\theta = a - \left\langle \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle$, $\mathbf{M} = [M_1^h, M_2^{n-h}]$, $\mathbf{m} = [m_1^h, m_2^{n-h}]$ (see [13]).

Remark 11. The assumption $m_i < M_i$ in point III Remark 10 can be relaxed to $m_i \leq M_i$. Indeed if $m_i = M_i, i = 1, 2$, the set $S_a^{[h]}$ reduces to the singleton $\{m_1 \mathbf{s^h} + m_2 \mathbf{v^h}\}$, while if $m_1 = M_1, m_2 < M_2$ the first h components of any $\mathbf{x} \in S_a^{[h]}$ are fixed and equal to m_1 and the maximal element of $S_a^{[h]}$ can be computed by the maximal element of $S_{a-hm_1} \in \mathbb{R}^{n-h}$ (see point II.). The case $m_2 = M_2, m_1 < M_1$ is similar.

3.2.2 Minimal elements

In this section we discuss only the computation of the minimal element of the set

$$S_a = \Sigma_a \cap \{\mathbf{x} \in {}^n : M_i \geq x_i \geq m_i, \ i = 1, ...n\}, \tag{19}$$

where $\mathbf{m} = [m_1, m_2, ..., m_n]^T$ and $\mathbf{M} = [M_1, M_2, ..., M_n]^T$ are two assigned vectors arranged in non-increasing order with $0 \leq m_i \leq M_i$, for all $i = 1, ...n$, and a is a positive real number such that $\langle \mathbf{m}, \mathbf{s^n} \rangle \leq a \leq \langle \mathbf{M}, \mathbf{s^n} \rangle$.

We have already recalled that the minimal element of Σ_a is $\mathbf{x}_*(\Sigma_a) = [(\frac{a}{n})^n]$. If it belongs to S_a then it is its minimal element, too. Otherwise we have to apply the following theorem.

Theorem 12. *([13]) Let $k \geq 0$ and $d \geq 0$ be the smallest integers such that*

1) $k + d < n$

2) $m_{k+1} \leq \rho \leq M_{n-d}$ *where* $\rho = \dfrac{a - \langle \mathbf{m}, \mathbf{s^k} \rangle - \langle \mathbf{M}, \mathbf{v^{n-d}} \rangle}{n-k-d}$.

Then

$$\mathbf{x}_*(S_a) = \mathbf{m} \circ \mathbf{s^k} + \rho(\mathbf{s^{n-d}} - \mathbf{s^k}) + \mathbf{M} \circ \mathbf{v^{n-d}} = [m_1, \cdots, m_k, \rho^{n-d-k}, M_{n-d+1} \cdots, M_n].$$

Remark 13.

In the following list we derive the minimal element of particular subsets of S_a useful in the sequel.

I. $S_a^{[h]} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_1 \geq x_1 \geq ... \geq x_h \geq m_1, M_2 \geq x_{h+1} \geq ... \geq x_n \geq m_2\}$

where $1 \leq h \leq n, 0 \leq m_2 \leq m_1, \ 0 \leq M_2 \leq M_1, \ m_i < M_i, i = 1, 2$ and $hm_1 + (n-h)m_2 \leq a \leq hM_1 + (n-h)M_2$.

i) If $m_1 \leq M_2$ then

$$\mathbf{x}_*(S_a^{[h]}) = \begin{cases} \left[\left(\frac{a}{n}\right)^n\right] & \text{if} \quad m_1 \leq \dfrac{a}{n} \leq M_2 \\ \left[m_1^h, \left(\frac{a-hm_1}{n-h}\right)^{n-h}\right] & \text{if} \quad \dfrac{a}{n} < m_1 \\ \left[\left(\frac{a-M_2(n-h)}{h}\right)^h, M_2^{n-h}\right] & \text{if} \quad \dfrac{a}{n} > M_2 \end{cases} . \tag{20}$$

ii) If $M_2 < m_1$ then

$$\mathbf{x}_*(S_a^{[h]}) = \begin{cases} \left[m_1^h, \left(\dfrac{a-hm_1}{n-h}\right)^{n-h}\right] & \text{if} \quad a < \widetilde{a} \\ \left[\left(\dfrac{a-M_2(n-h)}{h}\right)^h, M_2^{n-h}\right] & \text{if} \quad a \geq \widetilde{a} \end{cases} \tag{21}$$

(see [13]).

II. $S_a^1 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M \geq x_1 \geq ... \geq x_{n-1} \geq x_n \geq m\}$ where $0 \leq m < M$ and $m \leq \dfrac{a}{n} \leq M$. Then $\mathbf{x}_*(S_a^1) = \dfrac{a}{n}\mathbf{s^n} = \left[\left(\dfrac{a}{n}\right)^n\right]$ (see [104]).

III. $S_a^2 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \geq \alpha,\ i = 1, ...h\}$, where $1 \leq h \leq n$ and $0 < \alpha \leq a/h$. Then

$$\mathbf{x}_*(S_a^2) = \begin{cases} \left[\left(\dfrac{a}{n}\right)^n\right] & \text{if} \quad \alpha \leq \dfrac{a}{n} \\ (\alpha^h, \rho^{n-h}) \text{ with } \rho = \dfrac{a-\alpha h}{n-h} & \text{if} \quad \alpha > \dfrac{a}{n} \end{cases} ,$$

(see ([14]).

IV. $S_a^3 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \leq \alpha,\ i = h+1, ...n\}$ where $1 \leq h \leq (n-1)$ and $0 < \alpha < a$. Then

$$\mathbf{x}_*(S_a^3) = \begin{cases} \left[\left(\dfrac{a}{n}\right)^n\right] & \text{if} \quad \alpha \geq \dfrac{a}{n} \\ (\rho^h, \alpha^{n-h}) \text{ with } \rho = \dfrac{a-(n-h)\alpha}{h} & \text{if} \quad \alpha < \dfrac{a}{n} \end{cases} ,$$

(see ([14]).

Remark 14. We note that the minimal element of the set $S_a^{[h]}$ does not necessarily have integer components, while this is not the case for the maximal element. For our purposes it is crucial to find the minimal vector in S_a with integer components which can be constructed by the following procedure (see

Remark 12 in [13]). Let us consider, for instance, the vector $x_*(S_a^{[h]}) = \left[\left(\frac{a}{n}\right)^n\right]$ which corresponds to the case $m_1 \leq \frac{a}{n} \leq M_2$. If $\frac{a}{n}$ is not an integer, let us find the index k, $1 \leq k \leq n$, such that

$$\left(\left\lfloor \frac{a}{n} \right\rfloor + 1\right) k + \left\lfloor \frac{a}{n} \right\rfloor (n-k) = a$$

i.e., $k = a - \left\lfloor \frac{a}{n} \right\rfloor n$. The vector

$$\mathbf{x}_*^{\mathbf{1}} = \left[\left(\left\lfloor \frac{a}{n} \right\rfloor + 1\right)^k, \left(\left\lfloor \frac{a}{n} \right\rfloor\right)^{n-k}\right]$$

is the minimal element of $S_a^{[h]}$ with integer components. With slight modifications the same procedure can be applied also in the other cases discussed in (20), (21) or in Theorem 12.

3.3 A majorization procedure to get x_i's bounds

It may happen that the bounds on the variable x_i, $i = 1, \cdots, n$ are not directly available. To overcome this problem, we will now show that, if S assumes a particular expression, choosing the function $F(\mathbf{x}, \mathbf{p})$ as the $h-$component of the vector $\mathbf{x}$ and $\mathbf{p} = \mathbf{s}^n$, the solution of the problem (P) provides the required bounds.

To this aim we introduce a real, continuous, homogeneous of degree $\tau \geq 1$ and strictly Schur-convex function g. We refer the reader to [14] for the proofs of Lemma and Theorems stated below

Lemma 15. *(see Lemma 2.1 in [14]). Fix $b \in \mathbb{R}$ and consider the set*

$$S = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}_+^n : g(\mathbf{x}) = \sum_{i=1}^{n} x_i^\tau = b\}.$$

Then either $b = \frac{a^\tau}{n^{\tau-1}}$ or there exists a unique integer $1 \leq h^* < n$ such that:

$$\frac{a^\tau}{(h^*+1)^{\tau-1}} < b \leq \frac{a^\tau}{(h^*)^{\tau-1}},$$

where $h^* = \left\lfloor \sqrt[\tau-1]{\frac{a^\tau}{b}} \right\rfloor$.

We can now deduce upper and lower bounds for x_h (with $h = 1, ..., n$) by solving the following optimization problems $P(h)$ and $P^*(h)$:

$$\begin{array}{lr} \max(x_h) \text{ subject to } \boldsymbol{x} \in S & P(h) \\ \min(x_h) \text{ subject to } \boldsymbol{x} \in S & P^*(h) \end{array}$$

For the proof of the following Theorems, see [14], Theorems 3.1 and 3., respectively.

Theorem 16. *The solution of the optimization problem $P(h)$ is $(\frac{a}{n})$ if $b = \frac{a^\tau}{n^{\tau-1}}$.*
If $b \neq \frac{a^\tau}{n^{\tau-1}}$, the solution of the optimization problem $P(h)$ is α^* where

1. *for $h > h^*$, α^* is the unique root of the equation*

$$f(\alpha, \tau) = (h-1)\alpha^\tau + (a - h\alpha + \alpha)^\tau - b = 0 \tag{22}$$

in $I = \left(0, \frac{a}{h}\right]$;

2. *for $h \leq h^*$, α^* is the unique root of the equation*

$$f(\alpha, \tau) = h\alpha^\tau + \frac{(a - h\alpha)^\tau}{(n-h)^{\tau-1}} - b = 0 \tag{23}$$

in $I = \left(\frac{a}{n}, \frac{a}{h}\right]$.

Theorem 17. *The solution of the optimization problem $P^*(h)$ is $(\frac{a}{n})$ if $b = \frac{a^\tau}{n^{\tau-1}}$.*

If $b \neq \frac{a^\tau}{n^{\tau-1}}$, the solution of the optimization problem $P^*(h)$ is α^* where

1. *for $h = 1$, α^* is the unique root of the equation*

$$f(\alpha, \tau) = h^*\alpha^\tau + (a - h^*\alpha)^\tau - b = 0 \tag{24}$$

in $I = \left(\frac{a}{h^*+1}, \frac{a}{h^*}\right]$;

2. *for $1 < h \leq (h^* + 1)$, α^* is the unique root of the equation*

$$f(\alpha, \tau) = (n-h+1)\alpha^\tau + \frac{(a - (n-h+1)\alpha)^\tau}{(h-1)^{\tau-1}} - b = 0 \tag{25}$$

in $I = (0, \frac{a}{n}]$;

3. *for $h > (h^* + 1)$, α^* is zero.*

4. Topological indices

Structural properties of graphs can be characterized in terms of descriptors representing properties which are preserved by a graph isomorphism (namely graph invariants). In particular, we focus on topological indices and we classify them according the mathematical object they are based on. It is worth pointing out that we restrict our attention to those indices which can be formulated as Schur-convex (Schur-concave) functions of the degree sequence π as well as of the eigenvalues of some matrices associated to the graph G such as Adjacency, Laplacian, normalized Laplacian and transition matrices. The first category of descriptors can be grouped in two subsets: the degree-based indices over all vertices and the degree-based indices over all edges. Then we have the eigenvalues-based indices and this category also includes some weighted and unweighted resistance-based indices which can be reformulated in terms of eigenvalues of suitable matrices associated to G.

For reader's convenience we listed below the analyzed indices.

- First general and first multiplicative Zagreb indices;
- General Randić index;
- Generalized sum-connectivity index;
- Atom-bond connectivity index;
- Augmented Zagreb index;
- Energy index;
- Laplacian energy;
- Normalized Laplacian Index;
- Normalized Laplacian Energy;
- Normalized Laplacian Estrada index;
- HOMO-LUMO index;
- Kirchhoff index;
- Multiplicative degree-Kirchhoff index;
- Additive degree-Kirchhoff index;
- Weighted global cyclicity index.

4.1 Degree-based indices over all vertices

We explore a class of topological indices of particular interest found in the literature and depending on the degree sequence of a graph over all vertices.

4.1.1 First general and first multiplicative Zagreb indices[1]

The *first general Zagreb index* was firstly introduced by Li and Zheng ([95]) and it is defined as

$$M_1^\alpha = \sum_{i=1}^{n} d_i^\alpha \tag{26}$$

where α is an arbitrary real number with $\alpha \neq 0; 1$. For $\alpha = 2$ we get the *first Zagreb index* while for $\alpha = -1$ the *inverse degree*.
In [10] the authors, exploiting the fact that M_1^α is a Schur-convex (concave) function of the degree sequence either for $\alpha < 0$ or $\alpha > 1$ ($0 < \alpha < 1$), provided upper and lower bounds of M_1^α for the

[1] For details we refer the reader to [8] and [10].

classes of c-cyclic graphs with $0 \leq c \leq 6$. In particular, after characterizing c-cyclic graphs as those whose degree sequences belongs to particular subsets of $\mathbb{R}^n$, the maximal and minimal elements of these subsets with respect to the majorization order were identified and upper and lower bounds evaluated. For convenience, the reported results in Table 1 have been restricted to the first general Zagreb index with either $\alpha < 0$ or $\alpha > 1$ and $n \geq c+2$. When $0 < \alpha < 1$ the upper and lower bounds in Table 1 are turned over. Furthermore the specific case $\alpha = -1$ ([35], [36] and [94]) has been discussed. Notice that when more maximal elements are identified, the best choice depends on α.

c	Lower bounds	Upper bounds
1	$(n-1)^\alpha + 2^{\alpha+1} + (n-3)$	$n\,(2^\alpha)$
2	$(n-1)^\alpha + 3^\alpha + 2^{\alpha+1} + (n-4)$	$2\,(3^\alpha) + (2^\alpha)\,(n-2)$
3	$4\,(3^\alpha) + (2^\alpha)\,(n-4)$	$(n-1)^\alpha + 4^\alpha + 3\,(2^\alpha) + (n-5)$ $(n-1)^\alpha + 3^{\alpha+1} + (n-4)$
4	$2\,(3^{\alpha+1}) + (2^\alpha)\,(n-6)$	$(n-1)^\alpha + 5^\alpha + 2^{\alpha+2} + (n-6)$ $(n-1)^\alpha + 2^\alpha(2^\alpha+1) + 2\,(3^\alpha) + (n-5)$
5	$8\,(3^\alpha) + (n-8)\,2^\alpha$	$(n-1)^\alpha + 6^\alpha + 5\,(2^\alpha) + (n-7)$ $(n-1)^\alpha + 5^\alpha + 2\,(3^\alpha) + 2\,(2^\alpha) + (n-6)$ $(n-1)^\alpha + 2^{2\alpha+1} + 2\,(3^\alpha) + (n-8)$
6	$10\,(3^\alpha) + (n-10)\,2^\alpha$	$(n-1)^\alpha + 7 + 6\,(2^\alpha)\,(n-8)$ $(n-1)^\alpha + 6 + 2\,(3^\alpha) + 3\,(2^\alpha) + (n-7)$ $(n-1)^\alpha + 5 + 4 + 2\,(3^\alpha) + 2 + (n-6)$ $(n-1)^\alpha + 2^{2\alpha+2} + (n-5)$

Table 1. Bounds for M_1^α $(\alpha < 0 \vee \alpha > 1)$

Gutman [67] introduced the *first multiplicative Zagreb index*, defined as

$$\ln M_1 = 2\sum_{i=1}^{n} \ln(d_i) \tag{27}$$

and it is a Schur concave function of the degree sequence.

For c-cyclic graphs, $0 \leq c \leq 6$, bounds for the first multiplicative Zagreb index can be obtained by applying the same methodology described for the first general Zagreb index.

4.2 Degree-based indices over all edges

A class of topological indices depending on the degrees of nodes linked by an edge, is represented by the *General Randić index*, the *Generalized sum connectivity index*, the *Atom-bond connectivity index* and the *Augmented Zagreb index*.

4.2.1 General Randić index [2]

With respect to the degree sequence, one of the most popular index is the *General Randić index*:

$$R_\alpha(G) = \sum_{(v_i,v_j)\in E} (d_i d_j)^\alpha,$$

where α is a non zero real number ([18]). For a specific value of α, some very well known indices can be obtained: $\alpha = 1$, for example, corresponds to the Zagreb index $M_2(G)$ ([106]) while $\alpha = -1$ is the Randić index ([121]). In [13] the generalized Randić index has been rewritten as:

$$R_\alpha(G) = \frac{1}{2}\left(\sum_{(v_i,v_j)\in E} \left(d_i^\alpha + d_j^\alpha\right)^2 - \sum_{i=1}^{n} d_i^{2\alpha+1}\right). \tag{28}$$

Let $\pi = (d_1, d_2, .., d_n)$ be a fixed degree sequence and $\mathbf{x} \in \mathbb{R}^m$ be the vector whose components are $d_i^\alpha + d_j^\alpha$, with $(v_i, v_j) \in E$. Notice that by (4) $\sum_{i=1}^m x_i$ is a constant. Since $\sum\limits_{i=1}^{n} d_i^{2\alpha+1}$ is also a constant, $R_\alpha(G)$ is a Schur convex function of $\mathbf{x}$ and it is minimal (maximal) if and only $f(\mathbf{x}) = \sum\limits_{i=1}^{m} x_i^2 = \|\mathbf{x}\|_2^2$ is minimal (maximal).

Hence, considering a closed subset S of $\Sigma_a \subseteq \mathbb{R}^m$, where $a = \sum_{i=1}^n d_i^{\alpha+1}$, which admits $\mathbf{x}_*(S)$ and $\mathbf{x}^*(S)$ as extremal vectors with respect to the majorization order, the function f attains its minimum and maximum on S at $f(\mathbf{x}_*(S))$ and $f(\mathbf{x}^*(S))$, respectively. The general Randić index can be consequently bounded as follows:

$$\frac{\|\mathbf{x}_*(S)\|_2^2 - \sum\limits_{i=1}^{n} d_i^{2\alpha+1}}{2} \le R_\alpha(G) \le \frac{\|\mathbf{x}^*(S)\|_2^2 - \sum\limits_{i=1}^{n} d_i^{2\alpha+1}}{2}. \tag{29}$$

Using the information available on the degree sequence of G and characterizing suitably the set S, different numerical bounds can be derived.

For the particular case $\alpha = 1$, which corresponds to the Zagreb index $M_2(G)$, this methodology was applied in [63], and, more recently, in [13] where the authors get sharper bounds for the index M_2 in the case of a particular class of graphs having exactly h pendant vertices, i.e. vertices with degree one. The same procedure was applied in [11] for the Randić index:

$$R_{-1}(G) = \sum_{(i,j)\in E} \left(\frac{1}{d_i d_j}\right) = \frac{1}{2}\left(\sum_{(i,j)\in E} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)^2 - \sum_{i=1}^{n} \frac{1}{d_i}\right). \tag{30}$$

In this case, by (29), we have:

$$\frac{\|x_*(S)\|_2^2 - \sum\limits_{i=1}^{n} \frac{1}{d_i}}{2} \le R_{-1}(G) \le \frac{\|\mathbf{x}^*(S)\|_2^2 - \sum\limits_{i=1}^{n} \frac{1}{d_i}}{2}. \tag{31}$$

[2] For details we refer the reader to [8], [12] and [13].

4.2.2 Generalized sum-connectivity index [3]

In [48] the *Generalized sum-connectivity index*

$$\chi_\alpha(G) = \sum_{(v_i,v_j)\in E} (d_i + d_j)^\alpha .$$

has been proposed.
Notice that for $\alpha = 1$, $\chi_1(G)$ reduces to the first Zagreb index

$$M_1(G) = \sum_{(v_i,v_j)\in E} (d_i + d_j) = \sum_{i=1}^{n} d_i^2,$$

while for $\alpha = -\frac{1}{2}$ we have the Sum-connectivity index defined in [149].
Let π be a fixed degree sequence and $\mathbf{x} \in \mathbb{R}^m$ be the vector whose components are (d_i+d_j), $(v_i, v_j) \in E$. The function $f(\mathbf{x}) = \sum_{i=1}^{m} x_i^\alpha$ is strictly Schur-convex for $\alpha > 1$ or $\alpha < 0$, while it is strictly Schur-concave for $0 < \alpha < 1$. Since $\sum_{i=1}^{m} x_i = \sum_{i=1}^{n} d_i^2$ is a constant and considering a closed subset S of Σ_a, where $a = \sum_{i=1}^{n} d_i^2$, for $\alpha > 1$ or $\alpha < 0$, we get

$$\|\mathbf{x}_*(S)\|_\alpha^\alpha \leq \chi_\alpha(G) \leq \|\mathbf{x}^*(S)\|_\alpha^\alpha , \tag{32}$$

where $\|\cdot\|_\alpha$ stands for the $l_\alpha-$norm. For $0 < \alpha < 1$, the bounds are exchanged. Different bounds, depending on the choice of the set S, can be derived.

4.2.3 Atom-bond connectivity index[4]

The ABC index, proposed by Estrada et al. in [55], and reintroduced in [53] was defined as

$$ABC(G) = \sum_{(i,j)\in E} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}. \tag{33}$$

The index $ABC(G)$ has been studied in a large number of references of which we mention [59], [37] and [78] for their own interest and for many other related references found in them.

In the following we will present a new upper bound for $ABC(G)$ given in terms of the Randić index $R_{-1}(G)$. This upper bound yields a number of particular bounds (which improve all those in [109] and some in [77]) and maximal results as corollaries of numerous lower bounds for the Randić index found in the literature. We also find new lower bounds for $R_{-1}(G)$ through majorization, yielding additional upper bounds for $ABC(G)$.

In what follows we will assume that the graphs satisfy $n \geq 3$ in order to avoid cases where i and j are neighbours and $d_i = d_j = 1$. The first main result is a refinement of an argument found in [109].

[3]For details we refer to [8] and [12].
[4]For details we refer the reader to [11] and [109].

Proposition 18. *For any graph G we have*

$$ABC(G) \leq \sqrt{(n-1)(|E| - R_{-1}(G))}, \tag{34}$$

where $R_{-1}(G)$ has been defined in (30).

The inequality becomes an equality if G is either the complete graph or the star graph.

The maximality of the complete graph and the star graph will be seen below. The bound (34) is similar to a bound found by Horoldagva and Gutman with different means in [77] stating

$$ABC(G) \leq \sqrt{|E|(n - 2R_{-1}(G))}. \tag{35}$$

Bounds (34) and (35) are not comparable. A bit of algebra shows that our bound is better when $R_{-1}(G) \leq \dfrac{|E|}{2|E| - n + 1}$. Horoldagva and Gutman use their inequality (35) as an intermediate step in order to obtain yet another inequality for $ABC(G)$ in terms of the second Zagreb index, and use upper bounds on this index in order to get upper bounds on $ABC(G)$. Here we take the alternative path of producing upper bounds for $ABC(G)$ using (34) and (35) with the help of *lower* bounds for $R_{-1}(G)$. Perhaps the best such bound is given in [124], stating

$$R_{-1}(G) \geq \frac{n}{2d_1}, \tag{36}$$

where d_1 is the largest degree of the graph and where the equality is attained in case G is regular. This allows us to prove the following universal bounds

Proposition 19. *For any graph G we have*

$$ABC(G) \leq \sqrt{(n-1)\left(|E| - \frac{n}{2d_1}\right)} \leq n\sqrt{\frac{n-2}{2}}, \tag{37}$$

and

$$ABC(G) \leq \sqrt{|E|n\left(1 - \frac{1}{d_1}\right)} \leq n\sqrt{\frac{n-2}{2}}. \tag{38}$$

Again, the leftmost inequalities in (37) and (38) are not comparable, with (37) giving better bounds whenever $d_1 \geq n(1 - \frac{n-1}{2|E|})$. Now, for the complete graph K_n, it is easily seen that $ABC(K_n) = n\sqrt{\frac{n-2}{2}}$, so either (37) or (38) state that the complete graph is maximal for the ABC index among all graphs. In addition to the maximality of the complete graphs, we can prove another maximal result taking advantage of the literature on the Randić index. Reference [93] mentions that the minimum among trees of $R_{-1}(G)$ is attained by the star graph S_n, and its value is 1. Therefore, (34) implies that for any tree we have that

$$ABC(T) \leq \sqrt{(n-1)(n-2)}. \tag{39}$$

On the other hand, it is not difficult to compute that $ABC(S_n) = \sqrt{(n-1)(n-2)}$, and thus S_n is maximal for the ABC index among trees. This fact can also be shown using (35).

Furthermore, reference [93] founds that the minimum among unicyclic graphs of $R_{-1}(G)$ is attained by the graph S_n^* which consists of the graph S_n with two leaves connected by an edge. Using that $R_{-1}(S_n^*) = \frac{n-2}{n-1} + \frac{1}{4}$ and (35) we get that for unicyclic graphs

$$ABC(G) \leq \sqrt{\frac{n(2n^2 - 7n + 9)}{2(n-1)}}. \tag{40}$$

Notice, however, that in this case we cannot prove that S_n^* is maximal for the ABC index among unicyclic graphs, because $ABC(S_n^*) = (n-3)\sqrt{\dfrac{n-2}{n-1}} + \dfrac{3}{\sqrt{2}}$, which is strictly smaller than the upper bound (40) for $n \geq 4$.

C-cyclic and planar graphs

By applying (37) and (38), we provide the following bounds that improve those Propositions 2 and 3 in [109]:

Proposition 20. *If G is c-cyclic, $c \geq 0$, then*

$$ABC(G) \leq \sqrt{(n-1)\left(n-1+c-\frac{n}{2d_1}\right)}, \tag{41}$$

and

$$ABC(G) \leq \sqrt{n(n-1+c)\left(1-\frac{1}{d_1}\right)}. \tag{42}$$

If G is planar then

$$ABC(G) \leq \sqrt{(n-1)\left(3(n-2)-\frac{n}{2d_1}\right)} \leq \sqrt{\frac{6n^2-19n+2}{2}}. \tag{43}$$

The bound (41) is better than the bound (42) in case $d_1 \geq \dfrac{n(n-1+2c)}{2(n-1+c)}$. Thus (41) provides the better general bound when taking $d_1 = n-1$:

$$ABC(G) \leq \sqrt{(n-1)\left(n-1+c-\frac{n}{2(n-1)}\right)}, \tag{44}$$

There are tight bounds for the ABC index of c-cyclic graphs, for at least $c \leq 4$. For instance, reference [42], through a complex analysis, finds that for any tetracyclic graph with $n \geq 9$ the following tight bound holds:

$$ABC(G) \leq (n-6)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n+2}{5(n-1)}} + 4\sqrt{2}. \tag{45}$$

Our rightmost bound in (44) is slightly worse but asymptotically equivalent to (45): for $n = 10$ the respective values of these bounds are 10.58 and 9.94; for $n = 100$ they are 100.73 and 99.63, etc. Our bound (44) though not optimal, shows a reference value to be improved by any attempt to crack the best bound for c-cyclic graphs for $c \geq 5$.

As expected, for $c = 0$ and $c = 1$, (44) is worse than (39) and (40), respectively.

Chemical graphs

We briefly recall that a chemical graph is a graph with $d_1 \leq 4$. Of the two bounds (37) and (38), for $d_1 = 4$, (38) produces the best bound whenever $n \geq 9$, allowing us to state the following

Proposition 21. *For any chemical graph G with $n \geq 9$ we have*

$$ABC(G) \leq \sqrt{\frac{3n|E|}{4}}.$$

This yields as particular cases the bounds

$$ABC(T) \leq \sqrt{\frac{3n(n-1)}{4}} \tag{46}$$

for chemical trees T with $n \geq 9$,

$$ABC(U) \leq n\sqrt{\frac{3}{4}} \tag{47}$$

for chemical unicyclic graphs U with $n \geq 9$, etc.

Bounds (46) and (47) are roughly of order $.87n$. There are known bounds for the ABC index of c-cyclic chemical graphs, for $c = 0, 1, 2$, slightly better than ours, as in [24] and [61] (their orders are roughly $.79n$), found with laborious procedures that contrast with the simplicity of the proof of proposition 4. Even though proposition 4 may not get the best constants, it shows a path for better bounds of the ABC index to be found in the future for chemical c-cyclic graphs when $c \geq 3$.

It is possible to use majorization in order to find further lower bounds for the Randić index and thus new upper bounds for the ABC index. By using the leftmost inequality in (31) and by gathering a specific information available on the degree sequence of G, we can characterize suitably the set S and derive new different bounds.

The material thus far on the ABC index has been taken from [9]. We want to show now an alternative to the majorization we performed above on the Randić index, and that is to use majorization on the resistances, much as was done in Proposition 23. Then we can show the following

Proposition 22. *For any n-vertex G we have*

$$ABC(G) \leq \sqrt{\frac{d_1^2 - 1}{d_1^2}} \left(\sqrt{k} + \sqrt{\theta} + (|E| - k - 1)\sqrt{\frac{2}{n}} \right), \tag{48}$$

where

$$k = \lfloor \frac{n^2 - n - 2|E|}{n-2} \rfloor \quad \text{and} \quad \theta = n - 1 - k - \frac{2}{n}(|E| - k - 1).$$

This bound is attained by the complete graph K_n.

The upper bound (34) we obtained before is attained by both the complete graph and the star graph S_n. In the case of a tree T, our new bound states that

$$ABC(T) \leq \sqrt{\frac{d_1^2-1}{d_1^2}}(n-1) \leq \sqrt{\frac{(n-1)^2-1}{(n-1)^2}}(n-1) = \sqrt{n(n-2)},$$

so our new bound does not attain the value $ABC(S_n) = \sqrt{(n-1)(n-2)}$.

On the other hand, for a d-regular graph, the bound (34) becomes

$$ABC(G) \leq \sqrt{\frac{d^2-1}{d^2}}\sqrt{n(n-1)\frac{d}{2}},$$

which is worse than our (48) in case

$$\sqrt{n(n-1)\frac{d}{2}} \geq k + \sqrt{\theta} + (\frac{nd}{2} - k - 1)\sqrt{\frac{2}{n}}, \tag{49}$$

where $k = \lfloor\frac{n^2-n(d+1)}{n-2}\rfloor$ and $\theta = n-1-k-\left(d-2\frac{(k+1)}{n}\right)$.

This is easy to achieve if, say, $d=3$ and n is sufficiently large, because if that is the case, then the order of the left hand side of (49) is roughly $\sqrt{\frac{3}{2}}n$ whereas the order of the right hand side is roughly n.

Thus, the comments above show that our new bound and (34) are not comparable. Moreover, the same examples show that our new bound is not comparable to another similar upper bound found in [77]: $ABC(G) \leq \sqrt{|E|(n-2R_{-1}(G))}$.

Yet another upper bound in the literature, obtained in [38], states that

$$ABC(G) \leq p\sqrt{1-\frac{1}{d_1}} + \sqrt{[M_1(G)-2|E|-p(\delta_1-1)]\left(R_{-1}(G)-\frac{p}{d_1}\right)}, \tag{50}$$

where $M_1(G) = \sum_{i\in V} d_i^2$ is the first Zagreb index of G, p is the number of pendent vertices of and δ_1 is the minimal non-pendent degree. In case there are no pendent vertices, this upper bound becomes

$$ABC(G) \leq \sqrt{[M_1(G)-2|E|]\,R_{-1}(G)}. \tag{51}$$

The bound (50) is attained by $(1,\Delta)$-semiregular graphs, specifically by S_n and, as we have mentioned above, our new bound does not attain $ABC(S_n)$. On the other hand, if we consider, for n large and a multiple of 3, the graph G^* to be the symmetric barbell graph, composed of two copies of $K_{\frac{n}{3}}$ attached to each other through a linear graph of length $\frac{n}{3}$, then approximately, $|E| \sim \frac{n^2}{9}$, $k \sim \frac{7}{9}n$, $\theta \sim$ constant, and so asymptotically the bound (48) is equal to $\frac{\sqrt{2}}{9}n^{\frac{3}{2}}$.

Also, for this graph G^* we have $p=0$, $M_1(G^*) \sim \frac{2}{27}n^3$ and $R_{-1}(G^*) \sim \frac{1}{12}n$, so that the bound (51) is asymptotically equal to $\sqrt{\frac{2}{27}n^3\frac{1}{12}n} = \frac{1}{9\sqrt{2}}n^2$.

This shows that our new bound and the one found in [38] are not comparable.

4.2.4 Augmented Zagreb index[5]

The Augmented Zagreb Index of G, defined by

$$AZI(G) = \sum_{(i,j)\in E} \left(\frac{d_i d_j}{d_i + d_j - 2} \right)^3, \tag{52}$$

was introduced by Furtula et al. in [60] as an alternative to the ABC index, with a better predictive power for heat of formation in several compounds. In [60] and [79] a number of properties of this index were proven, among them several lower and upper bounds later improved in [136].

Majorization together with results (8) and (9) have been used to prove a lower bound not comparable to other similar bounds found in the references mentioned.

The proof of the next result is based on ideas that can be traced back to those used in [8] and [130].

Proposition 23. *For any n-vertex G we have*

$$AZI(G) \geq \left(\frac{d_1^2}{d_1^2 - 1} \right)^3 \frac{|E|^4}{(n-1)^3}. \tag{53}$$

This bound is attained by the complete graph K_n.

In the case of the complete graph K_n, $d_1 = n-1$, $|E| = \dfrac{n(n-1)}{2}$ and a bit of algebra shows that both the bound and the actual value $AZI(K_n)$ equal $\dfrac{n(n-1)^7}{16(n-1)^3}$.

Remarks. Our bound is smallest in case the graph is a tree T, when it becomes

$$AZI(T) \geq \left(\frac{d_1^2}{d_1^2 - 1} \right)^3 (n-1) \geq (n-1) \left[\frac{(n-1)^6}{n^3(n-2)^3} \right].$$

This bound, though giving the right order of magnitude, is weaker than those found in [60], [79] and [136] for general and chemical trees.

On the other hand, if we consider the n-vertex graph G_1 to be a complete K_{n-1} to which we add a vertex connected through two edges to two different vertices of the K_{n-1}, then our bound becomes

$$AZI(G_1) \geq \frac{(n-1)^3 \left(\binom{n-1}{2} + 2 \right)^4}{n^3(n-2)^3}$$

which is roughly of order n^5, whereas the lower bound given in theorem 2.8 of [136] becomes for this graph

$$AZI(G_1) \geq |E| \left(\frac{d_n^2}{2d_n - 2} \right)^3 = 2\binom{n-1}{2} + 4.$$

Also, the lower bound given in theorem 2.3 of [136] is not attained by K_n, as ours does. Therefore, these remarks show that our bound is not comparable to those in the cited references.

[5] For details we refer the reader to [118].

4.3 Eigenvalue-based indices

We now deal with a class of topological indices which can be formulated as Schur-convex (Schur-concave) functions of eigenvalues of some particular matrices associated to the graph G, like adjacency, Laplacian, and normalized Laplacian matrices. We present only some of the large number of indices of this kind studied in literature; the methodology to get upper and lower bounds can be easily adapted also to other indices.

4.3.1 Energy index[6]

The *Energy index* [66] is given by

$$E(G) = \sum_{i=1}^{n} |\lambda_i(A)| = \sum_{i=1}^{n} \sqrt{\lambda_i^2(A)}$$

and it is a Schur-concave function of the variables $\lambda_i^2(A), i = 1, \cdots, n$, where $\lambda_i(A)$ are the eigenvalues of the adjacency matrix. It is well known that $\sum_{i=1}^{n} \lambda_i^2(A) = 2m$ and $\lambda_1(A) \geq \frac{2m}{n}$ ([89], [88]).
If a sharper lower bound for $\lambda_1(A)$ is available, i.e. $\lambda_1(A) \geq k(\geq \frac{2m}{n})$, introducing the new variables $x_1 = \lambda_1^2(A)$ arranged in nondecreasing order

$$x_1 \geq k^2 \geq \left(\frac{2m}{n}\right)^2 \geq \frac{2m}{n}.$$

Applying Remark 13 (point III) with $a = 2m$, $h = 1$, $\alpha = k^2$, we get (see [12]) the following upper bound for the Energy index:

$$E(G) \leq k + \sqrt{(n-1)(2m-k^2)}. \tag{54}$$

In a similar way, by the equality $\lambda_1(A) = -\lambda_n(A)$, the following upper bound for bipartite graphs

$$E(G) \leq 2k + \sqrt{(n-2)(2m-2k^2)} \tag{55}$$

has been derived. New bounds for $E(G)$ can be derived as soon as a sharper lower bound of $\lambda_1(A)$ is available.

4.3.2 Laplacian energy[7]

The Laplacian energy was defined first in [73] as

$$LE(G) = \sum_{i=1}^{n} |\lambda_i(L) - d_G|, \tag{56}$$

where $d_G = \dfrac{2|E|}{n}$ is the average degree.

[6]For details we refer the reader to [12].
[7]For details we refer the reader to [115] and [116].

We can obtain a nice upper bound (see [115]) using the fact that the Laplacian eigenvalues are majorized by the degrees $d_1 \geq d_2 \geq \cdots \geq d_n$ of the graph (see the review [3], for instance) as follows:

$$(\lambda_1(L), \ldots, \lambda_n(L)) \trianglelefteq (d_1 + 1, d_2, \ldots, d_{n-1}, d_n - 1). \tag{57}$$

Proposition 24. *For any G we have*

$$LE(G) \geq 2 + \sum_{i=1}^{n} |d_i - d_G|. \tag{58}$$

The equality is attained by the star graph S_n.

The bound (58) improves the one found in [125] where the term 2 is missing.

We notice that the above argument has not used maximal elements. We do so next, using the material in [116].

Besides (58), there are other tight lower bounds for $LE(G)$. In [73] it was shown that

$$LE(G) \geq 2\sqrt{|E| + \frac{1}{2}\sum_{i=1}^{n}(d_i - d_G)^2}, \tag{59}$$

and the equality is attained by the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$. Also, in [146] it was proven that

$$LE(G) \geq 2d_G, \tag{60}$$

where the equality is attained by any regular complete k-partite graph, for $1 \leq k \leq n$. Finally, in [40] it was shown that

$$LE(G) \geq 2(d_1 + 1 - d_G), \tag{61}$$

where the equality is attained by S_n, and more generally, it was argued that for any $1 \leq k \leq n-1$ one has

$$LE(G) \geq 2(\sum_{j=1}^{k} d_j + 1 - kd_G). \tag{62}$$

It is worth to mention that for d-regular graphs, the bounds (58), (59), (60), (61) and (62) become 2, $\sqrt{2nd}$, 2d, 2 and 2, respectively, pointing to their not being comparable.

Now we will find a new general lower bound for the Laplacian energy of graphs satisfying a condition on the largest eigenvalue of their Laplace matrix, and as corollaries we obtain two new non comparable lower bounds for the Laplacian energy of bipartite graphs.

Proposition 25. *For any G, if there is α such that $\lambda_1(L) \geq \alpha \geq d_G\frac{n}{n-1}$ then we have*

$$LE(G) \geq \max\{2d_G, 2(\alpha - d_G)\}. \tag{63}$$

Now we can use a couple of lower bounds for $\lambda_1(L)$ known in the literature in order to find effortlessly two lower bounds for $LE(G)$; the first yields known results, the second is new.

Corollary 26. *(i) For any G we have*

$$LE(G) \geq \max\{2d_G, 2(d_1 + 1 - d_G)\};$$

(ii) For a bipartite G we have

$$LE(G) \geq 4\sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} - 2d_G, \tag{64}$$

and the equality is attained by $K_{\frac{n}{2},\frac{n}{2}}$.

Remarks. The lower bound in (i) implies at once the bounds (60) and (61).

It is obvious that the bounds given by proposition 1 and its corollary are always better than (60), and so we will compare (64) only to (59), (58), (61) and (62). For d-regular graphs, those latter bounds become $\sqrt{2nd}, 2, 2$ and 2, respectively, whereas our new bound becomes $2d$, so (64) is better than (59) if $d \geq \frac{n}{2}$ and worse if $d \leq \frac{n}{2}$, and thus (64) and (59) are not comparable. Also, (64) is better than (58), (61) and (62) for $d \geq 2$, that is, for all regular graphs on 3 or more vertices.

Bound (64) is not comparable to (61) or to (58) because both these bounds attain the equalities for the graph S_n, for which

$$LE(S_n) = \frac{2n^2 - 4n + 4}{n}, \tag{65}$$

whereas (64) becomes

$$LE(G) \geq 4\left(\sqrt{n-1} - \frac{n-1}{n}\right). \tag{66}$$

Bound (62) has a fluctuating behavior: it might improve when k increases, for small values of k, though eventually it starts to get worse, and when $k = n - 1$ it yields

$$LE(G) \geq 2\left(\frac{2|E|}{n} - d_n + 1\right),$$

which is not very good: for instance, in the case of S_n its expression is $LE(S_n) \geq \frac{4(n-1)}{n}$. Incidentally, we could even make (62) work even for $k = n$, when it becomes $LE(G) \geq 2$, which is of course worthless.

For completeness, notice that in the case of S_n, the bound (62) becomes, for $k = 2$ and $k = 3$,

$$LE(S_n) \geq \frac{2n^2 - 6n + 8}{n},$$

and

$$LE(S_n) \geq \frac{2n^2 - 8n + 12}{n},$$

respectively, and although progressively worse than the actual value (65), these bounds are still better than (66) and thus in general (62) and (64) are not comparable.

If we define t_i, the 2-degree of the vertex i, as the sum of the degrees of all the neighbors of i, then for any bipartite graph we have

$$\lambda_1(L) \geq \sqrt{\frac{\sum_{i=1}^{n}(d_i^2 + t_i)^2}{\sum_{i=1}^{n} d_i^2}}, \tag{67}$$

where the equality holds if and only if G is a semiregular bipartite graph. This immediately leads us to the following improvement of (64):

Corollary 27. *For any bipartite graph we have*

$$LE(G) \geq 2\sqrt{\frac{\sum_{i=1}^{n}(d_i^2 + t_i)^2}{\sum_{i=1}^{n} d_i^2}} - 2d_G, \tag{68}$$

where the equality is attained by $K_{\frac{n}{2},\frac{n}{2}}$ and S_n.

Also, in reference [76] they present the lower bound

$$\lambda_1(L) \geq 2 + \sqrt{\frac{1}{|E|}\sum_{u\sim v}(d_u + d_v - 2)^2}, \tag{69}$$

where the equality is attained by either a regular bipartite graph, or a semiregular bipartite graph, or the path with four vertices. Applying the Cauchy-Schwarz inequality we obtain

$$2 + \sqrt{\frac{1}{|E|}\sum_{u\sim v}(d_u + d_v - 2)^2} \geq 2 + \frac{1}{|E|}\sum_{u\sim v}(d_u + d_v - 2)$$

$$= \frac{1}{|E|}\sum_{u\sim v}(d_u + d_v) = \frac{1}{|E|}\sum_{i=1}^{n} d_i^2 = \frac{1}{|E|}\sqrt{\sum_{i=1}^{n} d_i^2}\sqrt{\sum_{i=1}^{n} d_i^2}.$$

Now we apply again the Cauchy-Schwarz inequality to one of the square root expressions and the above is bounded by

$$\frac{1}{|E|}\frac{1}{\sqrt{n}}\left(\sum_{i=1}^{n} d_i\right)\sqrt{\sum_{i=1}^{n} d_i^2} = 2\sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2}.$$

This means that we can improve (64) to

Corollary 28. *For any bipartite graph G we have*

$$LE(G) \geq 4 + 2\sqrt{\frac{1}{|E|}\sum_{u\sim v}(d_u + d_v - 2)^2} - 2d_G, \tag{70}$$

and the equality is attained by $K_{\frac{n}{2},\frac{n}{2}}$ and S_n.

Remarks. Bounds (68) and (70) coincide for all semiregular bipartite graphs (i.e., for all $K_{j,n-j}, 1 \leq j \leq n-1$), but they are not comparable. If we consider the n-gear graph G_n, that is, the n-wheel graph to which add a vertex between each pair of adjacent vertices of the outer cycle, then it is not difficult to see that (68) becomes

$$LE(G_n) \geq 4 + 2\sqrt{\frac{1}{3n}(n(n+1)^2 + 18n)} - 2d_G \sim 4 + \frac{2}{\sqrt{3}}n - 2d_G, \tag{71}$$

whereas (70) becomes

$$LE(G_n) \geq 2\sqrt{\frac{(n^2+3n)^2 + 389n}{n^2+13n}} - 2d_G \sim 2n - 2d_G. \tag{72}$$

So for this family of graphs (70) is better than (68). On the other hand, for the n-path graph P_n, it is easy to see that (68) becomes

$$LE(P_n) \geq 4 + 2\sqrt{\frac{4n-6}{n-1}} - 2d_G, \tag{73}$$

and (70) becomes

$$LE(P_n) \geq 2\sqrt{\frac{32n-70}{2n-3}} - 2d_G. \tag{74}$$

It is an elementary, if tedious, exercise to show that

$$4 + 2\sqrt{\frac{4n-6}{n-1}} > 2\sqrt{\frac{32n-70}{2n-3}},$$

for all $n \geq 3$ and thus for this family of graphs, (68) is better than (70).

The analysis of non comparability of (68) and (70) with respect to (59), (58), (61) and (62) follows as in the previous section for the bound (64) except for the cases when (58) and (61) turn out to be better than (68) and (70). This is achieved if we consider the n-gear graph, for which (61) becomes

$$LE(G_n) \geq 2(n+1) - 2d_G,$$

which is better than (71) and (72). Likewise, for the case of the n-path, (58) becomes

$$LE(P_n) \geq 2 + \frac{4(n-1)}{n},$$

which is clearly better than (73) and (74). Thus the refined bounds (68) and (70) are not comparable to those found in the literature.

4.3.3 Laplacian index [8]

The *Laplacian index* is given by the sum of the α-th power of the non-zero Laplacian eigenvalues ([97], [144])

$$s_\alpha(G) = \sum_{i=1}^{n-1} \lambda_i(L)^\alpha, \alpha \neq 0, 1.$$

[8]For details we refer the reader to [12].

Applying Remark 13 (point III) with $a = 2m, \alpha = 1 + d_1, h = 1$ and taking into account that $\frac{2m}{n-1} \leq (1 + d_1)$, by the Schur-convexity or Schur-concavity of the functions $s_\alpha(G)$ the bounds in [144], Theorem 3, can be easily recovered.

The above bounds can be improved by considering that $\lambda_2(L) \geq d_2$ (see [21]).
In this case, the minimal element can be computed applying the general result of Theorem 12 and the following bounds on $s_\alpha(G)$ hold (see [12]):

Theorem 29. *Let G be a simple connected graph such that $2m \leq 1 + d_1 + (n-2)d_2$,*

1. *if $\alpha < 0$ or $\alpha > 1$ then*

$$s_\alpha(G) \geq (1 + d_1)^\alpha + d_2^\alpha + \frac{(2m - 1 - d_1 - d_2)^\alpha}{(n-3)^{\alpha-1}}$$

2. *if $0 < \alpha < 1$ then*

$$s_\alpha(G) \leq (1 + d_1)^\alpha + d_2^\alpha + \frac{(2m - 1 - d_1 - d_2)^\alpha}{(n-3)^{\alpha-1}}.$$

4.3.4 Normalized Laplacian indices

In the following, we exploit the theoretical method described in Section 3.3 with the aim to provide some formulae that allow us to compute lower bounds for the first and the second eigenvalues of the normalized Laplacian matrix in a fairly straightforward way. These limitations on the eigenvalues are then used to assess bounds for the Normalized Laplacian indices reported in the next. We now present the framework we follow (see [30]) in order to provide new limitations for $\lambda_1(\mathcal{L})$ and $\lambda_2(\mathcal{L})$.

In this regard, we consider Theorem 17 limiting[9] the analysis when $\tau = 2$.
In this case we know indeed that $b = n + 2\sum_{(i,j)\in E} \frac{1}{d_i dj}$. For Lemma 15, when $b = \frac{n^2}{(n-1)}$ the solution of optimization problem $P^*(h)$ is $\left(\frac{n}{n-1}\right)$. This is the case of the complete graph K_n. Instead, when $b \neq \frac{n^2}{(n-1)}$, $h^* = \left\lfloor \frac{n^2}{b} \right\rfloor$.
To get a lower bound Q for $\lambda_1(\mathcal{L})$ for non-complete graphs, we solve equation (24) being $h = 1$. By some basic algebra, the acceptable solution in the proper interval I is equal to

$$Q = \frac{n + \sqrt{\frac{b(h^*+1)-n^2}{h^*}}}{1 + h^*}. \tag{75}$$

We can also derive a lower bound R for $\lambda_2(\mathcal{L})$. We still apply Theorem 17, considering the case $h = 2$. Since $h \leq (h^* + 1)$, we solve the equation (25) finding in the proper interval I the acceptable solution:

$$R = \frac{n - \sqrt{\frac{b(n-1)-n^2}{n-2}}}{n-1}. \tag{76}$$

[9] For values of $\tau \neq 2$, b depends on the graph's structure and topology. So the procedure can be only numerically applied: we need to compute the eigenvalues of normalized Laplacian matrix, but this information allows to directly obtain the index. In this case, the evaluation of bounds is useless.

Normalized Laplacian Index[10] The *Normalized Laplacian index* is defined as:

$$s_\alpha^*(G) = \sum_{i=1}^{n-1} \lambda_i^\alpha(\mathcal{L}), \alpha \neq 0, 1$$

given by the sum of the α-th powers of the non zero normalized Laplacian eigenvalues, first introduced by Bozkurt and Bozkurt in [20] and studied by the authors in [5] and [30].

By considering that $\lambda_1(\mathcal{L}) \geq t_1 \geq \frac{n}{n-1}$, by Remark 13 (point III) with $a = n$, $\alpha = t_1$, $h = 1$ and by the Schur-concavity or Schur-convexity of the function $s_\alpha^*(G)$, the following result holds:

Theorem 30. *Let G be a simple connected graph with $n \geq 3$ vertices.*

1. *If $\alpha < 0$ or $\alpha > 1$ then*
$$s_\alpha^*(G) \geq t_1^\alpha + \frac{(n-t_1)^\alpha}{(n-2)^{\alpha-1}},$$
2. *if $0 < \alpha < 1$ then*
$$s_\alpha^*(G) \leq t_1^\alpha + \frac{(n-t_1)^\alpha}{(n-2)^{\alpha-1}}.$$

By considering

$$t_1 = 1 + \sqrt{\frac{2}{n(n-1)} \sum_{(v_i,v_j)\in E} \frac{1}{d_i d_j}}\,, \tag{77}$$

in virtue of (7), we recover the same bounds as in Theorem 3.3 and 3.7 in [20].

By placing (75) in Theorem 30 we get a new bound for $s_\alpha^*(G)$. In [30], it has been proved that the value of (75) is greater than the value of (77) for non complete graphs, leading to an improvement of the existing bounds.

Taking into account the limitations on first and second eigenvalues of Normalized Laplacian matrix, since the condition $(n-1)Q > n$ is always satisfied we can apply Theorem 12. By the Schur-concavity or Schur-convexity of the function $s_\alpha^*(G)$, we get the following bounds

Theorem 31. *Let G be a simple connected graph with $n \geq 4$ vertices which is not complete and $\lambda_1(\mathcal{L}) \geq Q$, $\lambda_2(\mathcal{L}) \geq R$ with $Q + R(n-2) > n$.*

1. *If $\alpha > 1$ or $\alpha < 0$ then $s_\alpha^*(G) \geq Q^\alpha + R^\alpha + \frac{(n-Q-R)^\alpha}{(n-3)^{\alpha-1}}$;*
2. *If $0 < \alpha < 1$ then $s_\alpha^*(G) \leq Q^\alpha + R^\alpha + \frac{(n-Q-R)^\alpha}{(n-3)^{\alpha-1}}$.*

Considering Theorem 31, it is possible to obtain new bounds for $s_\alpha^*(G)$ by replacing the generic limitations Q and R with (75) and (76). In order to assess these bounds, both conditions of Theorem 31 must be satisfied (see [30] for further details). Notice that, due to Proposition 7, the bounds in the previous theorem perform equal or better than (16) and (17) in [20].

Finally, in case of bipartite graphs, bounds in Theorem 30 and 31 can be improved.

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[10] For details we refer the reader to [5] and [30].

Normalized Laplacian Energy [11] The *normalized Laplacian energy* of a graph, introduced by [22] and studied in [31], is denoted by:

$$NE(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1| \,. \tag{78}$$

In literature, (78) is also known as Randić energy (see [41] and [69]).

$NE(G)$ can be rewritten as a Schur-concave function of the variables $(\lambda_i(\mathcal{L}) - 1)^2$, $i = 1, \cdots, n$:

$$NE(G) = 1 + \sum_{i=1}^{n-1} \sqrt{(\lambda_i(\mathcal{L}) - 1)^2}. \tag{79}$$

If a lower bound for $\lambda_1(\mathcal{L})$ is available, i.e. $\lambda_1(\mathcal{L}) \geq t_1 \left(\geq \dfrac{n}{n-1}\right)$, introducing the new variables $x_i = (\lambda_i(\mathcal{L}) - 1)^2$ as a function of the eigenvalues $\lambda_i(\mathcal{L})$ arranged in non-increasing order, we get:

$$x_1 \geq k_1 = (t_1 - 1)^2 \,.$$

By applying Remark 13 (point III) with $a = 2\sum_{(i,j)\in E} \frac{1}{d_i d_j} - 1$, $\alpha = k_1$, $h = 1$, we derive

$$NE(G) \leq 1 + \sqrt{k_1} + \sqrt{(n-2)\,(a - k_1)}. \tag{80}$$

This bound could be computed by placing $k_1 = (Q-1)^2$, where Q is defined as in (75).

Considering also an additional information on $\lambda_2(\mathcal{L})$ (i.e. $\lambda_2(\mathcal{L}) \geq t_2$), we have $x_2 \geq (t_2 - 1)^2$.

Under the assumptions $t_1 \geq t_2$ and $t_1 + t_2(n-2) > a$, we can provide the bound:

$$NE(G) \leq 1 + \sqrt{k_1} + \sqrt{k_2} + \sqrt{(n-3)\,(a - k_1 - k_2)}, \tag{81}$$

where we can place $k_1 = (Q-1)^2$ and $k_2 = (R-1)^2$ (see (75) and (76))

Finally, for bipartite graphs, taking into account that $\lambda_1(\mathcal{L}) = 2$ and $\lambda_2(\mathcal{L}) \geq t_2$, under the assumption $\dfrac{a-2}{n-2} < t_2 \leq 2$ and we can provide the bound:

$$NE(G) \leq 2 + \sqrt{k_2} + \sqrt{(n-3)\,(a - k_2)}. \tag{82}$$

Normalized Laplacian Estrada index[12] The *normalized Laplacian Estrada index* has been proposed in [91] and it is defined as:

$$NEE(G) = \sum_{i=1}^{n} e^{(\lambda_i(\mathcal{L})-1)} = \frac{1}{e}\sum_{i=1}^{n} e^{\lambda_i(\mathcal{L})}. \tag{83}$$

In [74], an alternative definition of normalized Laplacian Estrada index has been provided:

$$\ell EE(G) = \sum_{i=1}^{n} e^{\lambda_i(\mathcal{L})}. \tag{84}$$

[11] For details we refer the reader to [31].
[12] For details we refer the reader to [31].

Notice that $NEE(G) = \frac{1}{e}\ell EE(G)$, any results derived for $NEE(G)$ can be trivially re-stated for $\ell EE(G)$ and viceversa.

Considering a limitation on $\lambda_1(\mathcal{L})$ ($\lambda_1(\mathcal{L}) \geq t_1 \geq \frac{n}{n-1}$, by means of Remark 13 (point III) with $a = n$, $\alpha = t_1$, $h = 1$, by the Schur-convexity of the function $NEE(G)$, we get the following bound:

$$NEE(G) \geq \frac{1}{e} + e^{t_1-1} + (n-2)e^{\frac{2-t_1}{n-2}}. \tag{85}$$

Setting $t_1 = \dfrac{n}{n-1}$, the authors in [31] derived the same result proved in [91], Theorem 3.1:

$$NEE(G) \geq (n-1)\, e^{\dfrac{1}{n-1}} + \frac{1}{e}. \tag{86}$$

Furthermore, (85) can be computed by using the lower bound Q (see (75)) for $\lambda_1(\mathcal{L})$. It has been shown in [30] that $Q \geq \frac{n}{n-1}$ and thus we assure that bound (85), by placing $t_1 = Q$, is sharper than (86) (see [12] and [13] for more theoretical details).

In a similar way, by the additional information $\lambda_2(\mathcal{L}) \geq t_2$, under the assumptions $t_1 \geq t_2$ and $t_1 + t_2(n-2) > n$, we can provide the following bound:

$$NEE(G) \geq \frac{1}{e} + e^{t_1-1} + e^{t_2-1} + (n-3)e^{\frac{3-t_1-t_2}{n-3}}. \tag{87}$$

By placing $t_2 = R$ (see (76)), it is possible to compute bound (87) that is tighter than (85) with $t_1 = Q$ and (86) (see [13], [12] and [30]).

Finally, for bipartite graphs, we can provide the following bound:

$$NEE(G) \geq \frac{1}{e} + e + e^{t_2-1} + (n-3)e^{\frac{1-t_2}{n-3}}, \tag{88}$$

where the lower bound $t_2 = R$ of $\lambda_2(\mathcal{L})$ derived in [30] can be also used to compute (88).

4.3.5 HOMO-LUMO index [13]

Median eigenvalues of the adjacency matrix of a molecular graph are strictly related to orbital energies and molecular orbitals. In this regard, the difference between occupied orbital of highest energy (HOMO) and unoccupied orbital of lowest energy (LUMO) has been investigated (see [58]). Motivated by the HOMO-LUMO separation problem, Jaklič et al. in [82] proposed the notion of HL-index that measures how large in absolute value are the median eigenvalues of the adjacency matrix.
The eigenvalues involved in the HOMO-LUMO separation are $\lambda_H(A)$ and $\lambda_L(A)$, where $H = \lfloor \frac{n+1}{2} \rfloor$ and $L = \lceil \frac{n+1}{2} \rceil$.

The HL-index of a graph is defined in [82] as:

$$HL(G) = \max\left(|\lambda_H(A)|, |\lambda_L(A)|\right).$$

Median eigenvalues of the normalized Laplacian matrix can be localized by applying the methodology recalled in Section 3.3. The additional information on median eigenvalues and the interlacing

[13] For details we refer the reader to [29].

between eigenvalues of normalized Laplacian and adjacency matrices turned out to be a handy tool for bounding the HL-index for both non-bipartite and bipartite graphs. According to [22] (see Theorem 2.2.1), the following relations hold:

$$\frac{|\lambda_{n-k+1}(A)|}{d_1} \leq |1-\lambda_k(\mathcal{L})| \leq \frac{|\lambda_{n-k+1}(A)|}{d_n}. \tag{89}$$

In [29], in virtue of (89) and by applying Theorems 16 and 17, the following propositions have been proved (for further details see [29]).

Proposition 32. *For a simple, connected and non-bipartite graphs*

$$0 \leq HL(G) \leq d_1 \max\left(|1-\alpha_1|, |1-\beta_1|, |1-\alpha_2|, |1-\beta_2|\right) \tag{90}$$

when n is even with

$$\alpha_1 = \frac{1}{n-1}\left(n+\sqrt{\frac{n-2}{n}\left(b_1(n-1)-n^2\right)}\right), \beta_1 = \frac{1}{n-1}\left(n-\sqrt{\frac{n-2}{n}\left(b_1(n-1)-n^2\right)}\right),$$

$$\alpha_2 = \frac{1}{n-1}\left(n+\sqrt{\frac{(n-4)}{(n+2)}(b_1(n-1)-n^2)}\right), \beta_2 = \frac{n}{n-1}\left(1-\sqrt{\frac{b_1(n-1)-n^2}{n(n-2)}}\right)$$

and

$$0 \leq R(G) \leq d_1 \max\left(|1-\alpha_3|, |1-\beta_3|\right) \tag{91}$$

when n is odd with

$$\alpha_3 = \frac{1}{n-1}\left(n+\sqrt{\frac{(n-3)}{(n+1)}(b_1(n-1)-n^2)}\right), \beta_3 = \frac{1}{n-1}\left(n-\sqrt{b_1(n-1)-n^2}\right),$$

where $b_1 = \sum_{i=1}^{n-1} \lambda_i^2(\mathcal{L}) = n + 2\sum_{(i,j)\in E} \frac{1}{d_i d_j}$.

Proposition 33. *For a simple, connected and bipartite graphs with n even we have:*

$$0 \leq HL(G) \leq d_1|1-\beta_1^{bip}| \tag{92}$$

where

$$\beta_1^{bip} = 1 - \sqrt{\frac{b_2}{n-2} - 1},$$

where $b_2 = \sum_{i=2}^{n-1} \lambda_i^2(\mathcal{L}) = n + 2\sum_{(i,j)\in E} \frac{1}{d_i d_j} - 4$.

In the following we obtain bounds on HL-index starting from relation

$$0 \leq HL(G) \leq \frac{E(G)}{n}, \tag{93}$$

provided in [92]. In virtue of relation (93) and by means of bounds (54) and (55) on the Energy index, we are now able to derive the following bounds for non-bipartite and bipartite graphs respectively.

Proposition 34.

1. *For a simple, connected and non-bipartite graph G:*

$$HL(G) \leq \frac{k}{n} + \frac{1}{n}\sqrt{(n-1)(2m-k^2)}; \tag{94}$$

2. *For a simple, connected and bipartite graph G:*

$$HL(G) \leq \frac{2k}{n} + \frac{1}{n}\sqrt{(n-2)(2m-2k^2)}, \tag{95}$$

where, by means of Theorem 17,

$$k = \frac{1}{1+h^*}\left(n + \sqrt{\frac{2m(1+h^*)-n^2}{h^*}}\right), h^* = \left\lfloor \frac{n^2}{2m} \right\rfloor.$$

In [29], it has been analytically proved that bounds (94) and (95) are tighter than or equal to bounds provided in [92].

4.4 Resistance-based indices

Among the various indices in Mathematical Chemistry, those indices based on the effective resistance R_{ij} between the node i and j of a connected undirected graph $G = (V, E)$ have received a lot of attention in the literature. The resistance indices, namely the Kirchhoff index and its generalizations, have undergone intense scrutiny in recent years because they have proven to be useful in discriminating among chemical molecules according to their cyclicity. A variety of techniques have been used, including graph theory, algebra (the study of the Laplacian and of the normalized Laplacian), electric networks, probabilistic arguments involving hitting times of random walks, and discrete potential theory (equilibrium measures and Wiener capacities), among others. The references that follow are a sample, by no means exhaustive, of these diverse techniques, whose end results usually follow either of these two paths: on the one hand, exact values for the index are obtained for graphs endowed with some form of symmetry or special property ([4], [62], [107], [132]). On the other hand, general bounds for the resistance indices, not containing effective resistances but a few invariants such as $|V|$, $|E|$, the degrees d_i etc., and sometimes extremal graphs, are found for specific families of graphs, as in [108], [118], [119], [133], [135], [148] and [150].

In what follows we adopt this latter approach, finding upper and lower bounds by using majorization techniques. The application of the majorization relies on the fact that these indices can be written as Schur-convex functions whose variables are eigenvalues of particular matrices as well as vertices degrees of the graphs. This subsection deals with the *Kirchhoff index* and some of its modifications, namely the *Multiplicative degree-Kirchhoff index* and the *Additive degree-Kirchhoff index*. Furthermore the *weighted global cyclicity index* will be discussed finding upper and lower bounds through the weighted majorization technique.

4.4.1 Kirchhoff index [14]

The Kirchhoff index $R(G)$ of a simple connected graph $G = (V, E)$ was defined by Klein and Randić in [87] as

$$R(G) = \sum_{i<j} R_{ij}, \tag{96}$$

where R_{ij} is the effective resistance between vertices i and j, which can be computed using Ohm's law. In addition to its original definition, it was shown in [70] and [151] that

$$R(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i(L)}, \tag{97}$$

where $\lambda_i(L)$ are the non-zero eigenvalues of the Laplacian matrix L.

If G is d-regular, then $L = dI - A$, $P = D^{-1}A = I - \frac{1}{d}L$ and

$$\lambda_{n-i+1}(P) = 1 - \frac{\lambda_i(L)}{d} \qquad i = 1, ..., n. \tag{98}$$

In this case, from (97), the alternative expression

$$R(G) = \frac{n}{d} \sum_{i=2}^{n} \frac{1}{1 - \lambda_i(P)}$$

in terms of the eigenvalues of the transition matrix P holds ([117]).
In case G is arbitrary, we do not have such a compact expression, but still we have the bounds given in [119], Corollary 2:

$$\left(\frac{n}{d_1}\right) \sum_{i=2}^{n} \left(\frac{1}{1 - \lambda_i(P)}\right) \leq R(G) \leq \left(\frac{n}{d_n}\right) \sum_{i=2}^{n} \left(\frac{1}{1 - \lambda_i(P)}\right). \tag{99}$$

All these expressions of $R(G)$ in terms of sums of inverses of eigenvalues can be used to find upper and lower bounds, as was done in [117], [148] and [150].

In [6] in order to get bounds for $R(G)$, the authors applied the majorization technique to the summations in (99).

We briefly recall the main results obtained in [6].

Lower bounds

Case 1): Assume to know that:

$$\lambda_n(P) \leq -\beta < 0,$$

then

$$R(G) \geq \frac{n}{d_1} \left[\frac{1}{1+\beta} + \frac{(n-2)^2}{n-1-\beta}\right]. \tag{100}$$

[14] For details we refer the reader to [6], [8], [28], [32], [110], [112], [117] and [119].

Case 2): Assume now that

$$\lambda_2(P) \geq \beta > 0. \tag{101}$$

then

$$R(G) \geq \frac{n}{d_1}\left[\frac{1}{1-\beta} + \frac{(n-2)^2}{n-1+\beta}\right]. \tag{102}$$

Now we exploit Case 1 above in order to get a general lower bound. In Section 2.2 we recall that for every matrix M with real eigenvalues $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ the following inequality is well-known

$$\lambda_n(M) \leq \mu - \frac{\sigma}{\sqrt{n-1}} \tag{103}$$

where $\mu = \frac{\mathrm{tr}(M)}{n}$ and $\sigma^2 = \frac{\mathrm{tr}(M^2)}{n} - \left(\frac{\mathrm{tr}(P)}{n}\right)^2$.

If M is a transition matrix P of a connected graph G, we observe that $\mathrm{tr}(P) = 0$ and $\mathrm{tr}(P^2) = 2\sum_{(v_i,v_j)\in E} \dfrac{1}{d_i d_j}$. Then $\mu = 0$ and

$$\sigma^2 = \frac{2}{n}\sum_{(v_i,v_j)\in E}\frac{1}{d_i d_j} = \left(\frac{2}{n}\right) R_{-1}(G).$$

Moreover, by the equality

$$\sigma^2 = \frac{\mathrm{tr}(P^2)}{n} = \frac{1+\sum_{i=2}^{n}\lambda_i^2}{n}$$

and the conditions on the eigenvalues of P, it easily follows that P has at least one eigenvalue whose absolute value is less than one. This gives $\sigma^2 < 1$. Notice that the upper bound $\sigma = 1$ is attained by any disconnected graph with an even number n of vertices and $\dfrac{n}{2}$ connected components , each of which of order two. In this case, the spectrum of P is $\left\{\underbrace{-1,-1,...,-1}_{n/2},\underbrace{1,1,.....1}_{n/2}\right\}$ and consequently $\sigma = 1$.

It is also worth noting that $\frac{1}{n-1}$ is the minimal value attainable by σ^2 among all connected graph of order n.

Applying now (100) with $\beta = \frac{\sigma}{\sqrt{n-1}}$, we get the following

Proposition 35. *([6]) For any simple connected graph G*

$$R(G) \geq \frac{n}{d_1}\left[\frac{1}{1+\frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n-1-\frac{\sigma}{\sqrt{n-1}}}\right]. \tag{104}$$

The next proposition contributes to show that the new bound (104) always performs better than well-known bound provided in [119] (Corollary 4) except in the case where $G = K_n$ for which the two bounds coincide.

Proposition 36. *([6]) Let G be a simple connected graph on n vertices, with $n \geq 3$. The lower bound of $R(G)$ in (104) is an increasing function of σ for $\dfrac{1}{\sqrt{n-1}} \leq \sigma < 1$, where the equality in the left side holds if and only if $G = K_n$.*

The new bound (104) always performs better than the well-known bound provided in [119], Corollary 4. More details may be found in [6].

Upper bounds

For a $d-$regular graph, Palacios in [117] found the following upper bound where, for simplicity, we write $\lambda_2(P) = \lambda_2$:

$$R(G) \leq \frac{n(n-1)}{d(1-\lambda_2)}. \tag{105}$$

The quantity $(1-\lambda_2)$ is known as *spectral gap*. It is noteworthy to underline that the bound (105) holds in general, for $d = d_n$, as can be seen from the r.h.s. (99).

By applying our procedure, it is possible to get an upper bound in terms of the spectral gap .

By using now (99) we get the following

Proposition 37. *([6]) For any simple connected graph G we have*

$$R(G) \leq \frac{n}{d_n}\left(\frac{n-k-2}{1-\lambda_2} + \frac{k}{2} + \frac{1}{\theta}\right), \tag{106}$$

where

$$k = \left\lfloor \frac{\lambda_2(n-1)+1}{\lambda_2+1} \right\rfloor \quad \textit{and} \quad \theta = \lambda_2(n-k-2) - k + 2.$$

The Kirchhoff index spawned a family of resistance indices such as the *Multiplicative degree-Kirchhoff index and the Additive degree-Kirchhoff index.* Here is another brief illustration of the majorization method applied to these indices.

4.4.2 Multiplicative degree-Kirchhoff index[15]

The Multiplicative degree-Kirchhoff index, proposed by Chen and Zhang in [25], is defined as

$$R^*(G) = \sum_{i<j} d_i d_j R_{ij}.$$

This index was looked at in [119], where the following expression in terms of the eigenvalues of the transition matrix P was given:

$$R^*(G) = 2|E| \sum_{j=2}^{n} \frac{1}{1-\lambda_j(P)}. \tag{107}$$

Furthermore, it was shown that

$$R^*(G) \geq \frac{2|E|(n-1)^2}{n}, \tag{108}$$

which is basically bound provided in [119] (Corollary 4), after replacing $\frac{n}{d_1}$ with $2|E|$. An upper bound of order n^5 for this index that is attained (up to the constant of the leading term) by the barbell graph was provided in [119] also. With electrical network techniques, the lower bound was improved in [118] to

$$R^*(G) \geq 2|E|\left(n-2+\frac{1}{d_1+1}\right). \tag{109}$$

[15]For details we refer to [6], [8], [111], [118] and [119].

It is clear, by looking at the expression (107), that we can obtain new upper and lower bounds for $R^*(G)$ by using the bounds on $R(G)$. Among these we mention explicitly the following results.

Proposition 38. *([6]) For any simple connected graph G we have*

$$R^*(G) \geq 2|E| \left[\frac{1}{1+\frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n-1-\frac{\sigma}{\sqrt{n-1}}} \right]. \tag{110}$$

This bound improves (109) if G has at least one vertex with degree $n-1$.

The only thing left to show is that (110) improves (109) under the given condition, which is clear because in that case (109) becomes (108), which is always less than (110).

Now we will give a general upper bound for this descriptor that gets us closer to the value $\frac{2}{243}n^5$ obtained for the barbell graph. The proof is inspired in that of an upper bound for the additive degree-Kirchhoff index found in [131].

Proposition 39. *For an n-vertex G we have*

$$R^*(G) \leq (n-1)^4 \quad \text{for } n \leq 48,$$

and

$$R^*(G) \leq \frac{n^5+50n^3-164n^2+165n-52}{54}, \quad \text{for } n \geq 49.$$

4.4.3 Additive degree-Kirchhoff index[16]

Gutman et al. defined in [68] the *Additive degree-Kirchhoff index* as

$$R^+(G) = \sum_{i<j} (d_i + d_j) R_{ij}, \tag{111}$$

and worked on the identification of graphs with lowest such degree among unicyclic graphs.

The additive degree Kirchhoff index is motivated by the degree distance of a graph as defined by Dobrynin and Kochetova in ([46]. It coincides with the additive degree-Kirchhoff index whenever the graph is a tree, and the former is always greater than or equal to the latter, because $d(i,j) \geq R_{ij}$ holds for any i, j in any graph G (see ([46] for other details).

It was shown in [108], using Markov chain theory, that for any graph G

$$R^+(G) \geq 2(n-1)^2, \tag{112}$$

and the lower bound is attained by the complete graph. Also, in [108] it was shown that for any G

$$R^+(G) \leq \frac{1}{3}(n^4 - n^3 - n^2 + n),$$

[16]For details we refer the reader to [7] and [108].

and it was conjectured that the maximum of $R^+(G)$ over all graphs is attained by the $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ barbell graph, which consists of two complete graphs on $\frac{n}{3}$ vertices united by a path of length $\frac{n}{3}$, and for which $R^+(G) \sim \frac{2}{27}n^4$. This conjecture was shown to be true asymptotically by Ilic and Ilic in [81].

We show next how majorization can be applied to bound the additive degree-Kirchhoff index. This approach can be pursued if we can identify a set of variables with constant sum and a Schur-convex function f to be optimized on the set S of these variables. In this case we know that the global minimum (maximum) of f is attained at the minimum (maximum) element of the set S with respect to the majorization order. For the detailed proof, we refer the reader to [7].

Theorem 40. *([7]) For any graph G with degree sequence $d_1 \leq d_2 \leq \cdots \leq d_n$, let*

$$\sum_{i<j} \frac{d_j}{d_i} = H. \tag{113}$$

Then

$$R^+(G) \geq n(n-3) + H + \left[\frac{n(n-1)}{2}\right]^2 \frac{1}{H}. \tag{114}$$

Majorization is also the main argument in yet another possible approach for obtaining lower bounds. In reference [108] it was shown that the following relationship between the additive and multiplicative degree-Kirchhoff indices holds :

$$R^+(G) = \frac{n}{2|E|} R^*(G) + \sum_{i,j} \pi_i E_i T_j, \tag{115}$$

where $E_i T_j$ is the expected value of the number of steps T_j that the random walk on G, started from vertex i, takes to reach vertex j. We recall that this random walk moves from a vertex v to any neighboring vertex w with uniform probabilities $p(v,w) = \frac{1}{d_v}$ and that the $n \times n$ matrix $P = [p(v,w)]$ of transition probabilities has a unique probabilistic left eigenvector $\pi = (\pi_i)$ (the stationary distribution), which is present in the summation in (115), and a spectrum $1 = \lambda_1 > \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_n \geq -1$ in terms of which $R^*(G)$ can be expressed as in (107) ([119]). With the preceding remarks and notation in [7] the authors proved the following result

Theorem 41. *For any graph G*

$$R^+(G) \geq n \left[\frac{1}{1 + \frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n-1-\frac{\sigma}{\sqrt{n-1}}}\right] + (n-1)^2, \tag{116}$$

We remark that we recover the universal bound (112) for the complete graph, for which $\sigma = \frac{1}{\sqrt{n-1}}$, and for all other graphs the bound is better than the universal one (112) (for details see [6]).

Finally, we turn to the analysis of some significant upper bounds which can be obtained by combining ideas from Markov chains and majorization. These bounds can be suitable expressed in terms of the spectral gap.

Recall that from (115) and subsequent comments we have

$$R^+(G) = \frac{n}{2|E|}R^*(G) + \sum_{j=1}^{n}\sum_{i=1}^{n}\pi_i E_i T_j = n\sum_{i=2}^{n}\frac{1}{1-\lambda_i} + \sum_{j=1}^{n}\sum_{i=1}^{n}\pi_i E_i T_j. \tag{117}$$

We want to find an upper bound for the summation with the hitting times in (117), for which we use some Markov chain theory found in reference [100], specifically:

$$\sum_i \pi_i E_i T_j = \frac{1}{\pi_j}\sum_{k=2}^{n}\frac{1}{1-\lambda_k}v_{kj}^2, \tag{118}$$

where v_{kj} is the j-th component of the eigenvector v_k associated to the eigenvalue λ_k (the vectors v_k can be chosen to be orthonormal), and

$$\sum_{k=2}^{n} v_{kj}^2 = 1 - \pi_j.$$

It is clear that (118) can be bounded as follows:

$$\frac{1}{\pi_j}\sum_{k=2}^{n}\frac{1}{1-\lambda_k}v_{kj}^2 \le \frac{1}{(1-\lambda_2)\pi_j}\sum_{k=2}^{n}v_{kj}^2 = \frac{1}{1-\lambda_2}\frac{1-\pi_j}{\pi_j}.$$

And so the sum of expected hitting times can be bounded as:

$$\sum_{j=1}^{n}\sum_{i=1}^{n}\pi_i E_i T_j \le \frac{1}{1-\lambda_2}\sum_j \frac{1-\pi_j}{\pi_j} = \frac{1}{1-\lambda_2}(2|E|\sum_j\frac{1}{d_j} - n).$$

Now use in (117) the upper bounds in [6] Section 3.2 for $\sum_{i=2}^{n}\frac{1}{1-\lambda_i}$, to obtain the following corollaries:

Corollary 42. *([7]) For any G we have*

$$R^+(G) \le n\left(\frac{n-k-2}{1-\lambda_2} + \frac{k}{2} + \frac{1}{\theta}\right) + \frac{1}{1-\lambda_2}(2|E|\sum_j\frac{1}{d_j} - n), \tag{119}$$

where $k = \left\lfloor \dfrac{\lambda_2(n-1)+1}{\lambda_2+1} \right\rfloor$ *and* $\theta = \lambda_2(n-k-2) - k + 2$.

Corollary 43. *([7]) For any bipartite G we have*

$$R^+(G) \le n\left(\frac{1}{2} + \frac{n-k-3}{1-\lambda_2} + \frac{k}{2} + \frac{1}{\theta}\right) + \frac{1}{1-\lambda_2}(2|E|\sum_j\frac{1}{d_j} - n), \tag{120}$$

where k and θ are defined above.

For the n-star graph we have that $\lambda_2 = 0$, $k = 1$ and $\theta = 1$ and therefore the bound (120) becomes $3n^2 - 7n + 4$ and the actual value is attained. This can be extended to the complete bipartite graph $K_{r,s}$, for arbitrary r, s, for which the bound (120) becomes

$$3r^2 + 3s^2 + 2rs - 3r - 3s, \tag{121}$$

whose order is always n^2, and improves the bound $2|E|(n-1)D = 4rs(r+s-1)$. The smallest value of (121) occurs for $r = s = \frac{n}{2}$, where it takes the value $n(2n-3)$, which is equal to the actual value of $R^+(G)$.

4.4.4 Some interplay of the three Kirchhoffian indices[17]

It is to be expected that the similarities in the definitions of the three Kirchhoffian indices will result in some equations involving two or three of them together. We explore that topic in this section.

One such relation is (115), that we may rewrite as

$$R^+(G) \geq \frac{n}{2|E|} R^*(G) + (n-1)^2. \tag{122}$$

Another such relation is given in the following

Proposition 44.

$$\frac{2}{d_n} R^*(G) \geq R^+(G) \geq \frac{2}{d_1} R^*(G). \tag{123}$$

Equations (122) and (123) together with lower bounds for $R^*(G)$ furnish new lower bounds for $R^+(G)$. For instance, using (137) we get the bounds

$$R^+(G) \geq n(n-2)^2 + (n-1)^2 + \frac{n(n-1)}{2|E|},$$

and

$$R^+(G) \geq \frac{2}{d_1}[n - 1 + 2|E|(n-2)].$$

With the notation $d_G = \dfrac{2|E|}{n}$ (that is the *average degree*) and starting again from (115) we can prove the relations

$$\frac{1}{d_G} R^*(G) + d_n R(G) \leq R^+(G) \leq \frac{1}{d_G} R^*(G) + d_1 R(G). \tag{124}$$

and

$$\left(\frac{1}{d_G} + \frac{1}{d_1}\right) R^*(G) \leq R^+(G) \leq \left(\frac{1}{d_G} + \frac{1}{d_n}\right) R^*(G). \tag{125}$$

In [150] they found this set of inequalities:

$$d_G d_n R(G) \leq R^*(G) \leq d_G d_1 R(G). \tag{126}$$

In [131] and [80] they came up, almost simultaneously, with the same idea of expressing

$$R^+(G) = d_G R(G) + n\mathrm{trace}(\mathbf{D}\mathbf{L}^{\#}), \tag{127}$$

where $\mathbf{L}^{\#}$ is Moore-Penrose inverse of $\mathbf{L}$. Using this characterization, these authors proved the inequalities

$$(d_n + d_G)\, R(G) \leq R^+(G) \leq (d_1 + d_G)\, R(G). \tag{128}$$

It is clear that (123), (124), (125), (126) and (128) are variations on the same theme of the interplay of the three Kirchhoffian indices, and we can use bounds for one of the indices in order to get bounds for another index.

[17] For details we refer the reader to [113] and [114].

In [114], starting again from (115), we were able to write

$$R^{+}(G)=\frac{1}{d_G}R^{*}(G)+2|E|\sum_{i=1}^{n}\frac{1}{\nu_i}-n, \tag{129}$$

where the ν_is are the eigenvalues of the *modified Laplacian matrix*

$$\mathbf{L}+\frac{1}{2|E|}\mathbf{DOD},$$

where $\mathbf{D}$ is the diagonal matrix whose diagonal values equal those of the diagonal of $\mathbf{L}$, and $\mathbf{O}$ is the $n\times n$ matrix of all whose entries are ones. Since $R^{*}(G)$ can be expressed in terms of the eigenvalues of the normalized Laplacian matrix, (129) is a representation of $R^{+}(G)$ in terms of the Laplacian matrix $\mathbf{L}$, as an alternative to the representation given in (127) in terms of the Moore-Penrose inverse of $\mathbf{L}$. Using the interlacing of the eigenvalues of $\mathbf{L}$ and those of $\mathbf{L}+\frac{1}{2|E|}\mathbf{DOD}$ it was shown in [114] that the following bound holds for any G:

$$\begin{aligned}R^{+}(G)\geq&\frac{R^{*}(G)}{d_G}+d_GR(G)\\&+\frac{2|E|}{d_n+\frac{1}{2}+\sqrt{(d_n-\frac{1}{2})^2+\sum_{i+1}^{n}d_i(d_i-d_n)}+\frac{1}{2|E|}\sum_{i=1}^{n}d_i^2}-n.\end{aligned} \tag{130}$$

Also it was shown that the new bound (130) improves the lower bounds in (124), (125) and (128).

For additional information the reader may check [113] and [114].

4.4.5 Weighted topological index[18]

In [86], by means of the concept of effective resistances, the global cyclicity index has been proposed:

$$C(G)=\sum_{(i,j)\in E}\frac{1}{R_{ij}}-m. \tag{131}$$

Yang in [130] studied this new cyclicity measure for connected graphs. Following Bianchi et al. ([13], [12]) and computing the extremal values of the Schur-convex function $f(R_{ij})=\sum_{(i,j)\in E}\dfrac{1}{R_{ij}}$ on the set

$$S=\left\{R_{ij}\in\mathbb{R}^m:\sum_{(i,j)\in E}R_{ij}=n-1,\frac{2}{n}\leq R_{ij}\leq 1\right\},$$

he obtained the following bounds for $C(G)$:

$$\frac{m(m-n+1)}{n-1}\leq C(G)\leq\frac{n(m-n+1)}{2}, \tag{132}$$

where $(m-n+1)$ is the well known cyclomatic number of a graph (see Theorem 3.13, 3.15 and Corollary 3.14 in [130]).

[18]For details we refer the reader to [9].

In [9] the authors defined the *weighted global cyclicity index* for a general network as:

$$CW(G) = \sum_{(i,j)\in E} \left(\frac{1}{R_{ij}} - \frac{1}{r_{ij}} \right),$$

where a resistance r_{ij}, $k \le r_{ij} \le K$ is associated to any edge.
Notice that the weighted global cyclicity index is a natural extension of the global cyclicity index (131), which can be recovered when $r_{ij} = 1$ for all $(i,j) \in E$.
Setting $x_{ij} = \dfrac{R_{ij}}{\sqrt{r_{ij}}}$ and $p_{ij} = \dfrac{1}{\sqrt{r_{ij}}}$, the weighted global cyclicity index can be written as a function of x_{ij} and p_{ij} as follows:

$$CW(G) = f(x_{ij}, p_{ij}) = \sum_{(i,j)\in E} \left(\frac{p_{ij}}{x_{ij}} - p_{ij}^2 \right).$$

Indeed, the weighted majorization technique proposed in Section 3 can be a fruitful tool to bound the weighted global cyclicity index, throughout the $p-$Schur convex functions.
The choice of the variables and of the weights, taking into account Theorem 3, assures that the function f is p-Schur convex, being

$$(x_{ij} - x_{i'j'}) \left(\frac{1}{p_{ij}} \frac{\partial f}{\partial x_{ij}} - \frac{1}{p_{i'j'}} \frac{\partial f}{\partial x_{i'j'}} \right) = \frac{(x_{ij} - x_{i'j'})^2 (x_{ij} + x_{i'j'})}{x_{ij}^2 x_{i'j'}^2} \ge 0$$

for all $(i,j), (i',j') \in E$.

Remark 45. Note that other possible choices of the variables and of the weights are not fruitful:

1. if we use $x_{ij} = R_{ij}$ as variables and $p_{ij} = \dfrac{1}{r_{ij}}$ as weights, the function $CW(G)$ is not p-Schur-convex.
2. if we use $x_{ij} = \dfrac{R_{ij}}{r_{ij}}$ as variables and $p_{ij} = 1$ as weights, the function $CW(G)$ is not Schur-convex.

We can now state the main result in [9].

Theorem 46. *Let $G = (V, E)$ a connected network with n vertices and m edges. Let r_{ij}, $k \le r_{ij} \le K$, be the resistances associated to any edge $(i,j) \in E$ and let*

$$C = \sum_{(i,j)\in E} \frac{1}{r_{ij}}, \qquad C' = \sum_{(i,j)\in E} \frac{1}{\sqrt{r_{ij}}}, \qquad C'' = \max \left\{ \frac{nK}{2k}, \frac{\sqrt{k}}{\sqrt{K}} + \frac{n\sqrt{K}}{2k\sqrt{k}} - \frac{1}{K} \right\}.$$

Then

$$\frac{(C')^2}{n-1} - C \le CW(G) \le C'' + \left(\frac{n\sqrt{K}}{2k} + \frac{\sqrt{k}}{K} \right) C' - \frac{n}{2k} - \frac{n^2 - n}{2\sqrt{k}\sqrt{K}} - C. \tag{133}$$

4.4.6 The electric viewpoint

The main theme of previous subsections has been majorization, though some other themes have been played along the way. In particular, we have used ideas from electric networks, not only in the framework of the Kirchhoffian descriptors that deal precisely with effective resistances between vertices, but also in descriptors such as the AZI index and the ABC index. Here we present a handful of additional electrical derivations that show the power of having different approaches to the subject matter.

The Kirchhoff index for graphs with diameter 2 The monotonicity law described in subsection 2.3 together with Foster's first law implies the following proposition which is well known (see [103] for an elaborate argument or [140] for a shorter proof with Laplacian eigenvectors) but whose brief electrical proof we include here for the sake of completeness:

Proposition 47. *The Kirchhoff index is strictly monotonic in the number of edges: if G' is the graph which results from adding a new edge to a graph G, then $R(G') < R(G)$.*

Proof. By definition

$$R(G) = S_1 + S_2 + S_3 + \cdots ,$$

where $S_k = \sum_{i<j:d(i,j)=k} R_{ij}$, for $k \geq 1$, $d(i,j)$ is the distance between i and j, and all but a finite number of summations S_k are not equal to zero.

When we add an edge to G in order to form G', and we compute $R(G') = S_1' + S_2' + S_3' + \cdots$, the number of summands in S_1' increases by 1 with respect to S_1 but the value of the sum stays the same: $S_1 = S_1' = n - 1$. However, at least one of the sums $S_2', S_3', \ldots$, loses one nonzero summand while all others, by the monotonicity law, are kept bounded by the corresponding summands in $S_2, S_3, \ldots$, and thus

$$R(G) = n - 1 + S_2 + S_3 + \cdots > n - 1 + S_2' + S_3' + \cdots = R'(G).$$

□

It is plain that for any graph G with diameter 2 we have

$$R(G) = n - 1 + S_2. \tag{134}$$

The idea now is to express $S_2 = \sum_{i<j:d(i,j)=2} R_{ij}$ in terms of (11). In that direction we first prove the following

Proposition 48. *For any graph G we have*

$$S_2 \leq d_1(n-2). \tag{135}$$

If G is geodetic (i.e., for every pair of vertices of G at distance 2 there is a single common neighboring vertex) and does not have any triangles then

$$S_2 \geq d_n(n-2). \tag{136}$$

Now we will exhibit the extremal graphs under consideration

Proposition 49. *If G has diameter equal to 2 then*

$$n - 1 + \frac{2}{n-2} \leq R(G) \leq (n-1)^2.$$

The upper bound is attained if and only if $G = S_n$, the n-star graph. The lower bound is attained if and only if $G = K_n^-$, the graph obtained deleting one edge from the complete graph K_n.

More results on this topic may be found in [110].

Another lower bound for the multiplicative degree-Kirchhoff index

Proposition 50. *For any n-vertex graph $G = (V, E)$ we have*

$$R^*(G) \geq n - 1 + 2|E|(n - 2). \tag{137}$$

The equality is attained by the complete graph K_n and the star graph S_n.

It is also clear that for K_n we have $2|E| = n(n-1)$ and the bound gives the precise value $R^*(G) = (n-1)^3$.

Also, for any G we have $|E| \geq n - 1$, and therefore applying directly (137) we have that for any graph G

$$R^*(G) \geq n - 1 + 2(n-1)(n-2) = (n-1)(2n-3) = R^*(S_n),$$

proving in a more direct way than in [118] that the minimal multiplicative degree-Kirchhoff index is attained by the star graph S_n.

Since $d_1 \leq n - 1$ it is clear that

$$2|E| \leq d_1 n \leq d_1 n - d_1 + n - 1 = (d_1 + 1)(n - 1),$$

and therefore (137) is always better than (109). More details on the subject can be found in [111].

More bounds for the Kirchhoff index The material in the following paragraphs is taken from [112]. We first give a lower bound that is attained by a large family of graphs. It would be interesting to characterize exactly the extent of this family.

Proposition 51. *For any n-vertex graph G we have*

$$R(G) \geq n - 1 + \frac{2}{d_1}\left(\binom{n}{2} - |E|\right). \tag{138}$$

This lower bound is attained by K_n.

We obtain immediately the following

Corollary 52. *For any d-regular graph we have*

$$R(G) \geq n - 1 + \frac{n}{d}(n - 1 - d). \tag{139}$$

We are going to show now that the equality in the lower bound (139) (and therefore in (138)) is attained not only by K_n but by a large family of regular graphs. Let $N(i)$ be the neighborhood of the vertex i, i.e., the set of its neighbors, and let the diameter D be defined as $D = \max_{i,j}\{d(i,j) : i, j \in V\}$. Then we have

Proposition 53. *The bound (139) is attained by any n-vertex d-regular graph G for which $D = 2$ and $|N(i) \cap N(j)| = d$ for all i, j such that $d(i,j) = 2$.*

To show that the set of graphs satisfying the previous proposition is nonempty consider, for $j \geq 1, p \geq 1$, the graph $G(j,p)$ on $n = (p+1)(j+1)$ vertices which is d-regular, with $d = j(p+1)$, defined by the neighbors of its vertices thus: the neighbors of vertex v come in $p+1$ bunches of j consecutive vertices (the first bunch would be $v+1, v+2, \ldots, v+j-1$) separated by a non-neighbor (the first non-neighbor would be $v+j$). Here the addition is mod n. The densest of these examples occurs when $p = 1$; in that case $d = n-2$ and $G(j,1)$ can be described thus: from the complete graph K_{2j} we delete the j edges $(i, i+j)$, for $1 \leq i \leq j$, i.e., any vertex is connected to all others but its "opposite vertex". The least dense example occurs when $j = 1$; in that case $d = \frac{n}{2}$ and $G(1,p)$ is the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$.

Going in the opposite direction, we first get a simple and general upper bound in the next

Proposition 54. *For any G we have*

$$R(G) \leq n - 1 + \left(\binom{n}{2} - |E| \right) R, \tag{140}$$

where $R = \max_{i,j} R_{ij}$.

Of course, the bound (140) is not very useful unless we have a good grip on the value of R. But for those graphs whose smallest degree is larger than $\lfloor \frac{n}{2} \rfloor$, we can show that $R(G)$ is *linear* in n. Specifically we obtain the following

Proposition 55. *For any G for which $d_n \geq \lfloor \frac{n}{2} \rfloor$ we have*

$$R(G) \leq 3n - 1. \tag{141}$$

It would be interesting to determine whether (141) is a tight bound.

Adapting the discussion in [23] to our context, it should be pointed out that there is a sharp threshold at $d_n = \lfloor \frac{n}{2} \rfloor$. Indeed, when going from $d_n = \lfloor \frac{n}{2} \rfloor - 1$ to $d_n = \lfloor \frac{n}{2} \rfloor$ the Kirchhoff index drops from an n^2 order to an n order, as the previous proposition and the following example show.

Example. To simplify the discussion, let us take n to be even. Consider $G_1 = G_2 = K_{\lfloor \frac{n}{2} \rfloor}$. Delete edges (a_i, b_i) from G_i for $i = 1, 2$, and join the resulting graphs with the edges (a_1, a_2) and (b_1, b_2). The n-vertex graph thus built is $(\lfloor \frac{n}{2} \rfloor - 1)$-regular, and if we choose $a \in G_1$, $b \in G_2$ then by shorting all vertices in each G_i, $i = 1, 2$ into single vertices, and applying the monotonicity principle we see that $R_{ab} \geq \frac{1}{2}$. Since there are roughly $\dfrac{n^2}{4}$ possibles choices for a and b, the Kirchhoff index of this graph is bounded below roughly by $\dfrac{n^2}{8}$.

4.5 Numerical results [19]

In this section we present some numerical examples which illustrate the majorization technique developed throughout the chapter. The numerical results obtained by our new method have been compared to

[19] For more details we refer the reader to [5], [6], [7], [10], [11], [12], [13], [28], [29], [30], [31], [32].

those of the literature. We restrict our attention to computing bounds of some particular graphs.

4.5.1 Atom-bond connectivity index

We provide some numerical examples, using majorization in order to obtain bounds on the Atom-bond connectivity index and then we compare our results to those proposed in the literature. In particular, we make use of the relation between $R_{-1}(G)$ and $ABC(G)$ index.

Example 1. Let us consider the family of trees $\mathcal{T}$ with 16 vertices, 10 pendant vertices and the degree sequence $\pi = (5,3,3,3,3,3,1,1,1,1,1,1,1,1,1,1)$. In this case $m = n-1 = 15$ (for more details see Section 4, Example i) in [12]).

The minimal element is

$$\mathbf{x}_*(\mathcal{T}) = \left[\underbrace{\frac{19}{15},\ldots,\frac{19}{15}}_{10},\underbrace{\frac{2}{3},\ldots,\frac{2}{3}}_{5}\right].$$

Replacing these values into (29) we obtain for any $T \in \mathcal{T}$:

$$R_{-1}(T) \geq 3.2,$$

so that (34) yields

$$ABC(T) \leq 13.304,$$

improving the value obtained with the general bound (39): $ABC(T) \leq 14.491$.

Example 2. We now deal with the family $\mathcal{U}$ of unicyclic graphs G, i.e. graphs for which $m = n$, with degree sequence $\pi = (3,3,3,3,2,2,2,2,2,1,1,1,1)$.

Since $\widetilde{a} > a$, the minimal element is:

$$\mathbf{x}_*(\mathcal{U}) = \left[\underbrace{\frac{4}{3},\ldots,\frac{4}{3}}_{4},\underbrace{\frac{23}{27},\ldots,\frac{23}{27}}_{9}\right]$$

Replacing these values into (29) we obtain for any $G \in \mathcal{U}$:

$$R_{-1}(G) \geq 2.904$$

and the bound (34) becomes

$$ABC(G) \leq 11.007$$

which is tighter than the bound in (41) involving d_1, that yields $ABC(G) \leq 11.402$.

Example 3. Let us consider the family $\mathcal{B}$ of bicyclic graphs, i.e. those where $m = n+1$, with degree sequence $\pi = (3,3,3,3,2,1,1)$.

We have that $\widetilde{a} > a$ and the minimal vector is:

$$\mathbf{x}_*(G) = \left[\underbrace{\frac{4}{3}, \ldots, \frac{4}{3}}_{2}, \underbrace{\frac{13}{18} \cdots \frac{13}{18}}_{6}\right]$$

so that for $G \in \mathcal{B}$ we have

$$R_{-1}(G) \geq 1.425,$$

and the inequality (34) yields

$$ABC(G) \leq 6.276,$$

which is tighter than the bound in (41) in terms of d_1, that yields $ABC(G) \leq 6.403$.

We can conclude that, for all the considered examples, proposed bound always performs better. It means that bound (35) modified with our methodology based on majorization technique is the best choice in these cases.

4.5.2 The Normalized Laplacian index

The proposed bounds have been evaluated on different graphs. We now focus only on non-bipartite graphs and we provide a comparison with the literature (see [20]).
In order to assure a robust analysis, graphs have been randomly generated following the Erdös-Rényi (ER) model $G_{ER}(n, q)$ (see [17], [27], [51] and [52]). Graphs have been obtained by using a MatLab code that gives back only connected graph based on the ER model (see [28] and [32]). In this fashion, the graph is constructed by connecting nodes randomly such that edges are included with probability independent from every other edge. The results are based on a classic assumption of a probability of existence of edges q equal to 0.5. We obtain indeed that the generated graphs have a number of edges not far from the half of its maximum value as proved in the literature (see for example [54]).

At this regard, in Table 5 in Appendix A, $s^*_\alpha(G)$ has been computed for several graphs by fixing α equal to 0.5. We report values of upper bounds based on (75) and (76) and the upper bound proposed in [20]. Relative errors r measures the absolute value of the difference between the upper bounds and $s^*_\alpha(G)$ divided by the value of $s^*_\alpha(G)$. We observe an improvement with respect to existing bounds according to all the analyzed graphs and the improvement appears reduced for very large graphs. However, for large graphs the formula provided in [20] already gives a very low relative error. Similar results have been obtained also for non-bipartite graphs (see [30]).

4.5.3 Normalized Laplacian Energy

We focus here on $NE(G)$ by comparing proposed bounds with those in the literature (Corollary 12 and 13 in [22]). In particular we analyze two alternative classes of graphs generated by using either the Erdös-Rényi (ER) model $G_{ER}(n, q)$ or the Watts and Strogatz (WS) model (see [139]). Both models have been generated by using a well-known package of R (see [33]) and by assuring that the graph obtained is connected. As usual, the ER is constructed by connecting nodes randomly such that edges are included with probability q independent from every other edge. The WS networks have been derived beginning by a simulated n-node lattice and rewiring each edge at random to a new target node with probability p.

Table 6 in Appendix A reports main results derived for graphs generated by a $ER(n, 0.5)$ model. We observe how both bounds (80) and (81) are tighter than those proposed in [22]. The improvement increases for greater number of vertices.

Graphs have been simulated by using also WS model with different rewiring probabilities p. As well-known, intermediate values of p result in small-world networks that share properties of both regular and random graphs. In [139], the authors show that these networks have small mean path lengths and high clustering coefficients. There is indeed a broad interval of p over which the average path is almost as small as random yet the clustering coefficient is significantly greater than random. These small-world networks result from the immediate drop in average path caused by the introduction of few long-range edges. In particular, we analyze the behaviour of bounds in this interval by considering graphs generated with a rewiring probability in the range $p \in (0.01, 0.1)$. At this regard, Table 9 reports bounds evaluated by considering $p = 0.1$. We observe in Table 7 (Appendix A) greater values of $NE(G)$. In this case, also the bound provided in Corollary 13 ([22]) gives better results than those observed for ER graphs. However it is confirmed the best approximation when bound (81) is used.

4.5.4 Normalized Laplacian Estrada Index

We focus here on $NEE(G)$ by comparing for non-bipartite graphs bounds (85) and (87) with (86) proposed in [91]. In [31], it has been already analytically proved that, when the additional information $\lambda_1((\mathcal{L})) \geq Q$ is considered, bound (85) with $t_1 = Q$ is tighter than (86). Both ER and WS models are analysed.

In Table 8 (Appendix A) we report the $NEE(G)$ index and the values of the three mentioned bounds evaluated on non-bipartite graphs generated by using ER model with different number of vertices and with q equal to 0.5. Relative errors r measures the absolute value of the difference between the lower bounds and $NEE(G)$ divided by the value of $NEE(G)$.

As expected, using bound (87) we observe an improvement with respect to existing bound according to all the analyzed graphs. The improvement is very significant for graphs with a small number of vertices, while it reduces for very large graphs. However, for large graphs formula (86) provided in [91] already gives a very low relative error.

Graphs have been simulated by using also WS model with different rewiring probabilities p. In particular, we analyze the behaviour of bounds by considering graphs generated with a rewiring probability $p = 0.1$ (see Table 9 in Appendix A). In this case, we observe greater relative errors especially for large graphs. Probably, being these networks very far from complete graphs, bounds tend to assure a weaker approximation. Similar results have been obtained by simulating WS graphs choosing different values of p that belong to the interval.

4.5.5 HOMO-LUMO index

In this subsection we compare our bounds ((90),(91) and (94)) with those existing in the literature (Theorem 1.3 in [82], Theorem 3.2 and 3.3 in [92]). Also in this case, we compute them for graphs generated by using the Erdös-Rényi (ER) model $G_{ER}(n,q)$ where edges are included with probability q independent from every other edge. Graphs have been derived randomly by using a well-known package of R (see [33]) and by ensuring that the graph is connected. Table 10 (Appendix A) compares alternative upper bounds of $HL(G)$ evaluated for simulated $G_{ER}(n,0.5)$ graphs with different number of vertices. It is noteworthy that bound (91) has the best performance for $n = 5$, while bound (94) is the sharpest one in all other cases. However, the improvements are very slight with respect to bound (Th.3.2 in [92]) when large graphs are considered.

We now report in Table 11 (Appendix A) a comparison of alternative bounds derived for bipartite graphs, varying the number of vertices and edges. In some selected cases (i.e. $n = 10$, $m = 25$ and $n = 20$, $m = 91$), our bound (92) performs better. In all the other cases, the tightest one is bound (95) based on energy index.

4.5.6 Additive Kirchhoff index

We report some examples when H can be easily computed.

For d-regular graphs we have $H = \dfrac{N(N-1)}{2}$. The lower bound (114) becomes $N(N-1)$ which is worse than bound (112).

Let us consider a semiregular graph G that has N_1 vertices with degree a and N_2 vertices with degree b, $a < b$, $N = N_1 + N_2$. Then $H = \frac{N(N-1)}{2} + \left(\frac{b}{a} - 1\right) N_1 N_2$.
We deal with two examples: i) a semiregular bipartite graph and ii) a semiregular not bipartite graph.

Example 5.6. Let us consider a semiregular bipartite graph with N_1=10 vertices with degree $a = 4$ and $N_2 = 4$ vertices with degree $b = 10$. For this graph we have $H = 151$, $\sigma = 0.47$ which imply

Formula	Lower bound
(112)	338
(116)	338.03
(114)	359.64

Table 2. Lower bound for $R^+(G)$

showing that the bound (114) performs better than the others.

Example 5.7. Let us take a semiregular graph G on N vertices (N even ≥ 8) that is the union of a complete $K_{N/2}$ and a $N/2$-cycle such that vertex i of the cycle is linked to vertex i of the complete graph with a single edge, for $1 \leq i \leq N/2$.

This graph has $N_1 = N_2 = N/2$, $a = 3$, $b = N/2$, thus $H = \frac{1}{24}N\left(6N + N^2 - 12\right)$. By (114) we get

$$R^+(G) \geq \frac{N\left(228N^2 - 1152N + 36N^3 + N^4 + 1152\right)}{24\left(6N + N^2 - 12\right)} \tag{142}$$

By Calculus, it is easy to show that , for $N > 8$, the bound (142) is better than (112).

Table 3 give a comparison between all lower bounds applicable to this example, for $N = 20$:

Formula	Lower bound
(112)	722
(116)	722.001
(142)	848.61

Table 3. Lower bound for $R^+(G)$

The bound (142) performs always better than (116) which in turn improves (112).

We consider a full binary tree T of depth $d > 1$ which has $N_1 = 2^d$ vertices of degree 1, one vertex (the root) of degree 2 and $N_2 = 2^d - 2$ vertices of degree 3. Then $H = \dfrac{N(N-1)}{2} + 2N_1 + \frac{3}{2}N_2 + 2N_1N_2$. Taking $d = 3$ we obtain the results summarized in the following table, which shows that our new bounds are better than the universal one (112):

Formula	Lower
(112)	392
(116)	392.14
(114)	406

Table 4. Lower bounds for $R^+(T)$

Appendix A

n	d_1	m	$s^*_\alpha(G)$	bound (75)	bound (76)	bound [20]	r(75)	r(76)	r([20])
4	2	3	3.35	3.44	3.43	3.46	2.86%	2.55%	3.47%
5	4	9	4.46	4.47	4.47	4.47	0.23%	0.21%	0.25%
6	3	6	5.30	5.47	5.46	5.48	3.13%	3.00%	3.27%
7	5	14	6.43	6.48	6.48	6.48	0.83%	0.81%	0.86%
8	5	13	7.33	7.48	7.48	7.48	2.02%	1.98%	2.06%
9	6	16	8.31	8.48	8.48	8.48	2.04%	2.01%	2.07%
10	8	25	9.39	9.51	9.48	9.52	1.36%	1.04%	1.37%
20	15	95	19.37	19.51	19.49	19.51	0.71%	0.62%	0.72%
30	19	209	29.36	29.50	29.50	29.50	0.49%	0.46%	0.49%
50	33	604	49.37	49.50	49.50	49.50	0.27%	0.26%	0.27%
100	60	2459	99.37	99.50	99.50	99.50	0.13%	0.12%	0.13%
200	116	10001	199.38	199.50	199.50	199.50	0.06%	0.05%	0.06%
300	179	22437	299.37	299.50	299.50	299.50	0.04%	0.04%	0.04%
500	279	62456	499.38	499.50	499.50	499.50	0.03%	0.02%	0.03%

Table 5. *Normalized Laplacian Index*: upper bounds for $s^*_\alpha(G)$ for $\alpha = 0.5$ and relative errors.

n	$NE(G)$	bound Cor. 12 in [22]	bound Cor. 13 in [22]	bound (80)	bound (81)
4	3.00	4	3.66	3.12	3.05
5	2.55	4	4.39	2.70	2.61
6	3.15	6	5.12	3.87	3.62
7	3.81	6	5.86	4.51	4.27
8	4.32	8	6.59	4.69	4.47
9	3.90	8	7.32	4.34	4.14
10	3.58	10	8.05	4.00	3.83
20	5.01	20	15.37	5.68	5.56
30	5.60	30	22.69	6.43	6.33
50	7.31	50	37.33	8.44	8.36
100	9.59	100	73.92	11.13	11.08

Table 6. *Normalized Laplacian energy*: upper bounds for $NE(G)$ for graphs generated by $ER(n, 0.5)$ model.

n	$NE(G)$	bound Cor. 12 in [22]	bound Cor. 13 in [22]	bound (80)	bound (81)
4	2	4	3.66	2.72	2.41
5	3.24	4	4.39	3.45	3.37
6	4	6	5.12	4.15	4.08
7	4.49	6	5.86	4.87	4.63
8	5.12	8	6.59	5.57	5.33
9	5.76	8	7.32	6.27	6.03
10	6.47	10	8.05	6.99	6.75
20	11.97	20	15.37	13.67	13.42
30	19.24	30	22.69	21.16	20.90
50	31.79	50	37.33	35.27	34.99
100	63.21	100	73.92	70.22	69.93

Table 7. *Normalized Laplacian energy*: upper bounds for $NE(G)$ for graphs generated by $WS(n, 0.1)$ model.

n	$NEE(G)$	bound (86)	bound (85)	bound (87)	r(86)	r(85)	r(87)
4	5.0862	4.5547	4.6783	4.7112	10.4488%	8.0184%	7.3717%
5	6.6073	5.5040	5.6407	5.6935	16.6991%	14.6301%	13.8304%
6	6.9783	6.4749	6.5088	6.5265	7.2140%	6.7287%	6.4748%
7	8.4965	7.4560	7.5345	7.5559	12.2457%	11.3223%	11.0700%
8	9.3463	8.4428	8.4778	8.4933	9.6663%	9.2921%	9.1266%
9	10.0295	9.4331	9.4456	9.4541	5.9466%	5.8219%	5.7365%
10	10.9027	10.4256	10.4334	10.4391	4.3768%	4.3048%	4.2528%
20	20.9252	20.3947	20.3963	20.3977	2.5353%	2.5274%	2.5206%
30	30.9411	30.3853	30.3860	30.3867	1.7963%	1.7940%	1.7919%
50	50.9236	50.3782	50.3784	50.3786	1.0710%	1.0705%	1.0701%
100	100.9001	100.3729	100.3730	100.3731	0.5225%	0.5224%	0.5223%

Table 8. *Normalized Laplacian estrada index*: lower bounds for $NEE(G)$ and relative errors for graphs generated by $ER(n, 0.5)$ model.

n	$NEE(G)$	bound (86)	bound (85)	bound (87)	r(86)	r(85)	r(87)
4	5.0862	4.5547	4.6783	4.7112	10.4488%	8.0184%	7.3717%
5	6.3276	5.5040	5.6002	5.6389	13.0165%	11.4961%	10.8843%
6	7.5967	6.4749	6.5492	6.5856	14.7666%	13.7886%	13.3087%
7	8.8273	7.4560	7.6023	7.6273	15.5347%	13.8778%	13.5948%
8	10.1431	8.4428	8.5646	8.5878	16.7630%	15.5621%	15.3339%
9	11.3946	9.4331	9.5349	9.5568	17.2145%	16.3209%	16.1287%
10	12.6329	10.4256	10.5736	10.5917	17.4727%	16.3005%	16.1573%
20	25.2327	20.3947	20.5345	20.5442	19.1737%	18.6195%	18.5813%
30	37.7967	30.3853	30.5175	30.5240	19.6086%	19.2590%	19.2418%
50	63.2448	50.3782	50.5227	50.5268	20.3442%	20.1157%	20.1092%
100	126.4764	100.3729	100.5201	100.5222	20.6390%	20.5226%	20.5209%

Table 9. *Normalized Laplacian estrada index*: lower bounds for $NEE(G)$ and relative errors for graphs generated by $WS(n, 0.1)$ model.

n	m	$HL(G)$	bound (90)/(91)	bound (94)	bound [82]	bound Th.3.2 in [92]	bound Th.3.3 in [92]
5	7	0.46	1.29	1.33	4	1.55	1.62
10	26	0.68	1.99	1.80	8	2.02	2.08
15	52	0.33	3.12	2.28	10	2.33	2.44
20	106	0.69	3.98	2.27	16	2.71	2.74
25	153	0.32	3.66	2.92	16	2.94	3.00
50	600	0.42	5.10	3.92	31	3.98	4.04
100	2,463	0.56	7.30	5.43	66	5.47	5.50
250	15,358	0.49	9.67	8.32	142	8.38	8.41
500	62,304	0.47	13.52	11.65	289	11.67	11.68
1000	249,556	0.50	17.92	16.29	549	16.30	16.31

Table 10. Upper bounds of $HL(G)$ for graphs generated by $G_{ER}(n, 0.5)$ model

n	m	$HL(G)$	bound (92)	bound (95)	bound Th.3.2 in [92]	bound Th.3.3 in [92]
10	13	0.46	1.75	1.47	1.52	1.62
10	25	0.00	0.00	1.00	1.00	1.62
20	45	0.10	2.97	1.90	1.94	2.08
20	91	0.00	1.04	1.16	1.77	2.08
50	315	0.06	3.82	2.86	2.95	3.00
50	560	0.00	1.74	1.34	2.39	3.00
100	1,248	0.03	4.72	4.00	4.01	4.04
100	2,254	0.03	2.36	1.48	2.99	4.04
250	7,839	0.02	7.52	5.91	6.07	6.09
250	14,083	0.03	3.60	1.79	4.22	6.09
500	31,321	0.04	9.29	8.20	8.39	8.41
500	56,231	0.01	5.01	2.16	5.64	8.41
1,000	124,887	0.02	12.68	11.66	11.67	11.68
1,000	225,145	0.01	7.02	2.65	7.58	11.68

Table 11. Upper bounds of $HL(G)$ for bipartite graphs

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Zagreb Indices: Bounds and Extremal Graphs

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Contents

1. Introduction

Let $G = (V, E)$ be a simple graph, i.e., graph without loops and multiple edges. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$. For $v_i \in V(G)$, by $d_i = d_i(G)$ we denote the degree of vertex v_i in G.

A sequence of positive integers $\pi(G) = (\delta_1, \delta_2, \ldots, \delta_n)$ is called the *degree sequence* of G if $\delta_i = d_i(G)$ holds for $i = 1, 2, \ldots, n$. Throughout this paper, we order the vertex degrees non-increasingly, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$.

The minimum and maximum degree of a vertex in a graph is denote by δ and Δ, respectively.

The girth of G is the length of shortest cycle contained in G. Let $N_i(v) = \{w \in V(G) | d(v, w) = i\}$, where $d(v, w)$ is the length of a shortest path connecting u and v. Define $n_i(v) = |N_i(v)|$. Also, instead of $N_1(v)$, it is often written $N(v)$ to denote the (open) neighborhood of the vertex v. The eccentricity $\varepsilon(v)$ of v is defined as $\varepsilon = \varepsilon(v) = \max_{w \in V(G)}\{d(v, w)\}$. The radius $r = r(G)$ and the diameter $D = D(G)$ are defined as the minimum and the maximum of $\varepsilon(v)$ over all vertices $v \in V(G)$, respectively.

The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent if and only if they are not adjacent in G.

For $S \subseteq V(G)$, let $G[S]$ be the subgraph induced by S.

The vertex-disjoint union of the graphs G and H is denoted by $G \cup H$. Let $G \vee H$ be the graph obtained from $G \cup H$ by adding all possible edges from vertices of G to vertices of H, i.e.,

$$G \vee H \cong \overline{\overline{G} \cup \overline{H}}\,.$$

The first and the second Zagreb index are defined as

$$M_1 = M_1(G) = \sum_{v_i \in V(G)} d_i^2 \qquad , \qquad M_2 = M_2(G) = \sum_{v_i v_j \in E(G)} d_i\, d_j \tag{1}$$

respectively.

The first Zagreb index $M_1(G)$ can also be expressed as [47]

$$M_1(G) = \sum_{v_i v_j \in E(G)} (d_i + d_j)\,. \tag{2}$$

As it is well-known, the number of vertices of odd degree in every graph must be even. Therefore, $M_1(G)$ must be an even number, as noted in [133].

2. Historical remarks

The Zagreb indices belong among the oldest and most studied molecular structure descriptors and found noteworthy applications in chemistry. It is generally accepted that these have been conceived in 1972 by Trinajstić and one of the present authors, and first published in the much quoted paper [71]. The nowadays standard notation M_1 and M_2 , as well as the definitions (1) were first time used in the paper [70].

Details on these vertex–based topological indices can be found in the reviews [37, 66, 116] published on the occasion of their 30th anniversary, as well as in the recent surveys [63, 69, 134].

The first survey on topological indices appeared in 1983 [11]. In it also M_1 and M_2 were mentioned and commented. The authors of [11] named them "*Zagreb group indices*", bearing in mind that these resulted from the work of a group of scholars at the "Rudjer Bošković" institute in Zagreb. The name remained, except that "*group*" was eventually dropped.

One of the first graph–based molecular structure descriptors (topological indices) was invented in 1947 by Platt [122]. The Platt index I_{Pl} is the count of the edges incident to an edge of the underlying graph, and its sum over all edges:

$$I_{Pl} = \sum_{v_i v_j \in E(G)} (d_i + d_j - 2) \, . \tag{3}$$

What was completely overlooked by the authors of the papers [70, 71], was the identity

$$M_1 = I_{Pl} + 2m$$

which straightforwardly follows from (3) and the relation (2).

In 1964, Gordon and Scantelbury [58] considered a graph invariant that sometimes is referred to as the Gordon–Scantelbury index I_{GS}. By definition, it is equal to the number of acyclic P_3-subgraphs contained in the graph G. For triangle–free graphs,

$$I_{GS} = \sum_{v_i \in V(G)} \binom{d_i}{2}$$

which leads to

$$M_1 = 2\, I_{GS} + 2m$$

implying that the first Zagreb index is essentially the same as the somewhat older Gordon–Scantelbury index. This too was missed by the authors of [70, 71].

More historical details on the Zagreb indices are found in [65].

3. On the maximum and minimum first Zagreb index of graphs with n vertices and m edges

A simple graph G on n vertices and m edges will be referred to as an (n, m)-graph. In this section we give a survey on upper and lower bounds for the first Zagreb index M_1 of (n, m)-graphs in terms of n and m, and give characterization of extremal graphs which attain these maximal (minimal) values. First, we deal with the upper bounds on M_1.

Székely et al. [131] gave the following upper bound for the sum of the squares of vertex degrees

$$M_1 = \sum_{1=1}^{n} d_i^2 \leq \left(\sum_{1=1}^{n} \sqrt{d_i} \right)^2 \tag{4}$$

and de Caen [42] proved that

$$M_1 = \sum_{1=1}^{n} d_i^2 \leq m \left(\frac{2m}{n-1} + n - 2 \right) \, . \tag{5}$$

De Caen pointed out that the bounds (4) and (5) are incomparable. Das [32] proved that the equality in (5) holds if and only if G is a star or a complete graph or a complete graph with one isolated vertex.

Das [32], Zhou [154], and Liu et al. [100] established some new upper bounds for M_1.

Theorem 3.1. [32, 100] *Let G be a connected graph with n vertices and m edges. Then*

$$M_1(G) \leq m(m+1) \tag{6}$$

with equality for $n > 3$ if and only if $G \cong K_3$ or $G \cong K_{1,n-1}$.

Theorem 3.2. [154] *Let G be a connected graph with n vertices and m edges. Then*

$$M_1(G) \leq n(2m-n+1) \tag{7}$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ or $G \cong mK_2$.

Remark. If $m = n-1$, then the bound (7) is equal to (6). If $m \geq n$, then $m(m+1) \geq n(2m-n+1)$ and thus the bound (7) is usually lower than the bound (6), as it was proven in [103].

Remark. If G is connected (n,m)-graph, then $m \leq \binom{n}{2}$, implying, as noted in [103], that

$$\begin{aligned} m\left(\frac{2m}{n-1}+n-2\right) &= mn+2m\left(\frac{m}{n-1}-1\right) \\ &\leq mn+n(n-1)\left(\frac{m}{n-1}-1\right) = n(2m-n+1)\,. \end{aligned}$$

Thus, the bound (5) is usually finer than the bound (7).

In the sequel, we outline the results concerned with the structure of (n,m)-graphs for which the maximum value of M_1 is attained.

Denote by $\mathcal{G}(n,m)$ the set of all simple (n,m)-graphs. The graph G is said to be optimal in $\mathcal{G}(n,m)$ if $M_1(G)$ is maximum. Denote by $\max(n,m)$ this maximum value.

A matrix formulation of these problems was first investigated by Schwarz [124] in 1964 by considering rearrangements of square matrices with non-negative elements in order to maximize the sum of elements of the matrix A^2. By papers of Katz [106], and later Aharoni [3], these problem were completely solved.

The graph formulation of these problems were first investigated by Ahlswede and Katona [4] in 1978. They solved an equivalent problem. In fact, they determined the maximum number of pairs of different edges that have a common vertex, given by

$$\sum_{v_i \in V} \binom{d_i}{2} = \frac{M_1}{2} - m\,.$$

Ahlswede and Katona proved that the maximum value $\max(n,m)$ is always attained at one or both of two special graphs in $\mathcal{G}(n,m)$ (Theorem 3.3).

The first of these special graphs, the quasi-complete graph, denoted by $QC(n,m)$, is the graph having the largest possible complete subgraph K_k.

The other special graph, called quasi-star graph and denoted by $QS(n,m)$, is the graph that has as many vertices of degree $n-1$ as possible. In fact, this graph is the complement of $QC(n,m')$, where $m' = \binom{n}{2} - m$.

After that, the problem of maximizing M_1 was investigated by Boesch et al. [16]. Also, Olpp [119], independently, was solving a question of Goodmen: maximize the number of monochromatic triangles in a two-coloring of the complete graph with a fixed number of red edges. Ollp showed that Goodman's problem is equivalent to finding the two-coloring that maximizes the sum of squares of the red degrees of the vertices, i.e., that maximizes M_1 of a subgraph consisted of red edges. In both papers, the result of Alshwede and Katona, that the maximum value of M_1 is always attained at one or both of two special graphs $QC(n,m)$ and $QS(n,m)$ in $\mathcal{G}(n,m)$ was reproven (Theorem 3.3).

In 1999, Peled et al. [121], and Byer [23], independently showed that all optimal graphs for which M_1 is maximum belong to one of the six classes of so-called threshold graphs. Byer solved another equivalent form of the problem. In fact, he studied the maximum number of paths of lengths two over all (n,m)-graphs, given by $M_1 - 2m$. However, in these papers it was not discussed when any of the six graphs, that achieve maximum, is optimal.

The problem was completely solved in 2009 by Ábrego et al. [2]. A related problem of determining in which of the graphs, $QC(n,m)$ or $QS(n,m)$, the maximum of M_1 is attained, was solved independently in [2] and [139].

As it was proven by Peled et al. [121], all optimal graphs belong to a class of special graphs called threshold graphs. The quasi-star and the quasi-complete graphs are among many threshold graphs in $\mathcal{G}(n,m)$. These graphs can be characterized in several equivalent ways. By [108] $G = (V,E)$ is a threshold graph if G can be constructed from K_1 by multiple adding of an isolated vertex or a vertex that is adjacent with any other vertex, i.e., as

$$G_1^*(a,b,c,d,\ldots) \cong K_a \vee (\overline{K}_b \cup (K_c \vee (\overline{K}_d \cup \cdots)))$$

or

$$G_2^*(a,b,c,d,\ldots) \cong \overline{K}_a \cup (K_b \vee (\overline{K}_c \cup (K_d \cup \cdots)))\,.$$

Theorem 3.3. [4, 16, 119] *Among the graphs from $\mathcal{G}(n,m)$, there exist threshold graphs*

$$QS(n,m) \cong G_1^*(a,b,1,d), \;\; QC(n,m) \cong G_2^*(a,b,1,d)$$

unique up to an isomorphism, such that at least one of them is optimal.

In fact, by Byer [23] and Peled et al. [121] it holds:

Theorem 3.4. [23, 121] *Let G be an optimal graph in $\mathcal{G}(n,m)$. Then $G \cong G_1^*(a,b,c,d)$ or $G \cong G_2^*(a,b,c,d)$ for $b=1$ or $c=1$ or $d=1$.*

By [108], the graph $G=(V,E)$ is a threshold graph if for every three distinct vertices $i,j,k \in V$, if $d_i \geq d_j$ and $jk \in E$, then $ik \in E$.

By the latter characterization of a threshold graph, its adjacency matrix has a special form. Its upper–triangular part is left justified and the number of zeros in each row of its upper–triangular part does not decrease. Having this in mind, a threshold graph can be represented by a partition $\pi = (a_0, a_1, \ldots, a_p)$ of m, all of whose parts are less than n, such that an upper–triangular part of its adjacency matrix is left justified and contains a_s ones in a row s. We denote by $Th(\pi)$ the threshold graph corresponding to a partition π, and say that the partition π is optimal if $Th(\pi)$ is an optimal graph. The diagonal sequence of a partition π is defined as the number of ones in the upper–triangular part of its adjacency matrix on each of the diagonal lines. By Theorem 3.4, there are at most six optimal partitions of graphs from $\mathcal{G}(n, m)$. Ábrego et al. [2] gave precise conditions to determine when each of these partitions is optimal.

Let $S_{n,m} = M_1(QS(n, m))$ and $C_{n,m} = M_1(QC(n, m))$. Then, by Theorem 3.3, the maximum value of M_1 equals to $S_{n,m}$ or $C_{n,m}$.

Theorem 3.5. [2] *Let n be a positive integer and m an integer such that $0 \leq m \leq \binom{n}{2}$. Let k, k', j, j' be the unique integers satisfying*

$$m = \binom{k+1}{2} - j\,, \ \text{with } 1 \leq j \leq k$$

and

$$m = \binom{n}{2} - \binom{k'+1}{2} + j'\,, \ \text{with } 1 \leq j' \leq k'\,.$$

Then every optimal partition π is one of the following six partitions:

1. $\pi_{1.1} = (n-1, n-2, \ldots, k'+1, j')$*, the quasi-star partition for* m*,*
2. $\pi_{1.2} = (n-1, n-2, \ldots, 2k'-j', 2k'-j'-2, \ldots, k'-1)$*, if* $k'+1 \leq 2k'-j'-1 \leq n-1$*,*
3. $\pi_{1.3} = (n-1, n-2, \ldots, k'+1, 2, 1)$*, if* $j' = 3$ *and* $n \geq 4$*,*
4. $\pi_{2.1} = (k, k-1, \ldots, j+1, j-1, \ldots, 2, 1)$*, the quasi-complete partition for* m*,*
5. $\pi_{2.2} = (2k-j-1, k-2, k-3, \ldots, 2, 1)$*, if* $k+1 \leq 2k-j-1 \leq n-1$*,*
6. $\pi_{2.3} = (k, k-1, \ldots, 3)$*, if* $j = 3$ *and* $n \geq 4$*.*

The partitions $\pi_{1.1}$ and $\pi_{1.2}$ always exist and at least one of them is optimal. Furthermore, $\pi_{1.2}$ and $\pi_{1.3}$ (if they exist) have the same diagonal sequence as $\pi_{1.1}$, and if $S_{n,m} \geq C_{n,m}$, then they are all optimal. Similarly, $\pi_{2.2}$ and $\pi_{2.3}$ (if they exist) have the same diagonal sequence as $\pi_{2.1}$, and if $S_{n,m} \leq C_{n,m}$, then they are all optimal.

In order to describe the behavior of $S_{n,m} - C_{n,m}$, we need the following definitions. Let $k_0 = k_0(n)$ be an integer such that

$$\binom{k_0}{2} \leq \frac{1}{2}\binom{n}{2} < \binom{k_0+1}{2}$$

and define the quadratic function

$$q_0(n) := \frac{1}{4}\left[1 - 2(2k_0-3)^2 + (2n-5)^2\right].$$

In addition, let

$$R_0 = R_0(n) = \frac{4\left[\binom{n}{2} - 2\binom{k_0}{2}\right](k_0-2)}{-1 - 2(2k_0-4)^2 + (2n-5)^2}\,.$$

Theorem 3.6. [2, 139] *Let n be a positive integer.*

(1) If $q_0(n) > 0$, then

$$\begin{aligned} S_{n,m} &\geq C_{n,m} \qquad \textit{for} \quad 0 \leq m \leq \frac{1}{2}\binom{n}{2} \\ S_{n,m} &\leq C_{n,m} \qquad \textit{for} \quad \frac{1}{2}\binom{n}{2} \leq m \leq \binom{n}{2}. \end{aligned}$$

$S_{n,m} \cong C_{n,m}$ *if and only if* $m \in \left\{0, 1, 2, 3, \frac{1}{2}\binom{n}{2}\right\}$ *or* $m = \binom{k_0}{2}$ *and* $(2n-3)^2 - 2(2k_0-3)^2 \in \{-1, 7\}$.

(2) If $q_0(n) < 0$, then

$$\begin{aligned} S_{n,m} &\geq C_{n,m} \qquad \textit{for} \quad 0 \leq m \leq \frac{1}{2}\binom{n}{2} - R_0 \\ S_{n,m} &\leq C_{n,m} \qquad \textit{for} \quad \frac{1}{2}\binom{n}{2} - R_0 \leq m \leq \frac{1}{2}\binom{n}{2} \\ S_{n,m} &\geq C_{n,m} \qquad \textit{for} \quad \frac{1}{2}\binom{n}{2} \leq m \leq \frac{1}{2}\binom{n}{2} + R_0 \\ S_{n,m} &\leq C_{n,m} \qquad \textit{for} \quad \frac{1}{2}\binom{n}{2} + R_0 \leq m \leq \binom{n}{2}. \end{aligned}$$

$S_{n,m} \cong C_{n,m}$ *if and only if* $m \in \left\{0, 1, 2, 3, \frac{1}{2}\binom{n}{2} - R_0, \frac{1}{2}\binom{n}{2}\right\}$.

(3) If $q_0(n) = 0$, then

$$\begin{aligned} S_{n,m} &\geq C_{n,m} \qquad \textit{for} \quad 0 \leq m \leq \frac{1}{2}\binom{n}{2} \\ S_{n,m} &\leq C_{n,m} \qquad \textit{for} \quad \frac{1}{2}\binom{n}{2} \leq m \leq \binom{n}{2}. \end{aligned}$$

$S_{n,m} \cong C_{n,m}$ *if and only if* $m \in \left\{0, 1, 2, 3, \binom{k_0}{2}, \ldots, \frac{1}{2}\binom{n}{2}\right\}$.

By using the fact that among the graphs from $\mathcal{G}(n,m)$ at least one of the graphs $QS(n,m)$ or $QC(n,m)$ is optimal, Nikiforov [115] obtained an upper bound for M_1, that is better than de Caen's (5), for the majority of graphs from $\mathcal{G}(n,m)$.

Theorem 3.7. [115] *For an integer n and $0 \leq m \leq \binom{n}{2}$, let*

$$F(n,m) = \begin{cases} 2m\sqrt{2m} & \textit{if } n^2/4 \leq m \\ (n^2-2m)\sqrt{n^2-2m} + 4mn - n^3 & \textit{if } m < n^2/4 . \end{cases}$$

Then

$$F(n,m) - 4m \leq \max\{S_{n,m}, C_{n,m}\} \leq F(n,m)\,.$$

Furthermore, if $n\sqrt{n} < m < \binom{n}{2} - n\sqrt{n}$, *then*

$$F(n,m) < m\left(\frac{2m}{n-1} + n - 2\right).$$

If we consider bipartite graphs with n vertices and m edges, then the graphs which attain maximum value of M_1 cannot be threshold graphs, since a bipartite graph does not contain a complete subgraph with more than two vertices. However, the structure of the extremal bipartite graphs whose M_1 is maximum is similar to the structure of threshold graphs. Let n, m, k be three positive integers. As in [30], we use $B(n,m)$ to denote a bipartite graph with n vertices and m edges, and $B(n,m,k)$ to denote a $B(n,m)$ with bipartition (X,Y) such that $|X| = k$, $|Y| = n-k$. By $\mathcal{B}(n,m,k)$ we denote the set of graphs of the form $B(n,m,k)$.

The sign of x, denoted by $sgn(x)$, is defined as 1, -1 and 0 when x is positive, negative and zero, respectively.

Suppose that n, m, k are three integers such that $n \geq 2$, $0 \leq m \leq \lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil$ and $\lceil\frac{n}{2}\rceil \leq k \leq n-1$ and let $m = qk + r$, where $0 \leq r < k$. Let $B^1(n,m,k)$ be a bipartite graph in $\mathcal{B}(n,m,k)$, such that q vertices from Y are adjacent to all the vertices in X and one more vertex from Y is adjacent to r vertices in X.

Theorem 3.8. [4] *For* $0 \leq m \leq \lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil$ *and* $\lceil\frac{n}{2}\rceil \leq k \leq n-1$, *the graph* $B^1(n,m,k)$ *has maximum* M_1 *among all bipartite graphs with* n *vertices,* m *edges and given bipartition* $(k, n-k)$.

This result was improved by Cheng [30] for bipartite graphs with arbitrarily bipartition.

Theorem 3.9. [30] *Let* n *and* m *be two integers such that* $n \geq 2$ *and* $0 \leq m \leq \lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil$. *Let*

$$k_0 = \max\left\{k | m = kq + r\ ,\ 0 \leq r < k\ ,\ \left\lceil\frac{n}{2}\right\rceil \leq k \leq n - q - sgn(r)\right\}. \tag{8}$$

Then, $M_1(B^1(n,m,k_0))$ *attains maximum value among all bipartite graphs with* n *vertices and* m *edges.*

As a consequence, the following upper bound for M_1 has been determined in [30].

Theorem 3.10. [30] *Let* n *and* m *be two integers such that* $n \geq 2$ *and* $0 \leq m \leq \lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil$ *and* G *is a bipartite graph with* n *vertices and* m *edges. Then the maximum possible value of* $M_1(G)$ *is*

$$\left\lfloor\frac{m}{k_0}\right\rfloor(k_0 - 1)\left(k_0 + \left\lfloor\frac{m}{k_0}\right\rfloor k_0 - 2m\right) + m^2 + m$$

where k_0 *is given by* (8).

Zhang and Zhou [151] slightly modified the previous result and proposed the following solution to the problem of finding all bipartite graphs with a given number of vertices and edges whose M_1 is maximum.

Theorem 3.11. [151]

(1) Let n and m be two integers such that $n \geq 2$ and $0 \leq m \leq n-1$. Suppose that $M_1(B^*)$ attains the maximum value among all bipartite graphs with n vertices and m edges. Then, $B^* \cong K_{1,m} \cup (n-m-1)K_1$.

(2) Let n and m be two integers such that $n \geq 2$ and $n \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$. Let k_0 being an integer given by (8)*. Suppose that $M_1(B^*)$ attains the maximum value among all bipartite graphs with n vertices and m edges. Then,*

(a) $B^* \cong B^1(n,m,k_0)$ or $B^* \cong B^1(n,m,n-k_0)$ if $m > (n-k_0)(k_0-1)$;

(b) $B^* \cong B^1(n,m,k_0)$ or $B^* \cong B^1(n,m,n-k_0)$ or $B^* \cong B^1(n,m,k_0-1)$ if $m = (n-k_0)(k_0-1)$;

(c) $B^* \cong B^1(n,m,k_0)$ if $m < (n-k_0)(k_0-1)$.

In the following, we turn our attention to the minimum of M_1. The Cauchy–Schwarz inequality yields a lower bound for M_1 given by

$$M_1 \geq \frac{4m^2}{n} \tag{9}$$

with equality if and only if the graph is regular. This bound was obtained several times in the literature [42, 85, 147] and it is close to the sharp lowest bound for M_1, determined in [32] and [62].

Theorem 3.12. [32, 62] *Let G be a simple (n,m)-graph. Then*

$$M_1 \geq 2m\left(\left\lfloor \frac{2m}{n} \right\rfloor + \left\lceil \frac{2m}{n} \right\rceil\right) - n\left\lfloor \frac{2m}{n} \right\rfloor \left\lceil \frac{2m}{n} \right\rceil \tag{10}$$

and the equality holds if and only if the degree of any vertex is either $\lfloor 2m/n \rfloor$ or $\lceil 2m/n \rceil$.

Cheng et al. [30] determined the minimum value of M_1 of bipartite graphs with n vertices and m edges.

Let $n \geq 2$ be an even integer and $t \leq n/2$ a nonnegative integer. By $B_{n,t}$ we denote the bipartite graph with vertices $x_1, x_2, \ldots, x_{n/2}, y_1, y_2, \ldots, y_{n/2}$ and edges x_iy_j with $i < j \leq i+t$ (where the addition is taken modulo $n/2$) for $i, j = 1, 2, \ldots, n/2$.

For two integers n and m such that $n \geq 2$ and $0 \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, let $2m = nt + r$, where $0 \leq r < n$. We define, as in [30], a bipartite graph $B^s(n,m)$ with n vertices and m edges as follows.

If n is even, then $B^s(n,m) \cong B_{n,t} \cup \{x_iy_j | \, 1 \leq i \leq r/2\}$.

If n is odd and $nt \leq 2m < nt + t$, let

$$B^s(n,m) \cong B^s(n-1, m-t+1) \cup \Big\{x_iy_0 | (n+r-t+1)/2 + 1 \leq i \leq (n+r+t-1)/2\Big\}$$

where the addition is taken modulo $(n-1)/2$.

If n is odd and $nt + t \leq 2m < nt + n - t - 1$, or $nt + n - t + 1 \leq 2m < nt + n$, let $B^s(n,m) = B^s(n-1, m-t) \cup \{x_iy_0 | (r-t)/2 + 1 \leq i \leq (r+t)/2\}$, where the addition is taken modulo $(n-1)/2$.

Theorem 3.13. [30] *Let n and m be two integers such that $n \geq 2$ and $0 \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$. Then $M_1(B^s(n,m))$ attains minimum value among all bipartite graphs with n vertices and m edges.*

As a consequence, the following lower bound for M_1 was obtained.

Theorem 3.14. [30] *If G is a bipartite (n,m)-graph, where $n \geq 2$ and $0 \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, then the minimum possible value of $M_1(G)$ is*

$$\begin{cases} (4m-n-nt)t+2m & \text{if } n \text{ is even; or } n \text{ is odd} \\ & \text{and } nt+t \leq 2m \leq nt+n-t-1 \\ (4m+1-nt)t & \text{if } n \text{ is odd and } nt \leq 2m < nt+t \\ (4m-n+1-nt)(t+1) & \text{if } n \text{ is odd and } nt+n-t+1 \leq 2m \leq nt+n \end{cases}$$

where $t = \lfloor 2m/n \rfloor$.

In [140] the relation between the M_1 index of an (n,m)-graph and the first three coefficient of its Laplacian polynomial was considered and as a consequence, a lower bound for M_1 was obtained and the corresponding extremal graphs were identified.

By [118], for an (n,m)-graph G, the first three coefficients of its Laplacian polynomial are given by

$$q_0(G) = 1 \;\;,\;\; q_1(G) = -2m \;\;,\;\; q_2(G) = 2m^2 - m - \frac{1}{2}\sum_{i=1}^{n} d_i^2\,.$$

The authors of [140, 141] used these coefficients to define the following invariant of a graph G

$$\mathcal{M}_1(G) = \frac{1}{2}M_1(G) - 2m$$

as well as the set $\mathcal{G}_i = \{G \,|\, G \text{ is connected}, \mathcal{M}_1(G) = i, i \geq -1, \text{ is an integer}\}$.

Before stating the result, we need several new definitions.

$L_{g,\ell}$ denotes the lollipop graph obtained from C_g and P_ℓ by identifying a vertex of C_g with an end-vertex of P_ℓ, where $g \geq 3$, $\ell \geq 2$ and $n = g + \ell - 1$.

$T_{\ell_1,\ell_2,\ldots,\ell_k}$ denotes the starlike tree of order n with a vertex u of degree k satisfying $T_{\ell_1,\ell_2,\ldots,\ell_k} - u = P_{\ell_1} \cup P_{\ell_2} \cup \ldots \cup P_{\ell_k}$, where $\ell_k \geq \cdots \geq \ell_2 \geq \ell_1 \geq 1$ and $n = \sum_{i=1}^{k} \ell_i + 1$. T_{ℓ_1,ℓ_2,ℓ_3} is also named a T-shape tree.

The centipede graph $P_{z_1,z_2,\ldots,z_t,\ell}^{a_1,a_2,\ldots,a_t}$ is defined as a path of ℓ vertices with pendent paths of z_i edges joining at vertex a_i for $i = 1,2,\ldots,t$, where $\{a_1,a_2,\ldots,a_t\} \subseteq \{2,\ldots,\ell-1\}$, $z_i \geq 1$ $(1 \leq i \leq t)$ and $n = \ell + \sum_{i=1}^{t} z_i$.

The sun-like graph $C_{z_1,z_2,\ldots,z_t,g}^{a_1,a_2,\ldots,a_t}$ is a cycle with girth g and with pendent paths of z_i edges joining at vertex a_i for $i = 1,2,\ldots,t$, where $\{a_1,a_2,\ldots,a_t\} \subseteq \{1,2,\ldots,g\}$, $z_i \geq 1$ $(1 \leq i \leq t)$ and $n = g + \sum_{i=1}^{t} z_i$.

By D_{ℓ,g_1,g_2} we denote the dumbbell graph obtained by joining two cycles C_{g_1} and C_{g_2} with a path of length ℓ, where $g_1, g_2 \geq 3$, $\ell \geq 1$ and $n = g_1 + g_2 + \ell - 1$.

The mirror graph $M_{\ell_1,\ell_2,\ell_3}^{g}$ is obtained from C_g and T_{ℓ_1,ℓ_2,ℓ_3} by identifying a vertex of C_g with an end-vertex of T_{ℓ_1,ℓ_2,ℓ_3}, where $\ell_i \geq 1$ $(1 \leq i \leq 3)$, $g \geq 3$ and $n = g + \sum_{i=1}^{3} \ell_i$.

The θ-graph $\theta_{i,j,k}$ consists of two vertices joined by three disjoint paths of orders i, j and k, where $n = i + j + k - 4$.

By $J^g_{\ell_1,\ell_2,\ldots,\ell_k}$ we denote a jellyfish graph obtained from C_g and $T_{\ell_1,\ell_2,\ldots,\ell_k}$, by identifying a vertex of C_g with the center of $T_{\ell_1,\ell_2,\ldots,\ell_k}$, where $g \geq 3$, $\ell_i \geq 1$ $(1 \leq i \leq k)$.

The fish graph $F^{g,l}_{\ell_1,\ell_2,\ell_3}$ is obtained from P_ℓ and $M^g_{\ell_1,\ell_2,\ell_3}$,by identifying an end-vertex of P_ℓ with a vertex of degree 2 which lies in the cycle of $M^g_{\ell_1,\ell_2,\ell_3}$, where $g \geq 3$, $\ell, \ell_1, \ell_2, \ell_3 \geq 1$.

By $K^{g,a_1,a_2}_{\ell,z_1,z_2}$ we denote the key graph obtained from C_g and $P^{a_1,a_2}_{z_1,z_2,\ell}$ by overlapping a vertex of C_g with an end-vertex of $P^{a_1,a_2}_{z_1,z_2,\ell}$, where $g \geq 3$ and $z_1, z_2 \geq 1$.

The double–starlike tree $S^l_{\ell_1,\ell_2,\ldots,\ell_k;h_1,h_2,\ldots,h_s}$ is obtained by joining the centers of the graphs $T_{\ell_1,\ell_2,\ldots,\ell_k}$ and $T_{h_1,h_2,\ldots,h_s}$ with a path P_ℓ, where $\ell_i, h_j \geq 1$.

These graphs are depicted in Fig. 1.

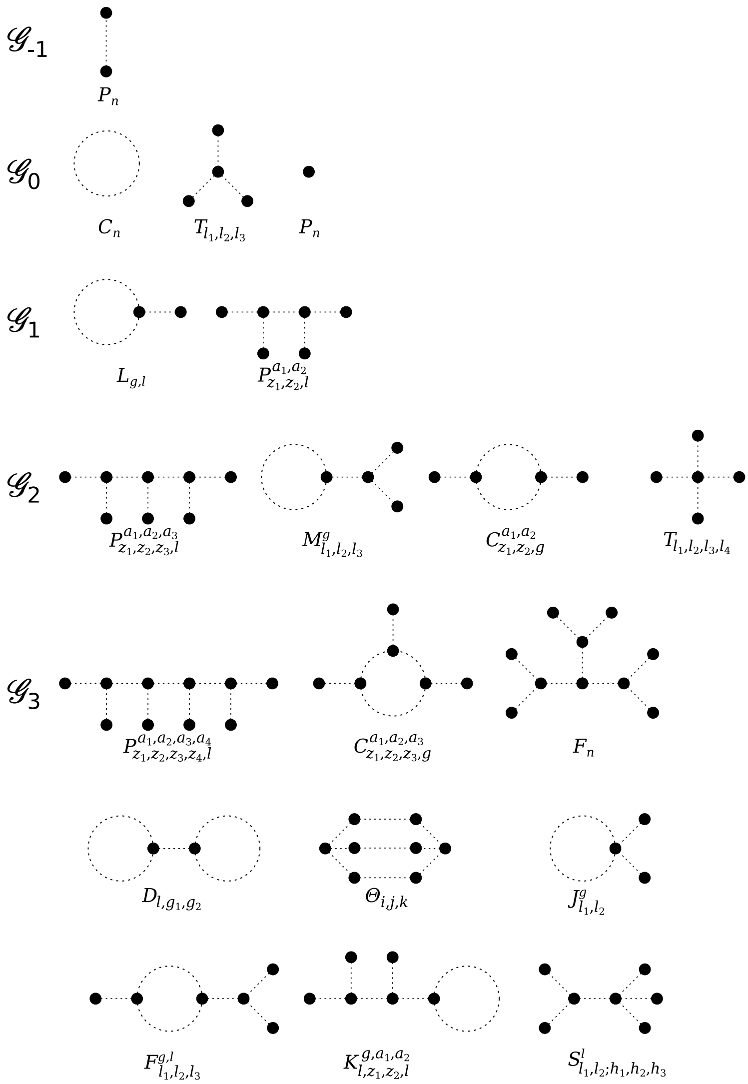

Fig. 1. The graphs occurring in Theorem 3.15.

Theorem 3.15. [140, 141] *Let G be a connected $(n,\, m)$-graph. Then*

(i) $M_1(G) \geq 4m-2$, and the equality holds if and only if $G \in \mathcal{G}_{-1} = \{P_n | n \geq 2\}$.

(ii) If $G \notin \mathcal{G}_{-1}$, then $M_1(G) \geq 4m$ with equality if and only if

$$G \in \mathcal{G}_0 = \Big\{P_1, C_n \,|\, n \geq 3\Big\} \cup \Big\{T_{\ell_1,\ell_2,\ell_3} \,|\, n \geq 4\Big\}.$$

(iii) If $G \notin \mathcal{G}_{-1} \cup \mathcal{G}_0$, then $M_1(G) \geq 4m+2$ with equality if and only if

$$G \in \mathcal{G}_1 = \Big\{L_{g,\ell} \,|\, n \geq 4\Big\} \cup \Big\{P^{a_1,a_2}_{z_1,z_2,\ell} \,|\, n \geq 6\Big\}.$$

(iv) If $G \notin \mathcal{G}_{-1} \cup \mathcal{G}_0 \cup \mathcal{G}_1$, then $M_1(G) \geq 4m+4$ with equality if and only if

$$G \in \mathcal{G}_2 = \Big\{C^{a_1,a_2}_{z_1,z_2,g}, T_{\ell_1,\ell_2,\ell_3,\ell_4} \,|\, n \geq 5\Big\} \cup \Big\{M^{g}_{\ell_1,\ell_2,\ell_3} \,|\, n \geq 6\Big\} \cup \Big\{P^{a_1,a_2,a_3}_{z_1,z_2,z_3,\ell} \,|\, n \geq 8\Big\}.$$

(v) If $G \notin \mathcal{G}_{-1} \cup \mathcal{G}_0 \cup \mathcal{G}_1 \cup \mathcal{G}_2$, then $M_1(G) \geq 4m+6$ with equality if and only if

$$G \in \mathcal{G}_3 = \Big\{C^{a_1,a_2,a_3}_{z_1,z_2,z_3,g}, P^{a_1,a_2,a_3,a_4}_{z_1,z_2,z_3,z_4,\ell}, F_n, D_{\ell,g_1,g_2}, J_{g,\ell_1,\ell_2}, \theta_{i,j,k}, F^{g,\ell}_{\ell_1,\ell_2,\ell_3}, S^{\ell,\ell_1,\ell_2}_{h_1,h_2,h_3}, K^{g,a_1,a_2}_{\ell,z_1,z_2}\Big\}.$$

The above theorem includes or extends some previously known results [45, 66, 93, 142].

For a graph G and $e = uv \in E(G)$, the degree of the edge e is defined as $d_G(e) = d(u) + d(v) - 2$.

The authors of [140] suggested the following construction that can characterize all connected graphs in $\mathcal{G}_k$. Using this construction they generalized the result of Theorem 3.15.

Construction A. [140] Suppose that $\mathcal{G}_{-1}, \mathcal{G}_0, \ldots, \mathcal{G}_{k-1}$ have been defined. For each graph $G \in \mathcal{G}_t$ $(1 \leq t \leq k-1)$, it is searched for all possible edges e such that $e \notin E(G)$ and $d_{G+e}(e) = k-t+1$ in order to construct the graph $G+e$ (some vertices are added if necessary). Collect these new graphs $G+e$ in $\mathcal{G}'_k$. By adding all possible edges of degree 1 to the graphs in $\mathcal{G}'_k$, we obtain all the graphs belonging to $\mathcal{G}_k$.

The following theorem generalizes Theorem 3.15.

Theorem 3.16. [140] *Let G be a connected (n, m)-graph.*

(i) $M_1(G) \geq 4m-2$ with equality if and only if $G \in \mathcal{G}_{-1}$.

(ii) If $G \notin \mathcal{G}_{-1} \cup \mathcal{G}_0 \cup \cdots \cup \mathcal{G}_{k-1}$ $(k \geq 0)$, then $M_1(G) \geq 4m+2k$ with equality if and only if $G \in \mathcal{G}_k$, and $\mathcal{G}_k$ is defined by Construction A.

For given n and m, the graphs with largest M_1-values are characterized in [45, 144]. Let $B_n^{(i)}$ be a graph of order n with $n+i$ edges and maximum degree $n-1$, second–maximum degree $2+i$, $i = 1,\, 2$.

Theorem 3.17. [45, 144] *Let G be a connected graph of order n with m edges $(n-1 \leq m \leq n+1)$. If M_1 is maximum, then:*

(i) *$G \cong K_{1,n-1}$ for $m = n-1$;*

(ii) *$G \cong K_{1,n-1} + e$ for $m = n$ where $e = uv$ with u, v as two pendent vertices in $K_{1,n-1}$;*

(iii) *$G \cong B_n^{(1)}$ for $m = n+1$.*

The following upper bound on M_1 is obtained in [144]:

Theorem 3.18. [144] *Let G be a connected graph of order n with m $(= n+2)$ edges. Then*

$$M_1(G) \leq n^2 - n + 24$$

with equality holding if and only if $G \cong B_n^{(2)}$ or $\overline{G} \cong (K_{n-4} \vee 3\,K_1) \cup K_1$.

For any integer m satisfying $n+3 \leq m \leq 2n-4$, we denote by $N_{n,\,m}^{n-1,\,m-n+2}$ a graph of order n and with m edges in which the maximum degree is $n-1$ and the second–maximum degree is $m-n+2$.

Theorem 3.19. [144] *Let G be a connected graph of order n with m edges, $n+3 \leq m \leq 2n-4$. Then*

$$M_1(G) \leq n(n-1) + (m-n+1)(m-n+6)$$

with equality holding if and only if $G \cong N_{n,m}^{n-1,m-n+2}$.

4. On graphs with given parameters whose M_1-value is extremal

In this section we give a survey of upper and lower bounds for M_1 of graphs with some fixed parameters.

Knowing the value of the maximum or minimum degree, the bound (5) can be sharpened.

Theorem 4.1. [32] *Let G be a connected graph with n vertices, m edges and minimum degree δ. Then*

$$\sum_{1=1}^{n} d_i^2 \leq 2mn - n(n-1)\delta + 2m(\delta - 1) \tag{11}$$

and the equality holds if and only if G is a star or a regular graph.

Theorem 4.2. [32] *Let G be a connected graph with n vertices, m edges and maximum degree Δ. Then*

$$M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right) - \Delta\left(\frac{4m}{n-1} - 2m_1 - \frac{n+1}{n-1}\,\Delta + n - 1\right) \tag{12}$$

where m_1 is the average degree of the vertices adjacent to the highest degree vertex. Moreover, equality in (12) *holds if and only if G is a star or a complete graph or a graph consisting of isolated vertices.*

Das [32] suggested that in the case of trees, the upper bound (12) is always better than de Caen's bound (5).

Theorem 4.3. [154] *Let G be an (n,m)-graph with minimum degree δ. Then*

$$M_1(G) \leq n(2m - \delta n) + \frac{n}{2}\left[\delta^2 + 1 + (\delta - 1)\sqrt{(\delta+1)^2 + 4(2m - \delta n)}\right]$$

and equality holds if and only if G is a regular graph or $K_{1,n-1}$.

Denote by $K^*_{2,n-2}$ a connected graph of order n obtained from the complete bipartite graph $K_{2,n-2}$ with two vertices of degree $n-2$ joined by a new edge. A kite $Ki_{n,\omega}$ is the graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an endpoint from the path.

Recently, Das et al. [41] determined an upper bound for M_1 in terms of n, m, and Δ.

Theorem 4.4. [41] *Let G be an (n,m)-graph with maximum degree Δ. Then*

$$M_1(G) \leq (n+1)m - \Delta(n-\Delta) + \frac{2(m-\Delta)^2}{n-2}$$

with equality holding if and only if $G \cong K^*_{2,n-2}$ or $G \cong K_n$ or $G \cong Ki_{n,n-1}$.

Additional extensions of de Caen's upper bound (5) are given in the following three theorems.

Theorem 4.5. [33] *Let G be a graph with n vertices, m edges, minimum degree δ, and maximum degree Δ. Then*

$$M_1 \leq m\left[\frac{2m}{n-1} + \frac{n-2}{n-1}\Delta + (\Delta-\delta)\left(1-\frac{\Delta}{n-1}\right)\right] \tag{13}$$

with equality if and only if G is a star or a regular graph or a complete graph $K_{\Delta+1}$ with $n-\Delta-1$ isolated vertices.

Note that by (13), it holds

$$M_1 \leq m\left[\frac{2m}{n-1} + (n-2) - \big[n-2-(\Delta-\delta)\big]\left(1-\frac{\Delta}{n-1}\right)\right]$$

and since $1-\Delta/(n-1) \geq 0$ and $n-2-(\Delta-\delta) \geq 0$ for connected or disconnected graphs, the upper bound (13) is always better than de Caen's bound (5), as proven in [33].

For $1 \leq \alpha \leq n-1$, the complete split graph $CS(n,\alpha)$ is the graph on n vertices consisting of a clique on $n-\alpha$ vertices and a stable set on the remaining α vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

Theorem 4.6. [31, 33] *Let G be a graph with n vertices, m edges, minimum degree δ, and maximum degree Δ. Then*

$$M_1 \leq \frac{2m\,[2m+(n-1)(\Delta-\delta)]}{n+\Delta-\delta} \tag{14}$$

with equality if and only if G is a star or a regular graph or a complete graph $K_{\Delta+1}$ with $n-\Delta-1$ isolated vertices.

If G is a connected graph, then the equality in (14) *holds if and only if G is a regular graph or $G \cong CS(n,\alpha)$, for an integer α.*

The upper bound given by (14) is better than the bound (5), since the right–hand side of the inequality (14) is a monotonically increasing function of $\Delta-\delta$ and $\Delta-\delta \leq n-2$.

In [33] Das also obtained the following upper bound on M_1.

Theorem 4.7. [33] *Let G be a graph with n vertices and m edges, minimum vertex degree δ and maximum vertex degree Δ. Then*

$$M_1 \leq 2m(\delta + \Delta) - n\delta\Delta \tag{15}$$

with equality if and only if G is a bidegreed graph, i.e., it has only two type of degrees, δ and Δ.

In [154], the above upper bound was improved by proving the following.

Theorem 4.8. [154] *Let G be a graph with n vertices and m edges, minimum vertex degree δ ($\delta \geq 1$), maximum vertex degree Δ and $\Delta > \delta$. Then*

$$M_1 \leq 2m(\delta + \Delta) - n\delta\Delta + (\delta - k)(\Delta - k) \tag{16}$$

where k is an integer defined via

$$2m - n\delta \equiv k - \delta\,(mod\,(\Delta - \delta)) \;\;,\;\; \delta \leq k \leq \Delta - 1$$

i.e.,

$$k = 2m - \delta(n-1) - (\Delta - \delta)\left\lfloor \frac{2m - n\delta}{\Delta - \delta} \right\rfloor \, .$$

Equality in (16) *is attained if and only if at most one vertex of G has degree different from δ and Δ.*

Recall that a chemical graph is a graph with $\Delta \leq 4$. From the previous theorem, the following corollary is immediately deduced.

Corollary 4.1. [154] *Let G be a chemical graph with $n \geq 2$ and m edges. Then*

$$M_1(G) \leq \begin{cases} 10m - 4n, & \text{if } 2m - n \equiv 0\,(mod\,3) \\ \\ 10m - 4n - 2 & \text{otherwise} \end{cases}$$

with equality if and only if either

(i) every vertex of G is of degree 1 or 4 (in which case it must be $2m - n \equiv 0$ (mod 3), or

(ii) one vertex of G has degree 2 or 3, and all other vertices are of degree 1 or 4.

In the paper [84], the following inequality, stronger than (15), has been obtained.

Theorem 4.9. [84] *Let G be a simple non-regular graph with n vertices and m edges, with a vertices of maximal degree Δ and b vertices of minimal degree δ. Then*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta - (n - a - b)(\Delta - \delta - 1) \tag{17}$$

with equality if and only if the vertex degrees are equal to δ, $\delta + 1$, $\Delta - 1$, or Δ.

Some additional upper bounds for M_1 were presented in [50, 84, 103, 112, 113].

Theorem 4.10. [103] *Let G be a connected (n,m)-graph. Then*

$$M_1 \leq \max\left\{m\left(\Delta+\delta-1+\frac{2m-\delta(n-1)}{\Delta}\right), m\left(\delta+1+\frac{2m-\delta(n-1)}{2}\right)\right\} \tag{18}$$

and the equality is attained, for example, by a star or a regular graph of order $n \geq 3$.

It was proven in [103] that for $n \geq 3$, the bound (18) is better than (6).

Theorem 4.11. [50, 84, 103] *Let G be connected (n,m)-graph. Then*

$$M_1(G) \leq \frac{2m^2}{n} + \left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right)\frac{m^2}{n} \tag{19}$$

with equality if and only if G is a regular graph or G is a bidegreed graph such that $\Delta+\delta$ divides δn and there are exactly $p = 2n/(\Delta+\delta)$ vertices of degree Δ and $q = \Delta n/(\Delta+\delta)$ vertices of degree δ.

In fact, the inequality in the previous relation was independently proven in [50, 84, 103], whereas the equality case was determined first in [103] and then corrected in [84]. As a simple corollary of the previous theorem, the following result was obtained.

Corollary 4.2. [84, 103] *Let G be a connected graph with n vertices and m edges. If $\delta = 1$, then*

$$M_1(G) \leq \frac{nm^2}{n-1}$$

with equality if and only if $G \cong K_{1,n-1}$. If $\delta \geq 2$, then

$$M_1(G) \leq \frac{(n+1)^2\, m^2}{2n(n-1)}$$

with equality if and only if $G \cong K_3$.

The upper bound (19) was improved in [112] in the following way.

Theorem 4.12. [112] *Let G be a connected (n,m)-graph, $n \geq 2$. Futher, let S be a subset of $I_n = \{1,2,\ldots,n\}$ that minimizes the expression $|\sum_{i\in S} d_i - m|$. Then*

$$M_1(G) \leq \frac{4m^2}{n}\left[1+\left(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\right)^2 \beta(S)\right] \tag{20}$$

where

$$\beta(S) = \frac{1}{2m}\sum_{i\in S} d_i\left(1-\frac{1}{2m}\sum_{i\in S} d_i\right)$$

and with equality as determined in Theorem 4.11.

As noted in [112], for each set $S \subset I_n$ it holds $\beta(S) \leq \frac{1}{4}$, implying that the inequality (20) is stronger than (19). Besides, by Theorem 4.12, the bounds from Corollary 4.2 were also improved:

Corollary 4.3. [112] *Let G be a connected graph with n vertices and m edges, $n \geq 2$. If $\delta = 1$, then*

$$M_1(G) \leq \frac{4m^2}{n}\left[1 + \frac{(n-2)^2}{(n-1)}\,\beta(S)\right]$$

with equality if and only if $G \cong K_{1,n-1}$. If $\delta \geq 2$, then

$$M_1(G) \leq \frac{4m^2}{n}\left[1 + \frac{(n-3)^2}{2(n-1)}\,\beta(S)\right]$$

with equality if and only if $G \cong K_3$.

The following upper bound for M_1 was obtained in [50].

Theorem 4.13. [50] *Let G be a simple (n,m)-graph. Then*

$$M_1(G) \leq \frac{4m^2}{n} + \frac{n}{4}\left(\Delta - \delta\right)^2. \tag{21}$$

This bound is improved as follows.

Theorem 4.14. [78, 112, 113] *Let G be a connected (n,m)-graph. Then*

$$M_1(G) \leq \frac{1}{n}\left[\alpha(n)(\Delta-\delta)^2 + 4m^2\right] \tag{22}$$

where the integer function $\alpha(n)$ is defined as

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

The equality holds if and only if G is a regular graph.

The above inequality was first obtained in the paper [78], but the function $\alpha(n)$ was erroneously defined via $\lceil x \rceil$. The correct proof was given in [112, 113] and the equality case was characterized only in [112]. It can be easily seen [112] that the inequality (22) is stronger than the inequality (21) for each odd n, $n \geq 3$.

An upper bound on the first Zagreb index $M_1(G)$ in terms of n, m, Δ, δ, and the second–maximum vertex degree Δ_2 was obtained in [39].

Theorem 4.15. [39] *Let G be a graph with n vertices ($n > 1$), m edges, maximum degree Δ, second–maximum degree Δ_2 and minimum degree δ. Then*

$$M_1(G) \leq \frac{(2m-\Delta)^2}{n-1} + \Delta^2 + \frac{n-1}{4}(\Delta_2 - \delta)^2. \tag{23}$$

Equality holds in (23) if and only if G is isomorphic to a graph H_1 such that $d_2(H_1) = d_3(H_1) = \cdots = d_n(H_1) = \delta$ or G is isomorphic to a graph H_2 such that $d_2(H_2) = d_3(H_2) = \cdots = d_{p+1}(H_2) = \Delta_2$ and $d_{p+2}(H_2) = d_{p+3}(H_2) = \cdots = d_{2p+1}(H_2) = \delta$, $n = 2p+1$.

The upper bound (23) was improved in the same paper.

Theorem 4.16. [39] *Let G be the same graph as in Theorem 4.15. Then*

$$M_1(G) \leq \Delta^2 + (\Delta_2 + \delta)(2m - \Delta) - (n-1)\Delta_2\,\delta\,. \tag{24}$$

Equality holds in (24) *if and only if G is isomorphic to a graph H such that $d_2(H) = d_3(H) = \cdots = d_p(H) = \Delta_2$ and $d_{p+1}(H) = d_{p+2}(H) = \cdots = d_n(H) = \delta$, $2 \leq p \leq n$.*

As it was outlined in [39], the bound (24) is always better than the bound (15). By [39], it holds

$$\begin{aligned} & 2m(\Delta + \delta) - n\Delta\delta \geq \Delta^2 + (\Delta_2 + \delta)(2m - \Delta) - (n-1)\Delta_2\,\delta \\ \Leftrightarrow\quad & 2m(\Delta - \Delta_2) + \Delta(\Delta_2 + \delta) - \Delta^2 - n\delta(\Delta - \Delta_2) - \Delta_2\,\delta \geq 0 \\ \Leftrightarrow\quad & (2m - \Delta - n\delta + \delta)(\Delta - \Delta_2) \geq 0 \Leftrightarrow \sum_{i=2}^{n}(d_i - \delta)(\Delta - \Delta_2) \geq 0 \end{aligned}$$

which is obviously always obeyed.

Similarly, it was proven in [39] that the bound (24) is always better than the bound (23).

Some further estimations of the first Zagreb index were proposed in [40]. For a vertex v_i of the graph G we denote by m_i the average degree of the vertices adjacent to v_i. Denote by μ and ν the maximum and minimum of m_i. Then it holds:

Theorem 4.17. [40] *Let G be a connected graph of order n with m edges. Then*

$$\frac{2m[2m - (\Delta - \nu)(n-1)]}{n + \nu - \Delta} \leq M_1(G) \leq \frac{2m[2m + (\mu - \delta)(n-1)]}{n + \mu - \delta}\,. \tag{25}$$

Equality on the left–hand side of (25) *holds if and only if G is regular. The right–hand side equality holds in* (25) *if and only G is either regular graph or $G \cong CS(n, \alpha)$.*

As noted in [40], Theorem 4.17 generalizes the previously obtained upper bound (14).

The irregularity index $t(G)$ of a graph G is defined as the number of distinct terms in the degree sequence of G. Before we state the next result, we need a few more definitions from [35].

Let Υ_2 be the class of graphs $H_1 = (V, E)$ such that H_1 is a graph of order n, irregularity index t, maximum degree Δ and

$$\Delta = t\ \ ,\ \ d_i = 1\ ,\ i = t+1, t+2, \ldots, n\,.$$

Let Υ_3 be the class of graphs $H_2 = (V, E)$ such that H_2 is a graph of order n, irregularity index t, maximum degree Δ and

$$d_i = \begin{cases} \Delta - i + 1 & ;\quad i = 1, 2, \ldots, t \\ \Delta & ;\quad i = t+1, t+2, \ldots, n\,. \end{cases}$$

Theorem 4.18. [35] *Let G be a graph of order n with irregularity index t and maximum degree Δ. Then*

$$M_1(G) \geq \frac{1}{6}\,t(t+1)(2t+1) + n - t$$

with equality if and only if $G \in \Upsilon_2$*, and*

$$M_1(G) \leq t(\Delta+1)^2 + \frac{1}{6}t(t+1)(2t+1) - (\Delta+1)t(t+1) + (n-t)\Delta^2$$

with equality if and only if $G \in \Upsilon_3$*.*

In the papers [154, 156, 158] Zhou et al. determined upper bounds for M_1 of K_{r+1}-free graphs with n vertices, where $r \geq 2$.

Theorem 4.19. [154] *Let* G *be a triangle–free* (n,m)*-graph. Then*

$$M_1(G) \leq mn \tag{26}$$

and equality holds if and only if G *is a complete bipartite graph.*

By Turán's theorem, for an (n,m)-triangle–free graph it holds $m \leq \lfloor \frac{n^2}{4} \rfloor$ with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$. Then, by the previous theorem, for an (n,m)-triangle–free graph it holds [154]

$$M_1(G) \leq n \left\lfloor \frac{n^2}{4} \right\rfloor$$

with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$.

Before we state the next results, we need few more definitions from [158]. By $\widetilde{W}_n$ we denote a graph, obtained by slightly redefining a class of graphs known as windmills. For n odd, $\widetilde{W}_n$ is a graph obtained by taking $\frac{n-1}{2}$ triangles all sharing one common vertex. For n even, $\widetilde{W}_n$ is a graph obtained from $\widetilde{W}_{n-1}$ by attaching a pendent vertex to a central vertex of $\widetilde{W}_{n-1}$. Also, let $even(n) = 1$ if n is even, and 0 otherwise.

Theorem 4.20. [158] *Let* G *be a quadrangle–free graph with* n *vertices and* $m > 0$ *edges. Then,*

$$M_1(G) \leq n(n-1) + 2m - 2\, even(n)$$

with equality if and only if $G \cong \widetilde{W}_n$*.*

The *Moore graph* is an r-regular graph with diameter k whose order is equal to

$$1 + r\sum_{i=0}^{k-1}(r-1)^i \,.$$

Hoffman and Singleton [75] proved that every r-regular Moore graph with diameter 2 must have $r \in \{2, 3, 7, 57\}$.

Theorem 4.21. [158] *Let* G *be a triangle– and quadrangle–free graph with* $n > 1$ *vertices. Then,*

$$M_1(G) \leq n(n-1)$$

with equality if and only if G *is a star* $K_{1,n-1}$ *or a Moore graph of diameter 2.*

Zhou [156] proved a general result concerning K_{r+1}-free graphs with n vertices, where $r \geq 2$. If $r \geq n$, then obviously $M_1(G) \leq M_1(K_n)$ with equality if and only if $G \cong K_n$. Thus, in the following theorem it is supposed that $2 \leq r \leq n-1$.

Theorem 4.22. [156] *Let G be a K_{r+1}-free graph with n vertices and $m > 0$ edges, where $2 \leq r \leq n-1$. Then, $M_1(G) \leq (2r-2)mn/r$ and the equality holds if and only if G is complete bipartite graph for $r = 2$ and a regular complete r-partite graph for $r \geq 3$.*

Besides, as a consequence, in the same paper [156] the following upper bound was obtained.

Theorem 4.23. [156] *Let G be a $K_{1,1,k+1}$- and $K_{2,\ell+1}$-free graph with n vertices and $m > 0$ edges, where $0 \leq k \leq \ell$. Then*

$$M_1(G) \leq 2(k+1-\ell)m + \ell n(n-1)$$

with equality if and only if each pair of adjacent vertices in G has exactly k common neighbors and each pair of non-adjacent vertices in G has exactly ℓ common neighbors.

In [100], upper bounds for M_1 were obtained in terms of the number of vertices, number of edges, and diameter (or girth). Recall that the girth $g = g(G)$ is the size of the smallest cycle in G.

Theorem 4.24. [100] *Let G be an (n,m)-graph with diameter D. Then*

$$M_1(G) = n(n-1)^2 \quad \text{if } D = 1$$

and

$$M_1(G) \leq m^2 - m(D-3) + (D-2) \quad \text{if } D > 1\,. \tag{27}$$

If $D = 2$, then equality in (27) holds if and only if either $G \cong K_{1,n-1}$ or $G \cong K_3$. If $D \geq 3$, then equality in (27) holds if and only if $G \cong P_{D+1}$.

Theorem 4.25. [100] *Let G be a connected (n,m)-graph with girth $g \geq 4$. Then $M_1(G) \leq m^2$ with equality if and only if $G \cong C_4$.*

In the paper [89], sharp upper bounds for M_1 and M_2 are given among n-vertex bipartite graphs with a given diameter D. Denote by $\mathcal{B}(n,D)$ the set of bipartite graphs on n vertices with diameter D. When $D = 1$, then the bipartite graph is just K_2. So, it is assumed that $D \geq 2$. If $G \in \mathcal{B}(n,D)$, then there exists a partition $V_0, V_1, \ldots, V_D$ of $V(G)$ such that $|V_0| = 1$ and $d(u,v) = i$ for each vertex $v \in V_i$ and $u \in V_0$, $i = 1, 2, \ldots, D$. Let $m_i = |V_i|$. Let $G[a,s,t,b]$ be a graph with $s = m_a = |V_a| > 1$, $t = m_{a+1} = |V_{a+1}| > 1$, $|V_j| = 1$ for $j \in \{0,1,\ldots,D\} \backslash \{a, a+1\}$, $a+b = D-1$, $s+t = n-D+1$, and two consecutive partition sets inducing a complete bipartite subgraph. Also, without loss of generality, it is assumed that $a \leq b$.

Theorem 4.26. [89] *Let $G \in \mathcal{B}(n,D)$ with the maximal M_1-value or M_2-value, then*

$$G \cong G\left\{a\,,\ \left\lfloor \frac{n-D+1}{2} \right\rfloor\,,\ \left\lceil \frac{n-D+1}{2} \right\rceil\,,\ b\right\}.$$

Furthermore, the parameters a and b satisfy the following conditions with respect to the diameter of G.

(i) if $D = 2$, then $a = 0$, $b = 1$;

(ii) if $D = 3$, then $a = 1$, $b = 1$;

(iii) if $D = 4$, then $a = 1$, $b = 2$;

(iv) if $D = 5$, then $a = 2$, $b = 2$;

(v) if $D = 6$, then $a = 2$, $b = 3$;

(vi) if $D \geq 7$, then $a \geq 3$, $b \geq 3$.

As a consequence, the bipartite graphs with largest, second–largest and smallest M_1-values (resp. M_2-values) have been characterized.

Theorem 4.27. [89] *Among all bipartite graphs of order $n \geq 2$, the graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ has the largest M_1– and M_2-values, whereas the path P_n has the smallest M_1– M_2-values.*

Theorem 4.28. [89] *Among all bipartite graphs with order $n > 2$, the graph $K_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n+2}{2} \rceil}$ has the second–largest M_1 values and M_2-values for even n, and the graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} - e$ has the second–largest M_1-values and M_2-values for odd n.*

For triangle– and quadrangle–free graphs, an upper bound for M_1 was established in terms of n and radius r.

Theorem 4.29. [145] *Let G be a triangle– and quadrangle–free connected graph with n vertices and radius r. Then, $M_1(G) \leq n(n + 1 - r)$ and the equality holds if and only if G is a Moore graph of diameter two or G is the 6-vertex cycle C_6.*

Morgan and Mukwembi [114] derived an upper bound for M_1 in terms of n, m, and the number of triangles t.

Theorem 4.30. [114] *Let G be an (n, m)-graph with t triangles. Then,*

$$M_1(G) \leq mn + 3t\,. \tag{28}$$

As noted in [114], the equality in (28) is attained by the complete graph K_n and the complete bipartite graph $K_{\frac{n}{2}, \frac{n}{2}}$. This bound is the generalization of the bound (26). Besides, for graphs with limited number of triangles, such as triangle–free graphs, the bound (28) is better than the de Caen's bound (5). Also, by [114], the bound (28) is better than Nikiforov' s bound (Theorem 3.7) for graphs with many edges.

By Theorem 4.30, the following corollary was obtained in [114].

Corollary 4.4. [114] *Let G be an (n, m)-graph with maximum degree Δ. Then,*

$$M_1(G) \leq m(n + \Delta - 1)\,.$$

A vertex of degree 1 (pendent vertex) is sometimes called a *leaf* vertex. The *leaf number* $L(G)$ of G is defined [114] as the maximum number of leaf vertices contained in a spanning tree of G. This graph invariant has applications in the optimization of centralized terminal networks [54].

In addition, the following upper bound for M_1 in terms of n, m, the number of triangles, and the leaf number has been obtained in [114].

Theorem 4.31. [114] Let G be an (n,m)-graph with t triangles and leaf number L. Then,

$$M_1(G) \leq m(L+2) + 3t\,.$$

Recall that a *matching* of a graph is a set of mutually independent edges in a graph, i.e., set of edges with no common vertices. The *matching number* $\beta(G)$ of the graph G is the number of edges in a maximum matching. Obviously, $\beta(G) = 0$ if and only if G is an empty graph. For a connected graph G with $n > 2$ vertices, $\beta(G) = 1$ if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$. A matching M is said to be an m-matching if $|M| = \beta(G) = m$. If $\beta(G) = n/2$, then the graph has a *perfect matching*.

Theorem 4.32. [51] *Let G be a connected graph with $n \geq 4$ vertices and matching number β, such that $2 \leq \beta \leq \lfloor n/2 \rfloor$. Let*

$$b = \frac{1}{18}\left(n + 3 + \sqrt{37n^2 - 30n + 9}\right).$$

Then the following holds:

(1) If $\beta = \lfloor n/2 \rfloor$, then

$$M_1(G) \leq n(n-1)^2$$

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

(2) If $b < \beta \leq \lfloor n/2 \rfloor - 1$, then

$$M_1(G) \leq n^2 - n + 8\beta^3 - 12\beta^2 + 4\beta$$

with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(3) If $\beta = b$, then

$$M_1(G) \leq bn^2 + b^2 n - 2bn - b^3 + b = n^2 - n + 8b^3 - 12b^2 + 4b$$

with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$ or $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(4) if $2 \leq \beta < b$, then

$$M_1(G) \leq \beta n^2 + \beta^2 n - 2\beta n - \beta^3 + \beta$$

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

A cut edge in a connected graph G is an edge whose deletion breaks the graph into two components. Denote by $\mathcal{G}_n^k$ the set of connected graphs with n vertices and k cut edges. The graph K_n^k is a graph obtained by joining k independent vertices to one vertex of K_{n-k} and the graph C_n^k is a graph obtained by identifying an end vertex of P_{k+1} with a vertex of C_{n-k} (this graph was mentioned before as a lollipop graph $L_{n-k,k+1}$).

Theorem 4.33. [52] *Let $G \in \mathcal{G}_n^k$. Then*

$$4n + 2 \leq M_1(G) \leq (n-k-1)^3 + (n-1)^2 + k$$

with left–hand–side equality if and only if $G \cong C_n^k$ and with right–hand–side equality if and only if $G \cong K_n^k$.

For any set W of vertices (edges) in a graph G, if G is connected and $G - W$ is disconnected, we say that W is a $|W|$-vertex (edge-) cut of G.

For $k \geq 1$, we say that a graph G is k-connected if either G is the complete graph K_{k+1}, or else it has at least $k+2$ vertices and contains no $(k-1)$-vertex cut. Similarly, for $k \geq 1$, a graph G is k-edge–connected if it has at least two vertices and does not contain an $(k-1)$-edge cut. The maximal value of k for which a connected graph G is k-connected is the connectivity of G, denoted by $\kappa(G)$. If G is disconnected, we define $\kappa(G) = 0$. The edge–connectivity $\kappa'(G)$ is defined analogously.

Denote by $\mathcal{V}_n^k$ the set of graphs of order n with $\kappa(G) \leq k \leq n-1$, and by $\mathcal{E}_n^k$ the set of graphs of order n with $\kappa'(G) \leq k \leq n-1$. Also, let G_n^k be a graph obtained by joining k edges from k vertices of K_{n-1} to an isolated vertex. Obviously, $G \in \mathcal{V}_n^k \subseteq \mathcal{E}_n^k$.

Li and Zhou in [92] investigated the Zagreb indices of $G \in \mathcal{V}_n^k$ (resp. $\mathcal{E}_n^k$) and gave sharp upper and lower bounds for $M_1(G)$ and $M_2(G)$, respectively. Besides, Hua in [81] independently obtained sharp upper bound for the first Zagreb index of graphs from $G \in \mathcal{V}_n^k$ (resp. $\mathcal{E}_n^k$).

Theorem 4.34. [81,92] Among all graphs G in $\mathcal{V}_n^k$ ($\mathcal{E}_n^k$), $k > 0$,

$$4n - 6 \leq M_1(G) \leq k(n-1)^2 + k^2 + (n-k-1)(n-2)^2$$

with left–hand side equality if and only if $G \cong P_n$ and right–hand side equality if and only if $G \cong G_n^k$.

A subset $S \subseteq V(G)$ of mutually non-adjacent vertices in a graph G is said to be an (vertex-) *independent set* in G, and the *independence number* $\alpha(G)$ is the maximum cardinality of an independent set in G. Besides, the so-called *vertex-independence number* and *edge-independence number* of a graph G can be defined as follows. Let S be an (vertex-) independent set of G. If for any vertex $x \in V(G) \setminus S$ it holds $N(x) \cap S \neq \emptyset$, then S is called maximal vertex–independent set of G. Let

$$i(G) = \min\{|S| \, : \, S \text{ is a maximal vertex–independent set of } G\}.$$

Then $i(G)$ is said to be the *vertex–independence number* of G.

A subset T of $E(G)$ is said to be an *edge–independent* set of G if T contains exactly one edge or any two edges in T (if such do exist) sharing no common vertices. Let T be an edge–independent set of G. For any $e \in E(G) \setminus T$, if $\{e\} \cup T$ is no longer an edge–independent set of G, then T is called a maximal edge–independent set of G.

Let

$$m(G) = \min\{|T| \, : \, T \text{ is a maximal edge–independent set of } G\}.$$

Then $m(G)$ is said to be the *edge–independence number* of G.

For a connected graph G it holds, as noted in [81], that $1 \leq i(G) \leq \lfloor \frac{n}{2} \rfloor$ and $1 \leq m(G) \leq \lfloor \frac{n}{2} \rfloor$. For $2 \leq k \leq (n-1)/2$, we define, as in [81], a graph $G_{n_1,n_2,\ldots,n_k}$ as follows.

For $2 \leq n_i \leq n-2k+2$, $i = 1,2,\ldots,k$, let K_{n_1}, $K_{n_2}, \ldots, K_{n_k}$ be complete graphs of orders $n_1, n_2, \ldots, n_k$, respectively, with $V(K_{n_i}) = \{v_{i1}, \ldots, v_{in_i}\}$. Let

$$G_{n_1,n_2,\ldots,n_k} = (K_{n_1} - \{v_{11}\}) \vee (K_{n_2} - \{v_{21}\}) \vee \cdots \vee (K_{n_k} - \{v_{k1}\}) \,.$$

For $k = 2$, let $\widetilde{G}_{n_1,n_2}$ be the graph obtained from G_{n_1,n_2} by adding to it the edge $v_{11}v_{21}$.

Sharp upper bounds for the first Zagreb index of graphs with given vertex- (edge-) independence number are obtained in [81].

Theorem 4.35. [81] *Let G be a connected graph with n vertices and $i(G) = k$ for $1 \leq k \leq \lfloor n/2 \rfloor$. Then the following holds:*

(i) If $k = 1$, then $M_1(G) \leq n(n-1)^2$ with equality if and only if $G \cong K_n$.

(ii) If $k = 2$, then $M_1(G) \leq (n-1)(n-2)^2 + 4$ with equality if and only if $G \cong \widetilde{G}_{2,n-2}$.

(iii) If $3 \leq k \leq (n-1)/2$, then $M_1(G) \leq (n-k)^3 + (n-2k+1)^2 + k - 1$ with equality if and only if $G \cong G_{2,\ldots,2,n-2k+2}$.

(iv) If $k = n/2$, then $M_1(G) \leq \frac{n^3}{4}$ with equality if and only if $G \cong K_{k,k}$.

Theorem 4.36. [81] *Let G be a connected graph with n vertices and $m(G) = k$. Then*

$$M_1(G) \leq 2k(n-1)^2 + 4k^2(n-2k)$$

with equality if and only if $G \cong K_{2k} \vee (n-2k)K_1$.

An outerplanar graph is a planar graph that has a planar drawing with all vertices on the same face. Thus, a graph is outerplanar if it can be embedded in the plane so that all its vertices lie on the outer face boundary. An edge of an outerplanar graph is said to be a chord if it joins two vertices of the outer face boundary of G, but is not itself an edge of the outer face boundary. A maximal outerplanar graph is an outerplanar graph such that all its faces, except eventually the outer face, are composed by three edges. Such a graph on n ($n \geq 3$) vertices has a plane representation as an n-gon triangulated by $n-3$ chords.

Denote by $P_{n,2}$ the graph obtained from P_n by adding new edges joining all pairs of vertices at distance 2 apart. Fig. 2 shows $P_{n,2}$ for the even and odd values of n.

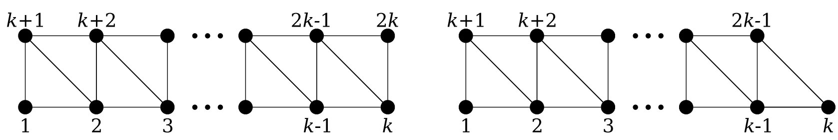

Fig. 2. The graph $P_{n,2}$ for $n = 2k$ and $2k-1$.

In thw paper [80], Hou et al. determined sharp upper bounds for M_1 among all (maximal) outerplanar graphs on n vertices, as well as among all $2k$-vertex conjugated (maximal) outerplanar graphs (i.e., outerplanar graphs on $2k$ vertices with perfect matchings).

Theorem 4.37. [80] *Let G be a maximal outerplanar graph on n ($n \geq 4$) vertices.*

(i) If $n = 6$, then $M_1(G) \leq 60$, with equality if and only if $G \cong K_1 \vee P_5$ or $G \cong H$, where H is the graph depicted in Fig. 3.

(ii) If $n \neq 6$, then $M_1(G) \leq n^2 + 7n - 18$ with equality if and only if $G \cong K_1 \vee P_{n-1}$.

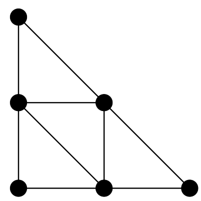

Fig. 3. The graph occurring in Theorem 4.37.

Theorem 4.38. [80] *Let G be conjugated maximal outerplanar graph on $2k$ vertices. Then*

$$32k - 38 \leq M_1(G) \leq 4k^2 + 14k - 18\,. \tag{29}$$

The left equality holds if and only if $G \cong P_{2k,2}$. If $k \neq 3$, then the right equality holds in (29) *if and only if $G \cong K_1 \vee P_{2k-1}$. If $k = 3$, then the right equality holds in* (29) *if and only if $G \cong K_1 \vee P_5$ or $G \cong H$ (where H is depicted in Fig. 3).*

Since by the definition of Zagreb indices it holds $M_i(G - e) < M_i(G)$, for $i = 1, 2$ and $e \in E(G)$, the extremal outerplanar graphs (with perfect matchings) whose M_i-values attain maximum must be maximal outer planar graphs. Thus, the statements of Theorems 4.37 and 4.38 still remain true for outerplanar graphs and conjugated outerplanar graphs, respectively. Similarly, the extremal outerplanar graphs (with perfect matchings) whose M_i-values attain minimum must be n-vertex trees, in fact n-vertex paths.

A graph is called a series–parallel if it does not contain a subdivision of K_4 [48]. For example, outerplanar graphs are series–parallel.

Theorem 4.39. [155] *Let G be a series–parallel graph with $n \geq 2$ vertices and m edges. Suppose that G has no isolated vertices. Then*

$$M_1(G) \leq n(m-1) + 2m$$

with equality for $n \geq 3$ if and only if G is isomorphic to $K_{1,1,n-2}$.

The *clique number* of G, denoted by $\omega(G)$, is the number of vertices in a largest clique of G. Let $\mathcal{W}_{n,k}$ be the set of connected n-vertex graphs with clique number k. The graphs with extremal (maximal and minimal) Zagreb indices belonging to $\mathcal{W}_{n,k}$ are characterized in [143]. Recall that the Turán graph $T_n(k)$ is a complete k-partite graphs whose partition sets differ in size by at most one. Obviously, for $k = 1$, the set $\mathcal{W}_{n,k}$ contains a single connected graph K_1. When $k = n$, the only graph in $\mathcal{W}_{n,k}$ is K_n. So, it may be assumed that $1 < k < n$ and let $n = kq + r$, where $0 \leq r < k$ and $q = \lfloor \frac{n}{k} \rfloor$.

Theorem 4.40. [143] *Let $G \in \mathcal{W}_{n,k}$. Then*

$$M_1(G) \leq (k-r) \left\lfloor \frac{n}{k} \right\rfloor \left(n - \left\lfloor \frac{n}{k} \right\rfloor \right)^2 + r \left\lceil \frac{n}{k} \right\rceil \left(n - \left\lceil \frac{n}{k} \right\rceil \right)^2$$

with equality if and only if $G \cong T_n(k)$.

In the following, we give a survey of results on the minimum of M_1 among the graphs with some given parameters.

Let Γ be the class of graphs $H = (V, E)$, where H is a graph of minimum vertex degree δ and maximum vertex degree Δ ($\Delta \neq \delta$) such that

$$d_2 = d_3 = \cdots = d_{n-1} = d_n = \delta \ , \ d_i = d_H(v_i) \ , \ i = 2, 3, \ldots, n \, .$$

Let Γ_2 and Γ_3 be the class of graphs such that $d_2 = d_3 = \cdots = d_{n-1} = \Delta_2$, $d_n = \delta$, with $d_1 = \Delta > d_i$, $i = 2, 3, \ldots, n$ and $d_i = \delta$ with $d_1 \geq d_2 > d_i$, $i = 3, 4, \ldots, n$, respectively. Das [32, 41] obtained the following lower bounds for M_1 which are better than (9).

Theorem 4.41. [32] *Let G be an (n, m)-graph with maximum degree Δ and minimum degree δ. Then*

$$M_1 \geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_2$.

Theorem 4.42. [41] *Let G be an (n, m)-graph with maximum degree Δ, second–maximum degree Δ_2 and minimum degree δ. Then*

$$M_1 \geq \Delta^2 + \frac{(2m - \Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2} (\Delta_2 - \delta)^2 \, .$$

The equality holds if and only if G is regular or $G \in \Gamma$.

Recently, Milovanović and Milovanović [112] proposed a new lower bound for M_1 better than (9). The conclusion related to the equality case was wrong in [112] and it was eventually corrected in [109], and the equality case additionally corrected in [36].

Theorem 4.43. [36, 109, 112] *Let G be an (n, m)-graph, $n \geq 2$, with maximum degree Δ and minimum degree δ. Then*

$$M_1 \geq \frac{4m^2}{n} + \frac{1}{2} (\Delta - \delta)^2$$

with equality if and only if G has the property $d_2 = d_3 = \cdots = d_{n-1} = (\Delta + \delta)/2$, which includes also the regular graphs.

In [36], the following strengthening of Theorem 4.43 was achieved:

Theorem 4.44. [36] *Let G be an (n,m)-graph, $n \geq 2$, with maximum degree Δ and minimum degree δ. Then*

$$M_1 \geq \frac{4m^2 + (n-1)(\Delta^2 + \delta^2) - 4m(\Delta + \delta) + 2\Delta\,\delta}{n-2}$$

with equality if and only if G has the property $d_2 = d_3 = \cdots = d_{n-1}$.

In the paper [109], the following lower bounds for M_1, better than (9), were also obtained.

Theorem 4.45. [109] *Let G be an (n,m)-graph, $n \geq 3$, with maximum degree Δ, minimum degree δ and the second–maximum degree Δ_2. Then*

$$M_1 \geq \Delta^2 + \Delta_2^2 + \frac{(2m - \Delta - \Delta_2)^2}{n-2}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_3$.

Corollary 4.5. [109] *With the assumptions as in Theorem 4.45, one has the inequality*

$$M_1 \geq \Delta^2 + \frac{(2m - \Delta)^2}{n-1}$$

with equality if and only if G is regular or $G \in \Gamma$.

A lower bound for M_1 of maximal outerplanar graphs was established in [80].

Theorem 4.46. [80] *Let G be maximal outerplanar graph on n vertices. Then*

$$M_1(G) \geq 16n - 38 \tag{30}$$

and the equality holds if and only if $G \cong P_{n,2}$.

In the paper [143], a sharp lower bound for M_1 of n-vertex graphs with a given clique number has been determined.

Theorem 4.47. [143] *Let $G \in \mathcal{W}_{n,k}$. Then*

$$M_1(G) \geq k^3 - 2k^2 - k + 4n - 4$$

with equality if and only if $G \cong Ki_{n,k}$, where $Ki_{n,k}$ is a kite.

The *local independence number* $\alpha(v)$ of a vertex v, is the independence number of the subgraph induced by the closed neighborhood of v. The *average local independence number* $\overline{\alpha}(G)$, of a graph G, is defined as $\frac{1}{n}\sum_{v \in V(G)} \alpha(v)$, [43].

In the paper [114], the following upper bound on the average local independence number in terms of n, m, the number of triangles t, and the first Zagreb index M_1 is obtained, from which the lower bound on M_1 can be deduced.

Theorem 4.48. [114] *Let G be connected (n,m)-graph with t triangles. Then*

$$\overline{\alpha}(G) \leq \sqrt{\frac{1}{n}(M_1 - 2m - 6t) + \frac{1}{4}} + \frac{1}{2}\,.$$

Also, it was proven in [50] that for an n-vertex graph G, $n \geq 3$, without isolated vertices, $M_1(G) \geq 3m$ and $M_2(G) \geq 2m$ with equality if and only if $G \cong P_3$.

5. Second Zagreb index

We first consider upper bounds for M_2.

Let G be an (n,m)-graph. Bollobás and Erdős [18] proved that if $m = k2$, then $M_2(G) \leq m(k-1)^2$, with equality if and only G is the union of the complete graph K_k and isolated vertices. This result can be reformulated as follows.

Theorem 5.1. [18] *Let G be a graph with n vertices and m edges. Then*

$$M_2(G) \leq m\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)^2$$

with equality if and only if m is of the form $m = \binom{k}{2}$ for some positive integer k, and G is the union of the complete graph K_k and isolated vertices.

For given n and m, the graphs with largest M_2-values are characterized in [45, 144].

Theorem 5.2. [45, 144] *Let G be a connected graph of order n with m edges, $n-1 \leq m \leq n+1$. If M_2 is maximum, then*

(i) $G \cong K_{1,n-1}$ *for* $m = n-1$*;*

(ii) $G \cong K_{1,n-1} + e$ *for* $m = n$ *where* $e = uv$ *with* u, v *as two pendent vertices in* $K_{1,n-1}$*;*

(iii) $G \cong B_n^{(1)}$ *for* $m = n+1$.

The following upper bound on M_2 is obtained in [144]:

Theorem 5.3. [144] *Let G be a connected graph of order n with m $(= n+2)$ edges. Then*

$$M_2(G) \leq n^2 + 4n + 22$$

with equality holding if and only if $\overline{G} \cong (K_{n-4} \vee 3\,K_1) \cup K_1$.

Denote by K_k^{n-k} the graph obtained by attaching $n-k$ pendent vertices to one vertex of K_k. For any positive integer $t < k$, let $K_k^{n-k}(t)$ be a graph obtained by adding t new edges between one pendent vertex in K_k^{n-k} and t vertices with degree $k-1$ in it. In particular, $\overline{(K_{n-4} \vee 3\,K_1) \cup K_1} \cong K_4^{n-4}$. For given n and m, the graph with largest M_2-values is characterized in [144]:

Theorem 5.4. [144] *Let G be a connected graph of order n with m edges, such that $m = n + \binom{k}{2} - k$, $k \geq 4$. If M_2 is maximum, then $G \cong K_k^{n-k}$.*

Xu, Das and Balachandran [144] gave the following conjecture:

Conjecture 5.1. *Let G be a connected graph of order n with m edges, $m \geq n+3$. If M_2 is maximum, then $G \cong K_k^{n-k}(t)$ if $m - n = \binom{k}{2} - k + t$ with $1 \leq t \leq k-1$ and $4 \leq k \leq n-2$.*

Bollobás, Erdős and Sarkar [19] proved the following:

Theorem 5.5. [19] *Let k and r be positive integers such that $0 < r \leq k$. Then all graphs G with $m = \binom{k}{2} + r$ edges and minimal degree at least one, satisfy*

$$M_2(G) \leq k^2 \binom{r}{2} + (k-1)^2 \binom{k-r}{2} + k(k-1)(k-r)r + kr^2$$

and the equality holds if and only if the graph G consists of a complete graph K_k together with an additional vertex joined to r vertices of K_k.

In the papers [154, 156, 158], results concerning upper bounds for the second Zagreb index of K_{r+1}-free graphs, $r \geq 2$, were obtained.

Theorem 5.6. [154] *Let G be a triangle–free graph with $m > 0$ edges. Then,*

$$M_2(G) \leq m^2$$

with equality if and only if G is the union of a complete bipartite graph and isolated vertices.

By Turán's theorem, for an (n, m)-triangle–free graph, $m \leq \lfloor \frac{n^2}{4} \rfloor$ with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$. Then, by the previous theorem, for an (n, m)-triangle–free graph it holds [154]

$$M_2(G) \leq \left\lfloor \frac{n^2}{4} \right\rfloor^2$$

with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$.

Recall that we use the notation $even(n) = 1$ if n is even and $even(n) = 0$, otherwise.

Theorem 5.7. [158]

(i) Let G be a quadrangle–free graph with n vertices and $m > 0$ edges. Then,

$$M_2(G) \leq mn + \binom{n}{2} - even(n)$$

with equality if and only if $G \cong \widetilde{W}_n$ for odd n, where $\widetilde{W}_n$ is the graph defined in Section 4 (in Theorem 4.20).

(ii) Let Let G be a triangle– and quadrangle–free graph with n vertices and $m > 0$ edges. Then,

$$M_2(G) \leq m(n-1)$$

with equality if and only if G is the star $K_{1,n-1}$ or a Moore graph of diameter 2.

More generally, it holds:

Theorem 5.8. [156] *Let G be a K_{r+1}-free graph with n vertices and $m > 0$ edges, where $2 \leq r \leq n-1$. Then*

$$M_2(G) \leq \frac{2}{r} m^2 + \frac{(r-1)(r-2)}{r^2} mn^2$$

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

As a consequence, the following theorem has been proved.

Theorem 5.9. [156] *Let G be a $K_{1,1,k+1}$- and $K_{2,l+1}$-free graph with n vertices and $m > 0$ edges, where $0 \leq k \leq l$. Then*

$$M_2(G) \leq m(k+1-l)^2 + l(n-1)m + \frac{1}{2}(k+1-l)ln(n-1)$$

with equality if and only if each pair of adjacent vertices in G has exactly k common neighbors and each pair of non-adjacent vertices in G has exactly l common neighbors.

In the paper [87], Lang et al. considered the second Zagreb index of bipartite graphs with a given number of vertices and edges and gave a necessary condition for a maximal M_2-value. Denote by $B(X,Y)$ a connected bipartite graph with a bipartition (X,Y) and by $\mathcal{B}(X,Y)$ the set of bipartite graphs $B(X,Y)$. In [87], the following ordered sets are defined. Let $\{u,v\} \in V(G)$. The pair of vertices $\{u,v\}$ is said to be ordered if $d(u) \geq d(v)$ implies $N_G(v) \subseteq N_G(u)$. A subset $S \subset V(G)$ is called an ordered set of vertices if any pair of vertices of S is ordered. Also, $B(X,Y)$ is said to be an ordered bipartite graph if X and Y are ordered sets of vertices. Otherwise, the graph $B(X,Y)$ is referred to as an unordered bipartite graph.

Theorem 5.10. [87] *Let m and n be two integers such that $n-1 \leq m \leq \lfloor n/2 \rfloor \lceil n/2 \rceil$. If $B(X,Y)$ attains the maximum value of the second Zagreb index in $\mathcal{B}(X,Y)$ with n vertices and m edges, then $B(X,Y)$ must be an ordered bipartite graph.*

Theorem 5.11. [87] *Let m, n and p be integers such that $m = (n-1)+(p-1)(n_2-1)+k$, where $p \geq 1$, $k \leq n_2 - 1$. If the graph $B(X,Y)$ with $|X| = n_1$ and $|Y| = n_2$ satisfies $|\{v \in X | d(v) = n_2\}| = p$, then*

$$M_2(G) \leq pn_1n_2 + p^2\,n_2^2 + n_1^2 + (k-p)n_1 + p(k-p)n_2 + (p+1)k(k+1)\,.$$

In the next theorem, in addition to n and m, the upper bounds depend also on the minimum vertex degree δ.

Theorem 5.12. [158] *(i) Let G be a quadrangle–free graph with n vertices, m edges and minimum vertex degree $\delta \geq 1$. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + (\delta-1)\left[\binom{n}{2} + m\right]$$

with equality if and only if G is isomorphic to a redefined windmill $\widetilde{W}_n$ (see Theorem 4.20) for odd n, or $\frac{n}{2}K_2$ for even n, or the star $K_{1,n-1}$.

(ii) Let G be a triangle– and quadrangle–free graph with n vertices, m edges, and minimum vertex degree $\delta \geq 1$. Then

$$M_2(G) \leq 2m^2 - (n-1)m\delta + (\delta-1)\binom{n}{2}$$

with equality if and only if G is the star $K_{1,n-1}$, or $\frac{n}{2}K_2$ for even n, or a G is a Moore graph of diameter 2.

In [157], an upper bound for M_1 in terms of n, m, the minimum vertex degree δ, and the maximum degree Δ was established (cf. Theorem 4.8). Fonseca and Stevanović [56] proved the analogous upper bound on M_2 for general values of n, m, δ, and Δ.

Theorem 5.13. [56] *Let G be a graph with n vertices, m edges, the minimum vertex degree δ and maximum vertex degree $\Delta > \delta + 1$. Then*

$$\begin{aligned} M_2 \;\leq\; & \frac{1}{2}\Big[(2m-k)(\Delta^2+\Delta\delta+\delta^2)-(n-1)\Delta\delta(\Delta+\delta)\Big] \\ + & \begin{cases} k\delta(k-\frac{\delta}{2}) & \textit{if } k \leq (\Delta+\delta)/2 \\ k\Delta(k-\frac{\Delta}{2}) & \textit{if } k > (\Delta+\delta)/2 \end{cases} \end{aligned} \tag{31}$$

where k is an integer defined via

$$2m - n\delta \equiv k - \delta\,(mod\,(\Delta-\delta))\ \ ,\ \ \delta \leq k \leq \Delta - 1$$

i.e.,

$$k = 2m - \delta(n-1) - (\Delta-\delta)\left\lfloor \frac{2m-n\delta}{\Delta-\delta} \right\rfloor .$$

A graph G attains equality in (31) *if and only if G does not contain an edge connecting a vertex of degree Δ to a vertex of degree δ and it contains at most one vertex of degree $k \neq \Delta, \delta$ such that*

(i) the vertex of degree k is adjacent to vertices of degree δ only, when $k < (\Delta+\delta)/2$;

(ii) the vertex of degree k is adjacent to a vertex of degree Δ only, if $k > (\Delta+\delta)/2$.

Remark. The case of equality in (31) implies that if $k \neq (\Delta+\delta)/2$, then the graph with the maximum value of M_2 for given n, m, Δ and δ is necessarily disconnected. If $k < (\Delta+\delta)/2$, then the vertices of degree Δ are adjacent only to vertices of degree Δ, while if $k > (\Delta+\delta)/2$, then the vertices of degree δ are adjacent only to vertices of degree δ. Only when $k = (\Delta+\delta)/2$, an M_2-maximal graph may be connected, as then the vertex of degree k may be adjacent both to vertices of degree Δ and to vertices of degree δ. The same situation is present in Theorem 4.8 as well. All this is not a mistake, but it just means that graphs attaining the maximum value of the first or second Zagreb index may happen to be disconnected multigraphs, as suggested in [56].

The appearance of disconnected multigraphs as extremal graphs for the second Zagreb index may be avoided in the case of trees (see Theorem 6.6).

In the papers [39, 41], Das et al. established some upper and lower bounds on $M_2(G)$ in terms of n, m, δ, Δ, and Δ_2.

Theorem 5.14. [39] *Let G be a graph with n vertices, m edges, maximum degree Δ, second–maximum degree Δ_2 and minimum degree δ. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta-1)\left[\frac{(2m-\Delta)^2}{n-1} + \Delta^2 + \frac{n-1}{4}(\Delta_2-\delta)^2\right]$$

with equality if and only if G is a regular graph or $G \cong K_{1,n-1}$ or $G \cong K_{p+1,p}$, $n = 2p+1$.

Theorem 5.15. [41] *Let G be a graph with n vertices, m edges, maximum degree Δ, second–maximum degree Δ_2 and minimum degree δ. Then*

(i)

$$\begin{aligned} M_2(G) &\geq 2m^2 - (n-1)m\Delta \\ &+ \frac{1}{2}(\Delta - 1)\left[\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2 - \delta)^2\right] \end{aligned}$$

with equality if and only if G is regular graph;

(ii)

$$\begin{aligned} M_2(G) &\leq 2m^2 - (n-1)m\delta \\ &+ \frac{1}{2}(\delta - 1)\left[(n+1)m - \Delta(n-\Delta) + \frac{2(m-\Delta)^2}{n-2}\right] \end{aligned}$$

with equality if and only if $G \cong K^*_{2,n-2}$ or $G \cong K_n$.

For triangle– and quadrangle–free graphs, an upper bound for M_2 was established in terms of n, m, and radius r.

Theorem 5.16. [145] *Let G be a triangle– and quadrangle–free connected graph with n vertices, m edges and radius r. Then, $M_2(G) \leq m(n+1-r)$ and the equality holds if and only if G is a Moore graph of diameter two or G is the 6-vertex cycle C_6.*

Extremal graphs whose M_2 is maximum among connected graphs with matching number β are characterized in [51].

Theorem 5.17. [51] *Let G be a connected graph with $n \geq 4$ vertices and matching number β, $2 \leq \beta \leq \lfloor n/2 \rfloor$. Let c be the largest root of the cubic equation*

$$16x^3 + 2x^2(n-13) + x(14n + 1 - 3n^2) - 2n^2 = 0\,.$$

Then the following holds:

(1) If $\beta = \lfloor n/2 \rfloor$, then

$$M_2(G) \leq \frac{1}{2}n(n-1)^3$$

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

(2) If $c < \beta \leq \lfloor n/2 \rfloor - 1$, then

$$M_2(G) \leq n^2 + 4n\beta^2 - 6n\beta - 20\beta^3 + 8\beta^4 + 14\beta^2 - \beta$$

with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(3) If $\beta = c$, then

$$M_2(G) \leq n^2 + 4nc^2 - 6nc - 20c^3 + 8c^4 + 14c^2 - c = \frac{1}{2}c(n-1)(1 - c - 2c^2 - n + 3cn)$$

with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$ or $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(4) If $2 \leq \beta < c$*, then*

$$M_2(G) \leq \frac{1}{2}\beta(n-1)(1-\beta-2\beta^2-n+3\beta n)$$

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

In [52] and [53], Feng et al. characterized the graphs from the set $\mathcal{G}_n^k$ of all connected graphs with n vertices and k cut edges whose M_2 is maximum (minimum).

Theorem 5.18. [52,53] *Let* $G \in \mathcal{G}_n^k$*, then*

$$4n+4 \leq M_2(G) \leq \frac{1}{2}(n-k-1)^3(n-k-2)+(n-1)^2$$

and the left equality holds if and only if $G \cong C_n^k$ *and the right equality holds if and only if* $G \cong K_n^k$.

Li and Zhou [92] determined sharp lower and upper bounds for the second Zagreb index of graphs with connectivity (edge–connectivity) at most k. Recall that we use $\mathcal{V}_n^k$ ($\mathcal{E}_n^k$) to denote the set of graphs of order n with $\kappa(G) \leq k \leq n-1$ ($\kappa'(G) \leq k \leq n-1$), and by G_n^k we denote a graph obtained by joining k edges from k vertices of K_{n-1} to an isolated vertex.

Theorem 5.19. [92] *Among all graphs* G *in* $\mathcal{V}_n^k$ ($\mathcal{E}_n^k$)*,* $k > 0$*, we have*

$$M_2(G) \geq 4n-8$$

and

$$M_2(G) \leq k^2(n-1)+\binom{k}{2}(n-1)^2+\binom{n-k-1}{2}(n-2)^2+k(n-k-1)(n^2-3n+2)$$

where the lower bound is attained if and only if $G \cong P_n$ *and the upper bound is attained if and only if* $G \cong G_n^k$.

As mentioned before, Hou et al. [80] determined sharp upper and lower bounds for M_2 among (maximal) outerplanar graphs on n vertices, as well as among conjugated (maximal) outerplanar graphs.

Theorem 5.20. [80] *Let* G *be a maximal outerplanar graph on* n *vertices,* $n \geq 4$*. Then*

(i) $M_2(G) \geq 32n-100$*, with equality if and only if* $G \cong P_{n,2}$.

(ii) If $n = 6$*, then* $M_2(G) \leq 96$*, with equality if and only if* $G \cong H$*, where* H *is the graph depicted in Fig. 3.*

(iii) If $n \neq 6$*, then* $M_2(G) \leq 3n^2+n-19$ *with equality if and only if* $G \cong K_1 \vee P_{n-1}$.

Theorem 5.21. [80] *Let* G *be conjugated maximal outerplanar graph on* $2k$ *vertices. Then*

$$64k-100 \leq M_2(G) \leq 12k^2+2k-19\,.$$

The left equality holds if and only if $G \cong P_{2k,2}$*. For* $k \neq 3$*, the right equality holds if and only if* $G \cong (K_1 \vee P_{2k-1})$*. For* $k = 3$*, the right equality holds if and only if* $G \cong H$ *(depicted in Fig. 3).*

As noted before, extremal (conjugated) outerplanar graphs whose M_2 is maximum coincide with those specified in Theorems 5.20 and 5.21. However, extremal (conjugated) outerplanar graphs whose M_2 is minimum are n-vertex paths.

Upper bounds on M_2 of series–parallel graphs were determined in [155].

Theorem 5.22. [155] *Let G be a series–parallel graph with $n \geq 2$ vertices and m edges. Suppose that G has no isolated vertices. Then*

$$M_2(G) \leq m^2 + \frac{1}{2}n(m-1)$$

with equality for $n \geq 3$ if and only if G is isomorphic to $K_{1,1,n-2}$.

Theorem 5.23. [155] *Let G be a series–parallel graph with $n \geq 2$ vertices, m edges and minimum vertex degree δ. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta-1)\big[n(m-1)+2m\big]$$

with equality if and only if G is isomorphic to $K_{1,1,n-2}$ or $K_{1,n-1}$ or $\frac{n}{2}K_2$ for even n.

Xu [143] obtained sharp upper and lower bounds for the second Zagreb index of graphs from the set $\mathcal{W}_{n,k}$ of n-vertex graphs with a clique number k.

Theorem 5.24. [143] *Let $G \in \mathcal{W}_{n,k}$. Then*

(1)

$$\begin{aligned} M_2(G) \ \leq \ & \binom{k-r}{2}\left\lfloor\frac{n}{k}\right\rfloor^2\left(n-\left\lfloor\frac{n}{k}\right\rfloor\right)^2 + r(k-r)\left\lfloor\frac{n}{k}\right\rfloor\left\lceil\frac{n}{k}\right\rceil\left(n-\left\lfloor\frac{n}{k}\right\rfloor\right)\left(n-\left\lceil\frac{n}{k}\right\rceil\right) \\ + \ & \binom{r}{2}\left\lceil\frac{n}{k}\right\rceil^2\left(n-\left\lceil\frac{n}{k}\right\rceil\right)^2 \end{aligned}$$

with equality if and only if $G \cong T_n(k)$;

(2)

$$M_2(G) \geq \binom{k}{2}(k-1)^2 + k^2 + 4(n-k) - 5$$

with equality if and only if $G \cong Ki_{n,k}$, where $Ki_{n,k}$ is a kite graph.

6. On extremal Zagreb indices of trees

A tree is a connected graph without cycles. In every tree $\delta = 1$. The tree with $\Delta = 2$ is the path P_n and the tree with $\Delta = n-1$ is the star $K_{1,n-1}$. In chemical trees it must be $\Delta \leq 4$. In the case of trees (both chemical and non-chemical), the relations (5) and (10) are significantly simplified and thus, the following result is straightforward.

Theorem 6.1. [66] *Let T be any tree of order n. Then*

$$4n - 6 \leq M_1(T) \leq n(n-1)$$

and the left equality holds if and only if $T \cong P_n$ and the right equality holds if and only if $T \cong K_{1,n-1}$.

Using the bound (18) from [103], the first four trees from the class $\mathcal{T}(n)$ of trees on n vertices whose M_1 is maximum were determined.

Theorem 6.2. [103] *Suppose that $T_1 \cong K_{1,n-1}$ and $T \in \mathcal{T}(n)$. If $n \geq 9$ and $T \in \mathcal{T}(n) \setminus \{T_1, T_2, T_3, T_4, T_5\}$, then $M_1(T_1) > M_1(T_2) > M_1(T_3) > M_1(T_4) = M_1(T_5) > M_1(T)$, where $T_2 - T_5$ are trees depicted in Fig. 4.*

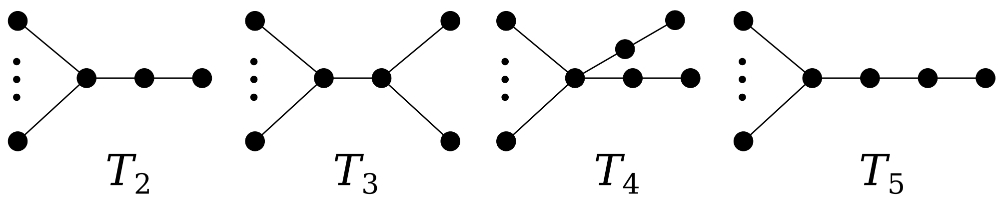

Fig. 4. The trees occurring in Theorem 6.2.

In [37], the trees with maximal and minimal value of the second Zagreb index are obtained as follows.

Theorem 6.3. [37] *Let T be any tree of order n, then*

$$4n - 8 \leq M_2(T) \leq (n-1)^2$$

and the left equality holds if and only if $T \cong P_n$ and the right equality holds if and only if $T \cong K_{1,n-1}$.

Das et al. [38] obtained the following upper bound on $M_1(T)$ in terms of n and Δ:

Theorem 6.4. [38] *Let T be a tree with n vertices and maximum degree Δ. Then*

$$M_1(T) \leq n^2 - 3n + 2(\Delta + 1)$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong P_4$.

In the paper [35], the authors gave some lower and upper bounds on the first Zagreb index $M_1(G)$ of graphs and trees in terms of number of vertices, irregularity index, maximum degree, and characterized extremal graphs. Let Υ_1 be the class of trees $T = (V, E)$ such that T is a tree of order n, irregularity index t, maximum degree Δ and

$$\Delta = t \ , \ d_i = 1 \, , \, i = t, t+1, \ldots, n \, .$$

Theorem 6.5. [35] *Let T be a tree of order n with irregularity index t and maximum degree Δ. Then*

$$M_1(T) \leq \left[n - 3 - \frac{t(t-3)}{2}\right] \Delta^2 - (t-1)(t-2)\Delta + \frac{1}{3}\left(t^3 - 3t^2 + 2t + 6\right)$$

with equality if and only if $G \in \Upsilon_1$.

A caterpillar or caterpillar tree is a tree in which all the pendent vertices are within distance 1 of a central path. In [133] it was noted that each even number, except 4 and 8 is the first Zagreb index of a caterpillar.

From Theorem 4.8, it can easily be deduced that for a tree T with n vertices and maximum degree $\Delta > 1$ it is satisfied

$$M_1(T) \leq 2(n-1)(1+\Delta) - n\Delta + (1-k)(\Delta - k)$$

where k is an integer defined via

$$k = n - 1 - (\Delta - 1)\left\lfloor \frac{n-2}{\Delta - 1} \right\rfloor .$$

Equality is attained if and only if at most one vertex of T has degree different from 1 and Δ.

Besides, Corollary 4.1 implies the upper bound for the first Zagreb index of chemical trees with $n \geq 2$ vertices. This upper bound is also obtained in [107]. As in [107], for $n = 3\ell \geq 6$ let $T_{3\ell}$ be the family of chemical trees with n vertices, such that $\ell - 1$ vertices have degree 4, one vertex has degree 2 and the remaining vertices are pendent. Denote by $\widetilde{T}_{3\ell}$ a subset of $T_{3\ell}$ such that for the unique vertex $v \in V(T)$, $T \in \widetilde{T}_{3\ell}$, of degree 2, exactly one of its neighbors is pendent. For $n = 3\ell + 1 \geq 7$, let $T_{3\ell+1}$ be the family of chemical trees with n vertices such that $\ell - 1$ vertices have degree 4, one vertex has degree 3 and the remaining vertices are pendent, while $\widetilde{T}_{3\ell+1}$ denotes the family of trees T from $T_{3\ell+1}$ such that for the unique vertex $v \in V(T)$ of degree 3 exactly one of its neighbors is pendent. Finally, for $n = 3\ell + 2 \geq 5$, let $T_{3\ell+2}$ denotes the family of chemical trees with n vertices such that ℓ vertices have degree 4, and the remaining vertices are pendent. Then,

$$M_1(T) \leq \begin{cases} 6n - 10 & \text{if } n \equiv 2 \,(\mathrm{mod}\, 3) \\ 6n - 12 & \text{otherwise} \end{cases}$$

with equality if and only if $T \in T_n$.

The trees with the maximum second Zagreb index among the trees with given n and Δ are determined in [56].

Theorem 6.6. [56] *Let T be a tree with n vertices and the maximum degree $\Delta \geq 2$. Then*

$$M_2(T) \leq \Delta(2n - \Delta - 1 - k) + k(k-1)$$

where

$$k \equiv n - 1 (\mathit{mod}\,(\Delta - 1))\,,\ 1 \leq k \leq \Delta - 1$$

i.e.,

$$k = n - 1 - (\Delta - 1)\left\lfloor \frac{n-2}{\Delta - 1} \right\rfloor .$$

Equality is attained if and only if T has at most one vertex of degree k that is adjacent to a single vertex of degree Δ, and all other vertices of T have degree either Δ or 1.

As a simple corollary of the previous theorem, an upper bound for the second Zagreb index of chemical trees, can easily be obtained. This upper bound was determined in [107].

$$M_2(T) \le \begin{cases} 8n - 24 & \text{if } n \equiv 2 \,(\mathrm{mod}\, 3) \\ 8n - 26 & \text{otherwise} \end{cases}$$

with equality if and only if $n \equiv 0, 1(\mathrm{mod}\, 3)$ and $G \in \widetilde{T}_n$, or $n \equiv 2(\mathrm{mod}\, 3)$ and $G \in T_n$.

In order to state the results from [138] we need the following notations. Denote by m_{ij} $(1 \le i, j \le \Delta)$ the number of edges that connect vertices of degrees i and j in a tree T, and by n_i $(i = 1, 2, \ldots, \Delta)$ the number of vertices of degree i.

Theorem 6.7. [138] *Let T be a tree with maximal second Zagreb index with n_i vertices of degree i and maximal degree Δ. Then,*

1) $m_{\Delta\Delta} = n_\Delta - 1$;

2) $m_{ij} = \min\left\{ n_i - \sum_{k=j+1}^{\Delta} m_{ik} \, , \, jn_j - \sum_{k=i+1}^{j} m_{kj} - \sum_{k=j}^{\Delta} m_{jk} \right\}$ for each $1 \le i < j \le \Delta$;

3) $m_{ii} = n_i - \sum_{k=i+1}^{\Delta} m_{ik}$ for each $i = 1, \ldots, \Delta - 1$.

Using this result, in the same paper, the authors presented a simple algorithm for calculating the maximal value of the second Zagreb index for trees with prescribed number of vertices of given degree. The user needs only to input values $n_1, n_2, \ldots, n_\Delta$ and the algorithm outputs the edge connectivity values m_{ij} as well as the maximal value of the second Zagreb index. The complexity of algorithm is proportional to Δ^3. Since the complexity is independent of the number of vertices, for chemical trees the algorithms works in constant time no matter how large the molecule is.

Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two different non-increasing degree sequences. We write $\pi \lhd \pi'$ if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$ and $\sum_{i=1}^{j} d_i \le \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is called to be a *majorization* [110]. Also, we use $\Gamma(\pi)$ to denote the class of connected graphs that have degree sequence π.

For a given degree sequence π, let $M_2(\pi) = \max\{M_2(G) | G \in \Gamma(\pi)\}$. A graph G is called an *optimal graph* in $\Gamma(\pi)$ if $G \in \Gamma(\pi)$ and $M_2(G) = M_2(\pi)$.

Liu and Liu [104] characterized optimal trees in the set of trees with a given degree sequence.

A sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called a *tree degree sequence* if there exists a tree T having π as its degree sequence, i.e., if and only if

$$\sum_{i=1}^{n} d_i = 2(n-1) . \tag{32}$$

In order to present the main results of the paper [104], we introduce some more notations. Assume that G is a rooted graph with root v_0. Let $h(v)$, also called *height* of a vertex v, be the distance between v and v_0 and $V_i(G)$ be the set of vertices at distance i from vertex v_0. Then, according to [152], a well-ordering $\prec$ of the vertices is called *breadth–first search* ordering with non-increasing degrees (BFS-ordering, for short) if the following holds for all vertices $u, v \in V(G)$:

(i) $u \prec v$ implies $h(u) \leq h(v)$;

(ii) $u \prec v$ implies $d(u) \geq d(v)$;

(iii) if there are two edges $uu_1 \in E(G)$ and $vv_1 \in E(G)$ such that $u \prec v$, $h(u) = h(u_1) + 1$ and $h(v) = h(v_1) + 1$, then $u_1 \prec v_1$.

A tree that has a BFS-ordering of its vertices is said to be a BFS-tree.

In order to solve the problem of finding optimal trees in $\Gamma(\pi)$, Liu and Liu [104] used the method of [152] to define a special tree $T^* \in \Gamma(\pi)$ as follows: Select a vertex v_0 in layer 0 and create a sorted list of vertices beginning with v_0. Choose d_1 new vertices in layer 1 adjacent to v_0, say $v_{11}, v_{12}, \ldots, v_{1d_1}$, then $d(v_0) = d_1$. Choose $d_2 + \ldots + d_{d_1} - d_1$ new vertices in layer 2 such that $d_2 - 1$ vertices, say $v_{21}, v_{22}, \ldots, v_{2,d_2-1}$, are adjacent to v_{11}, $d_3 - 1$ vertices are adjacent to v_{12}, …, $d_{d_1} - 1$ vertices are adjacent to v_{1d_1}. Then $d(v_{11}) = d_2$, $(v_{12}) = d_3, \ldots, d(v_{1,d_1}) = d_{d_1}$. Now choose $d_{d_1+1} - 1$ new vertices in layer 3 adjacent to v_{21} and hence $d(v_{21}) = d_{d_1+1}, \ldots$. Continue recursively with $v_{22}, v_{23}, \ldots$ until all vertices in layer 3 are processed. Repeat the above procedure until all vertices are processed. In this way, a BFS-tree $T^* \in \Gamma(\pi)$ is obtained. For example, for a given tree degree sequence $\pi_1 = (4, 4, \underbrace{3, \ldots, 3}_{4}, 2, 2, 2, \underbrace{1, 1, \ldots, 1}_{10})$ a BFS-tree T_1^* is depicted in Fig. 5.

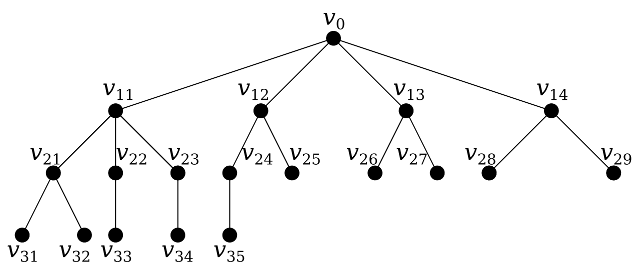

Fig. 5. The BFS-tree T_1^* with degree sequence $(4, 4, \underbrace{3, \ldots, 3}_{4}, 2, 2, 2, \underbrace{1, 1, \ldots, 1}_{10})$.

Theorem 6.8. [152] *For a given tree degree sequence π, there exists a unique BFS-tree T^* in $\Gamma(\pi)$, i.e., T^* is uniquely determined up to isomorphism.*

Now, the main result of paper [104] can be stated as follows.

Theorem 6.9. [104] *Given a tree degree sequence π, the BFS-tree T^* has the maximum second Zagreb index in $\Gamma(\pi)$.*

Hence, by Theorems 6.8 and 6.9, there is a unique BFS-tree that has the maximum M_2 in $\Gamma(\pi)$. On the other hand, this BFS-tree needs not be the only tree with the maximum M_2 in $\Gamma(\pi)$, as shown by an example in [104].

Theorem 6.10. [104] *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Let T^* and T^{**} be the trees with the maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then, $M_2(T^*) < M_2(T^{**})$.*

In addition, as a simple corollary of Theorem 6.10, it is reproved that the star $K_{1,n-1}$ has the maximum second Zagreb index among all n-vertex trees. Also, the following result is easily deduced.

Theorem 6.11. [104] *If T is a tree of order n with k pendent vertices, then $M_2(T) \leq M_2(F_n(k))$, where $F_n(k)$ is the tree on n vertices obtained by attaching k paths of almost equal lengths (i.e., paths whose lengths differ by at most one) to one common vertex.*

Denote by $\mathcal{T}_{n,k}$ the class of trees with n vertices and with exactly k vertices of maximum degree Δ ($k \leq n-2$). The extremal trees whose Zagreb indices are maximum (minimum) in $\mathcal{T}_{n,k}$ are characterized by Borovićanin and Aleksić Lampert [21]. Obviously, a path P_n is the unique element of $\mathcal{T}_{n,n-2}$. Thus, it may be assumed that $k \leq n-3$, in which case it was shown [21] that $1 \leq k \leq n/2 - 1$.

Theorem 6.12. [21] *Let $T \in \mathcal{T}_{n,k}$, where $1 \leq k \leq n/2 - 1$. Then*

$$M_1(T) \leq k\Delta^2 + p(\Delta-1)^2 + \mu^2 + n - k - p - 1$$

and the equality holds if and only if T has the vertex degree sequence

$$(\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta-1, \ldots, \Delta-1}_{p}, \mu, \underbrace{1, \ldots, 1}_{n-k-p-1})$$

where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1,\ p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and $\mu = n - 1 - k(\Delta-1) - p(\Delta-2)$.

Theorem 6.13. [21] *Let $T \in \mathcal{T}_{n,k}$ where $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$M_1(T) \geq 2k + 4n - 6$$

and the equality holds if and only if the tree T has the vertex degree sequence

$$(\underbrace{3, \ldots, 3}_{k}, \underbrace{2, \ldots, 2}_{n-2k-2}, \underbrace{1, \ldots, 1}_{k+2}).$$

Extremal trees which maximize (minimize) the second Zagreb index in the class $\mathcal{T}_{n,k}$ are characterized in the sequel.

Theorem 6.14. [21] *Let $T \in \mathcal{T}_{n,k}$, where $1 \leq k \leq n/2 - 1$. Then*

$$M_2(T) \leq (k-1)\Delta^2 + 2p(\Delta-1)^2 + \mu(\Delta+\mu-1) + \Delta(n-k-(\Delta-1)p-\mu)$$

where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$, $p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and $\mu = n - 1 - k(\Delta-1) - p(\Delta-2)$. The equality holds if and only if the following conditions are satisfied.

(i) The tree T has the vertex degree sequence

$$(\underbrace{\Delta,\ldots,\Delta}_{k},\underbrace{\Delta-1,\ldots,\Delta-1}_{p},\mu,\underbrace{1,\ldots,1}_{n-k-p-1})\,.$$

(ii) Every vertex of degree $\Delta-1$ is adjacent to a vertex of degree Δ and to $\Delta-2$ pendent vertices.

(iii) The vertex of degree μ (when $\mu>1$) is adjacent to a vertex of the degree Δ and to $\mu-1$ pendent vertices.

(iv) The remaining pendent vertices are attached to the vertices of degree Δ.

Theorem 6.15. [21] *Let $T\in\mathfrak{T}_{n,k}$, where $1\le k\le n/2-1$. Then*

$$M_2(T)\ge\begin{cases}3k+4n-10, & \text{if } n\ge 3k+1\\[2ex] 6k+3n-9, & \text{if } n<3k+1\,.\end{cases}$$

The equality holds if and only if the following three conditions are satisfied.

(i) The tree T has the vertex degree sequence $(\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n-2k-2},\underbrace{1,\ldots,1}_{k+2})$.

(ii) Between any two vertices of degree 3 in T there should be at least one vertex of degree 2, if possible.

(iii) The remaining vertices of degree 2 (if they exist) in T are placed either between two vertices of degree 2 or between a vertex of degree 2 and a vertex of degree 3.

Goubko [59] discovered an interesting property of trees with a given number of pendent vertices, which enabled him to determine a lower bound for M_1 of trees that depends only on the number of pendent vertices of a tree, irrespective the number of its vertices.

Theorem 6.16. [59, 67] *Let T be a tree with $n_1\ge 2$ pendent vertices and first Zagreb index M_1.*

(a) If n_1 is even, then $M_1(T)\ge 9n_1-16$ with equality if and only if all non-pendent vertices of T are of degree 4.

(b) If n_1 is odd, then $M_1(T)\ge 9n_1-15$, and the equality holds if and only if all non-pendent vertices of T, except one, are of degree 4, and a single vertex of T is of degree 3 or 5.

Although Goubko's theorem 6.16 provides simple structural conditions for graphs with minimal first Zagreb indices, it is restricted to graphs with very special number of vertices. In fact, this theorem determines extremal trees only if $n=\frac{3}{2}n_1-1$ and $n=\frac{3}{2}n_1$, respectively, and requires that n_1 be even. This limitation can be circumvented, as follows.

Theorem 6.17. [68] *Let T be a tree of order n with n_1 pendent vertices. Then*

$$M_1(T) \geq 4n - 6 + (n + n_1 - 4) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor^2 .$$

Equality is attained if and only if T consists of n_1 pendent vertices, $n_t = (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2$ vertices of degree $t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n - 2 - (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Sharp lower bounds for the second Zagreb index for trees with a given number of pendent vertices, were derived in papers [59,61]. The corresponding optimal trees were determined, too.

As in [28,59], a non-pendent vertex in a tree is called a stem vertex if it has incident pendent vertices. The edge connecting a stem with a pendent vertex will be referred to as a stem edge.

Theorem 6.18. [59,61] *For any tree T with $n_1 \geq 9$ pendent vertices $M_2(T) \geq 11n_1 - 27$. The equality holds if each stem vertex in T has degree 4 or 5, while other non-pendent vertices are of degree 3. At least one such tree exists for any $n_1 \geq 9$.*

An analogous type of problem was considered in the paper [60]. There a dynamic programming method was elaborated, enabling the characterization of trees with a given number of pendents, for which a vertex–degree–based topological index achieves its extremal value. This method was applied to the first and second Zagreb indices.

A vertex of a tree with degree at least three is called a branching vertex and a segment of a tree is a path-subtree whose terminal vertices are branching or pendent vertices.

In papers [20, 97], sharp lower and upper bounds on Zagreb indices of trees with fixed number of segments are determined and the corresponding extremal trees are characterized. As the number of segments in a tree is determined by the number of vertices of degree two (and vice versa), in this way also the extremal trees with prescribed number of vertices of degree two whose Zagreb indices are minimum (or maximum) are determined.

Denote, by $\mathcal{ST}_{n,k}$ the set of all n-vertex trees with exactly k segments. Then, as noted in [97], the path P_n is the unique element of $\mathcal{ST}_{n,1}$, the star S_n is the unique element of $\mathcal{ST}_{n,n-1}$ and the set $\mathcal{ST}_{n,2}$ is empty. Accordingly, only the set $\mathcal{ST}_{n,k}$ for $3 \leq k \leq n-2$ needs to be considered.

Theorem 6.19. [97] *Let $T \in \mathcal{ST}_{n,k}$, where $3 \leq k \leq n-2$. Then,*

$$4n + k^2 - 3k - 4 \geq M_1(T) \geq \begin{cases} 4n + k - 7 & \text{if } k \text{ is odd} \\ 4n + k - 4 & \text{if } k \text{ is even.} \end{cases}$$

The upper bound is attained if and only if T is a starlike tree of degree k. For odd k, the lower bound is attained if and only if T is an n-vertex tree with vertex degree sequence $(\underbrace{3, \ldots, 3}_{\frac{k-1}{2}}, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{\frac{k+3}{2}})$.

For even k the bound is attained if and only if T is an n-vertex tree with vertex degree sequence $(4, \underbrace{3, \ldots, 3}_{\frac{k-4}{2}}, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{\frac{k+4}{2}})$.

Denote by $\mathbb{ST}_O(n,k)$, for odd k, the set of all n-vertex trees with the degree sequence $(\underbrace{3,\ldots,3}_{\frac{k-1}{2}}, \underbrace{2,\ldots,2}_{n-k-1}, \underbrace{1,\ldots,1}_{\frac{k+3}{2}})$, whose vertices of degree 2 are placed between the vertices of degree 3 so that there is at least one vertex of degree 2 between any two vertices of degree 3, and the remaining vertices of degree 2 (if such do exist) are arranged arbitrarily so that a vertex of degree 2 has no pendent neighbor.

Denote by $\mathbb{ST}_E(n,k)$, for even k, the set of all n-vertex trees with the degree sequence $(4, \underbrace{3,\ldots,3}_{\frac{k-4}{2}}, \underbrace{2,\ldots,2}_{n-k-1}, \underbrace{1,\ldots,1}_{\frac{k+4}{2}})$, whose vertices are arranged as follows. The unique vertex of degree 4 has three pendent neighbors and a neighbor of degree 2. Then, the vertices of degree 2 are placed between the vertices of degree 3 (at least one vertex of degree 2 between any two vertices of degree 3, if it is possible) and the remaining vertices of degree 2 are arranged arbitrarily so that a vertex of degree 2 has no pendent neighbor.

Theorem 6.20. [20] *Let $T \in \mathcal{ST}_{n,k}$, where $3 \leq k \leq n-2$. Then*

$$M_2(T) \geq \begin{cases} \dfrac{8n+3k-23}{2}, & n \geq (3k-1)/2 \text{ and } k \text{ odd} \\ 3n+3k-12\,, & n < (3k-1)/2 \text{ and } k \text{ odd} \\ \dfrac{8n+3k-18}{2}, & n \geq (3k-2)/2 \text{ and } k \text{ even} \\ 3n+3k-10\,, & n < (3k-2)/2 \text{ and } k \text{ even}\,. \end{cases}$$

The equality holds if and only if $T \in \mathbb{ST}_O(n,k)$, for odd k, or $T \in \mathbb{ST}_E(n,k)$, for even k.

Theorem 6.21. [20] *Let $T \in \mathcal{ST}_{n,k}$, where $3 \leq k \leq n-2$. Then*

$$M_2(T) \leq \begin{cases} 2k^2-6k+4n-4\,, & n \geq 2k+1 \\ k(n-3)+2n-2\,, & n < 2k+1\,. \end{cases}$$

The upper bound is attained if and only if T is an n-vertex starlike tree of degree k, such that an arbitrary pendent vertex is adjacent to a vertex of degree 2, for $2k+1 \leq n$, or the central vertex of degree k has exactly $2k+1-n$ pendent neighbors, for $n < 2k+1$.

In the paper [20], sharp lower and upper bounds for Zagreb indices of trees with given number of branching vertices are determined, and the corresponding extremal trees characterized. For further details, see [20].

In the paper [40], extremal trees with maximal first (second) Zagreb index among trees of order n and independence number α are characterized. Let $S_{n,\alpha}$ be a tree (known as a spur) obtained from the star $K_{1,\alpha}$ by attaching a pendent edge to its $n-\alpha-1$ pendent vertices. If $\Delta = \alpha$ in a tree T of order n with independence number α, then $T \cong S_{n,\alpha}$.

Theorem 6.22. [40] *Let T be a tree of order n with independence number α. Then,*

$$M_1(T) \leq \alpha^2 - 3\alpha + 4n - 4$$

and

$$M_2(T) \leq n\alpha - 3\alpha + 2n - 2\,.$$

Equality in both inequalities holds if and only if $T \cong S_{n,\alpha}$.

In the paper [135], extremal trees with minimal first Zagreb index among trees of order n and independence number α are characterized. The extremal tree is the path P_n for $\alpha = \lceil n/2 \rceil$ and the star $K_{1,n-1}$ for $\alpha = n-1$. For $\lceil n/2 \rceil < \alpha < n-1$ define the set $\mathcal{T}_{n,\alpha}$ consisting of all trees $T = (V, E)$ with n vertices and independence number α such that the degrees of the vertices in its maximum independent set S differ by at most one, and such that the complement $\overline{S} = V \setminus S$ is also an independent set whose vertex degrees differ by at most one. In fact, the set $\mathcal{T}_{n,\alpha}$ consists of the coalescence of stars having almost equal order (i.e., differing by at most one), with the pair of leaves identified in neighboring stars (see Fig. 6).

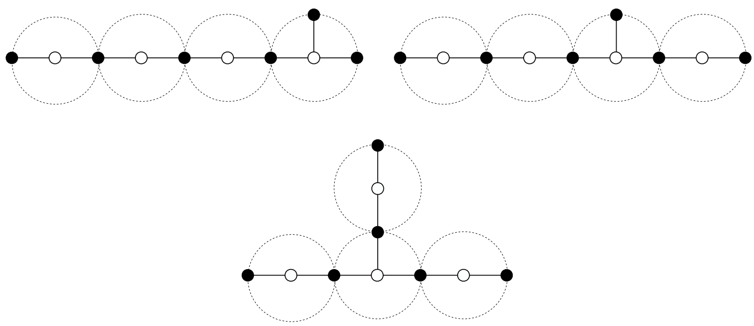

Fig. 6. Three non-isomorphic trees with $n = 10\,, \alpha = 6$ and minimum value of $M_1 = 36\,.$

The following holds:

Theorem 6.23. [135] *If T is a tree with n vertices and independence number α, then*

$$\begin{aligned} M_1(T) &\geq 2(n-1) - \alpha \left\lfloor \frac{n-1}{\alpha} \right\rfloor^2 - (n-\alpha) \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor^2 \\ &+ (2n-\alpha-2) \left\lfloor \frac{n-1}{\alpha} \right\rfloor + (n+\alpha-2) \left\lfloor \frac{n-1}{n-\alpha} \right\rfloor \end{aligned}$$

with equality if and only if $T \in \mathcal{T}_{n,\alpha}$.

As noted in [135], it appears that the problem of characterization of extremal trees with minimal second Zagreb index among trees of order n and independence number α cannot be solved as easily as it was the case with the first Zagreb index. Hence, the characterization of trees with minimal second Zagreb index remains an open problem.

The domination number $\gamma(G)$ of a graph G is the minimum cardinality of a subset D of $V(G)$ such that each vertex of G that is not contained in D is adjacent to at least one vertex of D. A subset D is called minimum dominating set of G.

In paper [21], upper bounds on Zagreb indices of trees in terms of domination numbers are presented. These bounds are strict and extremal trees are characterized. In addition, a lower bound for the first Zagreb index of trees with a given domination number is determined and the extremal trees are characterized.

Note that $\gamma(T) = 1$ if and only if $T \cong K_{1,n-1}$. It is well known [120] that every graph of order n without isolated vertices has domination number at most $\frac{n}{2}$. Also, it was proved by Fink et al. [55] that equality holds only for C_4 and for graphs of the form $H \circ K_1$, for some H.

Theorem 6.24. [21] *Let T be a tree with domination number γ. Then*

$$M_1(T) \leq (n-\gamma)(n-\gamma+1) + 4(\gamma-1)$$

and

$$M_2(T) \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1)\,.$$

Equality in both cases holds if and only if $G \cong S_{n,n-\gamma}$, where $S_{n,n-\gamma}$ is a spur obtained from the star $K_{1,n-\gamma}$ by attaching a pendent edge to its $\gamma-1$ pendent vertices.

In order to state the results from [21] concerning minimum first Zagreb index we need a few definitions.

Suppose first that $1 \leq \gamma \leq n/3$. Define $\mathcal{D}(n,\gamma)$ as a set of n-vertex trees T with domination number γ such that T consists of the stars of orders $\left\lfloor \frac{n-\gamma}{\gamma} \right\rfloor$ and $\left\lceil \frac{n-\gamma}{\gamma} \right\rceil$ with exactly $\gamma-1$ pairs of adjacent leaves in neighboring stars. Then, it holds:

Theorem 6.25. [21] *Let T be a tree on n vertices with domination number γ, where $1 \leq \gamma \leq n/3$. Then,*

$$M_1(T) \geq -\gamma \left\lfloor \frac{n-1}{\gamma} \right\rfloor^2 + (2n-\gamma) \left\lfloor \frac{n-1}{\gamma} \right\rfloor + 6(\gamma-1)\,.$$

The equality holds if and only if $T \in \mathcal{D}(n,\gamma)$.

Next, suppose that $\frac{n}{3} \leq \gamma \leq \frac{n}{2}$ and define $\mathcal{G}(n,\gamma)$ as a set of trees T on n vertices with domination number γ, such that every vertex from T has at most one pendent neighbor and

(i) there exists a minimum dominating set D of T containing $3\gamma-n-2$ vertices of degree 3 and $2n-4\gamma$ vertices of degree 2, while the set $\overline{D}$ contains $n-2\gamma+2$ vertices of degree 2 and $3\gamma-n$ pendent vertices, or

(ii) there exists a minimum dominating set D of T containing $n-2\gamma$ vertices of degree 2 and $3\gamma-n$ pendent vertices, while the set $\overline{D}$ contains $2n-4\gamma+2$ vertices of degree 2, $3\gamma-n-2$ vertices of degree 3 and every vertex from $\overline{D}$ has exactly one neighbor in D.

Theorem 6.26. [21] *Let T be a tree on n vertices with domination number γ, where $\frac{n}{3} \leq \gamma \leq \frac{n}{2}$. Then,*

$$M_1(T) \geq \begin{cases} 4n-6 & \text{if } \gamma = \left\lceil \dfrac{n}{3} \right\rceil \\ 2n+6\gamma = 10 & \text{if } \dfrac{n+3}{3} \leq \gamma \leq \dfrac{n}{2} \end{cases}$$

with equality if and only if $T \cong P_n$, for $\gamma = \lceil n/3 \rceil$, or $T \in \mathcal{G}(n,\gamma)$, otherwise.

Huang and Deng [83], and independently Li and Zhao [91] and Sun and Chen [128], characterized the trees with perfect matchings having the largest and the second largest Zagreb indices. Denote by $\mathcal{T}_m$ the set of trees with perfect matchings on $2m$ vertices. Let $T_m^1 \in \mathcal{T}_m$ be the tree on $2m$ vertices obtained by attaching a pendent edge together with $m-1$ paths of lengths 2 at a single vertex (see Fig. 7), and let $T_m^2 \in \mathcal{T}_m$ be the tree displayed in Fig. 7.

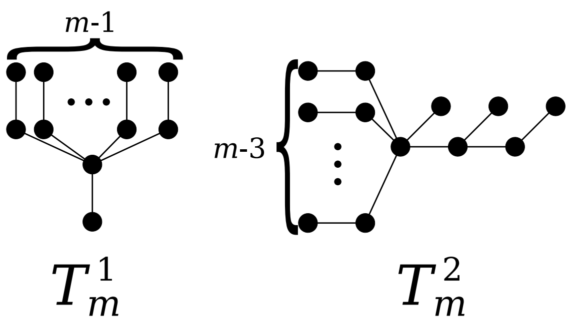

Fig. 7. The trees occurring in Theorem 6.27.

Theorem 6.27. [83, 91, 128]

a) Let T be any tree in $\mathcal{T}_m$, $m \geq 3$. If T is different from T_m^1, then $M_i(T) < M_i(T_m^1)$, $i = 1, 2$;

b) Let T be any tree in $\mathcal{T}_m \setminus \{T_m^1, T_m^2\}$, $m \geq 3$, then $M_i(T) < M_i(T_m^2)$.

At the end of this section we present results from [49] concerning the so-called k-trees, class of graphs which is the generalization of trees.

The k-tree T_n^k, $k \geq 1$, introduced in [12], is defined recursively as follows.

(i) The smallest k-tree is the k-clique K_k.

(ii) If G is a k-tree with n vertices and a new vertex v of degree k is added and joined to the vertices of a k-clique in G, then the larger graph is a k-tree with $n+1$ vertices.

The (k,n)-path P_n^k, has vertex set $\{v_1, v_2, \ldots, v_n\}$ where $G[\{v_1, v_2, \ldots, v_k\}] \cong K_k$. For $k+1 \leq i \leq n$, let vertex v_i be adjacent to the vertices $\{v_{i-1}, v_{i-2}, \ldots, v_{i-k}\}$.

A helpful characteristic of the k-path P_n^k is that we may order the vertices $v_1, v_2, \ldots, v_n$ so that $P_n^k - \{v_1, v_2, \ldots, v_i\}$ is a k-path on $n-i$ vertices for $1 \leq i \leq n-k-1$.

The (k,n)-star $S_{k,n-k}$, has vertex set $\{v_1, v_2, \ldots, v_n\}$ where $G[\{v_1, v_2, \ldots, v_k\}] \cong K_k$ and $N(v_i) = \{v_1, v_2, \ldots, v_k\}$ for $k+1 \leq i \leq n$.

The 3-path and the 3-star on 7 vertices are presented in Fig. 8.

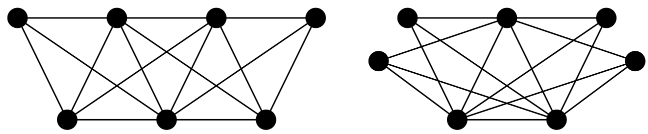

Fig. 8. The 3-path and 3-star with 7 vertices.

The first and second Zagreb indices of k-paths and k-stars are obtained in [49].

Theorem 6.28. [49] *Let P_n^k be the k-path on $n \geq k+3$ vertices. Then*

$$\begin{aligned} M_1(P_n^k) &= 2nk(n-2) - \frac{1}{3}n(n-1)(n-2) - \frac{1}{3}k(k+1)(2k-5) \\ & \qquad \textit{for } \ k+3 \leq n \leq 2k \ \textit{ and } \ k \geq 3 \\ M_1(P_n^k) &= 4nk^2 - \frac{1}{3}k(10k-1)(k+1) \ \textit{for } \ n \geq \max(4, 2k+1)\,. \end{aligned}$$

Theorem 6.29. [49] *Let P_n^k be the k-path on $n \geq k+3$ vertices. Then*

$$\begin{aligned} M_2(P_n^k) &= \frac{1}{2}(k^4 + 9k^3 + 12k^2 - 8k + 2), \ \ n = k+3 \\ M_2(P_n^k) &= \frac{1}{24}((10-4k)n^3 - n^4 + (54k^2 - 18k - 23)n^2 \\ &- (44k^3 + 66k^2 - 54k - 14)n + 7k^4 + 38k^3 + 5k^2 - 26k) \\ & \textit{for } \ k+4 \leq n \leq 2k \\ M_2(P_n^k) &= \frac{1}{24}(n^4 - (12k+6)n^3 + (54k^2 + 54k + 11)n^2 \\ &- (12k^3 + 162k^2 + 66k + 6)n - (25k^4 - 70k^3 - 109k^2 - 14k)) \\ & \textit{for } \ 2k+1 \leq n \leq 3k-1 \\ M_2(P_n^k) &= \frac{1}{24}(48nk^3 - 53k^4 - 46k^3 + 5k^2 - 2k) \ \textit{for } \ n \geq \max(5, 3k)\,. \end{aligned}$$

Theorem 6.30. [49] *Let $S_{k,n-k}$ be the k-star on $n \geq k+1$ vertices. Then*

$$\begin{aligned} M_1(S_{k,n-k}) &= n^2k + (k^2-2k)n - k^3 + 1 \\ M_2(S_{k,n-k}) &= \frac{1}{2}\left[(3k^2-k)n^2 - (2k^3+4k^2-2k)n + k(2k-1)(k+1)\right]. \end{aligned}$$

Sharp upper and lower bounds for M_1 and M_2 of k-trees are determined as follows.

Theorem 6.31. [49] *Let T_n^k be a k-tree on $n \geq k$ vertices. Then*

$$M_1(P_n^k) \leq M_1(T_n^k) \leq M_1(S_{k,n-k})$$

and

$$M_2(P_n^k) \leq M_2(T_n^k) \leq M_2(S_{k,n-k})$$

and the left–hand side equality in both inequalities is reached if and only if $T_n^k \cong P_n^k$ whereas the right–hand side equality holds if and only if $G \cong S_{k,n-k}$.

Accordingly, by this theorem, the results of the papers [37,66] (valid in the case $k=1$) are extended to the k-tree, $k>1$. Also, it can be proven that maximal outerplanar graphs are 2-trees, and consequently, the results obtained for k-trees also extend the result of Hou, Li, Song and Wei from [80], who determined sharp upper and lower bounds for M_1- and M_2-values of maximal outerplanar graphs.

7. On c-cyclic graph, $c \geq 1$

For connected graphs, the cyclomatic number, i.e., the number of independent cycles, is equal to $c = m-n+1$. Graphs with $c = 0,1,2,3,4$ are referred to as trees, unicyclic, bicyclic graphs, tricyclic and tetracyclic graphs, respectively.

Zhang and Zhang in [150] determined the first three unicyclic graphs from the class $\mathcal{U}(n)$ of all connected unicyclic graphs with n vertices whose M_1 is maximum (minimum). The part of this result, concerning the first three largest values of M_1, was reproved in [103] using a different approach.

Theorem 7.1. [103, 150] *Let $G \in \mathcal{U}(n)$. If $n \geq 9$ and $G \in \mathcal{U}(n) \setminus \{U_1,U_2,U_3,U_4\}$, then $M_1(U_1) > M_1(U_2) > M_1(U_3) = M_1(U_4) > M_1(G)$, where $U_1 - U_4$ are unicyclic graphs depicted in Fig. 9.*

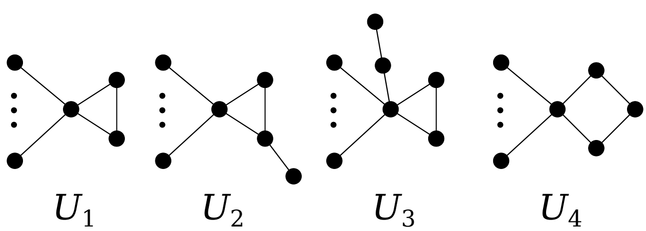

Fig. 9. The graphs occurring in Theorem 7.1.

Theorem 7.2. [150] *Let $G \in \mathcal{U}(n)$, $n \geq 7$. Then*

(i) $M_1(G)$ attains the smallest value if and only if $G \cong C_n$;

(ii) $M_1(G)$ attains the second smallest value if and only if G is a cycle C_{n-1} with a pendent edge attached;

(iii) $M_1(G)$ attains the third smallest value if and only if G is a cycle C_{n-2} with two pendent edges attached at different vertices.

Sharp bounds for the second Zagreb index of unicyclic graphs were established in the paper [146].

Let $\mathcal{U}_{n,k}$ be the set of unicyclic graphs with n vertices and k pendent vertices, $0 \leq k \leq n-3$. Denote by $C_q(p_1, p_2, \ldots, p_k)$, $k \geq 1$, a unicyclic graph with n vertices created from C_q by attaching paths of lengths $p_1, p_2, \ldots, p_k$ to one vertex of the cycle C_q, respectively, where $n = q + \sum_{i=1}^{k} p_i$, $p_i \geq 1$, $i = 1, 2, \ldots, k$. In addition, denote

$$\begin{aligned} \mathcal{U}^*_{n,0} &= \{C_n\} \\ \mathcal{U}^*_{n,k} &= \{C_q(p_1, p_2, \ldots, p_k) : p_i \geq 2, 1 \leq i \leq k, q \geq 3\} \ , \quad k \geq 1 \\ U^n_k &= C_3(1, 1, \ldots, 1, \underbrace{2, 2, \ldots, 2}_{n-k-3}) \end{aligned}$$

see Fig. 10. Obviously, $\mathcal{U}^*_{n,k} \subseteq \mathcal{U}_{n,k}$ and $U^n_k \in \mathcal{U}_{n,k}$.

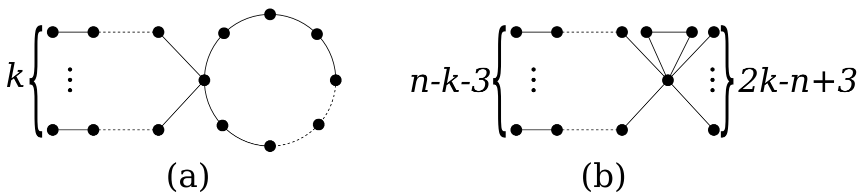

Fig. 10. (a) An element of $\mathcal{U}^*_{n,k}$, and (b) the graph U^n_k . These graphs are mentioned in Theorem 7.3.

Let $\mathcal{U}^+_{n,k}$ be the set of all graphs from $\mathcal{U}_{n,k}$ such that $\Delta(G) \leq 3$ and each pendent vertex of G is adjacent to another vertex of degree 3 and every pair of vertices of degree 3 are nonadjacent. Clearly, $\mathcal{U}^+_{n,0} = \{C_n\}$. As an illustration, in Fig. 11, the graphs $G_1, G_2, G_3, G_4 \in \mathcal{U}^+_{13,4}$ are presented.

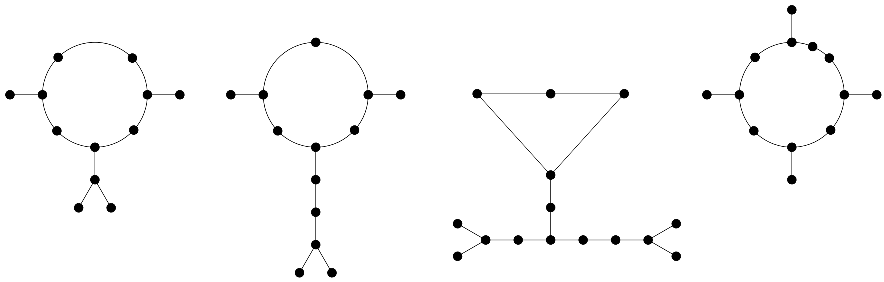

Fig. 11. For graphs belonging to the set $\mathcal{U}^+_{13,4}$. These graphs are mentioned in Theorem 7.4.

Theorem 7.3. [146] *Let* $G \in \mathcal{U}_{n,k}$, $0 \le k \le n-3$. *Then*

$$M_2(G) \le \begin{cases} 4n + 2k(k+1) & \text{if } n \ge 2k+3 \\ 4n + (n-1)k, & \text{if } n \le 2k+2 \,. \end{cases}$$

Equalities hold if and only if $G \in \mathcal{U}^*_{n,k}$, *for* $n \ge 2k+3$, *and* $G \cong U^n_k$, *for* $n \le 2k+2$.

Theorem 7.4. [146] *Let* $G \in \mathcal{U}_{n,k}$, $0 \le k \le n-3$. *Then*

$$M_2(G) \ge 4n + 3k$$

and the equality holds if and only if $n \ge 3k$ *and* $G \in \mathcal{U}^+_{n,k}$.

Let $\varphi(n,k) = 4n + 2k(k+1)$ and $\phi(n,k) = 4n + 3k$, where n and k are integers such that $0 \le k \le n-3$. The functions $\varphi(n,k)$ and $\phi(n,k)$ increase strictly monotonically in $0 \le k \le n-3$ [146]. As the set of all unicyclic graphs with n vertices is $\bigcup_{k=0}^{n-3} \mathcal{U}_{n,k}$, by Theorems 7.3 and 7.4, U^n_{n-3} and C_n have the maximum and the minimum second Zagreb index among all unicyclic graphs with n vertices [146].

In the paper [105], an extremal unicyclic graph that achieves the maximum second Zagreb index in the class of unicyclic graphs with given degree sequence is characterized.

Let $\pi = (d_1, d_2, \ldots, d_n)$ be a degree sequence of a c-cyclic graph, where c is an integer and $c \ge 0$, then

$$\sum_{i=1}^{n} d_i = 2(n+c-1) \ , \ \ d_1 \ge d_2 \ge c+1 \,. \tag{33}$$

We now present the construction of the graph $G^* \in \Gamma(\pi)$ as in [104, 105, 148, 152].

Select v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices $v_2, v_3, \ldots, v_{d_1+1}$ as the first layer such that

$$N(v_1) = \{v_2, v_3, \ldots, v_{d_1+1}\} \,.$$

Then append $d_2 - 1$ vertices to v_2, $d_3 - 2$ vertices to v_3,..., $d_{c+2} - 2$ vertices to v_{c+2} such that

$$\begin{aligned}
N(v_2) &= \{v_1, v_3, \ldots, v_{c+2}, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-c}\} \\
N(v_3) &= \{v_1, v_2, v_{d_1+d_2-c+1}, \ldots, v_{d_1+d_2+d_3-c-2}\} \\
&\ldots \\
N(v_{c+2}) &= \{v_1, v_2, v_{(\sum_{i=1}^{c+1} d_i)-3c+3}, \ldots, v_{(\sum_{i=1}^{c+2} d_i)-3c}\}\,.
\end{aligned}$$

After that, append $d_{c+3} - 1$ vertices to v_{c+3} such that

$$N(v_{c+3}) = \{v_1, v_{(\sum_{i=1}^{c+2} d_i)-3c+1}, \ldots, v_{(\sum_{i=1}^{c+3} d_i)-3c-1}\}\,.$$

Repeat the above procedure until all vertices are processed. As noted in [148], the vertices $v_1v_2v_3$, $\ldots, v_1v_2v_{c+2}$ form c triangles in G^* and G^* has a BFS-ordering. In particular, if $c = 0$ there are no triangles and the graph G^* coincides with the tree T^* specified in Theorem 6.9. If $c = 1$, then G^* is a unicyclic graph denoted by U^* whereas if $c = 2$, then G^* is bicyclic graph, denoted by B^*.

Let $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$, be an unicyclic degree sequence ($c = 1$ in (33)). Let U^* be the unique unicyclic graph such that the unique cycle of U^* is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$, and the remaining vertices appear in BFS-ordering with respect to C_3 starting from v_4 that is adjacent to v_1. In fact, U^* can be constructed by the BFS method as described above.

Theorem 7.5. [105] *If $d_n = 1$, then U^* achieves the maximum second Zagreb index in the class of unicyclic graph with degree sequence π.*

Remark. [105] For a given unicyclic degree sequence π, U^* is the unique BFS-graph with the maximum M_2 in $\Gamma(\pi)$, but it needs not be the unique unicyclic graph with maximum M_2 in $\Gamma(\pi)$, which is illustrated by an example in [105].

In addition, it is proven in [105], that if $\pi \lhd \pi'$, π and π' are unicyclic degree sequences and U^* and U^{**} have the maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, then $M_2(U^*) < M_2(U^{**})$.

As a simple corollary of Theorem 7.5, the result from [146], which is concerned with unicyclic graphs with n vertices and k pendent vertices whose second Zagreb index is maximum is reproven in [105]. Furthermore, the first to ninth largest second Zagreb indices together with the corresponding extremal unicyclic graphs in the class of unicyclic graphs with $n \geq 17$ vertices have been determined in [105].

Theorem 7.6. [105] *Let U be a unicyclic graph on $n \geq 17$ vertices. If $U \notin \{U_1, U_2, \ldots, U_{10}\}$, then $M_2(U) < M_2(U_{10}) < M_2(U_9) < M_2(U_8) < M_2(U_7) = M_2(U_6) < M_2(U_5) < M_2(U_4) < M_2(U_3) < M_2(U_2) < M_2(U_1)$, where $U_1 - U_{10}$ are unicyclic graphs displayed in Fig. 12.*

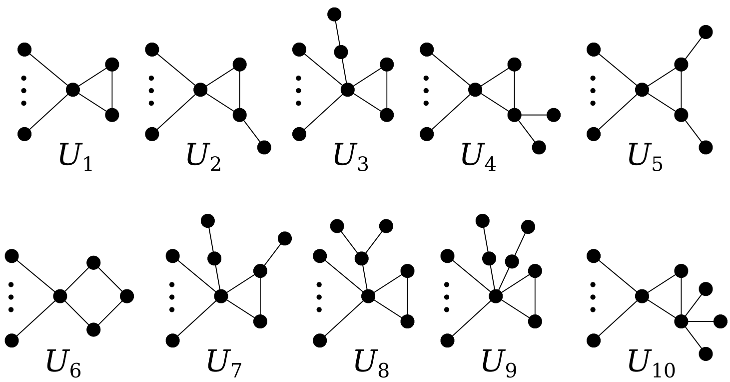

Fig. 12. The unicyclic graphs $U_1, U_2, \ldots, U_{10}$ occurring in Theorem 7.6.

In the paper [135], unicyclic graphs of order n and independence number α with minimal first Zagreb index are determined. Let $\mathcal{U}_{n,\alpha}$ denote the set consisting of all unicyclic graphs $G = (V, E)$ with n vertices and independence number α, such that the degrees of the vertices in its maximum independent set S differ by at most one among each other, and such that the complement $\overline{S} = V \backslash S$ is also independent set whose vertex degrees differ by at most one among each other. These graphs, in fact, consist of coalescence of stars, whose orders differ by at most one, with pairs of leaves identified in neighboring stars (see Fig. 13).

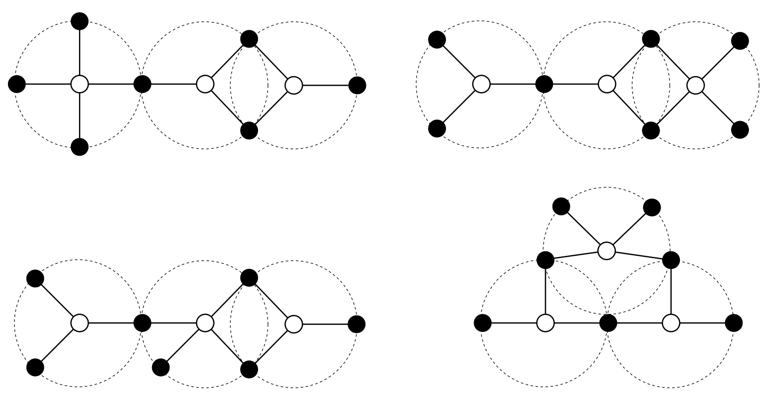

Fig. 13. Four non-isomorphic unicyclic graphs with $n = 10$, $\alpha = 7$ and minimum value of $M_1 = 50$.

Theorem 7.7. [135] *If G is a unicyclic graph with n vertices and the independence number α, then*

$$M_1(G) \geq 4n - 2\alpha - (n-\alpha)\left\lfloor \frac{n}{n-\alpha} \right\rfloor^2 + (n+\alpha)\left\lfloor \frac{n}{n-\alpha} \right\rfloor$$

with equality if and only if $G \in \mathcal{U}_{n,\alpha}$ when $\alpha \geq n/2$ and $G \cong C_{2\alpha+1}$ when $\alpha = (n-1)/2$.

Huang and Deng in [83] characterized unicyclic graphs with perfect matchings which attain the largest and the second largest values of Zagreb indices. Denote by $\mathcal{U}_m$ the set of unicyclic graphs with perfect matchings on $2m$ vertices. Let $U_m^1 \in \mathcal{U}_m$ be the graph on $2m$ vertices obtained from C_3 by attaching a pendent edge together with $m-2$ paths of lengths 2 at the vertex u (see Fig. 14). Let $U_m^2 \in \mathcal{U}_m$ be the graph on $2m$ vertices obtained from C_3 by attaching a pendent edge and $m-3$ paths of lengths 2 at the vertex u, and single pendent edges at the other vertices, respectively (see Fig. 14).

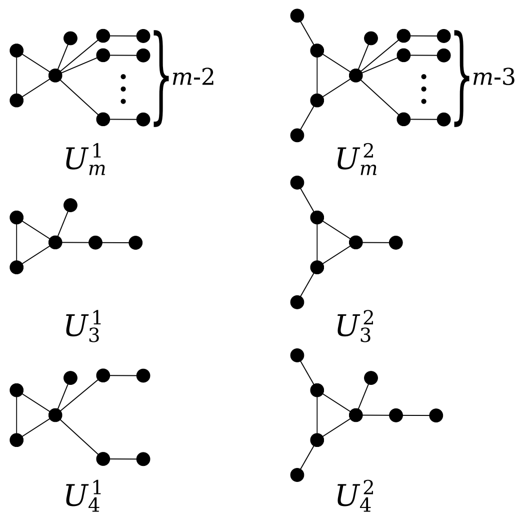

Fig. 14. The graphs occurring in Theorem 7.8.

Theorem 7.8. [83]

a) Let $G \in \mathcal{U}_m$. If $m = 2$ or $m \geq 5$, then U_m^1 and U_m^2 are the graphs with the largest and second largest Zagreb indices, respectively.

b) Let $G \in \mathcal{U}_3$. Then $M_1(G) < M_1(U_3^2) = M_1(U_3^1)$ and $M_2(G) < M_2(U_3^1) < M_2(U_3^2)$.

c) Let $G \in \mathcal{U}_4$. Then $M_1(G) < M_1(U_4^2) < M_1(U_4^1)$ and $M_2(G) < M_2(U_4^2) = M_2(U_4^1)$.

Horoldagva and Das in [76] gave lower bounds for M_1 of unicyclic graphs of order n with maximum degree Δ and cycle length k. Denote by $\mathcal{B}_n(k, \Delta)$ the set of graphs of order n obtained by attaching $\Delta - 2$ paths to one vertex of C_k.

Theorem 7.9. [76] *Let G be a connected unicyclic graph of order n with maximum degree Δ and cycle length k $(3 \leq k \leq n - \Delta + 2)$. Then*

$$M_1(G) \geq \Delta(\Delta - 3) + 4n + 2$$

with equality if and only if $G \in \mathcal{B}_n(k, \Delta)$.

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

Let G be a connected unicyclic graph of order n with maximum degree Δ and cycle length k. Then obviously $\Delta + k \leq n+2$. If $\Delta + k = n$ and the maximum degree vertex does not lie on the cycle of G, then G is isomorphic to $C_{n,\Delta}^k$. If $\Delta + k \geq n$ and G is different from $C_{n,\Delta}^k$, then the maximum degree vertex of G must lie on the cycle. In this case one can easily characterize graphs with minimum M_2. In [76], Horoldagva and Das obtained the following lower bound on $M_2(G)$ and characterize extremal graphs when $\Delta + k < n$.

Theorem 7.10. [76] *Let G be a connected unicyclic graph of order n with maximum degree Δ and cycle length k $(\Delta + k < n)$. Then*

$$M_2(G) \geq \begin{cases} \Delta(\Delta-3)+4n+6 & \text{if } \Delta \geq 5 \\ 4n+10 & \text{if } \Delta = 4 \\ 4n+4 & \text{if } \Delta = 3 \end{cases} \tag{34}$$

where Δ is the maximum degree in G. Moreover, the equalities hold in (34) if and only if $G \cong C_{n,\Delta}^k$, $G \cong C_{n,4}^k$ or $G \cong D_{n,4}^k$, $G \cong A_n^k$, respectively.

Zhao and Li [153] determined sharp lower and upper bounds for both M_1 and M_2 of n-vertex bicyclic graphs with k pendent vertices, as well as the corresponding extremal graphs which attain these bounds.

The set of n-vertex bicyclic graphs consists of graphs of two types: graphs whose two independent cycles have no common edge and graphs whose two independent cycles have at least one edge in common. The arrangement of cycles contained in a bicyclic graph has three possible cases [45,153], depicted in Fig. 15, and denoted by $B^1(a,b)$, $B^2(a,b,r)$ and $B^3(a,b,r)$, respectively.

Let $\mathcal{B}_{n,k}$ be a set of n vertex bicyclic graphs with k pendent vertices and let $\mathcal{B}_{n,k}^i$ be a subset of $\mathcal{B}_{n,k}$ consisting of those graphs G whose arrangement of cycles is B^i, where B^i is depicted in Fig. 15, for $i = 1, 2, 3$.

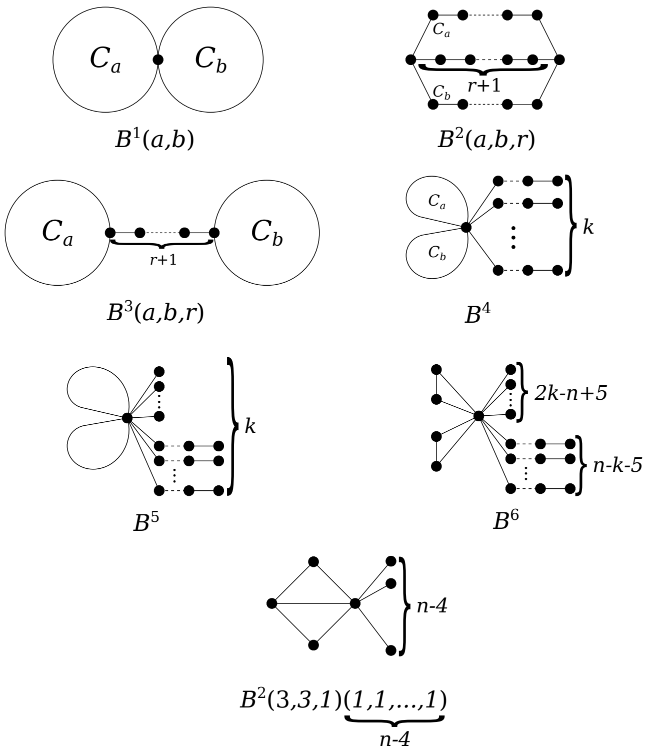

Fig. 15. The different types of bicyclic graphs.

Denote by $B^i(a,b)(p_1,p_2,\dots,p_k)$, $i=1,2,3$, $k\geq 1$, the n-vertex bicyclic graphs obtained from $B^1(a,b)$ and $B^i(a,b,r)$, $i=2,3$, respectively, by attaching k pendent paths of lengths $p_1,p_2,\dots,p_k$ to exactly one vertex of maximum degree in $B^1(a,b)$, i.e., in $B^i(a,b,r)$, $i=2,3$, where $p_j\geq 1$, $j=1,2,\dots,k$. Also, let

$$\begin{aligned}
\mathcal{B}^{*}_{n,k} &= \Big\{B^1(a,b)(p_1,p_2,\dots,p_k) : p_i\geq 2, 1\leq i\leq k\Big\}\\
\mathcal{B}^{**}_{n,k} &= \Big\{B^1(a,b)(p_1,p_2,\dots,p_k) : p_i\geq 1, 1\leq i\leq k\Big\}\\
B^n_k &= B^1(3,3)(\underbrace{1,\dots,1}_{2k-n+5},\underbrace{2,\dots,2}_{n-k-5}).
\end{aligned}$$

The graphs $B^4\in\mathcal{B}^{*}_{n,k}$, $B^5\in\mathcal{B}^{**}_{n,k}$ and $B^6\cong B^n_k$ are depicted in Fig. 15.

Let $\mathcal{B}^{+}_{n,k}$ be a set of graphs G from $\mathcal{B}^2_{n,k}\cup\mathcal{B}^3_{n,k}$ such that $\Delta(G)\leq 3$, each pendent vertex from G is adjacent to a vertex of degree 3 and every pair of vertices of degree 3 are nonadjacent. Also, let $\mathcal{B}^{++}_{n,k}$ be a set of graphs G from $\mathcal{B}_{n,k}$ such that $|d(u)-d(v)|\leq 1$ for all non-pendent vertices $u,v\in V(G)$.

Theorem 7.11. [153] *Let* $G \in \mathcal{B}_{n,k}$ *with* $0 \leq k \leq n-5$. *Then*

$$M_1(G) \leq 4n + k^2 + 5k + 12$$

with equality attained if and only if $G \in \mathcal{B}^{**}_{n,k}$.

Theorem 7.12. [153] *Let* $G \in \mathcal{B}_{n,k}$ *with* $0 \leq k \leq n-5$. *Then*

$$M_2(G) \leq \begin{cases} 4n + 2k^2 + 10k + 20 & \text{if } n \geq 2k+5 \\ \\ 6n + nk + k + 10 & \text{if } n \leq 2k+4\,. \end{cases}$$

Equalities hold if and only if $G \in \mathcal{B}^{*}_{n,k}$, *for* $n \geq 2k+5$, *and* $G \cong B^n_k$, *for* $n \leq 2k+4$.

Theorem 7.13. [153] *Let* $G \in \mathcal{B}_{n,k}$ *with* $0 \leq k \leq n-4$, $d = \left\lceil \frac{2k+2-n}{n-k} \right\rceil$. *Then*

$$M_1(G) \geq \begin{cases} 4n + 2k + 10 & \text{if } n \geq 2k+2 \\ \\ (-d^2 - d + 3)n + (d^2 + 3d + 2)k + (4d + 10) & \text{if } n \leq 2k+1\,. \end{cases} \tag{35}$$

Equalities in (35) *hold if and only if* $G \in \mathcal{B}^{++}_{n,k}$.

Theorem 7.14. [153] *Let* $G \in \mathcal{B}_{n,k}$ *with* $0 \leq k \leq n-4$, $d = \left\lceil \frac{2k+2-n}{n-k} \right\rceil$. *Then*

$$M_2(G) \geq 4n + 3k + 16\,.$$

Equality holds if and only if $n \geq 3k+3$ *and* $G \in \mathcal{B}^{+}_{n,k}$.

On the basis of Theorems 7.11 and 7.12, Zhao and Li [153] deduced that if $0 \leq k \leq n-5$, then each member $G \in \mathcal{B}^{**}_{n,n-5}$ and B^n_{n-5}, respectively, have the maximum first and second Zagreb indices among graphs from $\bigcup_{k=0}^{n-5} \mathcal{B}_{n,k}$, and furthermore

$$M_1(G) = n^2 - n + 12\,, \text{ for } G \in \mathcal{B}^{**}_{n,n-5}\,,\ M_2(B^n_{n-5}) = n^2 + 2n + 5\,.$$

If $k = n-4$, then [153]

$$G \cong B^2(3,3,1)(\underbrace{1,\ldots,1}_{n-4})\,, \text{ and } M_1(G) = n^2 - n + 14\,,\ M_2(G) = n^2 + 2n + 9\,.$$

Hence, the graph $B^2(3,3,1)(\underbrace{1,\ldots,1}_{n-4})$, depicted in Fig. 15, has the maximum M_1-value and M_2-value among all bicyclic graphs with n vertices, which represents in fact the reproved result of Deng [45]. The same result concerning bicyclic graphs with maximal M_1 was obtained independently in [27] using a different approach.

Also, it was easy to deduce [153] that each member in $\mathcal{B}^{++}_{n,0}$ (resp. $\mathcal{B}^{+}_{n,0}$) has the minimum first (resp. second) Zagreb index among all n-vertex bicyclic graphs, and in such a way the corresponding results of Deng [45] were reproved.

The study of optimal graphs in the set of all connected graphs with a given degree sequence π which satisfy some conditions was continued in the paper [148] and some results that generalize the main results of the papers [104, 105] were obtained. In addition, some optimal graphs in the set of bicyclic graphs with a given degree sequence were determined. First, it was proven:

Theorem 7.15. [148] *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a degree sequence. If it satisfies the following conditions*

(i) $\sum_{i=1}^{n} d_i = 2(n + c - 1)$, c is an integer and $c \geq 0$,

(ii) $d_1 \geq d_2 \geq c + 1$,

(iii) $d_3 \geq d_4 = d_5 = \cdots = d_{c+2}$, for $c \geq 1$,

(iv) $d_n = 1$,

then the graph G^*, constructed as described in the explanation of Theorem 7.5, is an optimal graph in $\Gamma(\pi)$, i.e., for any graph $G \in \Gamma(\pi)$, $M_2(G) \leq M_2(G^*)$.

The previous theorem implies the results of Theorems 6.9 and 7.5. Also, the corresponding result for bicyclic graphs was obtained. A bicyclic graph has the so-called bicyclic degree sequence π which satisfies the condition (33) for $c = 2$. We will use the notation from [153], introduced previously. By $B^2(a, b, 1)$ we denote a bicyclic graph such that two independent cycles C_a and C_b, contained in it, have exactly one edge in common. Also, let $B^3(a, b, 1)$ be a bicyclic graph formed by joining two independent cycles C_a and C_b by an edge (see Fig. 15, where $r = 1$). Finally, let $\mathcal{B}_\pi$ be the set of bicyclic graphs with a degree sequence π.

Theorem 7.16. [148] *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a bicyclic degree sequence and let k be the number of pendent vertices of a graph $G \in \mathcal{B}_\pi$.*

(1) If $d_n = 2$ and $d_2 \geq 3$, then $M_2(G) \leq 4n + 17$ with equality if and only if $G \cong B^3(a, b, 1)$ or $G \cong B^2(a, b, 1)$, where $a + b = n$ or $a + b - 2 = n$, respectively.

(2) If $d_n = 2$ and $d_2 = 2$, then $M_2(G) \leq 4n + 20$ with equality if and only if $G \cong B^1(a, b)$, where $a + b - 1 = n$.

(3) If $d_n = 1$, $d_2 = 2$ and $k \leq (n - 5)/2$, then $M_2(G) \leq 4n + 2k^2 + 10k + 20$ with equality if and only if $G \in \mathcal{B}^*_{n,k}$.

(4) If $d_n = 1$, $d_2 = 2$ and $k > (n - 5)/2$, then $M_2(G) \leq kn + 6n + k + 10$ with equality if and only if $G \cong B^n_k$;

(5) If $d_n = 1$ and $d_2 \geq 3$, then the graph B^*, defined previously (see the explanation of Theorem 6.9), is an optimal graph in the set $\mathcal{B}_\pi$.

Remark. [148] B^* is not the unique optimal graph in $\mathcal{B}_\pi$ for $d_n = 1$ and $d_2 \geq 3$, as illustrated by an example in [148].

Besides, in paper [148], it was proven:

Theorem 7.17. [148] *Let π and π' be two non-increasing bicyclic degree sequences. If $\pi \lhd \pi'$, then $M_2(\pi) \leq M_2(\pi')$, with equality if and only if $\pi = \pi'$.*

By Theorem 7.16 (parts (3) and (4)) the results of Theorem 7.12, concerned with bicyclic graphs with n vertices and k pendent vertices whose second Zagreb index is maximum are reproved.

Recall that Goubko (see Theorem 6.16) determined the lower bound for M_1 of trees with a given number of pendent vertices. This result was extended in [68] to any connected graph with a given number of pendents and fixed cyclomatic number.

Theorem 7.18. [68] *Let G be a connected graph with k pendent vertices and cyclomatic number c. Then,*

$$M_1(G) \geq 9k + 16(c-1)\,. \tag{36}$$

Equality in (36) *holds if and only if all non-pendent vertices of G are of degree 4, provided such graphs exist.*

The corresponding result for trees ($c = 0$) is stated in Theorem 6.17, and the result for unicyclic graphs is stated below.

Theorem 7.19. [68] *Let U be a unicyclic graph of order n with k pendent vertices. Then*

$$M_1(U) \geq 4n + (n+k)\left\lfloor \frac{n}{n-k} \right\rfloor - (n-k)\left\lfloor \frac{n}{n-k} \right\rfloor^2 .$$

Equality is attained if and only if U consists of k pendent vertices, $n_t = (n-k)\left\lfloor \frac{n}{n-k} \right\rfloor - k$ vertices of degree $t = \left\lfloor \frac{n}{n-k} \right\rfloor + 1$, and $n_{t+1} = n - (n-k)\left\lfloor \frac{n}{n-k} \right\rfloor$ vertices of degree $t+1$.

Unicyclic graphs of order n with k pendent vertices and minimal first Zagreb index, of the form specified in Theorem 7.19, exist for any value of n and k, provided $n \geq 3$ and $k \geq 0$.

Besides, in [68], the result from [153] were reproved, with some additional conditions proposed. In fact, it was shown in [68] that the extremal n-vertex bicyclic graphs with k pendent vertices which attain the minimum value of M_1, contain additional $n_t = (n-k)\left\lfloor \frac{n+2}{n-k} \right\rfloor - k - 2$ vertices of degree $t = \left\lfloor \frac{n+2}{n-k} \right\rfloor + 1 = d + 2$, and $n_{t+1} = n + 2 - (n-k)\left\lfloor \frac{n+2}{n-k} \right\rfloor$ vertices of degree $t + 1 = d + 3$, where $d = \left\lceil \frac{2k+2-n}{n-k} \right\rceil$ (cf. Theorem 7.13).

In the paper [132], Tache considered some degree–based topological indices for bicyclic graphs, including the first Zagreb index. Extremal bicyclic graphs with fixed number of pendents with maximal value of M_1 were determined, reproving in such a way the results from [153]. Besides, the results on extremal bicyclic graphs with fixed girth which attain the maximum value of M_1 were obtained.

Denote by $B^{*2}(a,b,r)$ a bicyclic graph $B^2(a,b,r)(\underbrace{1,\ldots,1}_{n-4})$ obtained by attaching k pendent edges to exactly one vertex of maximum degree to the graph $B^2(a,b,r)$ from Fig. 15.

Theorem 7.20. [132] *Let G be a bicyclic graph of order n and girth $g \geq 3$. If G maximizes the index M_1, then $G \cong B^{*2}(g,g,\frac{g}{2})$ for g an even number and $G \cong B^{*2}(g,g,\frac{g-1}{2})$ for g odd.*

Li and Zhao in [90] determined sharp upper bounds for M_1 and M_2 of bicyclic graphs with perfect matchings. Besides, in [90], sharp upper bounds for Zagreb indices of bicyclic graphs with an m-matching were also obtained.

Denote by $\mathfrak{B}_{n,m}$ the set of n-vertex bicyclic graphs with an m-matching, and let $B_{n,m}$, B_1, B_2, B_3 and B_4 be the graphs depicted in Fig. 16.

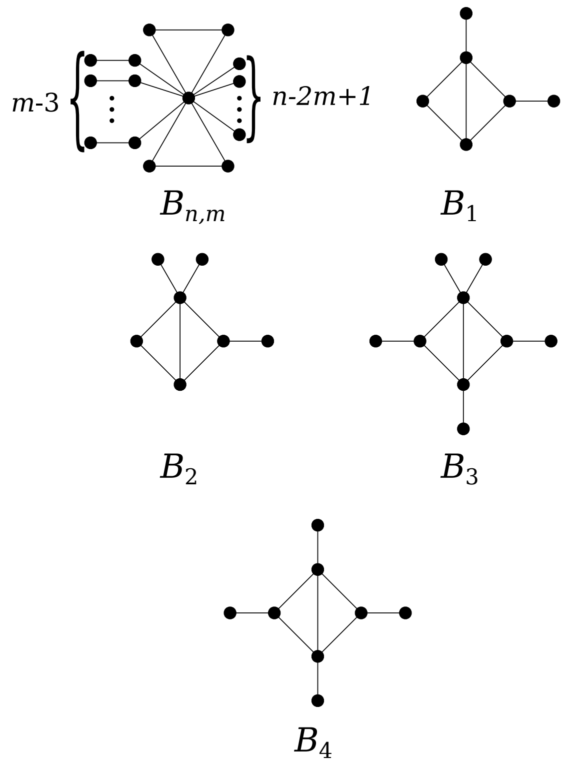

Fig. 16. Bicyclic graphs playing role in Theorems 7.21 and 7.22.

Let

$$
\begin{aligned}
f_1(n,m) &= (n-m+2)^2 + n + 3m + 2 \\
f_2(n,m) &= (n-m+2)(n+3) + 2m + 2\,.
\end{aligned}
$$

Theorem 7.21. [90] *Let $G \in \mathfrak{B}_{2m,m} \setminus \{B_1, B_4\}$, where $m \geq 3$. Then*

$$M_i(G) \leq f_i(2m,m)\ ,\ i = 1,2$$

and for each of the inequalities, the equality holds if and only if $G \cong B_{2m,m}$.

As noted in [90], $B_{6,3}$ has the maximum first Zagreb index in $\mathfrak{B}_{6,3}$, while B_1 has the maximum second Zagreb index in $\mathfrak{B}_{6,3}$. Also, $B_{8,4}$ has the maximum first Zagreb index in $\mathfrak{B}_{8,4}$, while B_4 has the maximum second Zagreb index in $\mathfrak{B}_{8,4}$.

For bicyclic graphs with an m-matching it holds

Theorem 7.22. [90] *Let $G \in \mathfrak{B}_{n,m} \setminus \{B_1, B_4\}$, where $m \geq 3$. Then*

$$M_i(G) \leq f_i(n,m)\ ,\ i = 1,2$$

and for each of the inequalities, the equality holds if and only if $G \cong B_{n,m}$.

Also, by [90], $B_{7,3}$ has the maximum first Zagreb index in $\mathfrak{B}_{7,3}$, while $B_{7,3}$ and B_2 both have the maximum second Zagreb index in $\mathfrak{B}_{7,3}$. Similarly, $B_{9,4}$ has the maximum first Zagreb index in $\mathfrak{B}_{9,4}$, while $B_{9,4}$ and B_3 both have the maximum second Zagreb index in $\mathfrak{B}_{9,4}$.

In the paper [44], the first and second maximum values of the first and second Zagreb indices of n-vertex tricyclic graphs are determined.

Let $q_n(n_1, n_2, n_3, n_4, n_5)$ be a graph obtained from a simple graph G with vertex set $V(G) = \{v_1, v_2, v_3, v_4, v_5\}$ and edge set $E(G) = \{v_1v_i, v_2v_j : 2 \leq i \leq 5, 3 \leq j \leq 5\}$ by adding $n_i - 1$ pendent vertices to vertex v_i, $1 \leq i \leq 5$, such that $n_1 \geq n_2 \geq n_3 \geq n_4 \geq n_5$ and $n_i \geq 1$ (see Fig. 17).

Denote by $K_n(n_1, n_2, n_3, n_4)$ a graph obtained from K_4 by adding $n_i - 1$ pendent vertices to vertex v_i, $1 \leq i \leq 4$, such that $n_i \geq 1$ and $n_1 = \max\{n_1, n_2, n_3, n_4\}$, see Fig. 17.

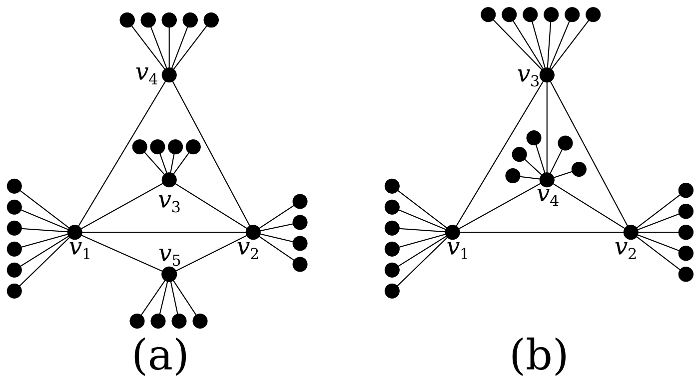

Fig. 17. (a) The graph $q_n(n_1, n_2, n_3, n_4, n_5)$; (b) The graph $K_n(n_1, n_2, n_3, n_4)$.

It was concluded in [44] that if the number of non-pendent vertices decreases, then the first and second Zagreb indices of the graphs under consideration will increase. This implies that the maximum of Zagreb indices among all tricyclic graphs is attained at graphs with a few number of non-pendent vertices. By inspecting all possible sets of tricyclic graphs with specified number of non-pendent vertices, the authors came to the following result.

Theorem 7.23. [44]

(i) Among all n-vertex tricyclic graphs, $n \geq 5$, $K_n(n-3, 1, 1, 1)$ and $q_n(n-4, 1, 1, 1, 1)$ have the maximum values of the first Zagreb index.

(ii) If $n = 6, 7$, then $K_6(2, 2, 1, 1)$ and $q_7(2, 2, 1, 1, 1)$ have the second–maximum value of the first Zagreb index. If $n \geq 5$, then $q_n(n-4, 1, 1, 1, 1)$ has the second–maximum value of the first Zagreb index.

(iii) The graph $K_n(n-3, 1, 1, 1)$ has the maximum value of the second Zagreb index.

(iv) For $n = 6, 7, 8$, the graph $K_n(n-4, 2, 1, 1)$ and for $n = 5$ and $n \geq 9$, the graph $q_n(n-4, 1, 1, 1, 1)$ have the second–maximum value of the second Zagreb index.

This research was continued and in the paper [72], using similar techniques, the first three maximum values of M_1 and the first and second maximum values of M_2 in the class of n-vertex tetracyclic graphs with $n \geq 6$ was determined. In order to state the obtained results we need few definitions.

Let F_5 be a graph obtained from K_4 by adding a vertex v_5 and connecting it to two vertices of K_4, whereas the vertices of F_5 are labeled so that $d(v_1) = d(v_2) = 4$, $d(v_3) = d(v_4) = 3$ and $d(v_5) = 2$, as shown in Fig. 18.

Define $F_n(n_1, n_2, n_3, n_4, n_5)$ as a graph, depicted in Fig. 18, obtained from F_5 by adding $n_i - 1$ pendent vertices to each v_i such that $n_i \geq 1$, $n_1 \geq n_2 \geq n_3 \geq n_4 \geq n_5$, $1 \leq i \leq 5$. Notice that $\sum_{i=1}^{5} n_i = n$.

Let W_5 be the wheel with center v_1 and construct a graph $W_n(n_1, n_2, n_3, n_4, n_5)$ from W_5 by adding $n_i - 1$ pendent vertices to each v_i such that $\sum_{i=1}^{5} n_i = n$, $n_1 = \max\{n_1, n_2, n_3, n_4, n_5\}$ and $n_i \geq 1$, $1 \leq i \leq 5$ (see Fig. 18).

Next, let $Q(6, 3, 3, 3, 3)$ is a tetracyclic graph, depicted in Fig. 18, such that all of its cycles of length 3 have a common edge. Construct the graph $Q_n(n_1, n_2, n_3, n_4, n_5, n_6)$ from $Q(6, 3, 3, 3, 3)$ by adding $n_i - 1$ pendent vertices to each v_i such that $\sum_{i=1}^{6} n_i = n$, $n_1 \geq n_2 \geq n_3$, $n_3 = \max\{n_3, n_4, n_5, n_6\}$ and $n_i \geq 1$, $1 \leq i \leq 6$.

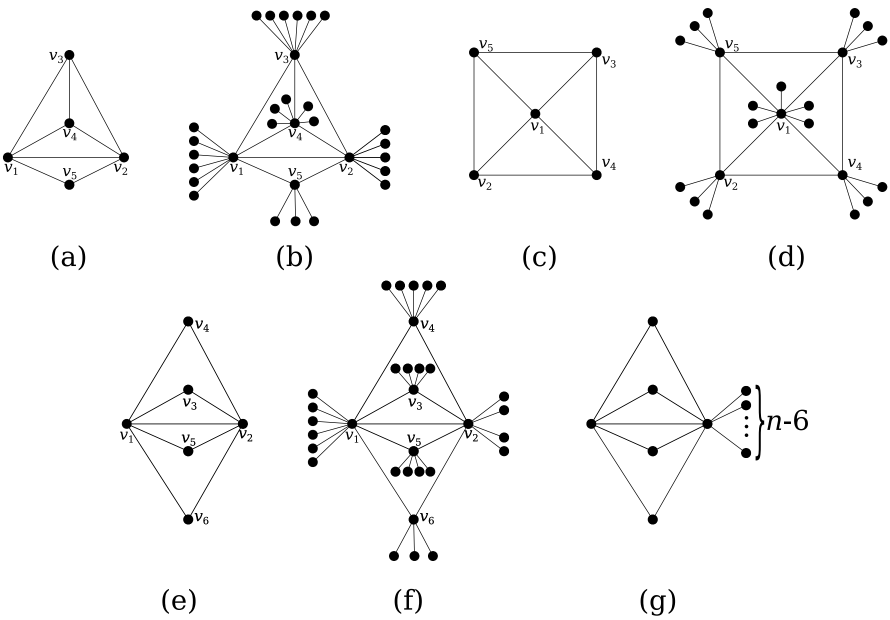

Fig. 18. (a) F_5 ; (b) $F_n(n_1, n_2, n_3, n_4, n_5)$; (c) W_5 ; (d) $W_n(n_1, n_2, n_3, n_4, n_5)$; (e) $Q(6, 3, 3, 3, 3)$ (f) $Q_n(n_1, n_2, n_3, n_4, n_5, n_6)$; (g) $Q_n(n - 5, 1, 1, 1, 1, 1)$.

By considering tetracyclic graphs with a few non-pendent vertices, the authors came to the following conclusions.

Theorem 7.24. [72] *The graph $Q_n(n-5,1,1,1,1,1)$ attains the maximum value of the first Zagreb index among all n-vertex tetracyclic graphs, $n \geq 6$. Moreover, $M_1(Q_n(n-5,1,1,1,1,1)) = n^2-n+36$.*

Theorem 7.25. *Among n-vertex tetracyclic graphs, $n \geq 6$, the graphs with the second–maximal M_1-values (cases a and b) and third–maximal M_1-values (cases c, d, e) are as follows:*

a) $F_n(n-4,1,1,1,1)$ with $M_1(F_n(n-4,1,1,1,1)) = n^2-n+34$, where $n \geq 6$ and $n \neq 8$;

b) $F_8(4,1,1,1,1)$ and $Q_8(2,2,1,1,1,1)$ with the first Zagreb index equal to 90;

c) $W_7(3,1,1,1,1)$ and $F_7(2,2,1,1,1)$ with the first Zagreb index equal to 74;

d) $W_9(5,1,1,1,1)$ and $Q_9(3,2,1,1,1,1)$ with the first Zagreb index equal to 104;

e) $W_n(n-4,1,1,1,1)$ with $M_1(W_n(n-4,1,1,1,1)) = n^2-n+32$, where $n = 8$ or $n \geq 10$.

Theorem 7.26. [72] *Among n-vertex tetracyclic graphs, $n \geq 6$, $F_n(n-4,1,1,1,1)$ has the maximum second Zagreb index equal to $M_2(F_n(n-4,1,1,1,1)) = n^2+6n+34$. The second–maximum value of M_2 is as follows:*

a) $Q_n(n-5,1,1,1,1,1)$ with second Zagreb index n^2+n+33, where $n \geq 6$ and $n \neq 7$;

b) $F_7(2,2,1,1,1)$ and $Q_7(2,1,1,1,1,1)$ with second Zagreb index 124.

A connected graph is a cactus if any of its cycles have at most one common vertex. In [88], Li et al. investigated the first and second Zagreb indices of cacti with k pendent vertices. If all cycles of the cactus G have exactly one common vertex, we say that they form a bundle. Denote by $\mathcal{C}_{n,k}$ the set of all connected cacti on n vertices with k pendent vertices.

Theorem 7.27. [88] *Let G be a graph in $\mathcal{C}_{n,k}$.*

(i) If $n-k \equiv 1 \ (mod\, 2)$, then $M_1(G) \leq n^2+2n-3k-3$ and $M_2(G) \leq 2n^2-(k+2)n-k$, with equality in both cases if and only if $G \cong C^1(n,k)$, where $C^1(n,k)$ is depicted in Fig. 19.

(ii) If $n-k \equiv 0 \ (mod\, 2)$, then $M_1(G) \leq n^2-3k$, with equality if and only if $G \cong C^2(n,k)$ or $G \cong C^3(n,k)$, where $C^2(n,k)$ and $C^3(n,k)$ are depicted in Fig. 19.

(iii) If $n-k \equiv 0 \ (mod\, 2)$, then $M_2(G) \leq 2n^2-(k+5)n+4$, with equality if and only if $G \cong C^2(n,k)$, where $C^2(n,k)$ is depicted in Fig. 19.

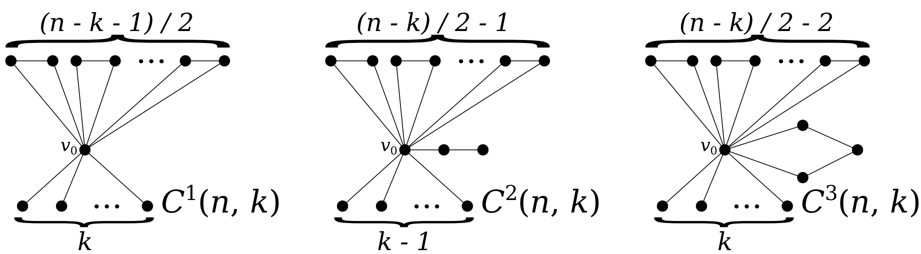

Fig. 19. Cacti occurring in Theorem 7.27.

As a consequence, the n-vertex cacti with maximal Zagreb indices were determined, as well as the cactus with the perfect matching having maximal Zagreb indices.

Theorem 7.28. [88] *Let G be connected cactus on n vertices.*

(i) $M_1(G) \leq n^2 + 2n - 3$ and $M_2(G) \leq 2n^2 - 2n$, for odd n, and the equality holds in both cases if and only if $G \cong C_n^1$, where C_n^1 is the graph depicted in Fig. 20.

(ii) $M_1(G) \leq n^2 + 2n - 6$ and $M_2(G) \leq 2n^2 - 3n - 1$, for even n, and the equality holds in both cases if and only if $G \cong C_n^2$, where C_n^2 is the graph depicted in Fig. 20.

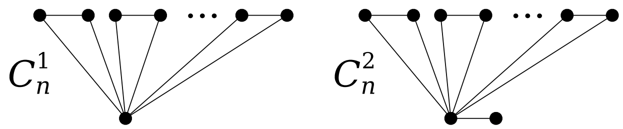

Fig. 20. Cacti occurring in Theorem 7.28.

Theorem 7.29. [88] *Let G be $2k$-vertex cactus with perfect matching. Then, $M_i(G) \leq M_i(C_{2k}^2)$ for $i = 1, 2$, and the equality holds if and only if $G \cong C_{2k}^2$.*

In addition, in [88], the authors determined sharp lower bounds for M_1 and M_2 of graphs from $\mathcal{C}_{n,k}$. It is assumed that for all $G \in \mathcal{C}_{n,k}$, G contains at least one cycle. Recall that by $\mathcal{U}_{n,k}^{+}$ we denote the set of unicyclic graphs G with n vertices and k pendent vertices, such that $\Delta(G) \leq 3$ and each pendent vertex of G is adjacent to another vertex of degree 3 and every pair of vertices of degree 3 are non-adjacent. Also, denote by $\mathcal{U}_{n,k}^{++}$ the set of unicyclic graphs G with n vertices and k pendent vertices, such that $\Delta(G) \leq 3$ and the number of vertices of degree 3 is equal to the number of pendent vertices k. Then, the following statement holds.

Theorem 7.30. [88] *Let $G \in \mathcal{C}_{n,k}$ and $0 \leq k \leq n - 3$. Then $M_1(G) \geq 4n + 2k$ with equality if and only if $n \geq 2k$ and $G \in \mathcal{U}_{n,k}^{++}$. In addition, $M_2(G) \geq 4n + 3k$ with equality if and only if $n \geq 3k$ and $G \in \mathcal{U}_{n,k}^{+}$.*

At the end of this section we mention few results from [45], [15], and [14] which provide a unified approach to the largest and smallest Zagreb indices of trees and cyclic graphs. In the paper [45], Deng introduced some transformations that increase (decrease) the Zagreb indices. First, we present two transformations from [45] which increase Zagreb indices.

Transformation A. Let uv be an edge of G, $d_G(v) \geq 2$, $N_G(u) = \{v, w_1, w_2, \ldots, w_t\}$ and $d_G(w_i) = 1$ for $i = 1, 2, \ldots, t$. Let

$$G' = G - \{uw_i \,|\, 1 \leq i \leq t\} + \{vw_i \,|\, 1 \leq i \leq t\}$$

see Fig. 21.

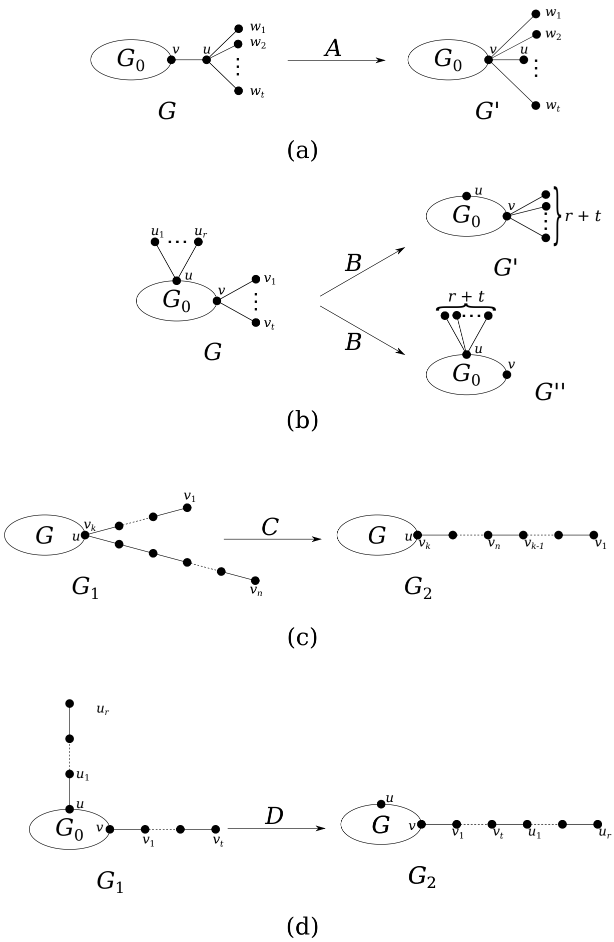

Fig. 21. The transformations A, B, C, and D.

Transformation B. Let u and v be two vertices in G with $u_1, u_2, \ldots, u_r$ being pendent vertices adjacent to u and $v_1, v_2, \ldots, v_t$ being pendent vertices adjacent to v. Let

$$\begin{aligned} G' &= G - \{uu_1, uu_2, \ldots, uu_r\} + \{vu_1, vu_2, \ldots, vu_r\} \\ G'' &= G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\} \end{aligned}$$

see Fig. 21.

It has been proven in [45], that for a graph G' obtained from G by the transformation A it holds $M_i(G') > M_i(G)$ $i = 1, 2$. Also, by [45], for the graphs G' and G'' obtained from G by the transformation B, it holds that either $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.

By using transformations A and B, results from [37, 66], concerning extremal trees with maximal values of Zagreb indices were reproven. Also, Deng [45] obtained the corresponding results for unicyclic and bicyclic graphs with maximal Zagreb indices and in such a way some previously known results from [103, 146, 150] were reproven.

Deng [45] also presented two transformations which decrease Zagreb indices.

Transformation C. Let $G \neq P_1$ be a connected graph and choose $u \in V(G)$. By G_1 is denoted the graph resulting from identifying u with the vertex v_k of a path $v_1 v_2 \ldots v_n$, $1 < k < n$. By G_2 is denoted the graph obtained from G_1 by deleting $v_{k-1}v_k$ and adding $v_{k-1}v_n$ (see Fig. 21).

Transformation D. Let u and v be two vertices in a graph G. G_1 denotes the graph that results from identifying u with the vertex u_0 of a path $u_0 u_1 \ldots u_r$ and identifying v with the vertex v_0 of a path $v_0 v_1 \ldots v_t$. Graph G_2 is obtained from G_1 by deleting uu_1 and adding $v_t u_1$ (see Fig. 21).

It was proven in [45], that for the graphs G_1 and G_2, obtained by transformation C, it holds $M_i(G_1) > M_i(G_2)$, $i = 1, 2$. Also, for graphs G_1 and G_2, obtained by transformation D, the following statement holds.

Theorem 7.31. [45] *Let G_1 and G_2 be the graphs depicted in Fig. 21. If $d_G(u) \geq d_G(v) > 1$, $r \geq 1$ and $t \geq 0$, then*

(i) if $t > 0$, then $M_1(G_1) > M_1(G_2)$ and $M_2(G_1) > M_2(G_2)$;

(ii) if $t = 0$ and $d_G(u) > d_G(v)$, then $M_1(G_1) > M_1(G_2)$;

(iii) if $t = 0$ and $\sum_{x \in N_G(u)-\{v\}} d_G(x) > \sum_{y \in N_G(v)-\{u\}} d_G(y)$, then $M_2(G_1) > M_2(G_2)$.

By using transformations C and D, and the previous theorem, trees, unicyclic and bicyclic graphs whose Zagreb indices are minimum can be obtained, as shown in [45], and in such a way some earlier known results for trees and unicyclic graphs have been confirmed [37, 66, 103, 150] and new results on extremal bicyclic graphs with minimal Zagreb indices, presented in the previous discussions, have been obtained.

In the papers [14, 15] Bianchi et al. established a unified approach aimed at determining upper and lower bounds for M_1 and M_2 of trees and c-cyclic graphs, $1 \leq c \leq 6$, by using of a majorization technique and Schur–convexity introduced in [110]. In fact, in the class of c-cyclic graphs, Bianchi et al. [14, 15] were interested in finding graphs associated to the maximal (minimal) degree sequence with respect to the majorization order. Before we present the results of [14, 15], we need few observations.

As mentioned before, the degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ of c-cyclic graph satisfies the condition $\sum_{i=1}^{n} d_i = 2(n+c-1)$, i.e., for short, $\pi \in \sum_{2(n+c-1)}$. Let now $F(d_1, d_2, \ldots, d_n)$ be any topological index which is a Schur–convex function of its arguments, defined on a subset $S \subseteq \sum_a$, where

$$\sum_a = \left\{ \mathbf{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n : x_1 \geq x_2 \geq \ldots \geq x_n \geq 0, \sum_{i=1}^{n} x_i = a \right\}.$$

Since the Schur–convex functions have the order preserving property, it holds

$$F(x_*(S)) \leq F(d_1, d_2, \ldots, d_n) \leq F(x^*(S))$$

where $x_*(S)$ and $x^*(S)$ are the minimal and maximal elements of S, respectively, with respect to the majorization order. Using these arguments, extremal degree sequences of c-cyclic graphs $(0 \leq c \leq 6)$

were determined and, consequently, extremal c-cyclic graphs with respect to M_1 were obtained in [14]. In such a way, some existing results mentioned previously [44, 66, 72, 103, 105, 150, 153] for $0 \le c \le 4$ were recovered and some new results were obtained as well. Here we mention only the new ones.

Since the upper and lower bounds for M_1 and corresponding extremal trees, unicyclic, and bicyclic graphs have already been presented, we start with tricyclic graphs.

Tricyclic graphs. The upper bounds for M_1 of tricyclic graphs and the corresponding extremal graphs have earlier been outlined (Theorem 7.23). Thus we present here only the lower bounds arising from considerations in the paper [14].

(i) For $n = 4$, there is only one tricyclic graph associated to the sequence $(3, 3, 3, 3)$, and thus $M_1 = 36$.

(ii) For $n \ge 5$, there is one minimal degree sequence $(\underbrace{3, \ldots, 3}_{4}, \underbrace{2, \ldots, 2}_{n-4})$, corresponding to the graph (a) in Fig. 22, for $n = 8$, hence $M_1 \ge 4n + 20$.

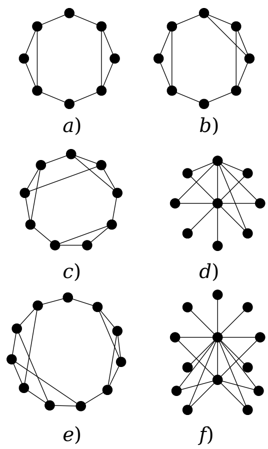

Fig. 22. Tricyclic and higher-cyclic graphs with minimal M_1, according to [14].

Tetracyclic graphs. Similarly to the previous case, we present only the lower bounds for M_1 of tetracyclic graphs, since the upper bounds and the corresponding extremal graphs have been presented in Theorem 7.24.

(i) For $n = 5$, the maximal degree sequence is $(4, 4, 3, 3, 2)$ and the minimal one is $(4, 3, 3, 3, 3)$, hence $52 \le M_1 \le 54$.

(ii) For $n \ge 6$ there is one minimal degree sequence $(\underbrace{3, \ldots, 3}_{6}, \underbrace{2, \ldots, 2}_{n-6})$ corresponding to the graph (b) in Fig. 22 for $n = 8$, hence $M_1 \ge 4n + 30$.

Pentacyclic graphs.

(i) For $n = 5$, there is only one pentacyclic graph with the degree sequence $(4,4,4,3,3)$, hence $M_1 = 66$.

(ii) For $n = 6$, there exist two maximal incomparable degree sequences $(5,5,3,3,2,2)$ and $(5,4,4,3,3,1)$, and one minimal degree sequence $(4,4,3,3,3,3)$. As suggested in [14], when more maximal (or minimal) elements are identified, the best one depends on the topological index under consideration. Hence, for M_1 it can easily be deduced that $68 \leq M_1 \leq 76$.

(iii) For $n = 7$, the minimal degree sequence is $(4,\underbrace{3,\ldots,3}_{6})$, whereas for $n \geq 8$, the minimal one is $(\underbrace{3,\ldots,3}_{8},\underbrace{2,\ldots,2}_{n-8})$.

For $n \geq 7$, there are three incomparable maximal degree sequences

$$(n-1,6,\underbrace{2,\ldots,2}_{5},\underbrace{1,\ldots,1}_{n-7})\ ,\ (n-1,5,3,3,2,2,\underbrace{1,\ldots,1}_{n-6})\ ,\ (n-1,4,4,3,3,\underbrace{1,\ldots,1}_{n-5})\,.$$

Thus, it is easily deduced that for $n = 7$ it holds $70 \leq M_1 \leq 92$ and for $n \geq 8$ we have $4n + 40 \leq M_1 \leq n^2 - n + 50$, wherein the graphs (c) and (d) in Fig. 22 achieve, for $n = 9$, the latter lower and upper bounds, respectively.

Hexacyclic graphs.

(i) For $n = 5$, there is only one hexacyclic graph associated to the degree sequence $(\underbrace{4,\ldots,4}_{5})$, hence $M_1 = 80$.

(ii) For $n = 6$, we have two incomparable maximal degree sequences $(5,5,4,3,3,2)$ and $(5,4,4,4,4,1)$, and one minimal degree sequence $(4,4,4,4,3,3)$. Simple calculation yields $82 \leq M_1 \leq 90$.

(iii) For $n = 7$, there exist three maximal incomparable degree sequences $(6,6,3,3,2,2,2)$, $(6,5,4,3,3,2,1)$, and $(6,4,4,4,4,1,1)$, and one minimal degree sequence $(4,4,4,3,3,3,3)$, from which one concludes that $84 \leq M_1 \leq 102$.

(iv) For $n = 8$ and $n = 9$, the minimal degree sequences are $(4,4,\underbrace{3,\ldots,3}_{6})$ and $(4,\underbrace{3,\ldots,3}_{8})$, respectively, whereas for $n \geq 10$, the minimal one is $(\underbrace{3,\ldots,3}_{10},\underbrace{2,\ldots,2}_{n-10})$. Thus, for $n = 8$ and 9, the the lower bounds for M_1 are 86 and 88, respectively, whereas for $n \geq 10$ it holds $M_1 \geq 4n + 50$, wherein the graph (e) in Fig. 22 achieves, for $n = 11$, the lower bound.

For $n \geq 8$, there are four incomparable maximal degree sequences

$$(n-1,7,\underbrace{2,\ldots,2}_{6},\underbrace{1,\ldots,1}_{n-8})\quad,\quad(n-1,6,3,3,2,2,2,\underbrace{1,\ldots,1}_{n-7})$$
$$(n-1,5,4,3,3,2,\underbrace{1,\ldots,1}_{n-6})\quad,\quad(n-1,\underbrace{4,\ldots,4}_{4},\underbrace{1,\ldots,1}_{n-5})$$

and hence, by a simple calculation, it holds $M_1 \leq n^2 - n + 66$ and the graph (f) in Fig. 22, achieves, for $n = 11$, this upper bound.

It was suggested in [14] that this approach can be extended to other topological indices whenever they can be expressed as Schur–convex or Schur–concave functions of the degree sequence of the graph.

An analogous approach was applied in the paper [15] where an analysis was presented aimed at establishing maximal and minimal vectors with respect to the majorization order under sharper constraints than those obtained by Marshall and Olkin [110]. This methodology was applied to the calculation of bounds for M_2 and it was shown that the bounds obtained by this technique are often sharper than those earlier communicated [39, 146, 153].

8. Zagreb coindices of graphs

In the paper [46], bearing in mind Eq. (2), Došlić introduced the Zagreb coindices, opposities to the Zagreb indices, defined by

$$\overline{M}_1(G) = \sum_{v_iv_j \notin E} (d_i + d_j) \qquad , \qquad \overline{M}_2(G) = \sum_{v_iv_j \notin E} d_i d_j \, .$$

The Zagreb coindices are closely related to the Zagreb indices [9]:

$$\overline{M}_1(G) = 2m(n-1) - M_1(G) \tag{37}$$

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}\, M_1(G)\, . \tag{38}$$

The Zagreb coindices of G are not the Zagreb indices of $\overline{G}$, since the defining sums run over $E(\overline{G})$, but the degrees are with respect to G. Still, those quantities are closely related. If we denote by $\overline{m}$ the number of edges in $\overline{G}$, then it holds, by [9],

$$M_1(\overline{G}) = M_1(G) + 2(n-1)(\overline{m} - m)$$

implying, as noted in [9], that

$$\overline{M}_1(G) = \overline{M}_1(\overline{G})\, .$$

Also, by [9], for the second Zagreb coindex we have

$$\overline{M}_2(G) = M_2(\overline{G}) - (n-1)M_1(\overline{G}) + \overline{m}(n-1)^2\, .$$

By (37), for trees, the sum $M_1(G) + \overline{M}_1(G) = 2(n-1)^2$ is constant for fixed n, implying that the problem of determining the minimum (maximum) first Zagreb coindex is equivalent to the problem of determining the maximum (minimum) first Zagreb index, which yields

Theorem 8.1. [10] *If T is an n-vertex tree, then $\overline{M}_1(K_{1,n-1}) \leq \overline{M}_1(T) \leq \overline{M}_1(P_n)$ and $\overline{M}_2(K_{1,n-1}) \leq \overline{M}_1(T) \leq \overline{M}_1(P_n)$.*

By Corollary 4.1 and Theorem 6.6, the following result concerning chemical trees, obtained in [56] by Fonseca and Stevanović, is immediately deduced.

$$\overline{M}_1(T) \geq 2(n-1)^2 - \begin{cases} 6n - 10 & \text{if } \; n \equiv 2 \,(\text{mod}\, 3) \\[2ex] 6n - 12 & \text{otherwise} \end{cases}$$

with equality as stated in Corollary 4.1.

Also, by relation (38) and Theorem 6.6, the lower bound for the second Zagreb coindex over chemical trees was obtained in [56] as follows

$$\overline{M}_2(T) \geq 2(n-1)^2 - \begin{cases} 11n - 29 & \text{if } n \equiv 2 \pmod 3 \\ 11n - 32 & \text{otherwise} \end{cases}$$

with equality if and only if either (i) every vertex of T is of degree 1 or 4 (in which case $n \equiv 2 \pmod 3$), or (ii) one vertex of T has degree 2 or 3 and it is adjacent to a single vertex of degree 4, while all other vertices are of degree 1 or 4.

In [10] the following results on Zagreb coindices of unicyclic and bicyclic graphs were obtained.

Theorem 8.2. [10] *If G is an n-vertex unicyclic graph, then $(n+2)(n-3) \leq \overline{M}_1(G) \leq 2n(n-3)$. Moreover, the left and right equalities hold if and only if G is isomorphic to $K_{1,n-1} + e$ and C_n, respectively.*

Theorem 8.3. [10] *If G is an n-vertex bicyclic graph, then $n^2 + n - 16 \leq \overline{M}_1(G) \leq 2n^2 - 4n - 12$. The left equality is satisfied if and only if G is isomorphic to $K_{1,n-1} + e + f$, where e and f are two edges with a common vertex forming two adjacent triangles in $K_{1,n-1}$. The right equality holds if and only if G is isomorphic to a graph constructed from C_p and C_q joined by a path P_{n-p-q}, $3 \leq p, q \leq n-3$ (see Fig. 23).*

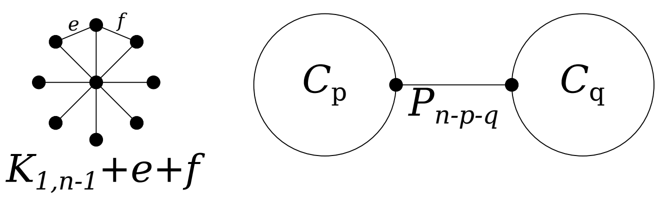

Fig. 23. Extremal graphs mentioned in Theorem 8.3.

Theorem 8.4. [10] *Suppose that G is a triangle– and quadrangle–free connected graph with n vertices, m edges and radius r. Then $\overline{M}_2(G) \geq 2m^2 - (n+1-r)(m + \frac{1}{2}n)$ with equality if and only if G is a Moore graph of diameter 2 or $G \cong C_6$.*

In addition, by [10], for a connected graph G it holds

$$\overline{M}_2(G) \leq 2m^2 - \frac{1}{2} \sum_{v \in V(G)} d(v)\big[d(v) + n_2(v)\big] - \frac{1}{2} \sum_{v \in V(G)} \big[d(v) + n_2(v)\big] .$$

The equality holds if and only if G is a triangle– and quadrangle–free connected graph.

Recently, Das et al. [41], by using the relation (37) and Theorem 4.4 obtained the following lower bound for $\overline{M}_1$ in terms of n, m and Δ.

Theorem 8.5. [41] *Let G be an (n, m)-graph with maximum degree Δ. Then*

$$\overline{M}_1(G) \geq (n-3)m + \Delta(n-\Delta) - \frac{2(m-\Delta)^2}{n-2}$$

with equality holding if and only if $G \cong K^*_{2,n-2}$ or $G \cong K_n$ or $G \cong Ki_{n,n-1}$.

Besides, in the paper [41], some upper and lower bounds on the second Zagreb coindex in terms of n, m, δ, Δ, and Δ_2 were established.

Theorem 8.6. citedasnum *Let G be an (n, m)-graph with minimal degree δ, maximum degree Δ and second–maximal degree Δ_2. Then*

(i)

$$\overline{M}_2(G) \geq \frac{1}{2}(n-3)m\delta + \frac{1}{2}\delta\Delta(n-\Delta) - \frac{\delta(m-\Delta)^2}{n-2}$$

with equality if and only if $G \cong K^*_{2,n-2}$ or $G \cong K_n$;

(ii)

$$\overline{M}_2(G) \leq m(n-1)\Delta - \frac{1}{2}\Delta^3 - \frac{\Delta(2m-\Delta)^2}{2(n-1)} - \frac{\Delta(n-2)}{(n-1)^2}(\Delta_2-\delta)^2$$

with equality if and only if G is a regular graph.

The lower bounds for Zagreb coindices of series–parallel graphs were determined in [10].

Theorem 8.7. [10] *Suppose that G is an (n, m)-series–parallel graph without isolated vertices. Then $\overline{M}_1(G) \geq m(n-4) + n$ and $\overline{M}_2(G) \geq (m-n)(m-1)$. The equality holds if and only if $G \cong K_2$ or $G \cong K_{1,1,n-2}$.*

In [82], two estimations on Zagreb coindices of connected graphs involving the number of pendent vertices were given.

Theorem 8.8. [82] *Let G be a connected graph of order n with n_1 pendent vertices. Then*

$$\begin{aligned} \overline{M}_1(G) &\geq -2n_1^2 + 3n\,n_1 - 4n_1 \\ \overline{M}_2(G) &\geq -\frac{3}{2}n_1^2 - \frac{5}{2}n_1 + 2n\,n_1 \,. \end{aligned}$$

As suggested in [82], when $n_1 = 0$, the complete graph K_n and the graph $\overline{K}_n$ attain both bounds. When $n_1 = 2$, the 4-vertex path P_4 attains both bounds in the previous theorem.

9. Nordhaus–Gaddum type of inequalities for Zagreb indices

In 1956, Nordhaus and Gaddum [117] established inequalities involving the chromatic number $\chi(G)$ of a graph G and its complement. Motivated by this result, different inequalities of that kind, known as

Nordhaus–Gaddum type inequalities, have been communicated in the literature. Here we present those pertaining to the first and second Zagreb indices.

Zhang and Wu in [149] established the following lower and upper bounds on $M_1(G) + M_1(\overline{G})$ and $M_2(G) + M_2(\overline{G})$, respectively, in terms of n only.

Theorem 9.1. [149] *Let G be a graph of order n, then*

$$\frac{n(n-1)^2}{2} \leq \; M_1(G) + M_1(\overline{G}) \; \leq n(n-1)^2$$

$$\binom{n}{2}\left(\frac{n-1}{2}\right)^2 \leq \; M_2(G) + M_2(\overline{G}) \; \leq \binom{n}{2}(n-1)^2 .$$

In both inequalities the left–hand–side equalities are attained if and only if $G \cong K_n$ and the right–hand–side equalities hold if and only if G is a $(\frac{n-1}{2})$-regular graph, with $n = 4k+1$, $k \geq 1$.

In the paper [39], Das et al. obtained the following upper bounds on $M_1(G)+M_1(\overline{G})$ (resp. $M_2(G)+M_2(\overline{G})$), in terms of n, m, δ, Δ, and Δ_2, by using Theorem 4.15.

Theorem 9.2. [39] *Let G be a graph with n vertices, m edges, maximum degree Δ, second–maximum degree Δ_2 and minimum degree δ. Then*

$$\begin{aligned} M_1(G) + M_1(\overline{G}) \; &\leq \; \frac{[n(n-2) - 2m + \delta + 1]^2}{n-1} + \Delta^2 + (n-1-\delta)^2 \\ &+ \; \frac{n-1}{4}\left[(\Delta-\delta)^2 + (\Delta_2-\delta)^2\right] \end{aligned}$$

with equality if and only if G is the path P_3 or G is a regular graph.

In addition,

$$\begin{aligned} M_2(G) + M_2(\overline{G}) \; &\leq \; \frac{n(n-1)^3}{2} + 2m^2 - 3m(n-1)^2 \\ &+ \; \left(n - \frac{3}{2}\right)\left[\frac{(2m-\Delta)^2}{n-1} + \Delta^2 + \frac{n-1}{4}(\Delta_2-\delta)^2\right] \end{aligned}$$

with equality if and only if G is isomorphic to a graph H_1, such that $d_2(H_1) = d_3(H_1) = \cdots = d_n(H_1) = \delta$ or G is isomorphic to a graph H_2 such that $d_2(H_2) = d_3(H_2) = \cdots = d_{p+1}(H_2) = \Delta_2$ and $d_{p+2}(H_2) = d_{p+3}(H_2) = \cdots = d_{2p+1}(H_2) = \delta$, $n = 2p+1$.

Recently, Das et al. in [41] established new lower and upper bounds on $M_1(G) + M_1(\overline{G})$ (resp. $M_2(G) + M_2(\overline{G})$) in terms of n, m, δ, Δ, and Δ_2.

Theorem 9.3. [41] *Let G be a graph with n vertices, m edges, maximum degree Δ, second–maximum degree Δ_2, and minimum degree δ. Then*

(i)

$$\begin{aligned} M_1(G) + M_1(\overline{G}) \; &\geq \; n(n-1)^2 - 4(n-1)m \\ &+ \; 2\left[\Delta^2 + \frac{(2m-\delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2-\delta)^2\right] \end{aligned}$$

with equality if and only if G is a regular graph or G is isomorphic to a graph H, such that $d_2(H) = d_3(H) = \cdots = d_n(H) = \delta$;

(ii)

$$M_1(G) + M_1(\overline{G}) \leq n(n-1)^2 - 2(n-3)m + 2\left[\frac{2(m-\Delta)^2}{n-2} - \Delta(n-\Delta)\right]$$

with equality if and only if $G \cong K_n$ or $G \cong K^*_{2,n-2}$ or $G \cong Ki_{n,n-1}$.

Theorem 9.4. [41] *Let G be a graph with n vertices, m edges, maximum degree Δ, second–maximum degree Δ_2, and minimum degree δ. Then*

(i)

$$\begin{aligned} M_2(G) + M_2(\overline{G}) \ &\geq \ \frac{n(n-1)^3}{2} + 2m^2 - 3m(n-1)^2 \\ &+ \ \left(n - \frac{3}{2}\right)\left[\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2 - \delta)^2\right] \end{aligned}$$

with equality if and only if G is a regular graph or G is isomorphic to a graph H, such that $d_2(H) = d_3(H) = \cdots = d_n(H) = \delta$;

(ii)

$$\begin{aligned} M_2(G) + M_2(\overline{G}) \ &\leq \ \frac{n(n-1)^3}{2} + 2m^2 - 3m(n-1)^2 \\ &+ \ \left(n - \frac{3}{2}\right)\left[(n+1)m - \Delta(n-\Delta) + \frac{2(m-\Delta)^2}{n-2}\right] \end{aligned}$$

with equality if and only if $G \cong K_n$ or $G \cong K^*_{2,n-2}$ or $G \cong Ki_{n,n-1}$.

In [82], several Nordhaus–Gaddum type bounds for the first Zagreb coindex were given. Let $even(n) = 1$ if n is even, and 0 otherwise.

Theorem 9.5. [82] *(i) If G is a graph with $n \geq 2$ vertices and m edges, then*

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 2mn - \frac{4m^2}{n-1}$$

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

(ii) If G is a connected K_{r+1}-free graph, $2 \leq r \leq n-1$, then

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 4m - \left(\frac{n}{r} - 1\right)$$

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

(iii) If G is a connected quadrangle–free graph, then

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 4mn - 2n^2 + 2n - 8m + 4\,even(n)$$

with equality if and only if G is a graph obtained from the star $K_{1,n-1}$ by adding $\lfloor (n-1)/2 \rfloor$ independent edges.

(iv) If G is a connected triangle– and quadrangle–free graph, then

$$\overline{M}_1(G) + \overline{M}_1(\overline{G}) \geq 2(n-1)(2m-n)$$

with equality if and only if $G \cong K_{1,n-1}$ or a Moore graph of diameter 2.

The corresponding Nordhaus–Gaddum type bounds for the second Zagreb coindices were determined in [79].

Theorem 9.6. [79] *Let G be a graph of order n containing m edges. Then*

$$\overline{M}_2(G) + \overline{M}_2(\overline{G}) \geq 2(m^2 + \overline{m}^2) - \binom{n}{2}(n-1)^2 - \frac{n(n-1)^2}{2} \tag{39}$$

and

$$\overline{M}_2(G) + \overline{M}_2(\overline{G}) \leq 2(m^2 + \overline{m}^2) - \binom{n}{2}\left(\frac{n-1}{2}\right)^2 - \frac{n(n-1)^2}{2}\,. \tag{40}$$

The equality in (39) is satisfied if and only if G is isomorphic to the complete graph K_n. The equality in (40) is satisfied if and only if $n \equiv 1$ (mod 4) and G is $\frac{n-1}{2}$-regular.

10. Relations between Zagreb indices

Recently, there has been much interest in comparing the values taken by the Zagreb indices M_1 and M_2 on the same graphs. Let

$$\Delta M(G) = M_2(G) - M_1(G)$$

and define the set $\Phi(z)$, for $z \in \mathbf{Z}$, as

$$\Phi(z) = \{G : G \text{ is connected and } \Delta M(G) = z\}\,.$$

If $G \in \Phi(z)$, it is said [111] that G is *z-Zagreb-balanced*.

Direct approaches to comparing Zagreb indices were used in [26, 136]. The case of trees was studied in [136]. The main result is that

$$M_1 - M_2 \leq d_v \tag{41}$$

where v is a vertex of degree $d_v \geq 2$. Thus, for a tree T, the difference $M_1 - M_2$ is bounded by the smallest degree of a non-pendent vertex of T.

In the paper [26], lower bounds on $\Delta M(G) = M_2 - M_1$ for cyclic graphs were studied.

Theorem 10.1. [26] *Let G be a simple and connected graph with n vertices and m edges.*

a) If $m \leq 6n/5$, then $\Delta M(G) \geq 6(m-n)$, with equality 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.

b) If $m \geq n$, then $\Delta M(G) \geq 11m - 12n$, with equality attained if and only if G is a graph with vertices of degree 2 and 3 only and, when $m \geq 6n/5$, no pair of vertices of degree 2 are adjacent.

From Theorem 10.1, the following result of Liu [98] can be deduced.

Theorem 10.2. [98] *Let G be a simple, connected and unicyclic graph. Then $M_1 \leq M_2$ with equality if and only if G is a cycle.*

In paper [111], two examples were provided showing that $\Phi(z)$ is non-empty for each $z \in \mathbf{Z}$. First, for a star $K_{1,z}$, $z \geq 1$, it holds $\Delta M(K_{1,z}) = -z$. Next, for $z \geq 0$, let $PC(z)$ be a tree on $3z+3$ vertices obtained from the path P_{2z+3} with vertex set $\{v_1, \ldots, v_{2z+3}\}$ by adding a pendent edge to vertices $v_3, v_5, \ldots, v_{2z+1}$. Then, $\Delta M(PC(z)) = z - 2$.

Hence, $\Phi(z)$ contains a star $K_{1,-z}$ for $z \leq -1$, and a tree $PC(z+2)$ for $z \geq -2$. Besides, two simple constructions of new elements of $\Phi(z)$ from the existing ones by adding an arbitrary number of new vertices were presented in [111]. Both of these constructions can be applied to the graph $PC(z+2) \in \Phi(z)$ for $z \geq -2$, provided that each set $\Phi(z)$, $z \geq -2$, is infinite.

Unlike the case $z \geq -2$, it was proven in [111] that $\Phi(z)$ contains only the star $K_{1,-z}$ for $z < -2$. In fact, it was proven that for a connected graph G, different from the star,

$$\Delta M(G) \geq -2\,.$$

Obviously, the previous inequality improves the inequality (41).

By considerations in [111], the first non-trivial sets $\Phi(z)$ are $\Phi(-2)$, $\Phi(-1)$ and $\Phi(0)$ and these have the property that all of their elements are trees, with exception of the cycles C_n which are the only non-tree elements of $\Phi(0)$. Also, it was proven in [111] that for a connected graph G which is neither a tree nor a cycle, it holds that $\Delta M(G) \geq 1$.

In order to present some further results on $\Delta M(G)$, recall that by the relations (1) and (2) it holds that [57]

$$\Delta M(G) = \sum_{v_i v_j \in E(G)} (d_i - 1)(d_j - 1) - m$$

i.e.,

$$\Delta M(G) = RM_2(G) - m$$

where $RM_2(G)$ is a vertex-degree-based graph invariant, introduced in [57] by

$$RM_2(G) = \sum_{v_i v_j \in E(G)} (d_i - 1)(d_j - 1)$$

and called *reduced second Zagreb index*.

Theorem 10.3. [57] *For almost all graphs and almost all edges $e \in E(G)$, the condition $RM_2(G) - RM_2(G-e) - 1 > 0$, i.e., $\Delta M(G) - \Delta M(G-e)$ is satisfied. Exceptionally:*

(a) $\Delta M(G) = \Delta M(G-e)$ holds if e is an edge between a pendent vertex u and a vertex v of degree two, and the other neighbor of v is also a vertex of degree two.

(b) $\Delta M(G) = \Delta M(G-e)$ holds if the graph G has a component which is a 4-vertex path, and e is the central edge of this path.

(c) $\Delta M(G) < \Delta M(G-e)$ holds if the graph G has a component which is a star, and e is an edge of this star.

Extremal trees of order n with maximal $\Delta M(G)$ were determined in [57].

Let n and k be fixed integers, $n \geq 4$, $2 \leq k \leq n-2$. Construct the set $\mathfrak{T}(n,k)$ of n-vertex trees by attaching (in any possible way) $n-k-1$ pendent vertices to the pendent vertices of the star $K_{1,k}$ on $k+1$ vertices.

Theorem 10.4. [57] *If T is a tree of order n, $n \geq 4$, then*

$$\Delta M(G) \leq \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil + 1 - n\,.$$

Equality holds if and only if $T \in \mathfrak{T}(,n/2)$ for even n, and $T \in \mathfrak{T}(n, \lfloor n/2 \rfloor) \bigcup \mathfrak{T}(n, \lceil n/2 \rceil)$ for odd n.

Let $C_{n,\Delta}^k$ be the unicyclic graph specified in connection with Theorem 7.10. Denote by $\mathcal{C}_\Delta$ the set $\{C_{n,\Delta}^k \mid 3 \leq k \leq n-\Delta-1\}$. The following lower bound on $M_2 - M_1$ is obtained in [76]:

Theorem 10.5. [76] *Let G be a unicyclic graph of order n with maximum degree Δ. Then*

$$M_2(G) - M_1(G) \geq \begin{cases} \Delta - 2 & \text{if} \quad d = 0 \\ \Delta & \text{if} \quad d = 1 \\ 2 & \text{if} \quad d > 1 \end{cases} \tag{42}$$

where d is the length of the shortest path from the maximum degree vertex u to the cycle $C(G)$ (The cycle of a graph G is denoted by $C(G)$.) The equalities hold in (42) 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.

For general graphs, the order of magnitude of M_1 is $O(n^3)$ whereas for M_2 is $O(mn^2)$, implying that M_1/n and M_2/m have the same orders of magnitude $O(n^2)$. This implies that is more convenient to compare M_1/n and M_2/m instead of M_1 with M_2. By using the AutoGraphiX conjecture–generating system [8, 24, 25] the following conjecture was obtained.

Conjecture 10.1. [8, 24, 25] *For all simple connected graphs with n vertices and m edges,*

$$\frac{M_1}{n} \leq \frac{M_2}{m} \tag{43}$$

with equality for complete graphs, among others.

The relation (43) is referred to as the *Zagreb indices inequality*. In 2007, Hansen and Vukičević [74] showed that this conjecture does not hold for general graphs but it is true for chemical graphs.

Theorem 10.6. [74] *For all chemical graphs G with n vertices and m edges, inequality* (43) *holds.*

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 $K_{1,4}$ and cycles $C_p, C_q, \ldots$ of any length.

Besides, Hansen and Vukičević [74] presented a non-connected counterexample (a star $K_{1,5}$ together with a cycle C_3) and a complicated connected counterexample with 46 vertices and 110 edges to Conjecture 10.1.

On the other hand, it was proven that there are some other classes of graphs for which the conjecture is true. Vukičević and Graovac in [136] first showed that relation (43) holds for all trees, with stars as extremal trees. Later, new proofs were given in [7, 127]. In the paper [98], it was shown that the conjecture is true for unicyclic graphs and the bound is tight with cycles as extremal graphs. In fact, as $m = n$ for unicyclic graphs, the relation (43) follows from Theorem 10.2.

Sun et al. [129] showed that the inequality (43) holds for bicyclic graphs except one class and characterized extremal graphs as well. Besides, counterexamples of bicyclic graphs were obtained from the excluded class. Using AutoGraphiX, Caporossi et al. [26] investigated the cases of bicyclic and tricyclic graphs and constructed counterexamples to Conjecture 10.1 in both cases. Also, in [26], an infinite family of counterexamples of c-cyclic graphs, for all $c \geq 2$ is obtained, which are constructed by joining complete bipartite graph $K_{2,c+1}$ and a star $K_{1,p}$ by an edge from a pendent vertex of $K_{1,p}$ to a vertex of the smallest side of $K_{2,c+1}$, see Fig. 24.

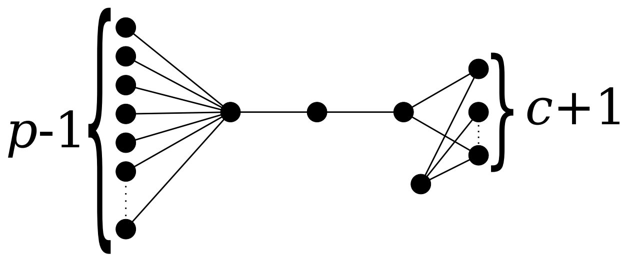

Fig. 24. An infinite family of counterexamples to Conjecture 10.1.

For other results concerning the validity or non-validity of (43) for various classes of graphs the reader is referred to [5, 6, 17, 73, 77, 85, 125, 130, 158]. These studies are summarized in two surveys [101, 102]. In addition, the equality case in (43) was also studied in [1, 137].

In the sequel, we present a few other results concerning the relations between M_1 and M_2.

For a connected graph G it was proven [37] that

$$M_1 + 2M_2 \leq 4m^2$$

with equality if and only if G is the complete graph K_n. Also, it was shown that [37]

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)M_1(G)$$

with equality if and only if G is isomorphic to $K_{1,n-1}$ or K_n.

In [123], Réti presented some new inequalities related to the first and second Zagreb indices.

Theorem 10.7. [123] *If G is a simple connected graph, then*

$$M_1(G) \geq \frac{M_2(G)}{\Delta} + \delta m$$

with equality if G is regular.

Theorem 10.8. [123] *If G is a simple connected graph, then*

$$M_1(G) \leq \frac{M_2(G)}{\delta} + \delta m \tag{44}$$

and

$$M_1(G) \leq \frac{M_2(G)}{\Delta} + \Delta m\,. \tag{45}$$

Equality in both cases holds if and only if G is a regular or bidgreed (biregular) graph with no adjacent vertices of the same degree.

From (44) and (45), the following relations were deduced [123].

Corollary 10.1. [123] *For a connected (n, m)-graph G with maximum degree Δ and minimum degree δ,*

$$M_1(G) \leq \frac{M_2(G)}{\delta} + \frac{2m^2}{n}$$

and

$$M_1(G) \leq \frac{nM_2(G)}{2m} + \Delta m$$

with equality in both cases if G is regular.

Corollary 10.2. [123] *For a connected graph G it holds*

$$M_1(G) \leq \frac{\Delta + \delta}{2} \left(\frac{M_2(G)}{\Delta\delta} + m \right)$$

and

$$M_1(G) \leq \sqrt{\left(\frac{M_2(G)}{\delta} + \delta m \right) \left(\frac{M_2(G)}{\Delta} + \Delta m \right)}\,.$$

Equality in both cases hold if G is regular or bidgreed (biregular) with no adjacent vertices of the same degree.

It was proven in [50] that for an arbitrary simple graph G it holds $M_1(G) \leq 2M_2(G)$ with equality if and only if G is an empty graph or the complete graph with two vertices.

The following results were also obtained in [50].

Theorem 10.9. [50]

$$M_1(G) \leq \frac{\Delta}{2} + \sqrt{\frac{\Delta^2}{4} + 2M_2(G) + 4m(m-1)\Delta^2}$$

with equality if and only if G is Δ-regular.

Theorem 10.10. [50]
$$M_1(G) \geq \frac{\delta}{2} + \sqrt{\frac{\delta^2}{4} + 2M_2(G) + 4m(m-1)\delta^2}$$
with equality if and only if G is δ-regular.

In the papers [40, 41], Das et al. established some new relations between the Zagreb indices.

Theorem 10.11. [40, 41] *Let G be a connected (n,m)-graph with maximum degree Δ and minimum degree δ. Then*
$$M_1(G)(\Delta-1) - 2M_2(G) \leq 2m[(n-1)\Delta - 2m]$$
and
$$2M_2(G) - \Delta^2\delta \geq \frac{(n-1)(M_1(G)-\Delta^2)^2}{(2m-\delta)(n-1)+(\Delta-\delta)\big[n(n-1)-2m\big]}\,. \tag{46}$$
Equality in both inequalities hold if and only if G is a regular graph.

Besides, in the same paper [41], a result better than (46) was obtained:

Corollary 10.3. [41] *Let G be a connected (n,m)-graph with maximum degree Δ and minimum degree δ. Then*
$$2M_2(G) - \Delta^2\delta \geq \frac{(n-1)(M_1(G)-\Delta\Delta_2)^2}{(2m-\delta)(n-1)+(\Delta-\delta)\big[n(n-1)-2m\big]}\,.$$
The above equality holds if and only if $G \cong K_{1,n-1}$ or G is a regular graph.

11. An exceptional property of first Zagreb index

The generalized version of the first Zagreb index, namely
$$Z_p = Z_p(G) = \sum_{v_i \in V(G)} d_i^p$$
where p is some real number, was first considered by Li et al. [94, 95], and the name *first general Zagreb index* was proposed for Z_p in [95]. Thus, the ordinary Zagreb index M_1 is the special case of Z_p, for $p = 2$. If we denote by n_k the number of vertices of G having degree equal to k, then
$$Z_p(G) = \sum_{k\geq 1} k^p\, n_k\,. \tag{47}$$

In what follows, it will be assumed, as in [64], that the exponent p in Eq. (47) is a positive integer. Since the case $p = 1$ is trivial ($Z_1(G) = 2m$), we assume that $p \geq 2$. Then, the following interesting result is obtained.

Theorem 11.1. [64] *Let G be a graph with n vertices, m edges, and n_ℓ vertices of degree ℓ, $\ell \neq 3$. Then, for $p \geq 3$,*
$$Z_p(G) \geq 2\cdot 3^p\,(m-n) + \Theta_p(\ell)\, n_\ell \tag{48}$$
where $\Theta_p(\ell) = \ell^p - 3^p\,\ell + 2\cdot 3^p$ is a polynomial of degree p in the variable ℓ. Equality is attained if and only if all the remaining $n - n_\ell$ vertices of G are of degree 3.

The equality case in (48) pertains to (n, m)-graphs with a fixed number of vertices of degree ℓ whose Z_p-value is minimal. The same graphs have minimal Z_p-values for all $p \geq 3$. If we focus to the case $\ell = 1$, then it holds:

Theorem 11.2. [64] *Let G be a graph with n vertices, m edges, and n_1 pendent vertices. Then, for $p \geq 3$,*

$$Z_p(G) \geq 2 \cdot 3^p\,(m-n) + (3^p+1)n_1\,. \tag{49}$$

Equality is attained if and only if all the remaining $n - n_1$ vertices of G are of degree 3.

This equality case pertains to (n, m)-graphs with a fixed number of pendent vertices whose Z_p-value is minimal and the same graphs have minimal Z_p-values for all $p \geq 3$.

The case $p = 2$, i.e., $Z_2 \equiv M_1$ is significantly different, as shown in [64], implying that the original first Zagreb index is a kind of exception in the class of its generalized counterparts.

Theorem 11.3. [64] *Let G be a graph with n vertices, m edges, and n_1 pendent vertices. Then, for $p = 2$,*

$$Z_p(G) \equiv M_1(G) \geq 16(m-n) + 9n_1\,.$$

Equality is attained if and only if the number of pendent vertices is even, and all the remaining $n - n_1$ vertices of G are of degree 4.

This equality case pertains to (n, m)-graphs with a fixed number of pendent vertices whose first Zagreb index is minimal; for illustrations see Fig. 25.

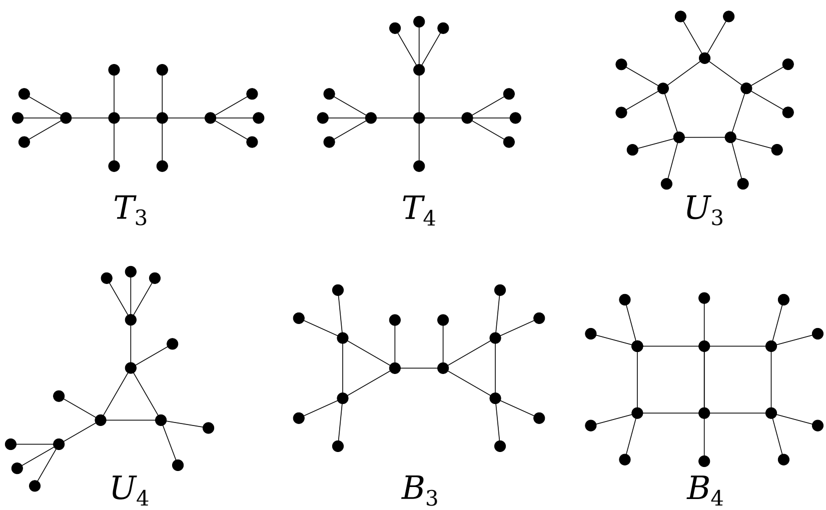

Fig. 25. Examples of trees (T_3, T_4), unicyclic graphs (U_3, U_4), and bicyclic graphs (B_3, B_4) with 10 pendent vertices, having minimal first Zagreb indices, but not minimal Z_p-values for $p = 2$.

The special case of Theorem 11.3 for trees was proven earlier by Goubko [59], who also characterized the trees with odd n_1 and minimal M_1-value (see also [67]). Analogous, but much more difficult results were obtained also for the second Zagreb index [59–61].

Ismailescu and Stefanica [86] characterized the graph with smallest $Z_p(G)$-values, $0 < p \leq 1/2$.

Theorem 11.4. [86] *Let G be a graph of order n with m edges, and let $0 < p \leq 1/2$. Let k be the unique positive integer such that $\binom{k-1}{2} < m \leq \binom{k}{2}$. If $Z_p(G)$ is minimum, then G is isomorphic to the graph with $n-k$ isolated vertices, a complete subgraph K_{k-1}, and one vertex of degree $m - \binom{k-1}{2}$ connected to vertices of the complete subgraph.*

In the same paper immediately after Theorem 11.4, the authors mentioned the following problem:

An interesting open question is to decide what happens if $\alpha \in (1/2, 1)$. Numerical computations strongly suggest that the result in Theorem 11.4 remains true.

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Upper and Lower Bounds for Merrifield–Simmons Index and Hosoya Index

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Abstract

In this chapter, we present a survey of extremal results for two closely related quantities: the Merrifield-Simmons index (number of independent sets) and the Hosoya index (number of matchings). Maxima and minima are given for many different classes of graphs, including general graphs with different restrictions, various classes of trees, unicyclic and bicyclic graphs. We also present common auxiliary results and techniques in this context.

Contents

1. Introduction

This chapter is devoted to two very similar quantities associated with a graph: the *Merrifield-Simmons index* and the *Hosoya index*. The former is the total number of independent sets of a graph, while the latter is the total number of matchings. Not only their definitions are very similar: as we will see in the following, they also have similar properties.

The Hosoya index was the first graph invariant to be called *topological index*, a term that is now commonly used to refer to many other invariants in the context of chemical graph theory. This name was introduced in Hosoya's seminal paper [50] in 1971. In this and subsequent work (see e.g. [51, 52]), he showed that certain physico–chemical properties of alkanes correlate well with the number of matchings in the associated molecular graph. Similar observations were made by Merrifield and Simmons, who investigated the number of independent sets in molecular graphs as part of a topological formalism, see [86–89] and in particular their book [90].

Merrifield-Simmons index and Hosoya index can also be seen as special values of two important graph polynomials. Let us first recall their definitions: denote by $i(G, k)$ the number of independent sets of cardinality k in a graph G (i.e., the number of ways to choose k pairwise non-adjacent vertices of G), and denote by $m(G, k)$ the number of matchings of cardinality k in G (i.e., the number of ways to choose k pairwise non-adjacent edges of G). The *independence polynomial* of G is given by

$$I(G, x) = \sum_{k \geq 0} i(G, k)x^k.$$

The *matching polynomial* of a graph is usually defined by

$$\mu(G, x) = \sum_{k \geq 0} (-1)^k m(G, k)x^{n-2k},$$

where n is the number of vertices of G. It is closely related to the *matching generating polynomial*

$$M(G, x) = \sum_{k \geq 0} m(G, k)x^k.$$

Indeed, it is easy to see that $\mu(G, x) = x^n M(-x^{-2})$. The matching polynomial has the remarkable property that its zeros are always real; for this and other interesting properties of the matching polynomial and the independence polynomial, we refer the interested reader to [30, 35, 64].

The Merrifield-Simmons index and the Hosoya index of a graph G can now be written as

$$\sigma(G) = \sum_{k \geq 0} i(G, k) = I(G, 1)$$

and

$$Z(G) = \sum_{k \geq 0} m(G, k) = M(G, 1) = i^{-n}\mu(G, i).$$

Remarkably, the graphs that maximize or minimize $\sigma(G)$ or $Z(G)$ are often even coefficient-wise extremal, i.e. they maximize or minimize $i(G,k)$ ($m(G,k)$, respectively) for every k. This is one of the motivations to consider poset structures on graphs in the following way (see [37,39] for early instances):

$$G \succ_i H \iff i(G,k) \geq i(H,k) \text{ for all } k,$$

and

$$G \succ_m H \iff m(G,k) \geq m(H,k) \text{ for all } k.$$

A greatest (least) element with respect to $\succ_i$ in a given set of graphs thus maximizes (minimizes) $i(G,k)$ for all k, and consequently maximizes (minimizes) $\sigma(G)$. An analogous statement holds for $\succ_m$. While a given set of graphs does not necessarily have to have a greatest or least element with respect to $\succ_i$ or $\succ_m$, it is indeed often the case that there are such elements, e.g. for trees of given size. However, we will focus on the total number of independent sets and matchings in this survey, even though many of the results listed in the following have stronger versions involving the partial orders $\succ_i$ and $\succ_m$.

The connection to the matching polynomial is relevant for another reason. It is well known that the matching polynomial of acyclic graphs (thus in particular trees) coincides with the characteristic polynomial $\phi(G,x)$ of the adjacency matrix $A(G)$:

$$\phi(G,x) = \det(xI - A(G)) = \mu(G,x) .$$

The sum of the absolute values of the eigenvalues of a graph is known as the *energy* [36, 41], see [73] for a comprehensive treatment. The eigenvalues are the zeros of the characteristic polynomial, and the celebrated Coulson formula relates the energy $E(G)$ of a graph G with the characteristic polynomial. This formula can be written in several different ways, for instance as

$$E(G) = \frac{2}{\pi} \int_0^\infty x^{-2} \ln \left(x^n |\phi(G, i/x)| \right) dx .$$

In view of the aforementioned identity between the characteristic polynomial and the matching polynomial, this becomes

$$E(T) = \frac{2}{\pi} \int_0^\infty x^{-2} \ln M(T, x^2)\, dx \tag{1}$$

if T is a tree. It is therefore not surprising that trees which maximize or minimize the Hosoya index also maximize/minimize the graph energy, and vice versa (see [66, 94, 142, 143] for some examples). This is even the case for some other classes of graphs, see [53]. For arbitrary graphs (not necessarily trees), the integral in (1) represents the *matching energy* that was recently introduced in [45]. Not surprisingly, the graphs that are extremal for the Hosoya index are also typically extremal with respect to the matching energy.

The Merrifield-Simmons index and the Hosoya index are connected in several ways: first of all, since the matchings of a graph G are precisely the independent sets of its line graph $L(G)$, we have the trivial relation

$$Z(G) = \sigma(L(G)) .$$

A different kind of relation is somewhat more complicated. It turns out that the graphs that maximize the Merrifield-Simmons index in a particular class of graphs are often also those that minimize the Hosoya index, and vice versa. However, it is generally not the case that $\sigma(G) \geq \sigma(H)$ implies $Z(G) \leq Z(H)$ or the other way around (see [121] for explicit counterexamples). It was also shown that the two indices are quite closely correlated for trees, see [120].

Early mathematical results on the Merrifield-Simmons index and the Hosoya index in the 1980s include the characterization of extremal graphs for the classes of trees, unicyclic graphs and bicyclic graphs. Some results were obtained independently by different (groups of) researchers, which is partly due to the fact that different names were sometimes used for the same concept. In the earliest occurrence of the Merrifield-Simmons index in the mathematical literature [101], it was dubbed *Fibonacci number* of a graph, which is due to the fact that the Merrifield-Simmons index of a path is always a Fibonacci number.

After a period of comparatively little activity, the topic has garnered considerable attention over the past ten years, with many new results. The survey paper [123] collected many of them, but the field has seen many interesting new developments since its publication. In this chapter, we will provide an updated survey including some recent results, without aiming to provide a comprehensive list of all theorems that can be found in the references listed at the end. In addition, this chapter provides selected proofs of central results in order to give an indication how bounds for the Merrifield-Simmons index and the Hosoya index are obtained.

2. Basic results: graphs and trees

In this section, we consider the most basic bounds for the Merrifield-Simmons index and the Hosoya index. Let us start with arbitrary graphs: it is obvious that adding edges decreases the number of independent sets and increases the number of matchings, while removing edges increases the number of independent sets and decreases the number of matchings. Hence the following elementary result is immediate:

Theorem 1 For every graph G with n vertices, we have

$$n+1 \leq \sigma(G) \leq 2^n\,,$$

with equality only for the complete graph K_n and the empty graph E_n respectively.
Moreover, we have

$$1 \leq Z(G) \leq \sum_{0 \leq k \leq n/2} \binom{n}{2k}(2k-1)!! = \sum_{0 \leq k \leq n/2} \frac{n!}{(n-2k)!k!2^k}\,,$$

with equality only for the empty and the complete graph respectively.

The values for the empty and the complete graph are trivial, perhaps with the exception of the Hosoya index of the complete graph: note here that $\binom{n}{2k}$ is the number of ways to choose the $2k$ vertices involved in the matching, while $(2k-1)!! = (2k-1)\cdot(2k-3)\cdots 3\cdot 1$ is the number of ways to form k pairs from $2k$ vertices.

The bounds that are attained by the empty graph can be improved if we assume the graph to be connected. The argument that removing edges decreases the Hosoya index while increasing the Merrifield-Simmons index shows that the extremal values must be attained for a tree. We have the following theorem:

Theorem 2 For every connected graph G with n vertices, we have

$$\sigma(G) \leq 2^{n-1}+1 \quad \text{and} \quad Z(G) \geq n\,,$$

with equality only for the star S_n in both cases.

Proof: For the Hosoya index, the bound is essentially trivial: note that every connected graph with n vertices has at least $n-1$ edges (exactly $n-1$ if the graph is a tree), thus at least n matchings: the empty set, and each single edge. Since the star is the only tree that has no other matchings because its edges are pairwise adjacent, it is the only connected graph with n vertices for which $Z(G) = n$.

The bound for the Merrifield-Simmons index is slightly more difficult to prove. As mentioned before, we can assume that the graph is a tree, so it suffices to prove the statement for trees, which is done by induction on n. The initial case $n = 1$ is trivial. For the induction step, consider a tree T with n vertices, and let v be a leaf of T. We denote its unique neighbor by w. There are two types of independent sets: those that contain v and those that do not. The number of independent sets that do not contain v is exactly the number of independent sets of $T \setminus v$. If v is contained in an independent set, then w is not, and the remaining vertices form an independent set of $T \setminus \{v, w\}$. Hence we have

$$\sigma(T) = \sigma(T \setminus v) + \sigma(T \setminus \{v, w\})\,.$$

By the induction hypothesis, we have $\sigma(T \setminus v) \leq 2^{n-2}+1$ (with equality only if $T \setminus v$ is a star), and Theorem 1 gives us $\sigma(T\setminus\{v, w\}) \leq 2^{n-2}$, with equality only if $T\setminus\{v, w\}$ is the empty graph. Combining the two gives us

$$\sigma(T) \leq 2^{n-1}+1\,,$$

with equality if and only if T is a star. This completes the proof. ∎

The induction step in the proof of Theorem 2 exhibits a special case of a formula that allows for the recursive calculation of the Merrifield-Simmons index. This (folklore) formula is given in the following lemma, along with an analogous formula for the Hosoya index. Here and in the following, we denote the (open) neighborhood of a vertex v, i.e., the set of all neighbors of v, by $N(v)$ and the closed neighborhood that also includes v itself by $N[v] = N(v) \cup \{v\}$.

Lemma 3 For every graph G and every vertex v of G, we have

$$\sigma(G) = \sigma(G \setminus v) + \sigma(G \setminus N[v])$$

and

$$Z(G) = Z(G \setminus v) + \sum_{w \in N(v)} Z(G \setminus \{v, w\}) .$$

Proof: For the first formula, we only need to split the set of all independent sets into those that do not contain v and those that do (and therefore do not contain any neighbor). The argument that gives us the second formula is similar: a matching either does not contain any of the edges incident with v, or exactly one of them. If the edge between v and w is contained in a matching, then the remaining edges must form a matching of $G \setminus \{v, w\}$. ■

In a similar way, one obtains the following theorem:

Lemma 4 For every graph G and every edge $e = vw$ of G, we have

$$\sigma(G) = \sigma(G \setminus e) - \sigma(G \setminus (N[v] \cup N[w])) ,$$

and

$$Z(G) = Z(G \setminus e) + Z(G \setminus \{v, w\}) .$$

Proof: For the first formula, note that all independent sets of $G \setminus e$ are also independent sets of G, except for those that contain both v and w. If both v and w are contained in an independent set, then no vertex of $N(v)$ or $N(w)$ is, so the number of these independent sets is $\sigma(G \setminus (N[v] \cup N[w]))$. The second formula is obtained in a similar way, by distinguishing between matchings that contain e and those that do not. ■

Finally, the following lemma is trivial:

Lemma 5 Let $G_1, G_2, \ldots, G_k$ be the connected components of a graph G. We have

$$\sigma(G) = \prod_{j=1}^{k} \sigma(G_j) \quad \text{and} \quad Z(G) = \prod_{j=1}^{k} Z(G_j) .$$

Among many other things, these formulas are useful in proving that the path is extremal for the family of all trees, as we will see in the following. Fibonacci numbers play an important role in this context: we define them by $F_0 = 0$, $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$.

Theorem 6 For every forest T with n vertices and in particular every tree, we have

$$\sigma(T) \geq F_{n+2} \quad \text{and} \quad Z(T) \leq F_{n+1} ,$$

with equality only for the path P_n in both cases.

Proof: Both inequalities are proven by means of a simple induction. They are easily verified for $n = 1$ and $n = 2$. For the induction step, we can assume that T is a tree, since adding edges decreases the Merrifield-Simmons index and increases the Hosoya index. Let v be a leaf of T and w its unique neighbor. Lemma 3 yields

$$\sigma(T) = \sigma(T \setminus v) + \sigma(T \setminus \{v, w\})$$

and

$$Z(T) = Z(T \setminus v) + Z(T \setminus \{v, w\}) .$$

Note that $T \setminus v$ and $T \setminus \{v, w\}$ are both forests, so we can apply the induction hypothesis to both of them. In view of the definition of the Fibonacci numbers, we obtain the desired inequalities immediately. Equality can only hold if both $T \setminus v$ and $T \setminus \{v, w\}$ are paths, which is only possible if T itself is a path. ■

Theorem 2 and Theorem 6 belong to the oldest results concerning the Merrifield-Simmons index, see [37, 39, 44, 101]. Tree-like classes such as unicyclic graphs were also already considered early – see Section 4. Before we discuss these results, let us consider some useful graph transformations that are known to decrease or increase the Merrifield-Simmons index and the Hosoya index.

3. Important transformations

In view of Theorem 2 and Theorem 6, it is perhaps not surprising that replacing a tree as part of a graph by a star of the same size increases the Merrifield-Simmons index and decreases the Hosoya index, while replacing a tree by a path of the same size decreases the Merrifield-Simmons index and increases the Hosoya index. Let us formulate this explicitly:

Lemma 7 Let G be a connected graph, let T be an induced subgraph of G that is a tree, and assume that T only shares a cutvertex v with the rest of the graph. Let G_1 and G_2 be the graphs that result from replacing T by a star (centred at v) and a path (with one end at v) respectively. The inequalities

$$\sigma(G_1) \geq \sigma(G) \geq \sigma(G_2)$$

and

$$Z(G_1) \leq Z(G) \leq Z(G_2)$$

hold. Both inequalities are strict unless G is isomorphic to either G_1 or G_2.

Proof: Let H be the "rest" of the graph G, i.e. G without the tree T, including the cutvertex v. By Lemma 3 and Lemma 5, we have

$$\begin{aligned}\sigma(G) &= \sigma(H \setminus v)\sigma(T \setminus v) + \sigma(H \setminus N[v])\sigma(T \setminus N[v]) \\ &= \sigma(H \setminus N[v])\sigma(T) + \big(\sigma(H \setminus v) - \sigma(H \setminus N[v])\big)\sigma(T \setminus v) .\end{aligned}$$

In view of Theorem 1, Theorem 2 and Theorem 6, the terms $\sigma(T)$ and $\sigma(T \setminus v)$ both attain their maximum when T is a star (centred at v), and they attain their minimum when T is a path (with v as one of its endpoints). The inequalities for the Merrifield-Simmons index follow immediately.

In a similar way, we get

$$Z(G) = Z(H \setminus v)Z(T) + \big(Z(H) - Z(H \setminus v)\big)Z(T \setminus v) ,$$

and $Z(T)$ and $Z(T \setminus v)$ are both maximized when T is a path and both minimized when T is a star, centred at v. ■

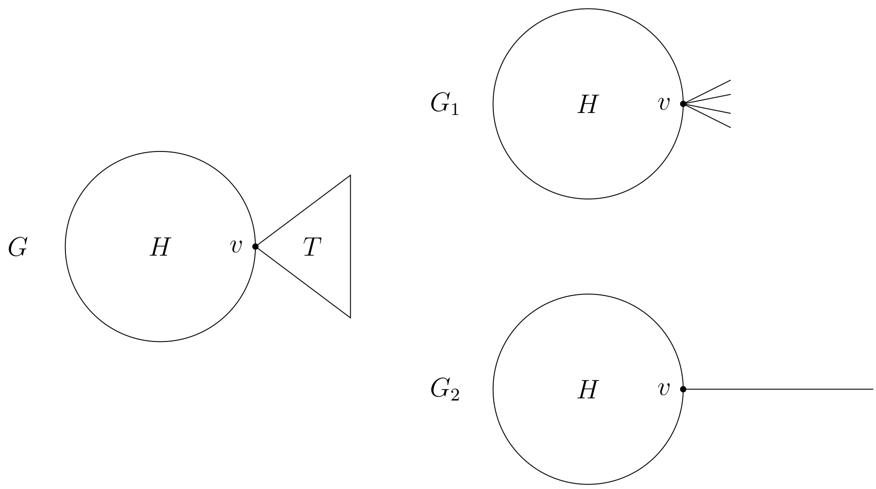

Figure 1. The transformations of Lemma 7.

The following lemma, which we provide without proof, deals with the operation of moving part of a graph from one place to another:

Lemma 8 Let G be a connected graph, and assume that H_1 and H_2 are induced subgraphs of G with at least two vertices, each of which only shares a cutvertex with the rest of the graph. Denote these cutvertices by v_1 and v_2. Let G_1 be the graph that is obtained by moving H_1 from v_1 to v_2, and let G_2 be the graph that results from moving H_2 from v_2 to v_1. The following two statements hold:

- Either $\sigma(G_1) > \sigma(G)$ or $\sigma(G_2) > \sigma(G)$.

- Either $Z(G_1) < Z(G)$ or $Z(G_2) < Z(G)$.

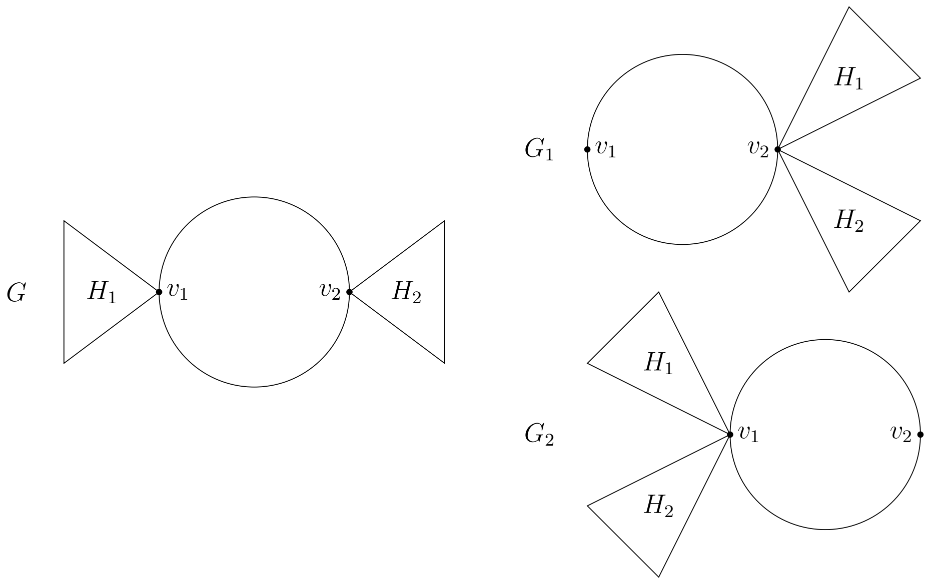

Figure 2. The transformations of Lemma 8.

A more general lemma of a similar nature that was specifically geared towards trees with degree restrictions can be found in [2, 47, 119].

The transformations of Lemma 7 and Lemma 8 apply not only to the Merrifield-Simmons index and the Hosoya index, but are useful in the study of many other graph invariants as well. Lemma 10 that follows below, on the other hand, is quite specific for Merrifield-Simmons index and Hosoya index. We first need a property of the Fibonacci numbers.

Lemma 9 For every integer $n \geq 2$, we have

$$F_1F_{n-1} \geq F_3F_{n-3} \geq F_5F_{n-5} \geq \cdots \geq F_{\lfloor n/2 \rfloor}F_{\lceil n/2 \rceil} \geq \cdots \geq F_6F_{n-6} \geq F_4F_{n-4} \geq F_2F_{n-2} \ .$$

Proof: Let $\phi = \frac{1+\sqrt{5}}{2}$ be the golden ratio, and $\bar{\phi} = -\frac{1}{\phi} = \frac{1-\sqrt{5}}{2}$. Binet's formula

$$F_n = \frac{1}{\sqrt{5}}\Big(\phi^n - \bar{\phi}^n\Big)$$

is well known. We also need the Lucas numbers $L_n = \phi^n + \bar{\phi}^n$. It is easy to verify that

$$F_kF_{n-k} = \frac{1}{5}\Big(L_n - (-1)^k L_{n-2k}\Big) \ .$$

Since the Lucas numbers L_{n-2k} are decreasing in k for $k \leq n/2$, the statement of the lemma follows immediately. ■

The following lemma is central for many results regarding the Merrifield-Simmons index and the Hosoya index, and it appears in different variants, see [46, 83, 121, 124, 144, 153, 163].

Lemma 10 Let G be a connected graph with at least two vertices, and choose a vertex $u \in V(G)$. Let $P(n, k, G, u)$ denote the graph that results from identifying u with the k-th vertex v_k of an n-vertex path (see Figure 3). Write n as $n = 4m + i$, $i \in \{1, 2, 3, 4\}$, $m \geq 0$. Then the inequalities

$$\begin{aligned}\sigma(P(n, 2, G, u)) > \sigma(P(n, 4, G, u)) > \ldots > \sigma(P(n, 2m + 2l, G, u)) > \\ \sigma(P(n, 2m + 1, G, u)) > \ldots > \sigma(P(n, 3, G, u)) > \sigma(P(n, 1, G, u)),\end{aligned}$$

and

$$\begin{aligned}Z(P(n, 2, G, u)) < Z(P(n, 4, G, u)) < \ldots < Z(P(n, 2m + 2l, G, u)) < \\ Z(P(n, 2m + 1, G, u)) < \ldots < Z(P(n, 3, G, u)) < Z(P(n, 1, G, u))\end{aligned}$$

hold, where $l = \lfloor \frac{i-1}{2} \rfloor$.

Proof: Applying Lemma 3 to the common vertex $u = v_k$, we obtain

$$\begin{aligned}\sigma(P(n, k, G, u)) &= \sigma(P_{k-1})\sigma(P_{n-k})\sigma(G \setminus u) + \sigma(P_{k-2})\sigma(P_{n-k-1})\sigma(G \setminus N[u]) \\ &= \sigma(P_n)\sigma(G \setminus N[u]) + \sigma(P_{k-1})\sigma(P_{n-k})\big(\sigma(G \setminus u) - \sigma(G \setminus N[u])\big) \\ &= F_{n+2}\sigma(G \setminus N[u]) + F_{k+1}F_{n-k+2}\big(\sigma(G \setminus u) - \sigma(G \setminus N[u])\big).\end{aligned}$$

By our assumptions on G, we have $\sigma(G \setminus u) - \sigma(G \setminus N[u]) > 0$. Therefore, the first set of inequalities follows easily from the previous lemma. The proof for the Hosoya index is similar. ∎

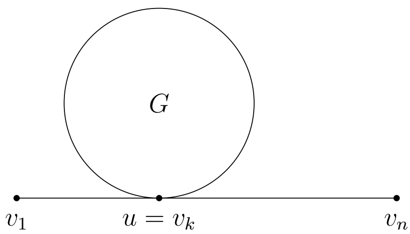

Figure 3. The graph $P(n, k, G, u)$ in Lemma 10.

The following lemma is of a similar nature; it was used specifically in connection with bicyclic graphs, see [18, 20, 21]:

Lemma 11 Let G be a connected graph with at least three vertices, and let u_1, u_2 be non-adjacent vertices of G. Let $P(n, k, l, G, u_1, u_2)$ denote the graph that is obtained by identifying u_1 with the vertex v_k and u_2 with the vertex v_l of an n-vertex path with vertices $v_1, \ldots, v_n$ (Figure 4). For every pair (k, l) with $1 < k < l < n$, at least one of the inequalities

$$\begin{aligned}\sigma(P(n, k, l, G, u_1, u_2)) > \sigma(P(n, 1, l - k + 1, G, u_1, u_2)), \\ \sigma(P(n, k, l, G, u_1, u_2)) > \sigma(P(n, n + k - l, n, G, u_1, u_2))\end{aligned}$$

holds. Likewise, at least one of the inequalities

$$Z(P(n,k,l,G,u_1,u_2)) < Z(P(n,1,l-k+1,G,u_1,u_2)),$$
$$Z(P(n,k,l,G,u_1,u_2)) < Z(P(n,n+k-l,n,G,u_1,u_2))$$

holds.

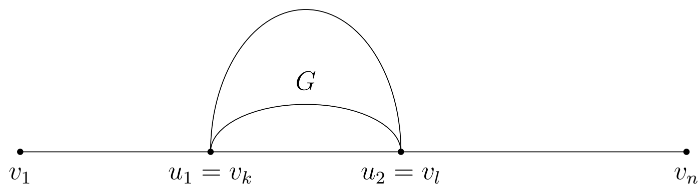

Figure 4. The graph $P(n,k,l,G,u_1,u_2)$ in Lemma 11.

The transformations presented in this section provide a "standard toolkit" that is useful for many different problems, not just concerning Merrifield-Simmons index or Hosoya index, but often also others. See [75, 79, 80] for some instances of a "unified" approach.

4. Tree–like classes of graphs

The transformations presented in the previous section are mostly geared towards graphs that are similar to trees in some sense. Once bounds for trees have been determined, a natural next step is to consider unicyclic graphs, which have exactly one cycle. These graphs will be the first topic in the following section.

4.1 Fixed cyclomatic number

Let G be a connected graph with n vertices and m edges. The *cyclomatic number* of G is $m-n+1$. In particular, a tree has cyclomatic number 0. A connected graph with cyclomatic number 1 is called *unicyclic*, a connected graph with cyclomatic number 2 *bicyclic*, etc. The following bounds were obtained by several different authors in various versions, see [21, 37, 39, 93, 95, 98, 144]:

Theorem 12 For every unicyclic graph G with n vertices ($n \geq 3$), we have the inequalities

$$\sigma(G) \leq 3 \cdot 2^{n-3} + 1 \quad \text{and} \quad Z(G) \geq 2n-2,$$

both with equality for the graph that results from adding an additional edge to a star. Moreover, we have

$$\sigma(G) \geq L_n \quad \text{and} \quad Z(G) \leq L_n,$$

both with equality if G is a cycle. In the case of the Hosoya index, the cycle is the unique graph that attains the bound L_n. In the case of the Merrifield-Simmons index, there is a second graph for which equality holds, consisting of a triangle with a path of length $n-3$ attached to it.

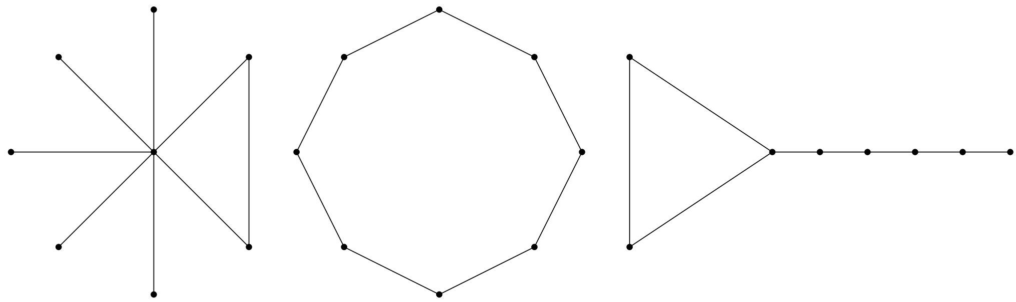

Figure 5. Extremal unicyclic graphs of order 8.

Similar results have been obtained for bicyclic graphs; for the maximum of the Merrifield-Simmons index and the minimum of the Hosoya index, we have the following theorem:

Theorem 13 ([19, 22]) For every bicyclic graph G with n vertices ($n \geq 4$), we have the inequalities

$$\sigma(G) \leq 5 \cdot 2^{n-4} + 1 \quad \text{and} \quad Z(G) \geq 3n - 4,$$

both with equality for the graph that results from adding two additional edges (with a common endvertex) to a star.

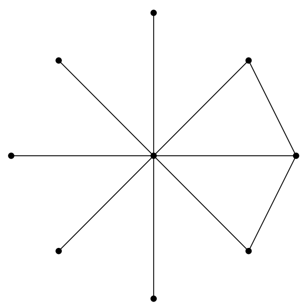

Figure 6. The graph of Theorem 13 (for $n = 9$).

It is noteworthy, however, that the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index are not attained by the same graphs any longer:

Theorem 14 ([20, 38, 106]) For every bicyclic graph G with n vertices ($n \geq 5$), we have the inequality

$$\sigma(G) \geq 5F_{n-2},$$

with equality if and only if G is a graph consisting of two triangles that are connected by a path of length $n - 5$. On the other hand, for every bicyclic graph G with n vertices ($n \geq 10$), we have

$$Z(G) \leq 7L_{n-4} + 3F_{n-4},$$

with equality if and only if G consists of a cycle of length 4 and a cycle of length $n - 4$, connected by an edge.

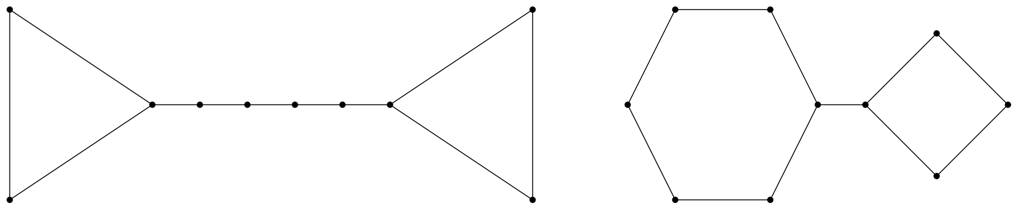

Figure 7. The graphs of Theorem 14 (for $n = 10$).

The second part of Theorem 14 above has an interesting history: it was given in [38], in fact in a stronger version involving the partial order $\succ_m$ mentioned in the introduction, correcting a wrong claim that was made in [37]. The problem was considered again in [18], but the extremal graphs determined there are incorrect, as one can verify easily by comparing them with those described in Theorem 14.

Tricyclic graphs have been investigated as well, and again the results are somewhat similar [24, 25, 43, 82, 169]. For general cyclomatic numbers (equivalently, for given number of vertices *and* edges), only partial results are available, and it is probably not feasible to characterise the extremal graphs in all possible cases. For small values of m, we have the following theorem:

Theorem 15 ([96, 113, 164]) For every connected graph G with n vertices and m edges, where $n-1 \leq m \leq 2n-3$, we have the inequality

$$\sigma(G) \leq 2^{n-2} + 2^{2n-3-m} + 1.$$

Equality holds if and only if G is the graph that consists of $m - n + 1$ triangles that share a common edge and $2n - m - 3$ edges attached to one of the two endpoints of this edge, except when $m = 2n - 4$, in which case there is another graph that also attains the bound.
Likewise, for every connected graph with n vertices and m edges, where $n - 1 \leq m \leq 2n - 3$, we have the inequality

$$Z(G) \geq mn - n^2 + 4n - 2m - 2.$$

Equality holds for the same graph as described above for $\sigma(G)$, except when $m = n + 2$, in which case there is another graph as well.

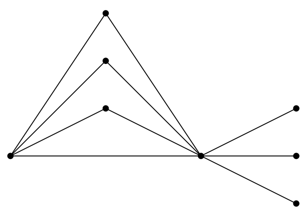

Figure 8. The graph of Theorem 15 (for $n = 8$ and $m = 10$).

In [113], a similar result is also given for the Hosoya index of graphs with "large" cyclomatic number (close to complete graphs). On the other hand, the following result of an asymptotic nature can be found in [122]:

Theorem 16 Let k be a fixed positive integer. For a graph G with n vertices and cyclomatic number k, we have

$$n \log \frac{1+\sqrt{5}}{2} + O(1) \leq \log \sigma(G) \leq n \log 2 + O(1).$$

Both O-constants only depend on k. Likewise, we have

$$\log n + O(1) \leq \log Z(G) \leq n \log \frac{1+\sqrt{5}}{2} + O(1),$$

again with both O-constants only depending on k.

4.2 Forests

Since most research focusses on connected graphs, there is little literature on forests. However, since the connected components of forests are trees, bounds for trees generally imply bounds for forests as well. In [76], all n-vertex forests with Merrifield-Simmons index of at least $\geq 2^{n-1} + 1$ are determined: they either consist of a star and an arbitrary number of isolated vertices, or of two isolated edges and a number of isolated vertices. Since every graph that contains a cycle has Merrifield-Simmons index of at most 2^{n-1}, these forests are in fact the only graphs whose Merrifield-Simmons index is greater than 2^{n-1}.

4.3 Quasi–trees

A *quasi-tree* is a graph with the property that one can remove one vertex to obtain a tree. Quasi-trees are considered in [69], where the following result is proved:

Theorem 17 For every quasi-tree G with n vertices ($n \geq 2$), we have the inequalities

$$\sigma(G) \geq F_{n+1} + 1$$

and

$$Z(G) \leq \frac{(n+4)F_n + 2nF_{n-1}}{5}.$$

Equality holds in both inequalities if and only if G is a fan, consisting of a path and an additional vertex connected to all vertices of the path by an edge.

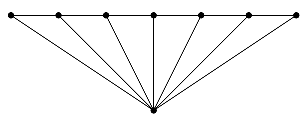

Figure 9. The fan (for $n = 8$).

The maximum of the Merrifield-Simmons index and the minimum of the Hosoya index are both essentially trivial: they are attained by the star.

Let us finally mention that quasi-unicyclic graphs have been considered as well, see [27].

5. Graphs with additional restrictions

5.1 General graphs

Let us now consider graphs with additional restrictions on various parameters. First of all, we consider graphs of given connectivity: recall that a graph is k-connected if one needs to remove at least k vertices to render it disconnected. A lower bound for the Merrifield-Simmons index and an upper bound for the Hosoya index have been provided in [138, 170]:

Theorem 18 ([138, 170]) Let G be a graph with n vertices and vertex connectivity (at most) k. The inequalities

$$\sigma(G) \geq 2n - k \quad \text{and} \quad Z(G) \leq Z(K_{n-1}) + kZ(K_{n-2})$$

hold. Equality holds in both cases if and only if G is a graph obtained from a complete graph K_n by removing $n-k-1$ edges with a common endvertex (equivalently, obtained from a complete graph K_{n-1} by adding a vertex and connecting it to k of the vertices of the complete graph).

Making use of the fact that the edge connectivity of a graph (the minimum number of edges that needs to be removed to render the graph disconnected) is always greater or equal to the vertex connectivity, one finds that Theorem 18 also holds if "vertex connectivity" is replaced by "edge connectivity".

Another very natural restriction is to include the independence number (greatest cardinality of an independent set) or the matching number (greatest cardinality of a matching). Since independent sets of a graph correspond to complete subgraphs in the complement, the following is a direct consequence of a theorem that was proved by Erdős [28, 29] (and rediscovered by Sauer [110] and Roman [109]): among graphs of order n without a complete subgraph of k vertices, the complete $(k-1)$-partite graph with the property that its partite sets are as equal in size as possible (any two only differ by at most one) has the greatest number of complete subgraphs, in fact of any order less than k.

Theorem 19 For every graph G with n vertices whose independence number is k, we have

$$\sigma(G) \leq \left(\left\lfloor \frac{n}{k} \right\rfloor + 1\right)^{k(\lfloor n/k \rfloor + 1) - n} \left(\left\lfloor \frac{n}{k} \right\rfloor + 2\right)^{n - k\lfloor n/k \rfloor}.$$

Equality holds if and only if G consists of $k(\lfloor n/k \rfloor + 1) - n$ complete graphs with $\lfloor n/k \rfloor$ vertices and $n - k\lfloor n/k \rfloor$ complete graphs with $\lfloor n/k \rfloor + 1$ vertices.

The lower bound is somewhat simpler, see [99]:

Theorem 20 For every G with n vertices whose independence number is k, we have

$$\sigma(G) \geq 2^{k-1}(n - k + 2).$$

Equality holds if and only if G consists of a complete graph with $n - k + 1$ vertices and $k - 1$ isolated vertices.

Bruyère and Mélot in [6] consider the same problem also for *connected graphs* (in addition to providing a proof of Theorem 19): they show that the extremal graphs in this case are quite similar to those in Theorem 19, with additional edges going out from one vertex of one of the larger components to one vertex of each other component. Moreover, the minimisation problem for trees with given independence number is studied in [5].

In the same vein, graphs with given matching number have been considered as well. In order to obtain an upper bound on the Merrifield-Simmons index or a lower bound on the Hosoya index under this condition, it suffices to look at trees (assuming that the graph is connected). This is because a maximum matching of any connected graph can be extended to a spanning tree that still has the same matching number. It has already been observed that removing edges always decreases the Hosoya index and increases the Merrifield-Simmons index, so one can simply consider the aforementioned spanning tree. The following theorem can then be obtained (see [54, 61, 154]):

Theorem 21 For every connected graph G with n vertices and matching number m, we have

$$\sigma(G) \leq 3^{m-1}2^{n-2m+1} + 2^{m-1} \quad \text{and} \quad Z(G) \geq 2^{m-2}(2n - 3m + 3).$$

Equality holds if and only if G is an extended star (see Figure 10), consisting of $m - 1$ paths of length 2 and $n - 2m + 1$ single edges, all joined at a common endpoint.

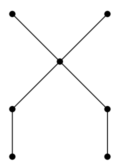

Figure 10. The extended star with 7 vertices and matching number 3.

Yu and Tian [154] even consider the more general situation where the cyclomatic number (equivalently, the number of edges) is prescribed in addition to the number of vertices and the matching number.
The minimum of the Merrifield-Simmons index and the maximum of the Hosoya index, on the other hand, have been determined in [170]. For the former, we have the following theorem:

Theorem 22 ([170]) Let G be a connected graph with n vertices and matching number m. If $m = \lfloor n/2 \rfloor$, then $\sigma(G) \geq n + 1$, with equality if and only if G is a complete graph. Otherwise, we have

$$\sigma(G) \geq m \cdot 2^{n+1-2m} + 1,$$

with equality if and only if G consists of a complete graph K_{2m} and a star with $n - 2m + 1$ vertices, whose centre is identified with one of the vertices of the complete graph.

The situation for the Hosoya index is somewhat more complicated. Here, there are two different types of extremal graphs.

Theorem 23 ([170]) Let n and m be positive integers with $n \geq 2m$, and let $G_1(n,m)$ be the graph described in Theorem 22, consisting of a complete graph K_{2m} and a star S_{n-2m+1} whose centre is identified with one of the vertices of the complete graph. Moreover, let $G_2(n,m)$ be the graph obtained by connecting a complete graph K_m and an empty graph E_{n-m} by all possible $m(n-m)$ edges. For every graph G with n vertices and matching number m, we have

$$Z(G) \leq \max\big(Z(G_1(n,m)), Z(G_2(n,m))\big).$$

Equality holds if and only if G is isomorphic to $G_1(n,m)$ or $G_2(n,m)$, whichever has the greater Hosoya index.

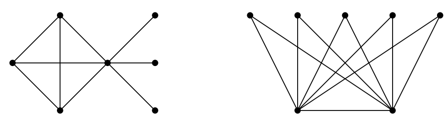

Figure 11. The graphs $G_1(7,2)$ and $G_2(7,2)$.

It was also shown in [170] that there exists a unique value m_0 depending on n such that $G_1(n,m)$ has greater Hosoya index when $m \geq m_0$, and $G_2(n,m)$ has greater Hosoya index otherwise. The asymptotic behaviour of m_0 as a function of n was considered as well. Let us also remark that upper bounds for the Hosoya index in terms of the number of edges and the matching number were also already provided in [42, 85].

Let us also mention results on graphs with given chromatic number, which were investigated in [140]: among graphs with given number of vertices and chromatic number k, the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index are both obtained for a complete k-partite graph whose partite sets are as equal as possible (known as a Turán graph, which is also the complement of the graph occurring in Theorem 19). The bipartite and tripartite graphs that yield the minimum of the Hosoya index and the maximum of the Merrifield-Simmons index are given in [140] as well (the bipartite case is also considered in [99]; if we assume connectedness, the star is the extremal bipartite graph).
We conclude this subsection with work on miscellaneous restrictions: here, one can mention Xu [135], who considers graphs with given clique number, Hua and Zhang [60], who are studying graphs with given number of cutvertices, a paper of Li and Zhang [65] on graphs with given minimum degree, and Wang's paper [130] on graphs with a perfect matching.

5.2 Trees

Trees are perhaps the class of graphs that has been studied most thoroughly, and several different restrictions have been considered. It is a recurring phenomenon that we have already observed in other instances that the extremal trees with respect to the Merrifield-Simmons index and the Hosoya index often coincide. Let us start with a result on trees with given diameter: recall that a *broom* $B_{n,k}$ is a tree that is obtained by appending a path of length $n-k$ to a star with k vertices.

Theorem 24 ([16, 63, 74, 97, 100, 143]) For a tree with n vertices and diameter d, we have the inequalities

$$\sigma(T) \leq 2^{n-d}F_{d+1} + F_d \quad \text{and} \quad Z(T) \geq (n-d)F_d + F_{d+1}.$$

Equality holds in both inequalities if and only if T is the broom $B_{n,n-d+1}$.

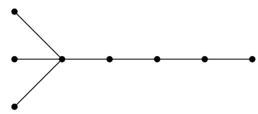

Figure 12. The broom $B_{8,4}$.

This result can be found in several papers by different authors: for the Merrifield-Simmons index in [63, 74, 100], and for the Hosoya index in [16, 97, 143]). In [63] (Merrifield-Simmons index), it is mainly shown as an auxiliary result, while in [143] (Hosoya index), it is actually a byproduct of a stronger statement that also establishes minimality of the energy. Liu et al. [81] even study the question in greater detail and also determine the second-largest/smallest value and more.

On the other hand, it seems that the analogous problem to find the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index for trees with given number of vertices and diameter is considerably harder, and only partial results for very small diameter (up to 5) are known – see [33, 63, 78, 94].

The *number of leaves* is another very natural additional parameter. It turns out that the broom occurs once again as extremal tree:

Theorem 25 ([97, 153]) For a tree with n vertices and k leaves, we have the inequalities

$$\sigma(T) \leq 2^{k-1}F_{n-k+2} + F_{n-k+1} \quad \text{and} \quad Z(T) \geq kF_{n-k+1} + F_{n-k}.$$

Equality holds in both inequalities if and only if T is the broom $B_{n,k}$.

Just like Theorem 24, this result was obtained independently in different papers, and it was also extended further, see [83, 129]. As before, it also appears to be much harder to determine the minimum of the Merrifield-Simmons index or the maximum of the Hosoya index. Here, only partial results are known if the number of leaves is either very small (up to 6, see [34, 127, 148]) or very large (more than half the vertices), see [23, 142].

The situation is quite different under another restriction: the maximum degree. Here, the minimum of the Merrifield-Simmons index and the maximum of the Merrifield-Simmons index can be obtained by a relatively straightforward application of Lemma 7 and Lemma 10. The final result reads as follows:

Theorem 26 ([121]) Let T be a tree with n vertices and maximum degree Δ. We have the inequalities

$$\sigma(T) \geq \begin{cases} 3^{n-\Delta-1}2^{2\Delta-n+1} + 2^{n-\Delta-1} & \Delta \geq \frac{n-1}{2}, \\ 3^{\Delta-1}F_{n-2\Delta+3} + 2^{\Delta-1}F_{n-2\Delta+2} & \text{otherwise.} \end{cases}$$

and

$$Z(T) \leq \begin{cases} 2^{n-\Delta-2}(3\Delta - n + 3) & \Delta \geq \frac{n-1}{2}, \\ 2^{\Delta-2}((\Delta+1)F_{n-2\Delta+2} + 2F_{n-2\Delta+1}) & \text{otherwise.} \end{cases}$$

For $\Delta \geq \frac{n-1}{2}$, equality holds in both cases if and only if T is an extended star consisting of $n - \Delta - 1$ paths of length 2 and $2\Delta - n + 1$ paths of length 1 sharing a common endpoint (see also Figure 10). Otherwise, equality holds if and only if T is an extended star consisting of $\Delta - 1$ paths of length 2 and a path of length $n - 2\Delta + 1$, again sharing a common endpoint.

The description of the trees with given number of vertices and maximum degree that maximize the Merrifield-Simmons index and minimize the Hosoya index is rather more involved. However, the extremal trees coincide again, as was shown in [47] (see also [31, 48]). They can be obtained as a special case of those trees that are extremal for a given degree sequence, so we will return to them later.

Fixing the maximum degree or the number of leaves are two instances of restricting the *degree sequence*. Andriantiana [2] studies the more general (and also more difficult) problem of prescribing the degree sequence of a tree completely. As it turns out, it is possible to characterise the trees that maximize the Merrifield-Simmons index and minimize the Hosoya index (once again, these are the same trees). The full characterisation is quite complicated (as is the somewhat technical proof):

Definition 1 ([2]) Let $(d_1, d_2, \ldots, d_k, 1, 1, \ldots, 1)$ be a degree sequence of a tree in non-increasing order ($d_k \geq 2$). We define a tree $\mathcal{M}(d_1, d_2, \ldots, d_k, 1, 1, \ldots, 1)$ associated with this sequence by the following recursive construction: if $k \leq d_k + 1$, then the tree $\mathcal{M}(d_1, d_2, \ldots, d_k, 1, 1, \ldots, 1)$ is obtained from a star S_{d_k+1} with d_k leaves by identifying $k-1$ of its leaves with the centres of $k-1$ stars $S_{d_1}, S_{d_2}, \ldots, S_{d_{k-1}}$. The non-leaves of this tree are assigned labels $v_1, \ldots, v_k$ in such a way that the degree of v_i is d_i for all i (in particular, v_k is the centre of the star S_{d_k+1} that started the construction).

If $k \geq d_k + 2$, then the tree $\mathcal{M}(d_1, d_2, \ldots, d_k, 1, 1, \ldots, 1)$ is obtained as follows: let l be the greatest integer such that v_l is a label in $\mathcal{M}(d_{d_k}, \ldots, d_{k-1}, 1, 1, \ldots, 1)$, and let s be the smallest integer such that v_s is adjacent to a leaf in $\mathcal{M}(d_{d_k}, \ldots, d_{k-1}, 1, 1, \ldots, 1)$. Now $\mathcal{M}(d_1, d_2, \ldots, d_k, 1, 1, \ldots, 1)$ is obtained from $\mathcal{M}(d_{d_k}, \ldots, d_{k-1}, 1, 1, \ldots, 1)$ by connecting a leaf that is adjacent to v_s to the centres of $d_k - 1$ disjoint stars $S_{d_1}, S_{d_2}, \ldots, S_{d_{d_k-1}}$. The centres of these stars receive the labels $v_{l+1}, \ldots, v_{l+d_k-1}$, in increasing order of degree.

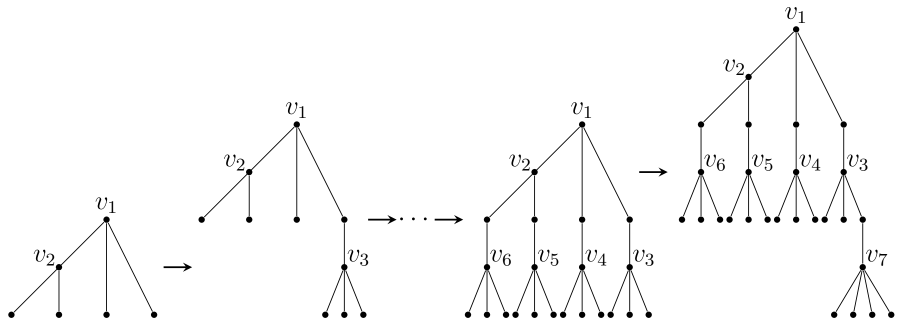

Figure 13. Construction of the tree $\mathcal{M}(5, 4, 4, 4, 4, 3, 3, 2, 2, 2, 2, 2, 1, 1, \dots, 1)$.

Figure 13 shows an example of the construction described above.

The central result of [2] reads as follows:

Theorem 27 ([2]) Let T be a tree with degree sequence $(d_1, d_2, \dots, d_n)$. We have the inequalities

$$\sigma(T) \leq \sigma\big(\mathcal{M}(d_1, d_2, \dots, d_n)\big)$$

and

$$Z(T) \geq Z\big(\mathcal{M}(d_1, d_2, \dots, d_n)\big).$$

Equality holds in both cases if and only if T is isomorphic to $\mathcal{M}(d_1, d_2, \dots, d_n)$.

What makes this theorem particularly powerful is the concept of *majorisation*: we say that a degree sequence $(d_1, d_2, \dots, d_n)$ *majorises* the degree sequence $(b_1, b_2, \dots, b_n)$ if we have

$$d_1 + d_2 + \cdots + d_k \geq b_1 + b_2 + \cdots + b_k$$

for all k. It was shown in [2] that

$$\sigma\big(\mathcal{M}(d_1, d_2, \dots, d_n)\big) \geq \sigma\big(\mathcal{M}(b_1, b_2, \dots, b_n)\big)$$

and

$$Z\big(\mathcal{M}(d_1, d_2, \dots, d_n)\big) \leq Z\big(\mathcal{M}(b_1, b_2, \dots, b_n)\big)$$

if $(d_1, d_2, \dots, d_n)$ majorises $(b_1, b_2, \dots, b_n)$, and it turns out that Theorem 24 and Theorem 25 follow as corollaries, as do the results of [47] (see also [84] for a less general result) on trees with given maximum degree: for given order n and maximum degree Δ, the tree that maximizes the Merrifield-Simmons index and minimizes the Hosoya index is $\mathcal{M}(\Delta, \Delta, \dots, \Delta, d, 1, 1, \dots, 1)$ (the value of $d \in \{1, 2, \dots, \Delta - 1\}$ is uniquely determined by n and Δ). The results of [77] on trees with a given number of vertices of degree 2 can be obtained from Theorem 27 as well.

Unfortunately, there is no simple formula for the Merrifield-Simmons index or the Hosoya index of $\mathcal{M}(d_1, d_2, \dots, d_n)$ in general. In [49], an asymptotic result is provided in the special case that only the maximum degree is prescribed.

It is not known whether the trees with given degree sequence that minimize the Merrifield-Simmons index or maximize the Hosoya index can be characterised as well. Little is known in general, but a complete solution is given in [3] for the case that the vertices of the tree can only have two different degrees (1 and another value d). Under this condition, caterpillar trees turn out to be extremal. Let us also mention in this context that [67] provides a somewhat complicated upper bound for the Hosoya index in terms of the degrees and the 2-degrees (sum of degrees of all neighbors).

Other restrictions on trees that have been considered in the literature include trees without a perfect matching [57, 80, 92] and trees with a given bipartition (sizes of the two sets in the unique 2-colouring) [150].

5.3 Unicyclic graphs

Several different restrictions have been considered for unicyclic graphs (as well as bicyclic graphs). The most natural condition is perhaps to fix the *girth*, i.e. the length of the unique cycle. We have the following bounds:

Theorem 28 ([21, 93, 95, 98, 124, 126, 151]) Let G be a unicyclic graph with n vertices and girth k ($3 \leq k \leq n$). We have

$$F_{k+1}F_{n-k+2} + F_{k-1}F_{n-k+1} \leq \sigma(G) \leq 2^{n-k}F_{k+1} + F_{k-1}.$$

The first inequality holds with equality for the graph that consists of a cycle of length k and a path of length $n-k$ attached to it. The second inequality holds with equality for the graph that consists of a cycle of length k and $n-k$ pendant edges attached to one of its vertices.

Likewise, we have

$$L_kF_{n-k+1} + F_kF_{n-k} \geq Z(G) \geq (n-k)F_k + L_k.$$

The first inequality holds with equality for the graph that consists of a cycle of length k and a path of length $n-k$ attached to it. The second inequality holds with equality for the graph that consists of a cycle of length k and $n-k$ pendant edges attached to one of its vertices.

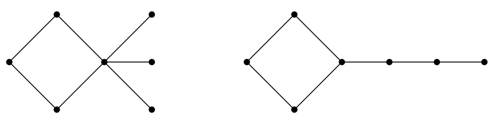

Figure 14. The extremal unicyclic graphs with 7 vertices and girth 4.

Of course, several other restrictions and additional conditions have been considered for unicyclic graphs as well: we mention the diameter [71], maximum degree [139], matching number or existence of a perfect matching [8, 166], number of pendant vertices [55, 58, 168] or the number of cutvertices [59]. Fully loaded unicyclic graphs, which are characterised by the property that each vertex on the cycle has degree at least 3, have been studied in [10, 56, 155]. [131] studies unicyclic *Hückel graphs*, which are characterised by the additional properties of having a perfect matching and maximum degree at most 3.

There are also several results on restricted bicyclic graphs. We mention in particular bicyclic graphs with given girth [115], diameter [72,136], matching number or existence of a perfect matching [26,167], maximum degree [137], and number of pendant vertices [152]. Moreover, bicyclic graphs with two elementary (disjoint) cycles are studied in [114].

We also remark that in many instances (in this and previous sections), more than the maximum and minimum for the respective class and index have been determined, but also second-largest/smallest, third-largest/smallest values, etc. See [62, 70, 118, 125, 129, 132, 141, 145–147, 149] for some notable examples of papers devoted to this task.

6. Other types of graphs

6.1 Hexagonal and other chains

Since hexagonal systems play an important role in mathematical chemistry (as representations of benzenoid hydrocarbons), they have been considered in the literature at quite an early stage. A hexagonal chain is obtained by starting with a single hexagon (6-cycle) and repeatedly attaching a new hexagon to the previous hexagon along an edge. The first important result on hexagonal chains reads as follows:

Theorem 29 ([40]) Let L_n be the linear hexagonal chain consisting of n hexagons, see Figure 15. For every hexagonal chain H consisting of n hexagons, we have

$$\sigma(H) \leq \sigma(L_n) \quad \text{and} \quad Z(H) \geq Z(L_n).$$

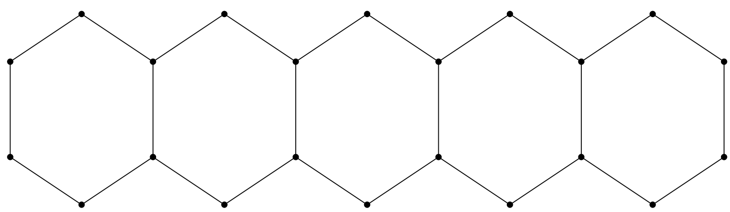

Figure 15. The linear hexagonal chain with 5 hexagons.

The following dual result was conjectured in [40] and finally proven in [159]:

Theorem 30 ([159]) Let Z_n be the zigzag hexagonal chain consisting of n hexagons, see Figure 16. For every hexagonal chain H consisting of n hexagons, we have

$$\sigma(H) \geq \sigma(Z_n) \quad \text{and} \quad Z(H) \geq Z(Z_n).$$

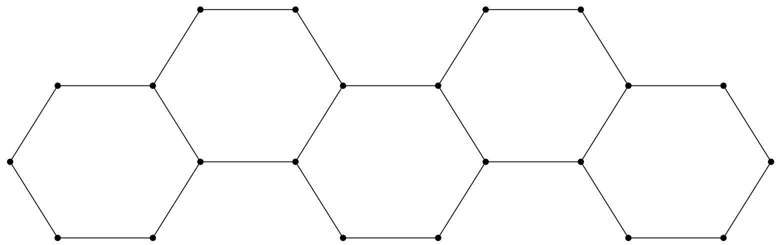

Figure 16. The zigzag hexagonal chain with 5 hexagons.

These theorems were further extended in many different ways, see [160–162], and many variants of hexagonal chains were studied, involving other types of polygons such as squares, pentagons and octagons as well. We refer the reader to [4, 7, 11–15, 68, 102–105, 111, 112, 117, 156, 157].

6.2 Outerplanar graphs

An outerplanar graph is a planar graph with the additional property that all its vertices lie on the outer face of some planar embedding. Alameddine [1] studies *maximal* outerplanar graphs, which are equivalent to triangulations of polygons. For these graphs, we have the following bounds:

Theorem 31 For every maximal outerplanar graph G with n vertices ($n \geq 3$), we have the bounds

$$a_n \leq \sigma(G) \leq F_n + 1,$$

where the sequence a_n is defined recursively by $a_0 = 1$, $a_1 = 2$, $a_2 = 3$ and $a_n = a_{n-1} + a_{n-3}$ for $n \geq 3$. Equality for the lower bound holds if and only if G is the "zigzag" graph shown in Figure 17, while equality for the upper bound holds if and only if G is a fan (see Figure 9).

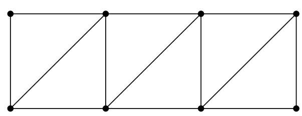

Figure 17. The (maximal) outerplanar graph with minimum Merrifield-Simmons index (for $n = 8$).

We remark that the lower bound is automatically also a lower bound for all outerplanar graphs (not necessarily maximal), since every outerplanar graph can be turned into a maximal outerplanar graph by adding edges. It is also noteworthy that the fan attains the *maximum*, while it also yields the *minimum* for quasi-trees, see Theorem 17. It would be very interesting to determine similar bounds for *planar* graphs, which appears to be more difficult.

6.3 Other special families

Theta graphs are graphs with two vertices that are connected by three pairwise edge-disjoint paths. They occur very naturally in the study of bicyclic graphs, but they have also been studied on their own right, as have generalisations [9, 91, 116].

Cacti, which are graphs with the property that each block (maximal 2-connected subgraph) is either a single edge or a cycle, have been the subject of investigation in [79, 128].

Many other parametrised special families consisting of suitable combinations of paths, cycles and stars have been investigated, see for instance [17, 107, 108, 134, 158, 165].

7. An inequality involving Merrifield–Simmons index and Hosoya index

Let us conclude this chapter with an inequality due to Fischermann, Volkmann and Rautenbach [32], which involves both the Merrifield-Simmons index and the Hosoya index.

Theorem 32 Let T be a tree with maximum degree Δ. We have

$$\frac{Z(T)}{\sigma(T)} \leq \begin{cases} \frac{2}{3} & \Delta = 1, \\ \frac{5}{8} & \Delta = 2, \\ \frac{\frac{\Delta}{2}+1}{(\frac{2}{3})^{\Delta}+1}, & \Delta \geq 3. \end{cases}$$

These inequalities are sharp: equality holds for the paths P_2 and P_4 and for all subdivided stars (obtained from a star by subdividing each edge into two edges).

We have seen many instances in this chapter where the extremal graphs with respect to the two indices were the same. It is therefore natural to assume that there is a strong correlation between the two, which also indicates that there might be many other interesting inequalities that the two quantities satisfy. One can also expect many similar results connecting Merrifield-Simmons index and Hosoya index to other graph invariants – see [133] for a recent effort in this direction.

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Some Bounds on Balaban Index

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Abstract

In this chapter we survey our recent results on Balaban index. First, we consider this index on r-regular graphs, for which we show that the Balaban index tends to zero as the number of vertices increases. We also present stronger results for cubic graphs, and in particular for fullerene graphs, and for nanotubical structures. The minimum value of Balaban index and corresponding extremal graphs are still unknown. Regarding this problem, we have shown that this value is of order $\Theta(n^{-1})$, and that in the class of balanced dumbbell graphs those with clique sizes $\sqrt[4]{\pi/2}\sqrt{n} + o(\sqrt{n})$ have asymptotically the smallest value. We introduced dumbbell-like graphs which are probably the extremal graphs for Balaban index. Various open problems and conjectures are proposed.

Contents

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1. Introduction

In this chapter we consider simple and connected graphs. For a graph G, by $V(G)$ and $E(G)$ we denote the vertex and edge sets of a graph G, respectively. Let $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$, by $\mathrm{dist}_G(u, v)$ we denote the distance from u to v in G. The *Balaban index*, $J(G)$, of a graph G is defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv} \frac{1}{\sqrt{w(u) \cdot w(v)}},$$

where the sum is taken over all edges $e = uv$ of G and for $x \in V(G)$, we have $w(x) = \sum_{y \in V(G)} \mathrm{dist}_G(x, y)$.

Balaban index is a topological index introduced by Alexandru T. Balaban near to 30 years ago [8,9]. This topological index was used successfully in QSAR/QSPR modeling [20,36]. Several recent uses can be found in [10,25,27]. In [11] two different approaches were presented for the calculation of Balaban index by taking into account the chemical nature of elements. In [12], Balaban index is compared with Wiener index regarding the alkanes, and it was obtained that Balaban index reduces the degeneracy of the later index and provides much higher discriminating ability. Therefore Balaban index is also called "sharpened Wiener index". See [13] for another reference that involves these two indicies and infinite polymers.

On other hand, mathematical properties of Balaban index are still not studied extensively. In Balaban, Ionescu-Pallas, Balaban [15], the behavior of J for various infinite families of graphs is discussed. In many of these cases, J tends to a constant finite value. For the study of this index over fullerene graphs see [16,23,26].

In [21] Dong and Guo considered extremal values of Balaban index in the class of connected graphs on n vertices. They stated that the path on n vertices attains the lower bound. Unfortunately, this statement turned out to be false as shown by Aouchiche, Caporossi and Hansen [5]. Thus the following problem from Dong and Guo [21,22] remains open:

Problem 1.1. *Among n-vertex graphs, find those with the minimum Balaban index.*

Among graphs on $n \geq 8$ vertices, Balaban index attains its maximum for the star S_n, where

$$J(S_n) = \sqrt{\frac{(n-1)^3}{2n-3}},$$

and for graphs on $n \leq 7$ vertices, Balaban index attains its maximum for the complete graph K_n, where

$$J(K_n) = \frac{n^3 - n^2}{2(n^2 - 3n + 4)},$$

see [22] and [31]. However, if we consider n-vertex trees, then the Balaban index attains its minimum for the path on n vertices P_n, see [17,35], and $\lim_{n\to\infty} J(P_n) = \pi$, see [15]. One may expect that, if G is an n-vertex r-regular graph, then $J(P_n) \leq J(G) \leq J(S_n)$ for large n. As we will see later, this is not the case.

In this chapter, we survey our recent results on Balaban index. First, we consider this index on r-regular graphs, for which we show that the Balaban index tends to zero as the number of vertices increases. In other words, zero is also an accumulation point for Balaban index. This was derived from an upper bound for Balaban index of r-regular graphs on n vertices from [29]. Even better upper bound was obtained for fullerene graphs. We evaluate the Balaban index for nanotubical structures in [4].

Although the Balaban index was introduced 30 years ago, its minimum value and corresponding extremal graphs are still unknown. We have shown that this value is of order $\Theta(n^{-1})$, and also that in the class of balanced dumbbell graphs those with clique sizes $\sqrt[4]{\pi/2}\sqrt{n} + o(\sqrt{n})$ and the path length $n - o(n)$ have asymptotically the smallest value. Next, we introduced dumbbell-like graphs, which are the graphs with the smallest Balaban index value known to us. We conclude the chapter with various open problems and conjectures.

2. Balaban index of regular graphs

In this section we concentrate on r-regular graphs with $r \geq 3$. A result from [29] gives a surprising upper bound for $J(G)$ for these graphs.

Theorem 2.1. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$J(G) \leq \frac{r^2(r-1)^2}{2(r-2)^2 \left\lfloor \log_{r-1} \frac{(r-2)n+2}{r} \right\rfloor} .$$

This result implies the following interesting consequence.

Corollary 2.1. *For r-regular graphs G on n vertices, where $r \geq 3$, it holds*

$$\lim_{n\to\infty} J(G) = 0.$$

In other words, Balaban index of regular graphs which are really big in the number of vertices, is close to 0. The number of such graphs is enormously large, and we conclude that the Balaban index does not distinguish them well.

Conclusion 2.2. *Balaban index does not distinguish well r-regular graphs on n vertices for $r > 2$ and large n.*

2.1 Fullerene graphs

Fullerenes [34] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces, and their corresponding graphs, fullerene graphs, are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces.

By Corollary 2.1, if $\mathcal{G}$ is the class of fullerenes, then

$$\lim_{n\to\infty} \{J(G);\, G \in \mathcal{G} \text{ and } |V(G)| = n\} = 0.$$

We remark that the upper bound given in Theorem 2.1 is very rough. For instance, if G is the well-known Buckminster fullerene, then our bound with $r = 3$ gives $J(G) \leq \frac{36}{2\lfloor \log_2 62/3 \rfloor} = 4.5$, while $J(G) = 0.91$.

Nevertheless, in [29] we give a better upper bound for the Balaban index of fullerene graphs, which tends to 0 for $n \to \infty$ much faster than $18/\lfloor \log_2 (n+2)/3 \rfloor$.

Theorem 2.3. *Let G be a fullerene graph on $n \geq 60$ vertices. Then*

$$J(G) \leq \frac{25}{\sqrt{n}}.$$

2.2 Cubic graphs with small value of Balaban index

There are cubic graphs for which the Balaban index tends to 0 even faster than for the fullerene graphs. While for fullerene graphs Balaban index is bounded by $25n^{-1/2}$, these cubic graphs have Balaban index $32n^{-1}$ and even less.

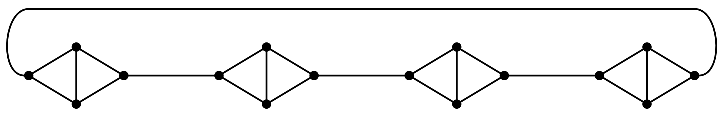

Figure 1. The graph H_{16}.

Let H_n be a graph obtained from $n/4$ copies of $K_4 - e$ (i.e., K_4 without one edge) which are joined by $n/4$ extra edges to form a connected cubic graph. Obviously, H_n has n vertices, see Figure 1 for H_{16}. We have the following statement in [29].

Proposition 2.4. *For positive n divisible by 4, it holds*

$$J(H_n) \leq \frac{32}{n}.$$

The last result means that if n approaches to ∞, then $J(H_n)$ approaches to 0 quite fast. However, among cubic graphs on n vertices H_n does not have the smallest value of Balaban index. We introduce a class of graphs L_n with $J(L_n) < J(H_n)$. Since it seems to be difficult to find a good upper bound for $J(L_n)$, in Table 1 below we present the values of $J(L_n)$ and $J(H_n)$ for a few small values of n divisible by 4, and the bound $\frac{32}{n}$.

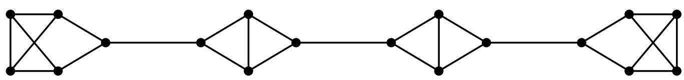

Figure 2. The graph L_{18}.

Let n be even and $n \geq 10$. If $4 \nmid n$, then L_n is obtained from $(n-10)/4$ copies of $K_4 - e$ joined into a path by edges connecting the vertices of degree 2, to which at the ends we attach two pendant blocks, each on 5 vertices, see Figure 2 for L_{18}. On the other hand, if $4 \mid n$, then L_n is obtained from $(n-12)/4$ copies of $K_4 - e$, joined into a path by edges connecting the vertices of degree 2, to which ends we attach two pendant blocks, one on 5 vertices and the other on 7 vertices, see Figure 3 for L_{20}.

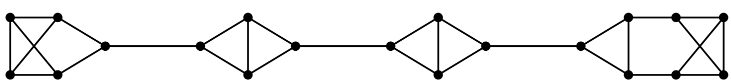

Figure 3. The graph L_{20}.

n	12	16	20	24	28
$32/n$	2.68	2	1.60	1.33	1.14
$J(H_n)$	1.50	1.19	1.00	0.85	0.75
$J(L_n)$	1.36	1.03	0.83	0.70	0.61

Table 1. Balaban index for H_n and L_n for small number of vertices.

We conclude the section with a conjecture about L_n from [29].

Conjecture 2.1. *Among n-vertex cubic graphs, L_n has the smallest Balaban index.*

2.3 Nanotubical structures

Here we consider graphs which are almost regular, namely the nanotubical graphs. These graphs are obtained by wrapping a long hexagonal grid into a tube so that hexagons with coodrinates (x, y) and $(x+k, y+l)$ are identified, and then possibly by closing the tube with patches (also called caps) see [4]. It is important to remark that from a mathematical point of view, nanotubical fullerenes are not well defined as the term "long" is not precise enough. In practice, the ratio

length of the cylindrical part : circumference of the cylindrical part

can be of order 100 000 000:1. It is a well known fact that in a nanotubical fullerene of type (k, l) on n vertices, the circumference of the cylindrical part is $(k + l)$ and the diameter of the cylindrical part is approximately $n/(k + l)$, since when n is large enough comparing to $k + l$, the caps are negligible small [2]. This encourages us to assume that nanotubical fullerenes of type (k, l) on n vertices satisfy

$$k + l \in o(n)\,.$$

In [4], infinite open nanotubes are considered. We have there the following result.

Theorem 2.5. *Let v be an arbitrary vertex in an infinite open (k, l)-nanotube. Denote by n_i the number of vertices at distance i from v. Then*

$$n_i(v) = \begin{cases} 3i, & i < k+l \\ 3i-(l+1), & i = k+l \\ 3i-2(l+2q), & i = k+l+q, \\ & 1 \le q \le k-l \\ 2(k+l), & i \ge 2k. \end{cases}$$

Moreover, if $i \ge 2k$, then at each side of the nanotube there are exactly $k + l$ vertices at distance i from v.

Using the above theorem we determined asymptotics for the Balaban index for nanotubical graphs. The leading term depends on the circumference of the cylindrical part of the nanotubical graph, but not on its specific type.

Theorem 2.6. *Let G be a nanotubical graph (open or not) of type (k, l) on n vertices. Then*

$$J(G) \sim \frac{9\pi(k+l)}{2n}.$$

3. Lower bounds

We start with a simple lower bound for the Balaban index in the class of graphs on n vertices from [28].

Theorem 3.1. *Let G be a graph on $n \geq 4$ vertices. Then*

$$J(G) \geq \frac{4}{n-1}\,.$$

A direct consequence of Theorem 3.1 and Proposition 2.4 is the following corollary.

Corollary 3.1. *As n increases, the minimum value of Balaban index in the class of graphs on n vertices tends to zero. More precisely, this value is of order $\Theta(n^{-1})$.*

Using more involved argument, we have proved the following lower bound in [28], which is for large n roughly twice the bound of Theorem 3.1.

Theorem 3.2. *Let G be a graph on n vertices, where n is big enough. Then*

$$J(G) \geq \frac{8}{n} + o(n^{-1}).$$

By Theorem 3.2, the asymptotic lower bound for $J(G)$ is $8/n$. Let us also mention that nanotubes of type (k, l) (regardless if they are open or not) have asymptotic value of Balaban index $\frac{9\pi(k+l)}{2n}$ by Theorem 2.6. Hence, nanotubes of specific type have also the minimum possible asymptotic value of Balaban index up to a multiplicative constant. However, in the sequel we show that there are graphs with even smaller value of Balaban index.

By the results and arguments from [28], one would expect that a graph with the minimum Balaban index will have $\Theta(n)$ edges, and vertices v with big value of $w(v)$. For small values of n we determined the extremal graphs and observed that they are either *dumbbell graphs* (i.e. graphs obtained from a path and two complete graphs, which are attached to the end-vertices of the path) or graphs similar to dumbbell graphs, see Figure 4. Motivated by this we studied the Balaban index of dumbbell graphs and graphs alike.

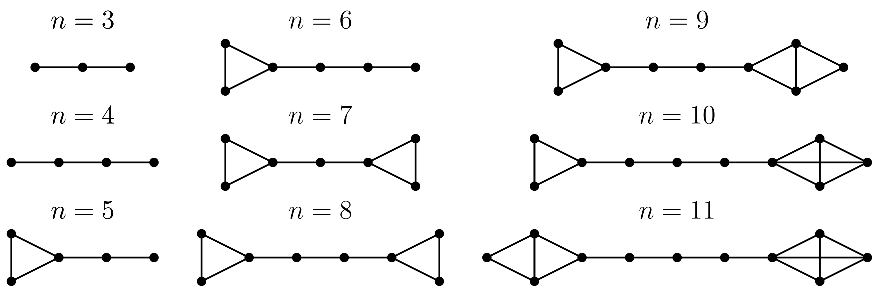

Figure 4. Graphs with the smallest value of Balaban index for $n \in \{3, 4, \dots, 10\}$. The case $n = 11$ was verified only for graphs with at most 22 edges in order to avoid the huge realm of graphs.

4. Bounds for balanced dumbbell graphs

First we define dumbbell graphs more precisely. Let K_a and $K'_{a'}$ be two disjoint complete graphs on a and a' vertices, respectively, and let P_b be a path on b vertices $(v_0, v_1, \dots, v_{b-1})$ disjoint from the cliques. The *dumbbell graph* $D_{a,b,a'}$ is obtained from $K_a \cup P_b \cup K'_{a'}$ by joining all vertices of K_a with v_0 and all vertices of $K'_{a'}$ with v_{b-1}. Thus, $D_{a,b,a'}$ has $a + b + a'$ vertices. In the literature, it is often assumed that $a = a'$, here we call such graphs *balanced dumbbell graphs*. In what follows, we always assume $a \le a'$.

Considering small values of n (up to 200), our computer tests show that among dumbbell graphs $D_{a,b,a'}$ on n vertices, the minimum value of Balaban index is achieved for those with

$$a' = a \quad \text{or} \quad a' = a + 1. \tag{1}$$

We strongly believe this is true in general, and henceforth, we state it as a conjecture.

Conjecture 4.1. *Among all dumbbell graphs $D_{a,b,a'}$ on n vertices, the minimum value of Balaban index is achieved for those with $a' = a$ or $a' = a + 1$.*

The rest of this section is devoted to determining the sizes of a and b for the optimal dumbbell graphs. When dealing with large graphs, there is not much difference between the cases $a' = a$ and $a' = a+1$, so for the sake of simplicity, we restrict ourselves to balanced dumbbell graphs. We denote such dumbbell graphs by $D_{a,b}$. Thus, $D_{a,b}$ stands for $D_{a,b,a}$ and it has $2a + b$ vertices. In [29] we proved the following statement:

Theorem 4.1. *Let $D_{a,b}$ be a balanced dumbbell graph on n vertices, where n is big enough, with the smallest possible value of Balaban index. Then a and b are asymptotically equal to $\sqrt[4]{\pi/2}\sqrt{n}$ and n, respectively. That is, $a = \sqrt[4]{\pi/2}\sqrt{n} + o(\sqrt{n})$ and $b = n - o(n)$.*

Observe that π appears in Theorem 4.1 naturally, since the extremal balanced dumbbell graphs contain a very long path. Theorem 4.1 yields the following consequence.

Corollary 4.1. *Let D be a balanced dumbbell graph on n vertices, where n is big enough, with the minimum value of Balaban index. Then*

$$J(D) \sim \frac{1}{n}\Big[\pi + 2\sqrt{2\pi} + 2\Big] \doteq \frac{10.15}{n}.$$

Comparing Corollary 4.1 with the lower bound presented in Theorem 3.2, we see that the asymptotic value of Balaban index for optimum balanced dumbbell graph is only about 1.27 times higher than our lower bound. Our expectation is that the optimal balanced dumbbell graph is not much different from the optimal dumbbell graph. Guided by this we present an alternative version of Conjecture 4.1.

Conjecture 4.2. *Among all dumbbell graphs $D_{a,b,a'}$ on n vertices, the minimum is achieved for one with $a = \sqrt[4]{\pi/2}\sqrt{n} + o(\sqrt{n})$, $a' = \sqrt[4]{\pi/2}\sqrt{n} + o(\sqrt{n})$ and $b = n - o(n)$.*

Observe that Conjecture 4.1 and Theorem 4.1 imply Conjecture 4.2.

5. Bounds for dumbbell–like graphs

Dumbbell-like graphs are obtained from dumbbell graphs by deleting edges connecting the last vertex of the path with the vertices of the clique. More precisely, let $D_{a,b,a'}$ be a dumbbell graph and let k satisfy $0 \le k < a'$. Recall that $a \le a'$ and all vertices of $K_{a'}$ are connected to v_{b-1}. The *dumbbell-like graph* $D^{-k}_{a,b,a'}$ is obtained from $D_{a,b,a'}$ by deleting k edges which connect v_{b-1} with k vertices of $K_{a'}$. Hence, the extremal graphs for $n = 9$ and $n = 11$ are dumbbell-like graphs $D^{-1}_{2,4,3}$ and $D^{-1}_{3,5,3}$, respectively, see Figure 4.

We have the following conjecture which is supported by our computer experiments.

Conjecture 5.1. *Dumbbell-like graphs attain the minimum value of Balaban index among graphs on n vertices.*

As mentioned above, it seems that among dumbbell graphs, those with the minimum Balaban index have cliques, sizes of which differ by at most one. Hence, they have a “balanced” form. One would therefore expect that, at least in the case when $a = a'$, extremal graphs can be obtained when we remove edges from both sides of dumbbell graph in a balanced way. That is, if we remove from $D_{a,b,a'}$ some edges connecting v_0 with vertices of K_a and some edges connecting v_{b-1} with vertices of $K_{a'}$. However, our computer experiments indicate that this is not the case and the minimum is obtained when we remove edges only from one side, i.e., by dumbbell-like graphs.

Now we modify the notation of dumbbell-like graphs slightly. The reason for this is that if we remove too many edges from $D_{a,b,a'}$, the dumbbell-like graph $D^{-k}_{a,b,a'}$ looks more like the dumbbell graph $D_{a,b+1,a'-1}$. In fact, $D^{-a'+1}_{a,b,a'}$ is the dumbbell graph $D_{a,b+1,a'-1}$. Therefore, if $k > \frac{a'-1}{2}$, instead of $D^{-k}_{a,b,a'}$ we use the notation $D^{a'-1-k}_{a,b+1,a'-1}$ if $a' > a$ and $D^{a'-1-k}_{a'-1,b+1,a}$ if $a' = a$. Observe that the upper index is positive in this modified notation. If a' satisfies $a \le a' \le a+1$, the dumbbell-like graph $D^{k}_{a,b,a'}$ may be viewed as obtained from the dumbbell graph $D_{a,b,a'}$ by adding k edges joining v_1 (the second vertex of the path) with k vertices of K_a.

In fact, the modified notation does not need to be restricted to the case $k > \frac{a'-1}{2}$. This notation suggests the following conjecture.

Conjecture 5.2. *Among dumbbell graphs on n vertices, let $D_{a,b,a'}$ be one with the minimum Balaban index. Then there is (possibly negative) ℓ such that among dumbbell-like graphs on n vertices $D^{\ell}_{a,b,a'}$ has the minimum value of Balaban index.*

We remark that Conjecture 5.2 was verified by computer for some values of n. Conjectures 4.1, 5.1 and 5.2 suggest a two-step process for finding graphs with the minimum Balaban index for given n:

(i) Find parameters a, b, a', where $a \le a' \le a+1$ and $a+b+a' = n$, such that $D_{a,b,a'}$ has the smallest Balaban index.

(ii) Find ℓ such that $D^{\ell}_{a,b,a'}$ has the smallest value of Balaban index.

Moreover, we believe the following conjecture holds.

Conjecture 5.3. *Dumbbell graphs asymptotically attain the minimum value of Balaban index among graphs on n vertices.*

6. Conclusion and further work

Using computers, for $n \le 11$ we found graphs with the minimum value of Balaban index. All these graphs but two are dumbbell graphs and the remaining two are dumbbell-like graphs. We found asymptotic lower and upper bounds for the minimum value of Balaban index and we have shown that they differ by a multiplicative constant 1.27. Finally, we studied dumbbell-like graphs.

Since we expect that balanced dumbbell graphs are asymptotically the best ones, we pose the following problem:

Problem 6.1. *Find a tighter lower bound for the minimum value of Balaban index among graphs on n vertices.*

As regards upper bounds for the smallest value of Balaban index, the following problems are interesting:

Problem 6.2. *Find a, b and a' such that among dumbbell graphs on n vertices $D_{a,b,a'}$ has the smallest value of Balaban index.*

Problem 6.3. *Find a, b, a' and ℓ such that among dumbbell-like graphs on n vertices $D^{\ell}_{a,b,a'}$ has the smallest value of Balaban index.*

Finally, the main problem still remains open although we believe that dumbbell-like graphs are the optimum ones:

Problem 6.4. *Among the graphs on n vertices, find those with the minimum value of Balaban index.*

Beside the above conjectures one can study some more related problems. As a diversity of the Balaban index J, further indices were developed omitting the fraction factor $m/(m-n+2)$ in front of the sum, and it would be interesting to *explore similar bounds for indices* introduced in [14].

6.1 On sum–Balaban index

A derived measure, so called *sum-Balaban* index, is defined as:

$$\mathrm{SJ}(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u)+w(v)}} \, .$$

Regarding this index we obtained some results where some of them are the counterparts of Theorems 2.6, 3.1, 3.2, and 4.1 for this index, [4, 31–33].

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Harary Index of Graphs

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Contents

1. Introduction

The topological index, also known as molecular descriptor, is a single number that can be used to characterize some property of the graph of a molecule [26, 27]. In 1947, Harold Wiener [31] introduced the Wiener index for calculating the boiling point of alkanes. Wiener index of a graph is defined as the sum of the distances between all unordered pairs of vertices of a graph. Probably, Wiener index is the first topological index used in Mathematical Chemistry.

Twenty five years ago, D. Plavšić et al. [22] introduced a topological index, which was named the Harary index in honour of Professor Frank Harary and presented in the Symposium held at the University of Saskatchewan, Saskatoon, Canada from September 12 to 14, 1991 to celebrate the 70$^{\text{th}}$ birthday of Prof. Frank Harary. At the same time the same topological index with different name called as reciprocal distance sum index was independently introduced by O. Ivanciuc et al. [14]. However the term Harary index nowdays is generally accepted for this molecular descriptor. Harary index of a graph is defined as the sum of the reciprocal of the distances between all unordered pairs of vertices of a graph.

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *order* of a graph G is the number of its vertices and the *size* of G is its number of edges. A graph G is said to be *connected* if every pair of vertices of G is joined by some path. The *distance* between the vertices v_i and v_j is the length of a shortest path joining them and is denoted by $d_G(v_i, v_j)$. The maximum distance between any two vertices is called the *diameter* of G and is denoted by $diam(G)$ [1]. The *degree* of a vertex v is the number of edges incident to it in G and is denoted by $d_G(v)$. A graph G is said to be *regular* if all its vertices have same degree. If G_1 and G_2 are isomorphic then it can be written as $G_1 \cong G_2$. As usual, we denote the complete graph by K_n, the cycle by C_n, the path by P_n, the complete bipartite graph by $K_{p,q}$ where $p + q = n$ and the star by $S_n = K_{1,n-1}$ on n vertices.

The *Wiener index* $W(G)$ of a connected graph G is defined as [31]

$$W(G) = \sum_{1 \le i < j \le n} d_G(v_i, v_j).$$

The *Harary index* of a connected graph G, denoted by $H(G)$, is defined as [14, 22]

$$H(G) = \sum_{1 \le i < j \le n} \frac{1}{d_G(v_i, v_j)}.$$

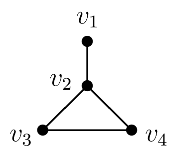

Figure 1. Graph G.

For a graph G given in Fig. 1, $H(G) = 1 + \frac{1}{2} + \frac{1}{2} + 1 + 1 + 1 = 5$ and $W(G) = 8$.

For any connected graph G, $H(G) \le W(G)$ with equality holds if and only if $G \cong K_n$. It is easy to see that

$$\begin{aligned}
H(K_n) &= \frac{n(n-1)}{2};\\
H(K_{p,q}) &= \frac{p(p-1)}{4} + \frac{q(q-1)}{4} + pq;\\
H(S_n) &= \frac{(n+2)(n-1)}{4};\\
H(P_n) &= 1 + n\sum_{k=2}^{n-1} \frac{1}{k};\\
H(C_n) &= \begin{cases} 1 + n\sum\limits_{k=1}^{n-2} \frac{1}{k}, & \text{if } n \text{ is even}\\ n\sum\limits_{k=1}^{n-1} \frac{1}{k}, & \text{if } n \text{ is odd.}\end{cases}
\end{aligned}$$

Harary index can be viewed as a graph invariant based on the reciprocal distance matrix of G [16, 19]. The important use of Harary index in Mathematical Chemistry is in the nonempirical quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) [22,26, 27].

A review of the Harary index and its applications can be found in [36]. In this chapter we focus on the bounds on the Harary index and extremal values.

One can easily observe that any edge addition will increase the Harary index and edge deletion decrease the Harary index. Thus if u and v are nonadjacent vertices of a connected graph G and $e \in E(G)$, then [33, 37]

$$H(G+uv) > H(G) \quad \text{and} \quad H(G-e) < H(G).$$

By above expressions, it easily follows that for any connected graph of order n, $H(G) \leq H(K_n) = \frac{n(n-1)}{2}$, with equlaity holds if and only $G \cong K_n$.

Let $d = diam(G)$. For any two vertices u and v of a connected graph G, $d_G(u,v) \geq 1$ and $d_G(u,v) \leq d$. Hence for any connected graph G of order $n \geq 2$ and having diameter d,

$$\frac{n(n-1)}{2d} \leq H(G) \leq \frac{n(n-1)}{2},$$

with equality on both sides holds if and only if $G \cong K_n$.

In a connected graph G on n vertices and with m edges, there are m pairs of vertices which are at distance 1 and the remaining $\binom{n}{2} - m$ pairs of vertices are at distance at least 2. Similarly $\binom{n}{2} - m$ pairs of vertices are at distance at most $d = diam(G)$. Hence for any connected graph G of order $n \geq 2$ and with m edges and diameter d,

$$\frac{n(n-1)}{2d} + m\left(1 - \frac{1}{d}\right) \leq H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2},$$

with equality on both sides holds if and only if $diam(G) \leq 2$.

2. Harary index of trees

Following theorem gives the lower and upper bounds for the Harary index of trees.

Theorem 2.1. [10] *Let T be a tree on n vertices. Then*

$$1 + n\sum_{k=2}^{n-1} \frac{1}{k} \leq H(T) \leq \frac{(n+2)(n-1)}{4},$$

with left equality holds if and only if $T \cong P_n$ and right equality holds if and only if $T \cong S_n$.

The Harary index increases by adding edges. Hence among all connected graphs, the extremal graph with the minimal Harary index must be tree. Thus, next Corollary follows from Theorem 2.1.

Corollary 2.1. [39] *Let G be a connected graph of order n. Then $H(G) \geq H(P_n)$, with equality holds if and only if $G \cong P_n$.*

A vertex v of a tree T is called a *branching point* if $d_T(v) \geq 3$. Let $T_n(n_1, n_2, \ldots, n_k)$ be a *star like tree* of order n obtained by inserting $n_1 - 1, n_2 - 1, \ldots, n_k - 1$ vertices into k edges of the star S_{k+1} respectively, where $n_1 + n_2 + \cdots + n_k = n - 1$. Note that any tree with exactly one branching point is a star like tree. Assume that T is any tree of order n with exactly two branching points v_1 and v_2 with $d_T(v_1) = r$ and $d_T(v_2) = t$. The orders of $r-1$ components which are paths of $T - v_1$ are $p_1, p_2, \ldots, p_{r-1}$, the order of the component which is not a path of $T - v_1$ is $p_r = n - p_1 - p_2 - \cdots - p_{r-1} - 1$. The orders of $t - 1$ components which are paths of $T - v_2$ are $q_1, q_2, \ldots, q_{t-1}$, the order of the component which is not a path of $T - v_2$ is $q_t = n - q_1 - q_2 - \cdots - q_{t-1} - 1$. We denote the tree T with two branching points as $T = T_n(p_1, p_2, \ldots, p_{r-1}; q_1, q_2, \ldots, q_{t-1})$ where $r \leq t$, $p_1 \geq p_2 \geq \cdots \geq p_{r-1}$ and $q_1 \geq q_2 \geq \cdots \geq q_{t-1}$. For convenience we use the symbol p_k^l to indicate that the number p_k is l times. For example $T_{16}(2, 2, 3, 3, 5) = T_{16}(2^2, 3^2, 5^1)$.

The ordering of trees with respect to Harary index has been given by K. Xu [32].

Theorem 2.2. [32] *Suppose that T is a tree of order $n \geq 16$. Then*

$$H(P_n) < H(T_n(n-3, 1^2)) < H(T_n(n-4, 2, 1)) < H(T_n(1^2; 1^2))$$

$$< H(T_n(n-5, 3, 1)) < H(T_n(1^2; 2, 1)) < H(T_n(n-4, 1^3)) < H(T).$$

Let $T_2, T_3, \ldots, T_8$ be the trees of order $n \geq 14$ as shown in Fig. 2.

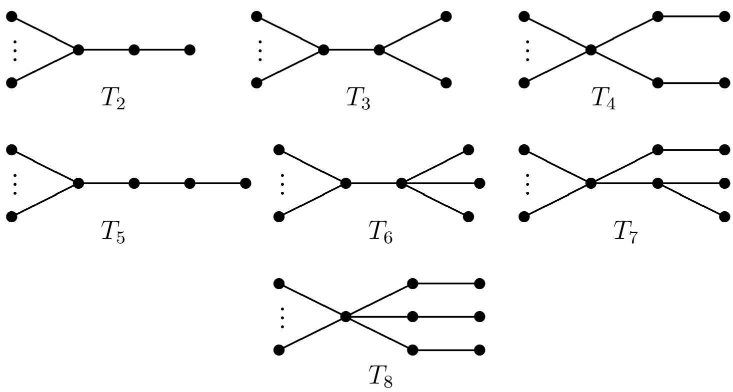

Figure 2.

Theorem 2.3. [32] *Suppose T is a tree of order $n \geq 16$ and $T \notin \{S_n, T_2, T_3, \ldots, T_8\}$. Then*

$$H(T) < H(T_8) < H(T_7) < H(T_6) < H(T_5) < H(T_4) < H(T_3) < H(T_2) < H(S_n).$$

A vertex having degree equal to 1 is called a *pendent* vertex. A set of vertices is *independent* if no two of them are adjacent. The largest number of vertices in such a set is called the *point independence number* of G. An independent set of edges of G has no two of its edges adjacent and the maximum cardinality of such a set is the *line independence number* or *matching number* of G.

Theorem 2.4. [13] *Let T be a tree with n vertices and k pendent vertices, where $2 \leq k \leq n-2$ and $0 \leq r < k$. Then*

$$H(T) \leq H\left(T_n\left(\left\lceil \frac{n}{k} \right\rceil^r, \left\lfloor \frac{n}{k} \right\rfloor^{k-r}\right)\right),$$

with equality holds if and only if $T \cong T_n\left(\left\lceil \frac{n}{k} \right\rceil^r, \left\lfloor \frac{n}{k} \right\rfloor^{k-r}\right)$.

The matching number of a tree $T_n(2^{\beta-1}, 1^{n-2\beta+1})$ is β.

Theorem 2.5. [5, 13] *Let T be a tree with n vertices and matching number β, where $2 \leq \beta \leq \lfloor n/2 \rfloor$. Then*

$$H(T) \leq H(T_n(2^{\beta-1}, 1^{n-2\beta+1})),$$

with equality holds if and only if $T \cong T_n(2^{\beta-1}, 1^{n-2\beta+1})$.

Corollary 2.2. [5, 13] *Let T be a tree with n vertices and point independence number α. Then*

$$H(T) \leq H(T_n(2^{n-\alpha-1}, 1^{2\alpha-n+1})),$$

with equality holds if and only if $T \cong T_n(2^{n-\alpha-1}, 1^{2\alpha-n+1})$.

The *complete Δ-ary tree*, denoted by $V_{n,\Delta}$, is defined as follows. Start with the root having Δ children. Every vertex different from root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. In the last level, while not all nodes have to exist, the nodes that do exist fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1. The complete Δ-ary tree is called *Volkmann tree* [9, 18].

Theorem 2.6. [8, 12, 13, 28] *Let T be a tree with n vertices and maximum degree $\Delta \geq 3$. Then*

$$H(T_n(n-\Delta, 1^{\Delta-1})) \leq H(T) \leq H(V_{n,\Delta}),$$

with left equality holds if and only if $T \cong T_n(n-\Delta, 1^{\Delta-1})$ and right equality holds if and only if $T \cong V_{n,\Delta}$.

The right hand side of Theorem 2.8 was conjectured in [13].

By Theorem 2.8, the following corollary can be easily obtained.

Corollary 2.3. [12] *Let G be a connected graph of order n and with maximum degree Δ. Then*

$$H(G) \geq H(T_n(n-\Delta, 1^{\Delta-1})),$$

with equality holds if and only if $G \cong T_n(n-\Delta, 1^{\Delta-1})$.

Theorem 2.7. [12, 13] *Let T be a tree with n vertices and diameter d, where $2 \leq d \leq n-2$. Then*

$$H(T) \leq H\left(T_n\left(\left\lceil \frac{d}{2} \right\rceil, \left\lfloor \frac{d}{2} \right\rfloor, 1^{n-d-1}\right)\right),$$

with equality holds if and only if $T \cong T_n\left(\left\lceil \frac{d}{2} \right\rceil, \left\lfloor \frac{d}{2} \right\rfloor, 1^{n-d-1}\right)$.

The *reciprocal complementary Wiener index* $RCW(G)$ of a graph G is defined as [15]

$$RCW(G) = \sum_{1 \le i < j \le n} \frac{1}{d + 1 - d_G(v_i, v_j)},$$

where d is the diameter of G.

Obviously $H(S_n) \le RCW(S_n)$ and $H(P_n) \ge RCW(P_n)$.

Denote by DS_{n_1,n_2} a *double star* obtained by adding a new edge between two central vertices of stars S_{n_1+1} and S_{n_2+1}.

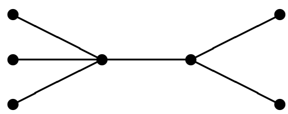

Figure 3. $DS_{3,2}$.

Das, Zhou and Trinajstić [6] obtained the bounds for the Harary index of double star.

Theorem 2.8. [6] *Let DS_{n_1,n_2} be a double star with $n_1 \ge 3$ and $n_2 \ge 2$. Then*

$$H(DS_{n_1,n_2}) \le RCW(DS_{n_1,n_2}),$$

with equality holds if and only if $n_1 = 3$ and $n_2 = 2$.

A *subdivision graph* $S(G)$ of a graph G is obtained by inserting new vertex on each edge of G.

Theorem 2.9. [6] *Let DS_{n_1,n_2} be a double star with $n_1 \ge 8n_2$. Then*

$$H(S(DS_{n_1,n_2})) \ge RCW(S(DS_{n_1,n_2})).$$

Let v be a vertex of a tree T and $d_T(v) = k + 1$. Suppose that $P^{(1)}, P^{(2)}, \dots P^{(k)}$ are pendent paths incident at v, with the starting points of paths $v_1, v_2, \dots, v_k$ respectively and length $n_i \ge 1$ ($i = 1, 2, \dots, k$). Let w be the neighbor of v distinct from v_i. Let $T' = \delta(T, v)$ be a tree obtained from T by removing the edges $vv_1, vv_2, \dots, vv_{k-1}$ and adding edges $wv_1, wv_2, \dots, wv_{k-1}$. We say that T' is a δ-transform of T.

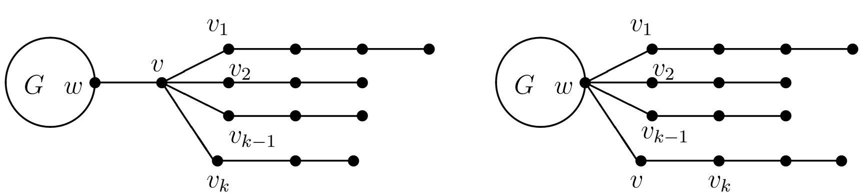

Figure 4. δ-transfromation on the vertex v.

Ilić, Yu and Feng [13] obtained several results on the Harary index of trees.

Theorem 2.10. [13] *Let T be a tree rooted at the center vertex u with at least two vertices of degree 3. Let $v \in \{z \mid d_T(z) \geq 3, z \neq u\}$ be a vertex with the largest distance $d_T(u,v)$ from the center vertex. Then for the δ-transform tree $T' = \delta(T,v)$, $H(T') > H(T)$.*

If v is the branching vertex of a star like tree $T_n(n_1, n_2, \ldots, n_k)$ then $T_n(n_1, n_2, \ldots, n_k) - v = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k}$, where $n_1 \geq n_2 \geq \cdots \geq n_k > 1$.

The star like tree $BT_{n,k} \cong T_n(n_1, n_2, \ldots, n_k)$ is balanced if all paths have almost equal length, that is $|n_i - n_j| \leq 1$ for $1 \leq i < j \leq k$.

The *broom* $B_{n,k}$ is a tree consisting of a star S_{k+1} and a path of length $n-k-1$ attached to an arbitrary pendent vertex of the star.

Let $x = (x_1, x_2, \ldots, x_n)$ and $y = (y_1, y_2, \ldots, y_n)$ be two integer arrays of length n. We say that x majorizes y and write $x \succ y$ if the elements of these arrays satisfy following conditions.

(i) $x_1 \geq x_2 \geq \cdots \geq x_n$ and $y_1 \geq y_2 \geq \cdots \geq y_n$.

(ii) $x_1 + x_2 + \cdots + x_k \geq y_1 + y_2 + \cdots + y_k$ for every $1 \leq k \leq n$.

(ii) $x_1 + x_2 + \cdots + x_n = y_1 + y_2 + \cdots + y_n$.

Theorem 2.11. [13] *Let $p = (p_1, p_2, \ldots, p_k)$ and $q = (q_1, q_2, \ldots, q_k)$ be two arrays of length $k \geq 2$, such that $p \prec q$ and $n = p_1 + p_2 + \cdots + p_k = q_1 + q_2 + \cdots + q_k$. Then*

$$H(T_n(p_1, p_2, \ldots, p_k)) \geq H(T_n(q_1, q_2, \ldots, q_k)).$$

Corollary 2.4. [13] *Let $T = T_n(n_1, n_2, \ldots, n_k)$ be a star like tree with n vertices and k pendent paths. Then*

$$H(B_{n,k}) \leq H(T) \leq H(BT_{n,k}).$$

Moreover, the left equality holds if and only $T \cong B_{n,k}$ and the right equality holds if and only if $T \cong BT_{n,k}$.

Theorem 2.12. [13] *Among all the trees on n vertices with k pendent vertices ($3 \leq k \leq n-2$), $BT_{n,k}$ is the unique tree having maximal Harary index.*

Note that

$$H(P_n) = H(BT_{n,2}) < H(BT_{n,3}) < \cdots < H(BT_{n,n-1}) = H(S_n).$$

If $\frac{n-1}{2} < k \leq n-1$, then the spur tree $A_{n,k}$ is obtained from the star S_{k+1} by adding a pendent edge to each of $n-k-1$ pendent vertices of the star S_{k+1} (see Fig. 5). Note that $A_{n,k} \cong BT_{n,k}$.

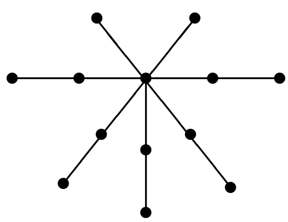

Figure 5. The spur tree $A_{13,7}$.

Theorem 2.13. [13] *Let T be a tree on n vertices with matching number β. Then*

$$H(T) \leq \frac{1}{24}(6n^2 - 4\beta n + \beta^2 + 9\beta + 10n - 22),$$

with equality holds if and only $T \cong A_{n,n-\beta}$.

Corollary 2.5. [13] *Let T be a tree on n vertices with perfect matching. Then*

$$H(T) \leq \frac{1}{4}(17n^2 + 58n - 88),$$

with equality holds if and only $T \cong A_{n,n/2}$.

Theorem 2.14. [13,28] *Let T be a tree on n vertices with point independence number α. Then*

$$H(T) \leq \frac{1}{24}(3n^2 + 2\alpha n + \alpha^2 - 9\alpha + 19n - 22),$$

with equality holds if and only $T \cong A_{n,\alpha}$.

Let $C_{n,k}(p_1, p_2, \ldots, p_{k-1})$ be a *caterpillar* on n vertices from a path $P_{k+1} = v_0 v_1 \cdots v_{k-1} v_k$ by attaching $p_i \geq 0$ pendent vertices to v_i, $1 \leq i \leq k-1$, where $n = k + 1 + \sum_{i=1}^{k-1} p_i$. Denote $C_{n,k,i} = C_{n,k}(\underbrace{0, 0, \ldots, 0}_{i-1}, n-k-1, 0, 0, \ldots, 0)$. Obviously $C_{n,k,i} = C_{n,k,n-i}$.

Theorem 2.15. [13] *Among all trees on n vertices and diameter d, $C_{n,d,\lfloor d/2 \rfloor}$ is the unique tree having maximal Harary index.*

Corollary 2.6. [13] *Let T be a tree on n vertices with radius $r \geq 2$ and diameter d. Then*

$$H(T) \leq H(C_{n,2r-1,\lfloor d/2 \rfloor}),$$

with equality holds if and only if $T \cong C_{n,2r-1,\lfloor d/2 \rfloor}$.

Note that $H(P_n) = H(C_{n,n-1,\lfloor (n-1)/2 \rfloor}) < \cdots < H(C_{n,3,1}) < H(C_{n,2,1}) = H(S_n)$.

Among all trees with n vertices, $C_{n,3,1}$ has the second maximal Harary index [13].

Theorem 2.16. [13] *Let T be a tree on n vertices with the maximum degree Δ. Then $H(T) \leq H(B_{n,\Delta})$, with equality holds if and only if $T \cong B_{n,\Delta}$, a broom.*

Note that $H(S_n) = H(B_{n,n-1}) > H(B_{n,n-2}) > \cdots > H(B_{n,3}) > H(B_{n,2}) = H(P_n)$.

Among all trees with n vertices, $B_{n,3}$ has the second minimum Harary index [13].

A branching point v of a tree T is said to be an *out branching point* if at most one of the components of $T - v$ is not a path, otherwise, v is an *in branching* point of T.

Consider the transformation $T \to T_A \to T_B \to T_C$ as shown in the Fig. 6, where T is a tree of order n and v is an out branching point of T with $d_T(v) = k$ and all the components $T_1, T_2, \ldots, T_k$ of $T - v$ except T_1 are paths.

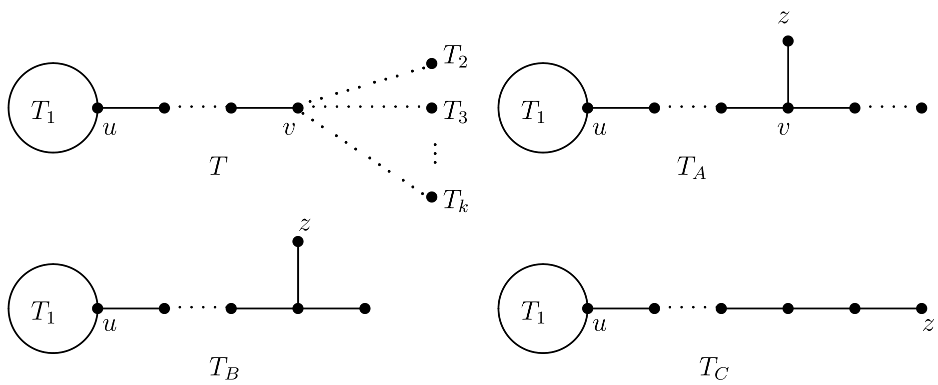

Figure 6.

Theorem 2.17. [32] *Let T be a tree of order n with v as its out branching point and $d_T(v) = k \geq 3$. Suppose that all components of $T - v$ except T_1 are paths. Then $H(T) \geq H(T_A) \geq H(T_B) > H(T_C)$ with $H(T) = H(T_A)$ (or $H(T) = H(T_B)$) if and only if $T \cong T_A$ (or $T \cong T_B$).*

The tree $T'_{n,s}$ is obtained from t paths of order $q+2$ and $s-t$ paths of order $q+1$ by identifying one end of each of the s paths. Here $n-1 = sq+t$, $0 \leq t < s$.

Theorem 2.18. [13] *Let T be a tree of order n with s pendent vertices. Then*

$$\begin{aligned} H(T) \leq H(T'_{n,s}) &= (s-1)\left(n-1+\frac{s}{2}\right)\sum_{i=1}^{2q+1}\frac{1}{i} - (s-2)(n-1-s)\sum_{i=1}^{q+1}\frac{1}{i} \\ &\quad + s\left(\frac{s-3}{2} - q\right) + \frac{t(t-1)}{4(q+1)}, \end{aligned}$$

with equality holds if and only if $T \cong T'_{n,s}$.

3. Harary index of unicyclic and bicyclic graphs

A *unicyclic graph* is connected graph of order n and with n edges. A *bicyclic graph* is a connected graph with n vertices and $n+1$ edges.

Denote by $C_k(n_1^{l_1}, n_2^{l_2}, \ldots, n_t^{l_t})$, the unicyclic graph obtained by attaching l_i paths of length n_i, $i = 1, 2, \ldots, t$ to one vertex of a cycle C_k, where $n_1 > n_2 > \cdots > n_t$. For example, the graph $C_5(4^1, 3^1, 2^2)$ is shown in the Fig. 7.

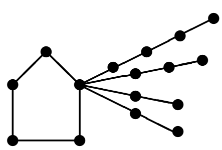

Figure 7. $C_5(4^1, 3^1, 2^2)$.

There are exactly two unicyclic graphs C_4 and $C_3(1^1)$ of order 4 with $H(C_4) = H(C_3(1^1))$.

Xu and Das [34] obtained the bounds for the Harary index of unicyclic graphs and bicyclic graphs.

Theorem 3.1. [34] *Let G be a unicyclic graph with $n \geq 5$ vertices. Then*

$$4 + \frac{2}{n-2} + n\sum_{i=1}^{n-3}\frac{1}{i} \leq H(G) \leq \frac{n^2+n}{4},$$

with the left equality holds if and only if $G \cong C_3((n-3)^1)$ and the right equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n \geq 5$.

The left equality of Theorem 3.1 was conjectured by Chen [2], as the extremal graph among all unicyclic graphs with minimal Harary index is a graph $C_3((n-3)^1)$. The right hand side of Theorem 3.1 was also proved in [2].

For $n = 5$ and $\beta = 2$, there are only two graphs C_5 and $C_3(1^2)$ which have the maximal Harary index among all unicyclic graphs of order 5 with matching number 2 [34].

In [7], Diudea et al. showed that the unique graph $C_3(1^{n-3})$ has the maximal Harary index among all unicyclic graphs of order n and with matching number 2.

The Theorem 3.2 gives extremal unicyclic graphs with maximal Harary index among all the unicyclic graphs with n vertices and matching number $\beta \geq 3$.

Theorem 3.2. [35] *Let G be a unicyclic graph with $n \geq 9$ vertices and matching number $\beta \geq 3$. Then*

$$H(G) \leq H(C_3(2^{\beta-2}, 1^{n-2\beta+1})),$$

with equality holds if and only if $G \cong C_3(2^{\beta-2}, 1^{n-2\beta+1})$.

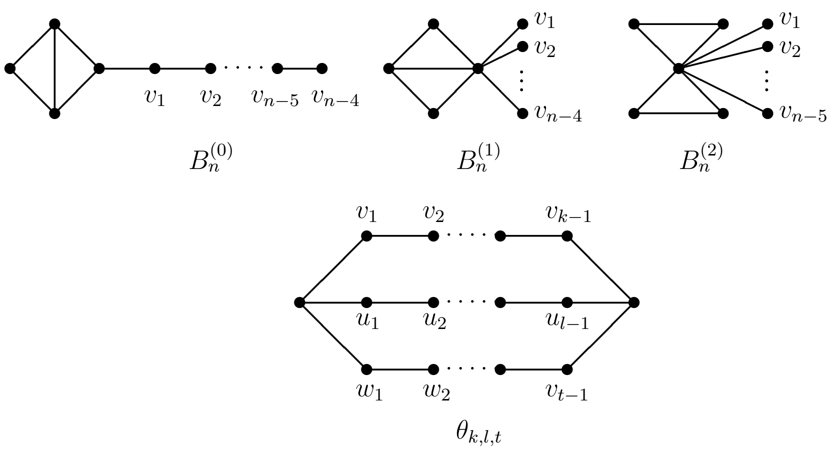

Figure 8.

Let $B_n^{(0)}$, $B_n^{(1)}$, $B_n^{(2)}$ and $\theta_{k,l,t}$ be the graphs as shown in the Fig. 8.

Theorem 3.3. [34] *Let G be a bicyclic graph with $n \geq 5$ vertices and $i \in \{1, 2, \}$. Then*

$$H(G) \leq \frac{n^2 + n + 2}{4},$$

with equality holds if and only if $G \cong B_n^{(i)}$ for $n \geq 7$ and $G \cong B_n^{(i)}$ or $G \cong \theta_{2,2,3}$ for $n = 6$ and $G \cong B_n^{(i)}$ or $G \cong \theta_{2,1,3}$ or $G \cong K_{2,3}$ for $n = 5$.

Theorem 3.4. [34] *Let G be a bicyclic graph of order $n \geq 5$. Then*

$$H(G) \geq n \sum_{i=1}^{n-4} \frac{1}{i} - n + \frac{19}{2} - \sum_{i=1}^{n-4} \left(\frac{3}{i} - \frac{2}{i+1} - \frac{1}{i+2} \right),$$

with equality holds if and only if $G \cong B_n^{(0)}$.

4. Harary index interms of graph parameters

Theorem 4.1. [25] *Let G be a connected graph of order n and maximum dgree $\Delta(G) \geq k \geq 2$. Then*

$$H(G) \geq k + \frac{1}{2} \binom{k-1}{2} + \frac{k-1}{n-k+1} + n \sum_{i=2}^{n-k} \frac{1}{i},$$

with equality holds if and only if $G \cong B_{n,k}$, a broom.

Denote G^* a graph with diameter d ($3 \leq d \leq 4$) and $|V(G^*)| \geq d + 2$, such that for any two distinct vertices $u \in V(G^*) \setminus V(P_{d+1})$ and $v \in V(G^*)$, $d_{G^*}(u, v) = 1$ or 2.

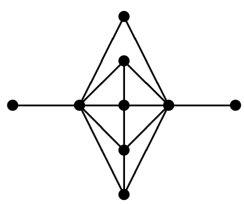

Figure 9. Example of G^*-type graph.

Theorem 4.2. [6] *Let G be a connected graph of order n with m edges and diameter d. Then*

$$H(G) \geq H(P_{d+1}) + \frac{n(n-1) + 2(m-d)(d-1)}{2d} - \frac{d+1}{2},$$

with equality holds if and only if G is a graph with diameter $d \leq 2$ or $G \cong P_n$ Moreover,

$$H(G) \leq H(P_{d+1}) + \frac{n(n-1) + 2m}{4} - \frac{d(d+3)}{2},$$

with equality holds if and only if G is a graph with diameter $d \leq 2$ or $G \cong P_n$ or G is isomorphic to some G^*-type graph.

Theorems 4.3 and 4.4 gives the bounds for Harary index interms of Wiener index.

Theorem 4.3. [33] *Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter d. Then*

$$(W(G) - m - d)\left(H(G) - m - \frac{1}{d}\right) \geq \left(\frac{n(n-1)}{2} - m - 1\right)^2,$$

with equality holds if and only if G has diameter at most 2.

Theorem 4.4. [4] *Let $G \neq K_n$ be a connected graph of order n, m edges and diameter d. Then*

$$m + \frac{\left(\frac{n(n-1)}{2} - m\right)^2}{W(G) - m} \leq H(G) \leq m + \frac{\left(\frac{n(n-1)}{2} - m\right)\left[2 + \left(\frac{n(n-1)}{2} - m - 1\right)\left(\frac{d}{2} + \frac{2}{d}\right)\right]}{2(W(G) - m)},$$

with equality on both sides holds if and only if G has diameter $d = 2$.

The first and second *Zagreb indices* of a graph G are defined as [11]

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

Denote by G^{**} a triangle and quadrangle free graph of diameter 4 and order $n \geq 6$ such that, for any two distinct vertices $u, v \in V(G^{**}) \setminus V(P_{d+1})$, $d_{G^{**}}(u, v) \leq 3$ where P_{d+1} is a path of order $d + 1$ in G^{**}.

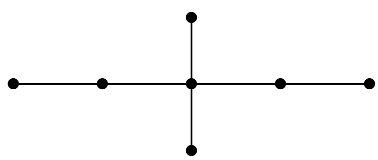

Figure 10. Example of G^{**}-type graph.

Following Theorems gives the Harary index interms of Zagreb indices.

Theorem 4.5. [6] *Let G be a triangle and quadrangle free graph with $n \geq 2$ vertices, m edges and diameter d. Then*

$$H(P_{d+1}) + \frac{d-2}{4d}M_1(G) + A_0 \leq H(G) \leq H(P_{d+1}) + \frac{1}{12}M_1(G) + A_1$$

where $A_0 = \frac{n(n-1)-2}{2d} + \frac{m}{2} - 2(d-1)$ and $A_1 = \frac{n(n-1)+1}{6} + \frac{m}{2} - \frac{d^2}{6} - d$. Moreover, the left equality holds if and only G is a graph of diameter at most 3 or a path P_n and right equality holds if and only if G is a graph of diameter at most 3 or a path P_n or G is isomorphic to a graph G^{**}-type.

Theorem 4.6. [39] *Let G be a triangle and quadrangle free graph with $n \geq 2$ vertices, m edges. Then*

$$H(G) \leq \frac{n(n-1)}{6} + \frac{m}{2} + \frac{M_1(G)}{12},$$

with equality holds if and only G is a graph of diameter at most 3.

Theorem 4.7. [5] *Let T be a tree of order n and with diameter d. Then*

$$\left(\frac{1}{3}-\frac{1}{d}\right)M_2(T)+\left(\frac{1}{2d}-\frac{1}{12}\right)M_1(T)+B_0\le H(T)\le\frac{1}{12}M_2(T)+\frac{1}{24}M_1(T)+B_1,$$

where $B_0=\frac{n^2}{2d}+\left(\frac{5}{6}-\frac{3}{2d}\right)n+\frac{1}{d}-\frac{5}{6}$ and $B_1=\frac{n^2}{8}+\frac{11n}{24}-\frac{7}{12}$. Moreover, the both equality holds if and only T is a tree with diameter at most 4.

Zhou and Trinajstić [40] obtained the bound for the Harary index interms of the maximum eigenvalue of the reciprocal distance matrix.

The *reciprocal distance matrix* $RD(G)=[rc_{ij}]$ of a graph G is an $n\times n$ matrix [16], where

$$rc_{ij}=\begin{cases}\frac{1}{d_G(v_i,v_j)}, & \text{if} \quad i\neq j\\ 0, & \text{otherwise.}\end{cases}$$

Theorem 4.8. [40] *Let G be a connected graph of order n and λ_1 be the maximum eigenvalue of the reciprocal distance matrix $RD(G)$ of G. Then*

$$H(G)\le\frac{n}{2}\lambda_1,$$

with equality holds if and only if $RD(G)$ has equal row sum.

Xu and Das [33] obtained the bounds for the Harary index interms of diameter, clique number and chromatic number.

Theorem 4.9. [33] *Let G be a connected graph with $n\ge 2$ vertices, m edges and diameter d. If there exists two nonadjacent vertices $u,v\in V(G)$, then*

$$\frac{1}{2}\le H(G+uv)-H(G)\le 1-\frac{1}{d}+\frac{n(n-1)-2m-2}{2}\left(\frac{1}{2}-\frac{1}{d}\right),$$

with left equality holds if and only if $d_G(u)=d_G(v)=1$ and $d_G(u,v)=2$ and right equality holds if and only if G has diameter 2.

Theorem 4.10. [33] *Let G be a triangle and quadrangle free graph with $n\ge 2$ vertices, m edges and diameter d. If there exists two nonadjacent vertices $u,v\in V(G)$, then*

$$\frac{1}{2}\le H(G+uv)-H(G)\le 1-\frac{1}{d}+\frac{n(n-1)-M_1(G)-2}{2}\left(\frac{1}{2}-\frac{1}{d}\right),$$

with left equality holds if and only if $d_G(u)=d_G(v)=1$ and $d_G(u,v)=2$ and right equality holds if and only if G has diameter 2.

The *kite graph* $Ki_{n,k}$ is obtained by identifying one vertex of the complete graph K_k with one pendent vertex of the path P_{n-k+1}.

The *Turán graph* $T_n(k)$ is complete multipartite graph formed by partitioning a set of n vertices into k subsets, with sizes as equal as possible. That is, it is a complete k-partite graph $K_{\lceil\frac{n}{k}\rceil,\lceil\frac{n}{k}\rceil,\ldots,\lfloor\frac{n}{k}\rfloor,\lfloor\frac{n}{k}\rfloor}$. The

Turán graph will have $n(mod\ k)$ subsets of size $\lceil \frac{n}{k} \rceil$ and $k - \lceil \frac{n}{k} \rceil$ subsets of size $\lfloor \frac{n}{k} \rfloor$. Each vertex has degree either $n - \lceil \frac{n}{k} \rceil$ or $n - \lfloor \frac{n}{k} \rfloor$.

The *chromatic number* of a graph G, denoted by $\chi(G)$ is the minimum number of colors require to color the vertices of G such that no two adjacent vertices have the same color.

A *clique* of a graph G is the subgraph of G which is complete graph. The *clique number* of G, denoted by $w(G)$ is the number of vertices in the largest clique of G.

Let $\mathscr{W}_{n,k}$ be the set of connected graphs of order n with clique number k. Let $\mathscr{X}_{n,k}$ be the set of connected graphs of order n with chromatic number k.

Theorem 4.11. [33] *Let $G \in \mathscr{X}_{n,k}$ and $0 \leq r < k$. Then*

$$H(G) \leq \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\left[(k-r)\left\lfloor \frac{n}{k} \right\rfloor^2 + r\left\lceil \frac{n}{k} \right\rceil^2\right],$$

with the equality holds if and only if $G \cong T_n(k)$.

Theorem 4.12. [33] *Let $G \in \mathscr{W}_{n,k}$ and $0 \leq r < k$. Then*

$$H(G) \leq \frac{n^2}{2} - \frac{n}{4} - \frac{1}{4}\left[(k-r)\left\lfloor \frac{n}{k} \right\rfloor^2 + r\left\lceil \frac{n}{k} \right\rceil^2\right],$$

with the equality holds if and only if $G \cong T_n(k)$.

Theorem 4.13. [33] *Let $G \in \mathscr{X}_{n,k}$. Then*

$$H(G) \geq \frac{k(k-1)}{2} + n\sum_{l=1}^{n-k} \frac{1}{l+1},$$

with the equality holds if and only if $G \cong Ki_{n,k}$, a kite graph.

Theorem 4.14. [33] *Let $G \in \mathscr{W}_{n,k}$. Then*

$$H(G) \geq \frac{k(k-1)}{2} + n\sum_{l=1}^{n-k} \frac{1}{l+1},$$

with the equality holds if and only if $G \cong Ki_{n,k}$, a kite graph.

The *vertex connectivity* of a graph is the minimum number of vertices whose removal yields the resulting graph disconnected or a trivial. The *edge connectivity* of a graph is the minimum number of edges whose removal yields the resulting graph disconnected or a trivial.

Li and Fan [17] obtained the extremal Harary index with respect to vertex connectivity and edge connectivity.

Let $K(n-1, r)$ be a graph obtained from K_{n-1} by adding a vertex together with edges joining this vertex to r vertices of K_{n-1}, where $1 \leq r \leq n-2$.

Theorem 4.15. [17] *For each $r = 1, 2, \ldots, n-2$ the graph $K(n-1, r)$ is the unique one with the maximum Harary index among all graphs of order n and vertex connectivity r.*

Theorem 4.16. [17] *For each* $r = 1, 2, \ldots, n-2$ *the graph* $K(n-1, r)$ *is the unique one with the maximum Harary index among all graphs of order* n *and edge connectivity* r.

Corollary 4.1. [17] *Let* G *be a graph of order* n *with vertex or edge connectivity* r*, where* $1 \leq r \leq n-2$. *Then*

$$H(G) \leq \frac{(n-1)^2 + r}{2},$$

with equality holds if and only if $G \cong K(n-1, r)$.

The second maximum Harary index among all graphs of order n with vertex connectivity r is reported in [17].

Ramane and Manjalapur [24] obtained the bounds for the Harary index interms of the eccentricities.

The *eccentricity* of a vertex v in G, denoted by $ecc(v)$, is the maximum distance from it to any other vertex. That is, $ecc(v) = \max\{d_G(u, v) \mid u \in V(G)\}$. The *radius* $r(G)$ of a graph G is the minimum eccentricity of the vertices. A vertex v is called *central vertex* of G if $ecc(v) = r(G)$. A graph G is said to be *self-centered* if every vertex of G is a central vertex. Thus in a self-centered graph, $r(G) = d(G)$. An *eccentric vertex* of a vertex v is a vertex farthest from v. An *eccentric path* $P(v)$ of a vertex v is a path of length $ecc(v)$, joining v and its eccentric vertex. For a given vertex, there may exists more than one eccentric paths.

Theorem 4.17. [24] *Let* G *be a connected graph with* n *vertices,* m *edges and* $e_i = ecc(v_i)$*,* $i = 1, 2, \ldots, n$. *Then*

$$H(G) \leq \frac{1}{4}\left[n(n-2) + 2m + 2\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{j} - \sum_{i=1}^{n} e_i\right],$$

with equality holds if and only if for every vertex v_i *of* G*, if* $P(v_i)$ *is one of the eccentric path of* v_i*, then for every* $v_j \in V(G)$ *which is not on* $P(v_i)$*,* $d_G(v_i, v_j) \leq 2$.

Corollary 4.2. [24] *Let* G *be a self-centered graph with* n *vertices,* m *edges and radius* r. *Then*

$$H(G) \leq \frac{1}{4}\left[n(n-r-2) + 2m + 2n\sum_{j=1}^{r}\frac{1}{j}\right],$$

with equality holds if and only if for every vertex v_i *of a self-centered graph* G*, if* $P(v_i)$ *is one of the eccentric path of* v_i*, then for every* $v_j \in V(G)$ *which is not on* $P(v_i)$*,* $d_G(v_i, v_j) \leq 2$.

Theorem 4.18. [24] *Let* G *be a connected graph with* n *vertices and* $e_i = ecc(v_i)$*,* $i = 1, 2, \ldots, n$. *Then*

$$H(G) \leq \frac{1}{2}\left[n(n-1) + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{j} - \sum_{i=1}^{n} e_i\right],$$

with equality holds if and only if for every vertex v_i *of* G*, if* $P(v_i)$ *is one of the eccentric path of* v_i*, then for every* $v_j \in V(G)$ *which is not on* $P(v_i)$*,* $d_G(v_i, v_j) = 1$.

Corollary 4.3. [24] *Let G be a self-centered graph with n vertices and radius r. Then*

$$H(G) \leq \frac{n}{2}\left[n-r-1+\sum_{j=1}^{r}\frac{1}{j}\right],$$

with equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d_G(v_i, v_j) = 1$.

Theorem 4.19. [24] *Let G be a connected graph with n vertices, m edges and diameter d. Let $e_i = ecc(v_i)$, $i = 1, 2, \ldots, n$. Then*

$$H(G) \geq \frac{1}{2d}\left[n(n-d)+2m(d-1)+d\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{j}-\sum_{i=1}^{n}e_i\right],$$

with equality holds if and only if diameter $d \leq 2$.

Corollary 4.4. [24] *Let G be a self-centered graph with n vertices and radius r. Then*

$$H(G) \geq \frac{1}{2r}\left[n(n-2r)+2m(r-1)+nr\sum_{j=1}^{r}\frac{1}{j}\right],$$

with equality holds if and only if G is self-centered graph with radius $r \leq 2$.

5. Harary index of some class of graphs

A graph G is called *quasi-tree graph* if there exists a vertex $v \in V(G)$ such that $G - v$ is a tree. Clearly any tree is a quasi-tree graph, since the deletion of any pendent vertex will deduce another new tree. A graph G is called *k-generalized quasi-tree graph* [38] if there exists a subset $V_k \subset V(G)$ with $|V_k| = k$ such that $G - V_k$ is a tree but, for any subset $V_{k-1} \subset V(G)$ with cardinality $k-1$, $G - V_{k-1}$ is not a tree.

For $k \geq 2$, we denote by $QT^{(k)}(n)$ the set of k-generalized quasi-tree graphs of order n. Let $C_k((n-k)^1)$ be a graph obtained by attaching a path of length $n-k$ to any one vertex of the cycle C_k. We denote by $C_{3,3}^{n-5}$ (see Fig. 11) a graph obtained by connecting two vertex-disjoint triangles by a path of length $n-5$.

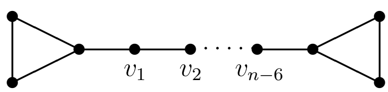

Figure 11. $C_{3,3}^{n-5}$.

Any tree is called a trivial quasi-tree graph and other quasi-tree graphs are called non-trivial quasi-tree graphs.

Xu, Wang and Liu [38] obtained the Harary index of quasi-tree graphs.

The *join* of two graphs G_1 and G_2 is a graph $G_1 \vee G_2$ obtained from G_1 and G_2 by joining every vertex of G_1 to all vertices of G_2. Let $\overline{G}$ be the complement of G.

Theorem 5.1. [38] *Let G be a non-trivial quasi-tree graph of order $n \geq 4$. Then*

$$3 + n\sum_{k=2}^{n-2}\frac{1}{k} \leq H(G) \leq \frac{(n-2)(n+5)}{4} + 1,$$

with left equality holds if and only if $G \cong C_3((n-3)^1)$ and right equality holds if and only if $G \cong K_2 \vee \overline{K_{n-2}}$.

Theorem 5.2. [38] *Let G be a 2-generalized quasi-tree graph of order $n \geq 6$. Then*

$$H(G) \geq 5 + n\sum_{k=2}^{n-3}\frac{1}{k} + \frac{1}{n-3},$$

with equality holds if and only if $G \cong C_{3,3}^{n-5}$ (Fig. 11).

Theorem 5.3. [38] *For any graph $G \in QT^{(k)}(n)$ with $n \geq 6$,*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{(k+1)(n-k-1)}{2} + \frac{k(k+1)}{4},$$

with equality holds if and only if $G \cong K_{k+1} \vee \overline{K_{n-k-1}}$.

A graph G is said to be *bipartite* if its vertex set $V(G)$ can be partitioned into two sets V_1 and V_2 such that every edge of G has one end in V_1 and other end in V_2.

Cui and Liu [3] obtained the bounds for the Harary index of bipartite graphs.

Theorem 5.4. [3] *Let G be a connected bipartite graph of order n with bipartite sets V_1 and V_2 where $|V_1| = p$, $|V_2| = q$ and $p + q = n$. Then*

$$H(G) \leq \frac{n}{8}\left[n - 2 + \sqrt{n^2 + 2pq}\right],$$

with equality holds if and only if $G \cong K_{p,q}$, a complete bipartite graph.

Theorem 5.5. [3] *Let G be a connected bipartite graph of order n with bipartite sets V_1 and V_2 where $|V_1| = p$, $|V_2| = q$ and $p + q = n$. Let Δ_1 and Δ_2 be maximum degrees among vertices in V_1 and V_2 respectively. Then*

$$H(G) \leq \frac{n}{8}(n-2) + \frac{n}{24}\sqrt{25 + 9n^2 + 8p\Delta_1 + 8q\Delta_2 + 16\Delta_1\Delta_2 - 25n - 5pq},$$

with equality holds if and only if $G \cong K_{p,q}$ or G is a semi regular graph with vertex eccentricity equal 3.

The bounds on Harary index among all k^{th} power of trees have been reported by Su, Xiong and Gutman [25].

The k^{th} power of G, denoted by G^k, is a graph with vertex set $V(G^k) = V(G)$ such that two vertices are adjacent in G^k if and only if they are at distance at most k in G [25].

Theorem 5.6. [25] *For any tree T of order n,*

$$H(P_n^k) \leq H(T^k) \leq H(S_n^k),$$

with left equality holds if and only if $T^k \cong P_n^k$ and right equality holds if and only if $T^k \cong S_n^k$.

Corollary 5.1. [25] *Let G be a connected graph of order n. Then*

$$H(P_n^k) \leq H(G^k).$$

Problem 5.7. [25] *Characterize the graphs G_1 and G_2 of the same order such that $H(G_1) \leq H(G_2)$ implies $H(G_1^k) \leq H(G_2^k)$.*

A connected graph G is called *cactus* if each block of G is either an edge or a cycle. Denote by $\mathscr{C}(n,r)$ the set of connected cacti possessing n vertices and r cycles. Let $C^0(n,r)$ be the cactus graph obtained from a star S_n by adding r independent edges between the leaves of S_n.

Theorem 5.8. [30, 41] *Let G be any graph in $\mathscr{C}(n,r)$. Then*

$$H(G) \leq \frac{1}{4}(n-2r-1)(n-2r-2) - r^2 + (n-1)(r+1),$$

with equality holds if and only if $G \cong C^0(n,r)$.

Theorem 5.9. [29] *Among all cacti of order $2n$ and with a perfect matching, the graph $C^0(2n, n-1)$ is the unique graph having the maximal Harary index.*

A *cut vertex* of a graph is a vertex whose removal increases the number of components of the graph. An edge is said to be *cut edge* if its removal increases the number of components of the graph.

Let $C^*_{n,k}$ be a cactus obtained by identifying the vertex of degree $n-4$ of $C^0(n-3, \frac{n-k-4}{2})$ with one vertex of C_4 (see Fig. 12, for an example).

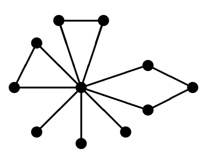

Figure 12. The cactus $C^*_{11,3}$.

Theorem 5.10. [29] *Among all cacti of order $2n$ and with k cut edges, the graph $C^0(n, \frac{n-k-1}{2})$ is the unique graph with maximal Harary index when $n-k$ is odd and $C^*_{n,k}$ uniquely has the maximal Harary index if $n-k$ is even.*

Theorem 5.11. [29] *Among all cacti of order $2n$ and with k pendent vertices, the graph $C^0(n, \frac{n-k-1}{2})$ is the unique graph with maximal Harary index when $n-k$ is odd and $C^*_{n,k}$ uniquely has the maximal Harary index if $n-k$ is even.*

Denote $C^{\dagger}(2n, r)$ a graph of order $2n$ obtained by adding $n - r - 1$ paths of length 2 at the vertex of maximum degree in $C^{0}(2r + 2, r)$.

Theorem 5.12. [41] *Let $G \in \mathscr{C}(2n, r)$ with a perfect matching. Then*

$$H(G) \leq \frac{1}{24}(n - r - 1)(23n + 17r - 2) + 2n + r^2 - 1,$$

with equality holds if and only if $G \cong C^{\dagger}(2n, r)$.

Let $1 \leq k \leq n$ and Kc_n^k be the graph obtained by attaching k pendent vertices to one vertex of the complete graph K_{n-k}.

Theorem 5.13. [37] *Among all connected graphs with n vertices and k cut edges, the graph Kc_n^k uniquely has the maximal Harary index.*

The *Moore graph* [20] is a regular graph of degree r with diameter d and girth $2d + 1$, whose order attains the upper bound

$$1 + r\sum_{i=0}^{d-1}(r - i)^i.$$

Theorem 5.14. [39] *Let G be a connected triangle and quadrangle free graph with $n \geq 2$ vertices and m edges. Then*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2},$$

with equality holds if and only if G is a star or a Moore graph of diameter 2.

Theorem 5.15. [8] *Let G be a connected triangle and quadrangle free graph with $n \geq 4$ vertices and matching number β, where $2 \leq \beta \leq \lfloor n/2 \rfloor$.*

(i) *If $\beta = \lfloor n/2 \rfloor$, then $H(G) \leq H(K_n)$ with equality holds if and only if $G \cong K_n$.*

(ii) *If $\frac{2n}{5} < \beta \leq \lfloor n/2 \rfloor - 1$, then $H(G) \leq H(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

(iii) *If $2 \leq \beta < \frac{2n}{5}$, then $H(G) \leq H(K_\beta \vee \overline{K_{n-\beta}})$ with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

(iv) *If $\beta = \frac{2n}{5}$, then $H(G) \leq H(K_\beta \vee \overline{K_{n-\beta}}) = H(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$ or $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

For a vertex $v_i \in V(G)$, we define

$$Q_G(v_i) = \sum_{v_j \in V(G)} \frac{d_G(v_i, v_j)}{1 + d_G(v_i, v_j)}.$$

Theorem 5.16. [33] *Let G be a connected graph with n vertices and $v_iv_j \in E(G)$. Then*

$$H(G) \geq H(G - v_i) + n - 1 - Q_{G-v_i}(v_j),$$

with equality holds if and only if v_i is a pendent vertex of G.

Let G be a graph with $v_i \in V(G)$. For two integers $l \geq k \geq 1$, let $G_{k,l}$ be the graph obtained from G by attaching at v_i two new paths $P' : v_i u_1 u_2 \cdots u_k$ and $P'' : v_i u'_1 u'_2 \cdots u'_l$ of length k and l, respectively, where $u_1, u_2, \ldots, u_k$ and $u'_1, u'_2, \ldots, u'_l$ are new distinct vertices.

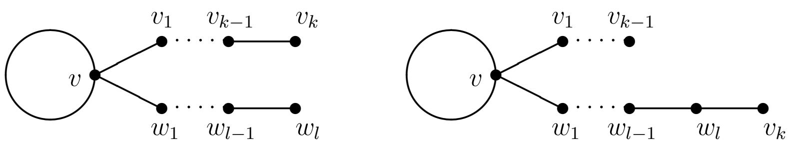

Figure 13. Graphs $G_{k,l}$ and $G_{k-1,l+1}$.

Theorem 5.17. [32] *Let $G \neq K_1$ be a connected graph. If $l \geq k \geq 1$, then*

$$H(G_{k,l}) > H(G_{k-1,l+1}).$$

Theorem 5.18. [33] *Let $G \neq K_1$ be a connected graph of order $n > 2$ and v_i, v_j be its distinct vertices with $Q_G(v_i) = Q_G(v_j)$. Suppose $G^*_{s,t}$ is a graph obtained from G by attaching at v_i one path $P(v_i)$: $v_i u_1 u_2 \cdots u_s$ and at v_j the other path $P(v_j) : v_j u'_1 u'_2 \cdots u'_t$. If $s \geq t \geq 1$, then $H(G^*_{s,t}) > H(G^*_{s+1,t-1})$.*

Following Corollary follows from Theorem 5.19.

Corollary 5.2. [33] *Let G be a connected graph of order $n > 2$ and v_i, v_j be its distinct vertices with $Q_G(v_i) = Q_G(v_j)$. Suppose $G^*_{s,t}$ is a graph obtained from G by attaching at v_i one path of length s and at v_j the other path of length t. Let G_{s+t} be a graph obtained from G by attaching at v_i (or v_j) a path of length $s+t$. Then $H(G^*_{s,t}) > H(G_{s+t})$.*

Theorem 5.19. [13] *Let G_0 be a connected graph and $u \in V(G_0)$. Let G_1 be the graph obtained from G_0 by attaching a tree T ($T \neq P_k$ and $T \neq S_k$) of order k to u, G_2 be the graph obtained from G by identifying u with end vertex of a path P_k, G_3 is the graph obtained from G_0 by identifying u with the center of a star S_k. Then $H(G_2) < H(G_1) < H(G_3)$.*

Theorem 5.20. [32] *Let G_1 and G_2 be two graphs of same order and with v_i as a pendent vertex of G_i and $u_i v_i \in E(G_i)$ for $i = 1, 2$. If $H(G_2 - v_2) \geq H(G_1 - v_1)$ and $Q_{G_1 - v_1}(u_1) \geq Q_{G_2 - v_2}(u_2)$, then $H(G_2) \geq H(G_1)$ with the equality holds if and only if the above two equalities holds simultaneously.*

Suppose that G is a graph with $v_1 \in V(G)$ and $v_2, v_3, \ldots, v_{t+s}$ are distinct new vertices (not in G). Let G' be the graph obtained from G by attaching at v_1 a new path $P : v_1 v_2 \cdots v_{t+s}$. Let $M_{t,t+s} = G' + v_t u_0$ and $M_{t+i,t+s} = G' + v_{t+i} u_0$, where $1 \leq i \leq s$ and u_0 is a new vertex not in G'.

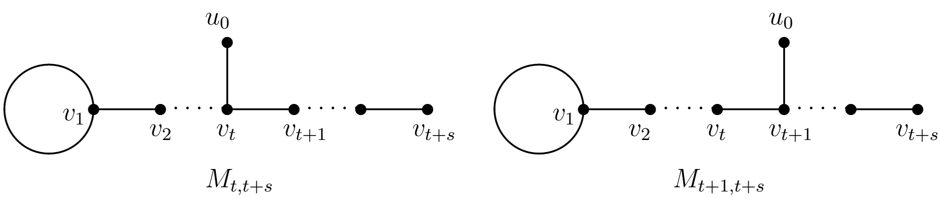

Figure 14.

Theorem 5.21. [32] *Let G be a connected graph of order $n \geq 2$. If $t > s > 1$, then*

$$H(M_{t,t+s}) > H(M_{t+i,t+s}), \quad \textit{for} \quad 1 \leq i \leq s.$$

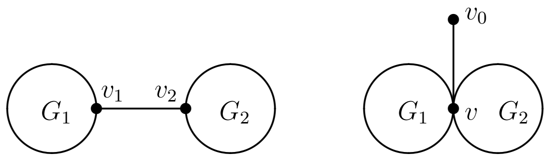

Figure 15. G and G'.

Theorem 5.22. [37] *Let $v_1v_2 \in E(G)$ be a cut edge in G, and $G - v_1v_2 = G_1 \cup G_2$ with $n_i = |V(G_i)| \geq 2$ for $i = 1, 2$. Suppose that $v_i \in V(G_i)$, $i = 1, 2$. Assume that G' is a graph obtained from G by identifying vertices v_1 and v_2 (the new vertex is labeled as v) and attaching a pendnet vertex v_0 to this identified vertex v (See Fig. 15). Then $H(G) < H(G')$.*

Let G_1 and G_2 be two connected graphs with $V(G_1) \cap V(G_2) = \{v\}$. Let G_1vG_2 be a new graph with its vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. By applying Theorem 5.24, the following result follows.

Corollary 5.3. [32] *Let G be graph and T_k be a tree of order k with $V(G) \cap V(T_k) = \{v\}$. Then $H(GvT_k) \leq H(GvS_k)$, where v is identified with the center of the star S_k in GvS_k. Moreover, the equality holds if and only if $T_k \cong S_k$.*

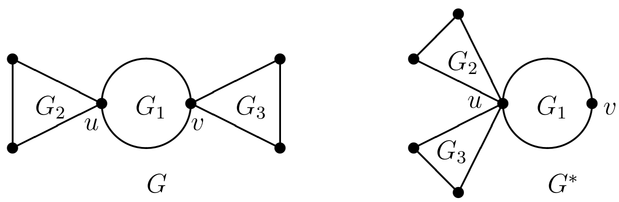

Figure 16.

Theorem 5.23. [37] *Let G_1, G_2 and G_3 be three connected graphs with disjoint vertex sets. Suppose that u and v are two vertices of G_1, v_0 is a vertex of G_2, u_0 is the vertex of G_2. Let G be the graph obtained from G_1, G_2 and G_3 by identifying v with v_0 and u with u_0 respectively. Let G^* be the graph obtained from G_1, G_2 and G_3 by identifying three vertices v, v_0 and u_0 (or by identifying the vertices u, v_0 and u_0) (see Fig. 16). Then $H(G^*) > H(G)$.*

The *line graph* of G is a graph $L(G)$ whose vertex set is in one-to-one correspondence with the edge set of G and two vertices in $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. Ramane and Manjalapur [23] obtained the Harary index for the line graphs.

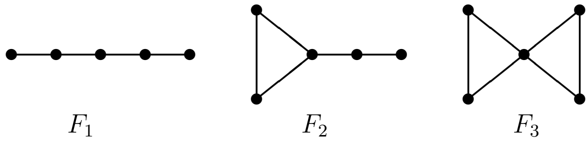

Figure 17. The graphs F_1, F_2 and F_3.

Theorem 5.24. [23] *Let G be a connected graph with n vertices and m edges. Let $d_G(v_i)$ be the degree of a vertex v_i in G and $L(G)$ be the line graph of G. Then*

$$H(L(G)) \leq \frac{1}{4}\left[m^2 - 3m + \sum_{i=1}^{n}(d_G(v_i))^2\right],$$

with equality holds if and only if none of the three graphs F_1, F_2 and F_3 of Fig. 17 is an induced subgraph of G.

Corollary 5.4. [23] *If G is a connected regular graph of degree r on n vertices and $L(G)$ is the line graph of G, then*

$$H(L(G)) \leq \frac{1}{16}[nr(nr + 4r - 6)],$$

with equality holds if and only if G is a regular graph of degree r and none of the three graphs F_1, F_2 and F_3 of Fig. 17 is an induced subgraph of G.

For a vertex $v \in V(G)$, denote by $N_G(v)$ the neighborhood of v in G. For a subset $W \subset V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W together with the edges incident with them. For a subset $E_1 \subset E(G)$, denote by $G - E_1$ the subgraph of G obtained by deleting the edges of E_1.

Theorem 5.25. [17] *Let G_1, G_2 and P_s be pairwise vertex disjoint connected graphs, where G_1 contains an edge uv such that $N_{G_1}(u) \setminus \{v\} = N_{G_1}(v) \setminus \{u\} = \{w_1, w_2, \ldots, w_k\}$ ($k \geq 1$), G_2 contains a shortest path $P_t = x_1x_2 \cdots x_t$ from x_1 to x_t, $P_s = z_1z_2 \cdots z_s$, and $t \geq s + 2$. Let G be obtained from G_1 by identifying u with x_1 of G_2 and identifying v with z_1 of P_s and let $G' = G - \{vw_1, vw_2, \ldots, vw_k\} + \{x_2w_1, x_2w_2, \ldots, x_2w_k\}$. Then $H(G) < H(G')$.*

Corollary 5.5. [17] *Let G be a connected graph containing an edge uv such that $N_G(u) \setminus \{v\} = N_G(v) \setminus \{u\} \neq \phi$. Let $G(t, s)$ be obtained from G by attaching a path P_t at u and a path P_s at v. If $t \geq s + 2 \geq 3$, then $H(G(t, s)) < H(G(t - 1, s + 1))$.*

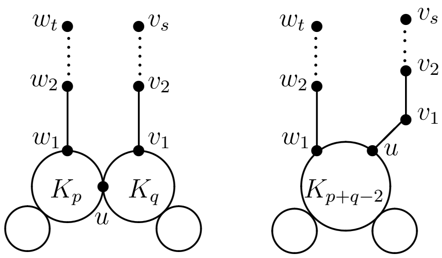

Figure 18. G and G' of Theorem 5.31.

The graphs G and G' of Fig. 18 possess the same number of cut vertices.

Theorem 5.26. [17] *Let K_puK_q be the graph obtained by identifying one vertex of K_p with one vertex of K_q at u, $p \geq 3$, $q \geq 3$. Let G be obtained from K_puK_q by attaching a path P_t at some vertex $w_1 \in V(K_p) \setminus \{u\}$ and a path P_s at some vertex $v_1 \in V(K_q) \setminus \{u\}$ and possibly attaching some connected graphs at vertices of $V(K_puK_q) \setminus \{u, v_1, w_1\}$ where $t \geq s \geq 1$ and let G' be obtained from G by deleting the edges of K_q incident to v_1 except v_1u and adding all possible edges between each of $V(K_q) \setminus \{v_1\}$ and each of $V(K_p)$ (see Fig. 18). Then $H(G) < H(G')$.*

Let $KP(n, k)$ be the graph obtained from K_{n-k} by attaching $n - k$ paths of almost equal lengths to its vertices respectively.

Theorem 5.27. [17] *Among all graphs with n vertices and k cut vertices, where $0 \leq k \leq n - 2$, the maximal Harary index is attained uniquely at the graph $KP(n, k)$.*

Theorem 5.28. [17]

$$H(K_n) = H(KP(n, 0)) > H(KP(n, 1)) > \cdots > H(KP(n, n-2)) = H(P_n).$$

Theorem 5.29. [17] *If a graph G of order $n \geq 3$ contains cut vertices or cut edges, then $H(G) \leq H(KP(n, 1))$, with equality holds if and only if $G \cong KP(n, 1)$.*

Theorem 5.30. [17] *Let $G_{n_1,n_2,n_3} = (K_{n_1} \cup K_{n_2}) \vee K_{n_3}$. If $n_1 \geq n_2 \geq 2$ and $n_3 \geq 1$, then $H(G_{n_1,n_2,n_3}) < H(G_{n_1+1,n_2-1,n_3})$.*

6. Haray index of graph operations

Das et al. [4] obtained the bounds for the Harary index of corona product and of Cartesian product.

Let G_1 be the graph with n_1 vertices and m_1 edges. Let G_2 be the graph with n_2 vertices and m_2 edges. The *corona product* $G_1 \circ G_2$ of G_1 and G_2 is obtained by taking one copy of G_1 and n_1 copies of G_2, and then joining i-th vertex of G_1 to every vertex of i-th copy of G_2, $i = 1, 2, \ldots, n_1$. The graph $G_1 \circ G_2$ has $n_1(n_2 + 1)$ vertices and $m_1 + n_1m_2 + n_1n_2$ edges.

Theorem 6.1. [4] *Let G_i be the graph with n_i vertices, m_i edges and diameter d_i, $i = 1, 2$. Let $G_1 \neq K_{n_1}$. Then the lower and upper bounds for $H(G_1 \circ G_2)$ are*

$$\begin{aligned} H(G_1 \circ G_2) \geq & \left[\frac{1}{W(G_1) - m_1} + \frac{n_2}{W(G_1) - 2m_1 + \frac{n_1(n_1-1)}{2}} \right. \\ & \left. + \frac{m_2^2}{W(G_1) - 3n_1 + n_1(n_1 - 1)} \right] \left(\frac{n_1(n_1 - 1)}{2} - m_1 \right)^2 \\ & + m_1 \left(1 + \frac{n_2}{2} + \frac{n_2^2}{3} \right) + \frac{1}{4}(n_2 + 3)n_1n_2 + \frac{1}{2}n_1m_2. \end{aligned}$$

Moreover,

$$H(G_1 \circ G_2) \le \left(\frac{n_1(n_1-1)}{2} - m_1\right)\left[\frac{2 + \left(\frac{n_1(n_1-1)}{2} - m_1 - 1\right)\left(\frac{d_1}{2} + \frac{2}{d_1}\right)}{2(W(G_1) - n_1)}\right.$$

$$+ \frac{n_2\left(2 + \left(\frac{n_1(n_1-1)}{2} - m_1 - 1\right)\left(\frac{d_1+1}{3} + \frac{3}{d_1+1}\right)\right)}{2\left(W(G_1) - 2m_1 + \frac{n_1(n_1-1)}{2}\right)}$$

$$\left. + \frac{n_2^2\left(2 + \left(\frac{n_1(n_1-1)}{2} - m_1 - 1\right)\left(\frac{d_1+2}{4} + \frac{4}{d_1+2}\right)\right)}{2(W(G_1) - 3m_1 + n_1(n_1-1))}\right]$$

$$+ m_1\left(1 + \frac{n_2}{2} + \frac{n_2^2}{3}\right) + \frac{1}{4}(n_2+3)n_1n_2 + \frac{1}{2}n_1m_2.$$

Equality holds in both cases if and only if $d_1 = 2$.

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 two vertices (u_i, v_j) and (u_k, v_l) are adjacent in $G_1 \times G_2$ if $u_i = u_k$ and v_j is adjacent to v_l in G_2 or $v_j = v_l$ and u_i is adjacent to u_k in G_1.

Theorem 6.2. [4] *Let G_i be the graph with n_i vertices, m_i edges and diameter d_i, $i = 1, 2$. Let $u_1, u_2, \ldots, u_{n_1}$ be the vertices of G_1. Then*

$$H(G_1 \times G_2) \ge n_1H(G_2) + n_2H(G_1) + n_2(n_2-1)\sum_{1 \le i < k \le n_1} \frac{1}{d_{G_1}(u_i, u_k) + d_2},$$

and

$$H(G_1 \times G_2) \le n_1H(G_2) + n_2H(G_1) + n_2(n_2-1)\sum_{1 \le i < k \le n_1} \frac{1}{d_{G_1}(u_i, u_k) + 1}.$$

Equality in both cases holds if and only if $G_2 \cong K_{n_2}$, a complete graph on n_2 vertices.

Interchanging G_1 and G_2, the Theorem 6.2 holds good, with equality if and only if $G_1 \cong K_{n_1}$.

Theorem 6.3. [4] *Let G_i be the connected graph with n_i vertices, m_i edges and diameter d_i, $i = 1, 2$. Let $G_i \ne K_{n_i}$. Then*

$$H(G_1 \times G_2) > n_1m_2 + n_2m_1 + \frac{n_2(n_2-1)m_1}{d_2+1} + \frac{\left(\frac{n_2(n_2-1)}{2} - m_2^2\right)n_1}{W(G_2) - m_2}$$

$$+ \left[\frac{n_2}{W(G_1) - m_1} + \frac{n_2(n_2-1)}{W(G_1) + \frac{n_1(n_1-1)}{2}d_2 - (d_2+1)m_1}\right]$$

$$\times \left(\frac{n_1(n_1-1)}{2} - m_1^2\right).$$

Moreover,

$$\begin{aligned} H(G_1 \times G_2) &< n_1 m_2 + n_2 m_1 + \frac{n_2(n_2-1)m_1}{2} \\ &+ \frac{n_1\left(\frac{n_2(n_2-1)}{2} - m_2\right)\left[2 + \left(\frac{n_2(n_2-1)}{2} - m_2\right)\left(\frac{d_2}{2} + \frac{2}{d_2}\right)\right]}{2(W(G_2) - m_2)} \\ &+ \left[\frac{n_2\left(2 + \left(\frac{n_1(n_1-1)}{2} - m_1 - 1\right)\left(\frac{d_1}{2} + \frac{2}{d_1}\right)\right)}{2(W(G_1) - m_1)}\right. \\ &+ \left.\frac{n_2(n_2-1)\left(2 + \left(\frac{n_1(n_1-1)}{2} - m_1 - 1\right)\left(\frac{d_1+1}{3} + \frac{3}{d_1+1}\right)\right)}{2\left(W(G_1) + \frac{n_1(n_1-1)}{2} - 2m_1\right)}\right] \\ &\times \left(\frac{n_1(n_1-1)}{2} - m_1\right). \end{aligned}$$

7. Nordhaus–Gaddum type results

In this section we report the Nordhaus-Gaddum [21] type results with respect to Harary index.

Theorem 7.1. [39] *Let G be a connected graph of order $n \geq 5$ and its complement $\overline{G}$ be the connected graph. Then*

$$1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1}\frac{1}{k} \leq H(G) + H(\overline{G}) \leq \frac{3n(n-1)}{4},$$

with left equality holds if and only if $G \cong P_n$ or $G \cong \overline{P_n}$ and with right equality holds if and only if both G and $\overline{G}$ have diameter 2.

Theorem 7.2. [6] *Let G be a connected graph of order $n \geq 2$ with a connected complement $\overline{G}$. If the graph G has diameter d, then*

$$H(G) + H(\overline{G}) \leq H(P_{d+1}) + \frac{3n(n-1)}{4} - \frac{d(d+3)}{4},$$

with equality holds if and only if both G and $\overline{G}$ have diameter 2 or $G \cong P_n$.

Since $H(P_n) < \frac{(n-1)(n+2)}{4}$, for $n > 4$, the upper bound in Theorem 7.2 is better than that in Theorem 7.1.

Theorem 7.3. [6] *Let G be a connected graph of order $n \geq 2$ with a connected complement $\overline{G}$. Denote by d and $\overline{d}$ the diameter of G and $\overline{G}$ respectively. Then*

$$H(G) + H(\overline{G}) \geq H(P_{k+1}) + \frac{n(n-1)}{2}\left(1 + \frac{1}{k}\right) - 3k + \frac{7}{2},$$

where $k = \max\{d,\ \overline{d}\}$. Moreover, the equality holds if and only if both G and $\overline{G}$ have diameter 2.

Theorem 7.4. [6] *Let G be a triangle and quadrangle free graph with $n \geq 2$ vertices, m edges and with a connected complement $\overline{G}$. Then*

$$H(G) + H(\overline{G}) \leq \frac{1}{6} M_1(G) + \frac{7n(n-1)}{12} + \frac{n(n-1)^2}{12} - \frac{m(n-1)}{3},$$

with equality holds if and only if both G and $\overline{G}$ have diameter at most 3.

Recall that the k^{th} power of a connected graph G is a graph G^k with vertex set $V(G^k) = V(G)$ such that two vertices are adjacent in G^k if and only if they are at distance at most k in G.

Theorem 7.5. [25] *Let G be a connected graph of order $n \geq 9$ and a connected complement $\overline{G}$. Then*

$$\binom{n}{2} + \sum_{j=1}^{n-1} \frac{n-j}{\lceil \frac{j}{k} \rceil} = H(P_n^k) + H(\overline{P_n}^k) \leq H(G^k) + H(\overline{G}^k) \leq n\binom{n}{2}.$$

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The Harmonic Index

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Contents

1. Introduction to the harmonic index

The topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index $R(G)$ [75] introduced by the chemist Milan Randić in 1975. There are many papers and a couple of books dealing with this index (see, e.g., [43, 57, 76] and the references therein).

During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors that resemble the original *Randić* *index*, which is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ denotes the degree of a vertex u of the graph G and uv the edge connecting the vertices u and v. Randić noticed that this index was well correlated with a variety of physico-chemical properties of alkanes: boiling point, enthalpy of formation, surface area, solubility in water, etc. Eventually, this index became one of the most successful molecular descriptors in structure property and structure activity relationship studies [40, 55, 56, 72], and scores of its pharmacological and chemical applications have been reported. Mathematical properties of this descriptor have also been studied extensively, as summarized Gutman [43, 57].

Two of the main successors of the Randić index are the *first and second Zagreb indices*, denoted by M_1 and M_2, respectively, and defined as

$$M_1(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big) = \sum_{u \in V(G)} d(u)^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

(see, e.g., [18, 42]). The Zagreb indices and their variants have been used to study molecular complexity and chirality whilst the overall Zagreb indices exhibit a potential applicability for deriving multilinear regression models. Various researchers also use the Zagreb indices in their QSPR and QSAR studies. Mathematical properties of the Zagreb indices were also subjects of several studies.

Other indices motivated in studying and predicting the properties of the molecules, are the *sum-connectivity index* $\chi(G)$ and the *general sum-connectivity index* $\chi_\alpha(G)$, proposed by Zhou and Trinajstić in [107, 108], and defined as

$$\chi(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^{-1/2}, \qquad \chi_\alpha(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^{\alpha},$$

where α is a real number. It has been found that the general sum-connectivity index and the Randić index correlate well between themselves and with the π-electronic energy of benzenoid hydrocarbons [64, 65]. Some mathematical properties of these indices were given in [30–33, 80, 107, 108].

In 1987 [36], Fajtlowicz introduced the *harmonic index* $H(G)$ of a graph G, defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

(Note that the harmonic index can be viewed as a particular case of the general sumconnectivity index, since $H(G) = 2\,\chi_{-1}(G)$.)

Although this quantity was first mentioned in a mathematical paper [36] in 1987, it did not attract the attention of scholars until quite recently. In the last few years, a remarkably large number of studies of the properties of the harmonic index have appeared (see, e.g., [24, 63, 94, 95, 97, 100, 101, 104, 109]). The chemical applicability of the harmonic index was also recently investigated [39, 48]. The harmonic index has reasonably good correlation abilities; in fact, it gives similar correlations with physical and chemical properties compared with the well-known Randić index.

Finding bounds for indices of a given class of graphs, as well as related problem of finding the graphs with extremal indices, attracted the attention of many researchers, and many results have been obtained. In particular, estimating bounds for $H(G)$ are of great interest, and many results have been obtained. For example, Favaron, Mahéo and Saclé [37] considered the relationship between the harmonic index and the eigenvalues of graphs, and Zhong and Xu [100, 101, 104] determined the minimum and maximum values of the harmonic index for connected graphs, trees, unicyclic graphs, and bicyclic graphs, and characterized the corresponding extremal graphs, respectively. It turns out that trees with maximum and minimum harmonic index are the path P_n and the star S_n, respectively.

Ilić [53] and Xu [97] independently proved an inequality involving the harmonic index and the first Zagreb index.

Estrada, Torres and Rodríguez [35] introduced the atom-bond connectivity (ABC) index, which has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. Zhong and Xu [105] have recently shown a relationship between $H(G)$ and $ABC(G)$.

Chang and Zhu [13] found the minimum values of the harmonic index for graphs with minimum degree at least two and for triangle-free graphs with minimum degree at least k $(k \geq 1)$, and characterized the corresponding extremal graphs. Moreover, Wu, Tang and Deng [94, 95] also considered the relation between the harmonic index and the girth of a graph.

Deng, Balachandran, Ayyaswamy and Venkatakrishnan considered the relation connecting the harmonic index $H(G)$ and the chromatic number $\chi^*(G)$ and proved that $\chi^*(G) \leq 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index [24]. (This inequality strengthens a result relating the Randić index and the chromatic number conjectured by the system AutoGraphiX and proved by Hansen and Vukicević [51].) The same authors in [25] determined the trees with the second-the sixth maximum harmonic indices, unicyclic graphs with the second-the fifth maximum harmonic indices, and bicyclic graphs with the first-the fourth maximum harmonic indices.

Li and Shiu [59] studied the harmonic index subject to perturbations and provided a simpler method for determining unicyclic graphs with maximum and minimum harmonic index among all unicyclic graphs. Another important work from the numerical point of view is developed by Lv and Li [66] which study the relationship between the harmonic index and the matching number for trees, and determine the trees with minimum harmonic index among trees with a perfect matching. Also they study the same relationship for unicyclic graphs. The graphs with minimum harmonic index among all unicyclic graphs with a perfect matching and with a given matching number are determined in [67].

Liu [60] proposed a conjecture concerning the relation between the harmonic index and the diameter of a connected graph, and showed that the conjecture is true for trees. Likewise Deng, Tang and Zhang [26] considered the harmonic index $H(G)$ and the radius $r(G)$ and strengthened some results relating the Randić index and the radius in [61, 99].

The two next sections contain bounds for the harmonic index involving other topological indices and some important parameters of graphs, respectively. The last section deals with some inequalities involving the natural generalization of the harmonic index: the general sum-connectivity index. We have included the results that we believe are the most important. Other results can be found in the bibliography at the end of the chapter.

Notations. Throughout this work, $G = (V(G), E(G))$ denotes a (nonoriented) finite simple (without multiple edges and loops) nontrivial ($E(G) \neq \emptyset$) graph. In many cases, we deal with connected graphs. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \dots, G_r$, then $H(G) = H(G_1) + \cdots + H(G_r)$. Furthermore, every molecular graph is connected.

We use S_n, P_n and K_n to denote the star, the path and the complete graph with n vertices, respectively. K_{n_1,n_2} will denote the complete bipartite graph.

If G_1 and G_2 are isomorphic graphs, then we write $G_1 \cong G_2$.

2. Relations between the harmonic index and other topological indices

2.1 Inequalities relating the harmonic and the Randić indices

Among the topological indices based on end-vertex degrees of edges, probably, the best known such descriptor is the Randić connectivity index $R(G)$ [75] introduced by the chemist Milan Randić in 1975. This index became one of the most successful molecular descriptors in structure property and structure activity relationship studies [40, 55, 56, 72, 76], and scores of its pharmacological and chemical applications have been reported. Mathematical properties of this descriptor have also been studied extensively, see [43, 57].

The following result provides bounds for the harmonic index by using the Randić index [105, Theorem 3.1]. The upper bound was proved before in [97, Theorem 2.1] for the case of connected graphs.

Theorem 2.1. *[105, Theorem 3.1] If G is a nontrivial graph with n vertices, then*

$$\frac{2\sqrt{n-1}}{n} R(G) \leq H(G) \leq R(G).$$

The lower bound is attained if and only if $G \cong S_n$, and the upper bound is attained if and only if all connected components of G are regular.

Proof. Let us consider the function

$$f(x,y) = \frac{\dfrac{2}{x+y}}{\dfrac{1}{\sqrt{xy}}} = \frac{2\sqrt{xy}}{x+y}$$

with $1 \leq x \leq y \leq n-1$. Since

$$\frac{\partial f(x,y)}{\partial x} = \frac{\sqrt{y}\,(y-x)}{\sqrt{x}\,(x+y)^2} \geq 0 \qquad \textit{and} \qquad \frac{\partial f(x,y)}{\partial y} = \frac{\sqrt{x}\,(x-y)}{\sqrt{y}\,(x+y)^2} \leq 0,$$

we have $f(x, y)$ is strictly increasing in x and strictly decreasing in y. Hence, the minimum value of $f(x, y)$ is attained for $(x, y) = (1, n-1)$, and the maximum value is attained for $x = y$ (for each $1 \le x \le n-1$). Thus,

$$\frac{2\sqrt{n-1}}{n} = f(1, n-1) \le f(x, y) \le f(x, x) = 1.$$

Fix $uv \in E(G)$. By the symmetry between u and v, we can assume that $1 \le d(u) \le d(v) \le n-1$. Consequently,

$$\frac{2\sqrt{n-1}}{n} \le \frac{H(G)}{R(G)} \le 1,$$

with the left equality if and only if $(d(u), d(v)) = (1, n-1)$ for every $uv \in E(G)$, and the right equality if and only if $d(u) = d(v)$ for every $uv \in E(G)$. This proves the theorem. ■

The argument in the proof of Theorem 2.1 allows to obtain the following improvement.

Theorem 2.2. *If G is a nontrivial graph with maximum degree Δ and minimum degree δ, then*

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} R(G) \le H(G) \le R(G).$$

The lower bound is attained if and only if one vertex has degree Δ and the other vertex has degree δ for every edge of G, and the upper bound is attained if and only if all connected components of G are regular.

2.2 Relations between harmonic and Zagreb indices

Recall that the *first Zagreb index* [18, 42] of a graph G is defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{uv \in E(G)} \big(d(u) + d(v)\big).$$

The Zagreb indices and their variants have been used to study molecular complexity and chirality whilst the overall Zagreb indices exhibit a potential applicability for deriving multilinear regression models. Various researchers also use the Zagreb indices in their QSPR and QSAR studies. Mathematical properties of the Zagreb indices were also subjects of several studies.

Ilić and Xu independently proved the following inequality involving the harmonic and the first Zagreb indices.

Theorem 2.3. *[53] [97, Theorem 2.5] Let G be a graph with $m \ge 1$ edges. Then*

$$H(G) \ge \frac{2m^2}{M_1(G)}$$

with equality if and only if $d(u) + d(v)$ is a constant for every $uv \in E(G)$.

Proof. Using the formula $M_1(G) = \sum_{uv\in E(G)}(d(u) + d(v))$ and the Cauchy-Schwarz inequality, we have

$$\Big(\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}\Big)\Big(\sum_{uv\in E(G)} \frac{d(u)+d(v)}{2}\Big) \geq \Big(\sum_{uv\in E(G)} 1\Big)^2 = m^2$$

or, equivalently,

$$H(G) \geq \frac{2m^2}{M_1(G)}$$

with equality if and only if $d(u) + d(v)$ is a constant for each $uv \in E(G)$. ■

Denote by $\overline{M}_1(G) = \sum_{uv\notin E(G)}(d(u) + d(v))$ the *first Zagreb coindex* [5, 29]. This invariant was formally introduced in [29] in the hope that it will improve our ability to quantify the contributions of pairs of non-adjacent vertices to various properties of molecules. Furthermore, it allowed to obtain more compact expressions for the vertex-weighted Wiener polynomials of some composite graphs.

Lemma 2.4. *[20, Lemma 3] Let G be a nontrivial graph with n vertices and m edges. Then $\overline{M}_1(G) + M_1(G) = 2m(n-1)$.*

Theorem 2.3 and Lemma 2.4 have the following consequence.

Corollary 2.1. *[97, Corollary 2.1] Let G be a nontrivial graph with n vertices and m edges. Then*

$$H(G) \geq \frac{2m^2}{2m(n-1) - \overline{M}_1(G)}$$

with equality if and only if $d(u) + d(v)$ is a constant for each $uv \in E(G)$.

In order to obtain bounds for $H(G)$, we need the following classical result, known as Polya-Szegö inequality (see [50, p.62]).

Lemma 2.5. *If $0 < n_1 \leq a_j \leq N_1$ and $0 < n_2 \leq b_j \leq N_2$ for $1 \leq j \leq k$, then*

$$\Big(\sum_{j=1}^{k} a_j^2\Big)^{1/2}\Big(\sum_{j=1}^{k} b_j^2\Big)^{1/2} \leq \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)\Big(\sum_{j=1}^{k} a_jb_j\Big).$$

Theorem 2.6. *If G is a nontrivial graph with $m \geq 1$ edges, maximum degree Δ and minimum degree δ, then*

$$H(G) \leq \frac{(\Delta+\delta)^2 m^2}{2\Delta\delta M_1(G)}$$

and the equality is attained if G is regular.

Proof. Since

$$\sqrt{\delta} \leq \sqrt{\frac{d(u)+d(v)}{2}} \leq \sqrt{\Delta}, \qquad \frac{1}{\sqrt{\Delta}} \leq \sqrt{\frac{2}{d(u)+d(v)}} \leq \frac{1}{\sqrt{\delta}},$$

Lemma 2.5 gives

$$H(G)\,\frac{M_1(G)}{2} = \Big(\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}\Big)\Big(\sum_{uv\in E(G)} \frac{d(u)+d(v)}{2}\Big)$$
$$\leq \frac{(\Delta+\delta)^2}{4\Delta\delta}\Big(\sum_{uv\in E(G)} 1\Big)^2 = \frac{(\Delta+\delta)^2}{4\Delta\delta} m^2,$$

and the inequality holds.

If the graph G is regular (i.e., $\Delta = \delta$), then $H(G) = \frac{m}{\Delta}$, $M_1(G) = 2\Delta m$, and we have the equality.
■

2.3 Inequalities relating the harmonic and the sum–connectivity indices

Recall that the *sum-connectivity index* $\chi(G)$ is defined as

$$\chi(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{-1/2},$$

It has been found that the sum-connectivity index correlates well with the π-electronic energy of benzenoid hydrocarbons [64,65]. Some mathematical properties of this index were given in [30–32,80,107].

In this section, we present some inequalities relating the harmonic index and the sumconnectivity index.

Theorem 2.7. *[105, Theorem 4.1] If G is a connected graph with $n \geq 3$ vertices, then*

$$\sqrt{\frac{2}{n-1}}\,\chi(G) \leq H(G) \leq \frac{2}{\sqrt{3}}\,\chi(G).$$

The lower bound is attained if and only if $G \cong K_n$, and the upper bound is attained if and only if $G \cong P_3$.

Proof. Let us define the function

$$f(x,y) = \frac{\frac{2}{x+y}}{\frac{1}{\sqrt{x+y}}} = \frac{2}{\sqrt{x+y}}$$

with $1 \leq x \leq y \leq n-1$ and $y \geq 2$. Since $f(x,y)$ is strictly decreasing in both x and y, the minimum value of $f(x,y)$ is $f(n-1,n-1)$, and the maximum value of $f(x,y)$ is $f(1,2)$. Hence,

$$\sqrt{\frac{2}{n-1}} = f(n-1,n-1) \leq f(x,y) \leq f(1,2) = \frac{2}{\sqrt{3}}.$$

Fix $uv \in E(G)$. By symmetry, we can assume that $1 \leq d(u) \leq d(v) \leq n-1$. Since G is a connected graph with $n \geq 3$ vertices, we have $d(v) \geq 2$. Thus,

$$\sqrt{\frac{2}{n-1}} \leq \frac{H(G)}{\chi(G)} \leq \frac{2}{\sqrt{3}}.$$

The left equality holds if and only if $(d(u),d(v)) = (n-1,n-1)$ for every $uv \in E(G)$, and the right equality holds if and only if $(d(u),d(v)) = (1,2)$ for every $uv \in E(G)$. This finishes the proof. ■

If the graph G has minimum degree $\delta \geq 2$, then we can improve the upper bound in Theorem 2.7.

Corollary 2.2. *[105, Corollary 4.2] Let G be a connected graph with minimum degree at least $k \geq 2$. Then*

$$H(G) \leq \sqrt{\frac{2}{k}}\,\chi(G)$$

with equality if and only if G is a k-regular graph.

Theorem 2.7 and Corollary 2.2 can be generalized as follows.

Corollary 2.3. *Let G be a graph with maximum degree Δ and minimum degree $\delta \geq 2$. Then*

$$\sqrt{\frac{2}{\Delta}}\,\chi(G) \leq H(G) \leq \sqrt{\frac{2}{\delta}}\,\chi(G).$$

Each bound is attained if and only if G is a regular graph.

Let G be any nontrivial graph. Denote by $m_{i,j}$ the number of edges connecting a vertex of degree i with a vertex of degree j in G. If $f(x, y)$ is a symmetric function, then the vertex-degree based topological index

$$F(G) = \sum_{uv \in E(G)} f(d(u), d(v))$$

can be written as

$$F(G) = \sum_{1 \leq i \leq j \leq n-1} f(i, j)\, m_{i,j}.$$

If the equality $m_{1,2} = 0$ holds for a graph G, then we can improve the upper bound in Theorem 2.7 in the following way.

Theorem 2.8. *[82, Corollary 4] Let G be a connected graph with $n \geq 3$ vertices and $m_{1,2} = 0$. Then*

$$H(G) \leq \chi(G)$$

with equality if and only if $G \cong S_4$ or $G \cong C_n$.

Proof. We can write

$$H(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{2m_{i,j}}{i+j}, \qquad \chi(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{m_{i,j}}{\sqrt{i+j}},$$

and so

$$H(G) - \chi(G) = \sum_{1 \leq i \leq j \leq n-1} \left(\frac{2}{i+j} - \frac{1}{\sqrt{i+j}} \right) m_{i,j}.$$

Since $m_{1,1} = m_{1,2} = 0$, it suffices to consider $1 \leq i \leq j \leq n-1$ with $i + j \geq 4$. We have

$$\frac{2}{i+j} - \frac{1}{\sqrt{i+j}} \leq 0 \quad \Leftrightarrow \quad i + j \geq 4.$$

Hence, $H(G) \leq \chi(G)$ with equality if and only if $G \cong S_4$ or $G \cong C_n$. ■

The argument in the proof of Theorem 2.8 has the following consequence.

Corollary 2.4. *[82, Corollary 6] Let G be a connected graph with $n \geq 3$ vertices and $d(u) + d(v) \leq 4$ for any $uv \in E(G)$. Then*

$$H(G) \geq \chi(G)$$

with equality if and only if $G \cong S_4$ or $G \cong C_n$.

2.4 Inequalities relating the harmonic and the ABC indices

The *atom-bond connectivity index* of a nontrivial graph G, denoted by $ABC(G)$, is defined [17, 23, 45, 46, 96] as

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

In the paper [48], the atom-bond connectivity index appears as the second-best vertex-degree-based molecular structure-descriptor. Consequently, this index is useful in designing quantitative structureproperty relations.

Theorem 2.9. *[49, Proposition 1] Let G be a graph with $n \geq 3$ vertices. Then*

$$\frac{3\sqrt{2}}{4} H(G) \leq ABC(G) \leq \gamma\, H(G),$$

where

$$\gamma = \begin{cases} \sqrt{2n-4} & if \quad 3 \leq n \leq 6, \\ \dfrac{n}{2}\sqrt{\dfrac{n-2}{n-1}} & if \quad n \geq 7. \end{cases}$$

The lower bound is attained if and only if every connected component of G is isomorphic to P_3. If $3 \leq n \leq 6$ (respectively, $n \geq 7$), then the equality in the upper bound holds if and only if $G \cong K_n$ (respectively, $G \cong S_n$).

Proof. Fix $uv \in E(G)$. By symmetry, we may assume that $1 \leq d(u) \leq d(v) \leq n-1$. Since G is a connected graph with $n \geq 3$ vertices, we have $d(v) \geq 2$.

Let us define the function

$$Q(x, y) = \frac{\sqrt{\dfrac{x+y-2}{xy}}}{\dfrac{2}{x+y}} = \frac{x+y}{2}\sqrt{\frac{x+y-2}{xy}}$$

with $1 \leq x \leq y \leq n-1$ and $y \geq 2$. Since

$$\frac{\partial Q(x, y)}{\partial y} = \frac{x(y+2) + y^2 - x^2 + y(y-2)}{4y\sqrt{xy(x+y-2)}} > 0,$$

$Q(x, y)$ is strictly increasing in y. Hence, the minimum value of $Q(x, y)$ is either $Q(1, 2)$ or $Q(2, 2)$, and its maximum value is $Q(x, n-1)$ for some $1 \leq x \leq n-1$, which still needs to be determined.

Since

$$Q(1,2)=\frac{3\sqrt{2}}{4}<\sqrt{2}=Q(2,2),$$

Q attains its minimum value for $(x,y)=(1,2)$. Therefore, $\frac{ABC(G)}{H(G)}\geq\frac{3\sqrt{2}}{4}$ with equality if and only if $(d(u),d(v))=(1,2)$ for every $uv\in E(G)$, i.e., every connected component of G is isomorphic to P_3.

Let us consider the function

$$Q(x,n-1)=\frac{x+n-1}{2}\sqrt{\frac{x+n-3}{(n-1)x}}.$$

Thus,

$$\frac{dQ(x,n-1)}{dx}=\frac{2x^2+(n-3)x-(n-1)(n-3)}{4x\sqrt{(n-1)x(x+n-3)}}.$$

Note that the roots of $2x^2+(n-3)x-(n-1)(n-3)=0$ are

$$x=\frac{-(n-3)\pm\sqrt{(n-3)(9n-11)}}{4}.$$

If $n=3$ or $n=4$, then $\frac{dQ(x,n-1)}{dx}>0$ for $x\in(1,n-1]$. Hence, $Q(x,n-1)$ is strictly increasing in x, and the maximum value of $Q(x,y)$ is $Q(n-1,n-1)=\sqrt{2n-4}$. If $n\geq 5$, then $Q(x,n-1)$ is strictly decreasing in

$$1\leq x\leq\frac{-(n-3)+\sqrt{(n-3)(9n-11)}}{4},$$

and strictly increasing in

$$\frac{-(n-3)+\sqrt{(n-3)(9n-11)}}{4}\leq x\leq n-1.$$

Then the maximum value of $Q(x,n-1)$ is

$$\begin{aligned}\max\left\{Q(1,n-1),Q(n-1,n-1)\right\}&=\max\left\{\frac{n}{2}\sqrt{\frac{n-2}{n-1}},\sqrt{2n-4}\right\}\\&=\begin{cases}\sqrt{2n-4} & if \quad n=5,6,\\ \frac{n}{2}\sqrt{\frac{n-2}{n-1}} & if \quad n\geq 7.\end{cases}\end{aligned}$$

Therefore, if $3\leq n\leq 6$, then $\frac{ABC(G)}{H(G)}\leq\sqrt{2n-4}$ with equality if and only if $(d(u),d(v))=(n-1,n-1)$ for every $uv\in E(G)$, i.e., $G\cong K_n$. If $n\geq 7$, then

$$\frac{ABC(G)}{H(G)}\leq\frac{n}{2}\sqrt{\frac{n-2}{n-1}}$$

with equality if and only if $(d(u),d(v))=(1,n-1)$ for every $uv\in E(G)$, i.e., $G\cong S_n$. ■

Similarly, we can improve the lower bound in Theorem 2.9 by Corollary 2.2 and [105, Corollary 6.2].

Corollary 2.5. *[105, Corollary 7.2] Let G be a connected graph with minimum degree at least $k \geq 2$. Then*

$$\sqrt{2k-2}\, H(G) \leq ABC(G)$$

with equality if and only if G is a k-regular graph.

Molecular graphs

A nontrivial connected graph with maximum degree at most four is a *molecular graph* representing hydrocarbons [90].

Let us recall the definition of the function

$$Q(x,y) = \frac{\sqrt{\dfrac{x+y-2}{xy}}}{\dfrac{2}{x+y}} = \frac{x+y}{2}\sqrt{\frac{x+y-2}{xy}}. \tag{1}$$

In the case of molecular graphs, the analysis of the relation between the harmonic and ABC indices is much simpler, since in these graphs we have just nine different types of edges. The respective Q-values are given in Table I.

The argument in the proof of Theorem 2.9 and the values from Table I allow to obtain the following result.

Proposition 2.10. *[49, Proposition 2] Let G be any molecular graph with $n > 2$ vertices. Then*

$$Q(1,2)H(G) \leq ABC(G) \leq Q(4,4)H(G),$$

where the values of $Q(i,j)$ are given in Table I. The equality $ABC(G) = Q(1,2)H(G)$ occurs if and only if G is the molecular graph of propane. In the case of ordinary molecular graphs, the equality $ABC(G) = Q(4,4)H(G)$ is not possible, but could be satisfied if G is the graph representation of a diamond-like nanostructure [27, 28].

For benzenoid systems, in which only (2,2)-, (2,3)- and (3,3)-type edges occur (i.e., the only non-zero multipliers are $m_{2,2}, m_{2,3}, m_{3,3}$) [15, 44, 73, 74], the following special case of Proposition 2.10 holds.

Proposition 2.11. *[49, Proposition 3] Let G be the molecular graph of a benzenoid system. Then*

$$Q(2,2)H(G) \leq ABC(G) \leq Q(3,3)H(G),$$

where the values of $Q(i,j)$ are given in Table I. The equality $ABC(G) = Q(2,2)H(G)$ occurs if and only if G is the molecular graph of benzene. The equality $ABC(G) = Q(3,3)H(G)$ occurs in the cases of nanotubes and nanotoruses, as well as fullerenes [27, 28].

TABLE I. The values of the auxiliary function Q in (1), for all possible edge-types that may occur in molecular graphs; i, j are the degrees of the end-vertices of the respective edges.

i, j	$Q(i, j)$
1,2	1.061
1,3	1.633
1,4	2.165
2,2	1.414
2,3	1.768
2,4	2.121
3,3	2.000
3,4	2.259
4,4	2.449

2.5 Relations between harmonic and geometric–arithmetic indices

The *first geometric-arithmetic index* GA_1 was introduced by Vukicević and Furtula in [92] as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{\frac{1}{2}(d(u) + d(v))}.$$

Although GA_1 was introduced in 2009, there are many papers dealing with this index (see, e.g., [19, 21, 22, 77–79, 92] and the references therein). The GA_1 index gives better correlation coefficients than Randić index for the properties of octanes, but the differences between them are not significant. However, the predicting ability of the GA_1 index compared with Randić index is reasonably better (see [21, Table 1]). Furthermore, the graphic in [21, Fig.7] (from [21, Table 2], [89]) shows that there exists a good linear correlation between GA_1 and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972). Hence, one can think that GA_1 index should be considered in the QSPR/QSAR researches.

In this section, we include some relations between the harmonic index and the first geometric-arithmetic index.

Theorem 2.12. *[82, Corollaries 1 and 2] Let G be a connected graph with $n \geq 2$ vertices. Then*

$$\frac{GA_1(G)}{n-1} \leq H(G) \leq GA_1(G). \tag{2}$$

The first equality occurs if and only if $G \cong K_n$. The second equality occurs if and only if $G \cong K_2$.

Proof. For any $uv \in E(G)$ we have $1 \leq d(u)d(v) \leq (n-1)^2$. Consequently,

$$\frac{1}{n-1} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)} \leq \frac{2}{d(u) + d(v)} \leq \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

and

$$\frac{GA_1(G)}{n-1} \leq H(G) \leq GA_1(G). \tag{3}$$

The first equality occurs if and only if $d(u) = d(v) = n-1$ for any $uv \in E(G)$, which implies $G \cong K_n$. The second equality occurs if and only if $d(u) = d(v) = 1$ for any $uv \in E(G)$, which implies $G \cong K_2$. ∎

By using the inequalities $\delta^2 \le d(u)d(v) \le \Delta^2$ in the argument in the proof of Theorem 2.12, we obtain the following improvement.

Theorem 2.13. *[77, Proposition 3.9] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ. Then*

$$\frac{GA_1(G)}{\Delta} \le H(G) \le \frac{GA_1(G)}{\delta} \tag{4}$$

and the equality in each inequality is attained if and only if G is regular.

Theorem 2.14. *[80, Theorem 2.23] Let G be a nontrivial graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$H(G) + \frac{1}{\sqrt{\Delta\delta}}\, GA_1(G) \le \frac{2m}{\delta},$$

and the equality holds if and only if G is regular.

Proof. Note that $\big(\sqrt{d(u)} - \sqrt{\delta}\,\big)\big(\sqrt{\Delta} - \sqrt{d(v)}\,\big) \ge 0$. Therefore,

$$\sqrt{\Delta}\,\big(\sqrt{d(u)} + \sqrt{d(v)}\,\big) \ge \sqrt{\Delta}\,\sqrt{d(u)} + \sqrt{\delta}\,\sqrt{d(v)} \ge \sqrt{d(u)d(v)} + \sqrt{\Delta\delta}.$$

Since $\sqrt{d(w)} \le d(w)/\sqrt{\delta}$ for every vertex $w \in V(G)$, we obtain

$$\begin{aligned}
\sqrt{d(u)d(v)} + \sqrt{\Delta\delta} &\le \sqrt{\frac{\Delta}{\delta}}\,(d(u)+d(v)),\\
\frac{1}{\sqrt{\Delta\delta}}\,\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)} + \frac{2}{d(u)+d(v)} &\le \frac{2}{\delta},\\
H(G) + \frac{1}{\sqrt{\Delta\delta}}\, GA_1(G) &\le \frac{2m}{\delta}.
\end{aligned}$$

If the graph is regular, then $GA_1(G) = m$ and $H(G) = m/\delta$, and the equality holds. If the equality is attained, then $\sqrt{d(w)} = d(w)/\sqrt{\delta}$ for every vertex $w \in V(G)$; thus, $d(w) = \delta$ for every $w \in V(G)$ and G is regular. ∎

The argument in the proof of Theorem 2.1 has the following useful consequence.

Lemma 2.15. *Let f be the function $f(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then $\frac{2\sqrt{ab}}{a+b} \le f(x,y) \le 1$. The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$.*

We need the following particular case of Jensen's inequality.

Lemma 2.16. *If f is a convex function in an interval I and $x_1, \dots, x_m \in I$, then*

$$f\Big(\frac{x_1 + \cdots + x_m}{m}\Big) \le \frac{1}{m}\,\big(f(x_1) + \cdots + f(x_m)\big).$$

Recall that a (Δ,δ)-*biregular graph* is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ.

Theorem 2.17. *Let G be a nontrivial graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$H(G) \geq \frac{2\sqrt{\delta}\, m^2}{\sqrt{\Delta}\,(\Delta+\delta) GA_1(G)}$$

and the equality holds if and only if G is regular.

Proof. Since $f(x) = 1/x$ is a convex function in $\mathbb{R}_+$, Lemma 2.16 gives

$$\frac{m}{\sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}} \leq \frac{1}{m} \sum_{uv\in E(G)} \frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}} \frac{d(u)+d(v)}{2} \frac{2}{d(u)+d(v)},$$

Lemma 2.15 and the inequality $d(u)+d(v) \leq 2\Delta$ give

$$\frac{m^2}{GA_1(G)} \leq \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\, \Delta H(G),$$

and we obtain the desired inequality.

If the graph is regular, then $H(G) = m/\Delta$, $GA_1(G) = m$ and we have the equality. If the equality holds, then $d(u) = d(v) = \Delta$ for every $uv \in E(G)$; hence, G is regular. ∎

2.6 Relations between harmonic and modified Narumi–Katayama indices

The *modified Narumi-Katayama index*

$$NK^*(G) = \prod_{u\in V(G)} d(u)^{d(u)} = \prod_{uv\in E(G)} d(u)d(v)$$

is introduced in [41], inspired in the Narumi-Katayama index defined in [70].

Next, we prove an inequality relating the harmonic and the modified Narumi-Katayama indices.

Theorem 2.18. *[80, Theorem 2.22] Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$H(G) \geq \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\, m\, NK^*(G)^{-1/(2m)}$$

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

Proof. Using Lemma 2.15 and the fact that the geometric mean is at most the arithmetic mean, we obtain

$$\begin{aligned}\frac{1}{m} H(G) &= \frac{1}{m} \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)} \geq \frac{1}{m} \sum_{uv\in E(G)} \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \frac{1}{\sqrt{d(u)d(v)}} \\ &\geq \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \Big(\prod_{uv\in E(G)} (d(u)d(v))^{-1/2} \Big)^{1/m} = \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} NK^*(G)^{-1/(2m)}.\end{aligned}$$

If the graph is regular or biregular, then $H(G) = 2m/(\Delta+\delta)$, $NK^*(G) = (\Delta\delta)^m$ and we have the equality.

If the equality holds, then we have $d(u) = \delta$ and $d(v) = \Delta$ or vice versa for every $uv \in E(G)$; hence, G is regular or biregular. ∎

3. General bounds for the harmonic index

Theorem 2.1 allows to obtain a well-known upper bound for the harmonic index in terms of n (see also [63, Theorem 2.2]).

Theorem 3.1. *Let G be a nontrivial graph with n vertices. Then*

$$H(G) \le \frac{n}{2}$$

with equality if and only if G contains no isolated vertices and all connected components of G are regular.

Proof. Theorem 2.1 gives

$$H(G) \le R(G) \le \frac{n}{2}$$

with equalities if and only if G contains no isolated vertices and all connected components of G and $\overline{G}$ are regular. ■

There are several results studying how the harmonic index behaves when the graph is subject to perturbations (see Theorems 3.2, 3.6 and 3.29). The first one deals with the behavior of the harmonic index when we join two pendent paths.

Theorem 3.2. *[53, Theorem 3.1] 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 the vertex w pendent paths $P = wv_1v_2 \dots v_p$ and $Q = wu_1u_2 \dots u_q$ of lengths p and q, respectively. If $p, q > 0$, then*

$$H(G(p,q)) < H(G(p+q,0)).$$

Proof. By symmetry, we can assume that $p \ge q > 0$. Since G is a nontrivial connected graph, we have $x = d(w) > 2$, and after transformation the vertex degree of w decreases by one and the weights of the edges in G either remain the same or decrease (the later are the edges adjacent to w). We will consider the difference $\Delta = H(G(p+q,0)) - H(G(p,q))$ in three cases.

Case 1. $p = q = 1$.

$$\Delta > \frac{1}{x+1} + \frac{1}{3} - \frac{1}{x+1} - \frac{1}{x+1} = \frac{1}{3} - \frac{1}{x+1} > 0.$$

Case 2. $p > q = 1$.

$$\Delta > \frac{1}{x+1} + \frac{1}{3} + \frac{p-1}{4} - \frac{1}{x+1} - \frac{1}{x+2} - \frac{p-2}{4} - \frac{1}{3} = \frac{1}{4} - \frac{1}{x+2} > 0.$$

Case 3. $p \ge q > 1$.

$$\Delta > \frac{1}{x+1} + \frac{1}{3} + \frac{p+q-2}{4} - \frac{2}{x+2} - \frac{p+q-4}{4} - \frac{2}{3} = \frac{1}{6} - \frac{2}{x+2} + \frac{1}{x+1} > 0.$$

This completes the proof. ■

By repetitive application of this transformation on branching vertices that are on the largest distance from the center of T, we have the following consequence, that improves Theorem 3.1 for trees.

Corollary 3.1. *[53, Corollary 3.2] Let T be a tree with $n \geq 3$ vertices. Then*

$$H(T) \leq \frac{4}{3} + \frac{n-3}{2}$$

with equality if and only if $T \cong P_n$.

This corollary generalizes [101, Theorem 2], by including the case $n = 3$, and provides a shorter proof.

Theorem 3.1 has the following direct consequence (see also [52, Theorem 6] and [100, Theorem 2]).

Corollary 3.2. *Let G be a connected unicyclic graph with $n \geq 3$ vertices. Then*

$$H(G) \leq \frac{n}{2}$$

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

Theorem 3.1 can be improved for bicyclic graphs.

Let us denote by $\mathcal{B}_n$ the set of bicyclic graphs obtained from C_n by adding an edge between two non-adjacent vertices, and by $\mathcal{B}'_n$ the set of bicyclic graphs with n vertices obtained by connecting two disjoint cycles by means of a new edge.

Theorem 3.3. *[52, Theorem 7] [109, Theorem 2.2] Let G be a connected bicyclic graph with $n \geq 4$ vertices. Then*

$$H(G) \leq \frac{n}{2} - \frac{1}{15}$$

with equality if and only if $G \in \mathcal{B}_n \cup \mathcal{B}'_n$.

Recall that Theorem 2.3 gives the inequality

$$H(G) \geq \frac{2m^2}{M_1(G)}$$

with equality if and only if $d(u) + d(v)$ is a constant for every $uv \in E(G)$.

There are many upper bounds for the first Zagreb index, from which we may deduce lower bounds for the harmonic index by Theorem 2.3. The next three examples appear in [105].

Corollary 3.3. *Let G be a graph with $m \geq 1$ edges containing no isolated vertices. Then*

$$H(G) \geq \frac{2m}{m+1}$$

with equality if and only if $G \cong S_{m+1}$ or $G \cong K_3$.

Proof. For each $uv \in E(G)$, we have $d(u) + d(v) \leq m + 1$ with equality if and only if every other edge of G is adjacent to the edge uv. Then

$$M_1(G) \leq \sum_{uv \in E(G)} (m + 1) = m(m + 1),$$

and thus Theorem 2.3 gives

$$H(G) \geq \frac{2m}{m + 1}$$

with equality if and only if G has no two independent edges, i.e., $G \cong S_{m+1}$ or $G \cong K_3$. ■

The distance, $d(u, v)$, between two vertices u and v in a graph G is the number of edges in a shortest path connecting them. We denote by $D(G)$ the diameter of graph G, i.e., $D(G) := \max\{d(u, v) \,|\, u, v \in V(G)\}$.

Corollary 3.4. *Let G be a triangle-free and quadrangle-free graph with n vertices and $m \geq 1$ edges. Then*

$$H(G) \geq \frac{2m^2}{n(n - 1)}$$

with equality if and only if $G \cong S_n$ or G is a Moore graph of diameter 2.

Proof. We have $M_1(G) \leq n(n - 1)$ with equality if and only if $G \cong S_n$ or G is a Moore graph of diameter 2 [106], and thus Theorem 2.3 gives the result. ■

Corollary 3.5. *Let G be a graph with n vertices, $m \geq 1$ edges, maximum degree Δ and minimum degree δ. Then*

$$H(G) \geq \frac{2m^2}{2m(\Delta + \delta) - n\Delta\delta}$$

with equality if and only if one vertex has degree Δ and the other vertex has degree δ for every edge of G.

Proof. $M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$ with equality if and only if G has only two types of degrees Δ and δ [16], and thus Theorem 2.3 gives the result. ■

Proposition 3.4. *[53] Let G be a graph such that $d(u) + d(v) \leq n$ for all edges $uv \in E(G)$. Then*

$$H(G) \geq \frac{2m}{n}$$

with equality if and only if $d(u) + d(v) = n$ for all edges $uv \in E(G)$.

Proof. Since $d(u) + d(v) \leq n$ for every $uv \in E(G)$, we have

$$H(G) \geq \sum_{uv \in E(G)} \frac{2}{n} = \frac{2m}{n}.$$

The equality holds if and only if $d(u) + d(v) = n$ for every $uv \in E(G)$. ■

In triangle-free graphs no two neighboring vertices have a common neighbor, and therefore all triangle-free graphs satisfy $d(u) + d(v) \le n$ for every $uv \in E(G)$. Hence, we have the following consequence.

Corollary 3.6. *[53] Let G be a nontrivial triangle-free graph with n vertices. Then*

$$H(G) \ge \frac{2(n-1)}{n}$$

with equality if and only if G is isomorphic to a complete bipartite graph.

Corollary 3.7. *[53, Corollary 2.1] Let T be a nontrivial tree with n vertices. Then*

$$H(T) \ge \frac{2(n-1)}{n}$$

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

Corollary 3.7 is generalized in [101, Theorem 3] for connected graphs. Using Corollary 3.3, we can generalize [101, Theorem 3] to graphs with n vertices containing no isolated vertices, and the unique extremal graph is still S_n.

Theorem 3.5. *[105, Theorem 2.2] Let G be a nontrivial graph with n vertices containing no isolated vertices. Then*

$$H(G) \ge \frac{2(n-1)}{n}$$

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

Proof. First suppose that G is a connected graph. Let m be the number of edges of G, thus $m \ge n-1$. Since $\frac{2m}{m+1}$ is strictly increasing in $m \ge 1$, Corollary 3.3 gives $H(G) \ge \frac{2m}{m+1} \ge \frac{2(n-1)}{n}$ with equalities if and only if $G \cong S_{m+1}$ and $m = n-1$, i.e., $G \cong S_n$.

So we may assume that G is disconnected. Let $G_1, G_2, \ldots, G_k$ be the connected components of G with $n_i = |V(G_i)|$ for each $1 \le i \le k$. Since G contains no isolated vertices, we have $n_i \ge 2$ and $\sum_{i=1}^{k} n_i = n$. Thus,

$$H(G) = \sum_{i=1}^{k} H(G_i) \ge \sum_{i=1}^{k} \frac{2(n_i-1)}{n_i}.$$

Since $n_i \ge 2$, we obtain

$$\begin{aligned} &\frac{2(n_1-1)}{n_1} + \frac{2(n_2-1)}{n_2} - \frac{2(n_1+n_2-1)}{n_1+n_2} = \\ &\qquad = 2\,\frac{(n_1n_2-n_1-n_2)(n_1+n_2)+n_1n_2}{n_1n_2(n_1+n_2)} > 0. \end{aligned}$$

We conclude that

$$\begin{aligned} H(G) &> \frac{2(n_1+n_2-1)}{n_1+n_2} + \sum_{i=3}^{k} \frac{2(n_i-1)}{n_i} > \frac{2(n_1+n_2+n_3-1)}{n_1+n_2+n_3} + \sum_{i=4}^{k} \frac{2(n_i-1)}{n_i} \\ &> \cdots > \frac{2(n_1+n_2+\cdots+n_k-1)}{n_1+n_2+\cdots+n_k} = \frac{2(n-1)}{n}. \end{aligned}$$

■

Let us define the *weight* of an edge $uv \in E(G)$ as

$$\frac{2}{d(v)+d(u)}.$$

The next result also studies how the harmonic index behaves when the graph is subject to perturbations. In fact, it deals with the behavior of the harmonic index if we remove an edge of maximal weight.

Theorem 3.6. *[13, Lemma 2.1] Let uv be an edge of maximal weight in a graph G with $m \geq 2$ edges. Then*

$$H(G - uv) < H(G).$$

Theorem 3.6 is used in the proof of the following result.

Given positive integers n and δ with $n \geq 2\delta$, let us denote by $K^*_{\delta,n-\delta}$ the graph obtained from a complete bipartite graph $K_{\delta,n-\delta}$ by joining each pair of vertices in the part with δ vertices by a new edge.

Theorem 3.7. *[13, Theorem 2.2] Let G be a graph with $n \geq 4$ vertices and minimum degree $\delta \geq 2$. Then*

$$H(G) \geq 4 + \frac{1}{n-1} - \frac{12}{n+1}$$

with equality if and only if $G \cong K^*_{2,n-2}$.

The following technical result will be used in the proof of Theorem 3.9 below.

Lemma 3.8. *[13, Lemma 3.1] The harmonic index of a graph G without isolated vertices can be rewritten as*

$$H(G) = \frac{n}{2} - \frac{1}{2} \sum_{1 \leq i < j \leq n-1} \Big(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \Big) m_{i,j}.$$

Proof. The harmonic index can be rewritten as

$$H(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{2m_{i,j}}{i+j} = \sum_{1 \leq i < j \leq n-1} \frac{2m_{i,j}}{i+j} + \sum_{i=1}^{n-1} \frac{m_{i,i}}{i}. \tag{5}$$

If we denote by n_i the number of vertices with degree i, then

$$\sum_{j=1, j\neq i}^{n-1} m_{i,j} + 2m_{i,i} = i n_i,$$

$$n_i = \frac{1}{i} \Big(\sum_{j=1, j\neq i}^{n-1} m_{i,j} + 2m_{i,i} \Big).$$

Since G does not have isolated vertices, the equality $n_1 + n_2 + \cdots + n_{n-1} = n$ holds. This fact and $m_{i,j} = m_{j,i}$ give

$$\sum_{1 \leq i < j \leq n-1} \Big(\frac{1}{i} + \frac{1}{j} \Big) m_{i,j} + 2 \sum_{i=1}^{n-1} \frac{m_{i,i}}{i} = n.$$

Hence, (5) allows to conclude

$$n - 2H(G) = \sum_{1 \le i < j \le n-1} \Big(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}\Big) m_{i,j}$$

and this finishes the proof. ∎

The following results improve Theorem 3.5 for triangle-free graphs.

Theorem 3.9. *[13, Theorem 3.2] Let G be a triangle-free graph with n vertices and minimum degree $\delta \ge k \ge 1$. Then*

$$H(G) \ge \frac{2k(n-k)}{n}$$

with equality if and only if $G \cong K_{k,n-k}$.

Proof. Let us denote by m the number of edges of G. Since G is triangle-free, we have $d(u) + d(v) \le n$ for every $uv \in E(G)$.

If $m > k(n-k)$, then

$$H(G) \ge \frac{2m}{n} > \frac{2k(n-k)}{n}$$

and equality is not possible.

Hence, we may assume that $m \le k(n-k)$. Since G is a triangle-free graph, the maximum degree of G is at most $n - \delta$ (in particular, we have $n \ge 2\delta$). By Lemma 3.8, $H(G)$ can be rewritten as

$$\begin{aligned} H(G) &= \frac{n}{2} + \frac{1}{2} \sum_{\delta \le i < j \le n-\delta} \Big(\frac{4}{i+j} - \frac{1}{i} - \frac{1}{j}\Big) m_{i,j} \\ &\ge \frac{n}{2} + \frac{1}{2} \sum_{\delta \le i < j \le n-\delta} \Big(\frac{4}{n} - \frac{1}{i} - \frac{1}{n-i}\Big) m_{i,j} \end{aligned}$$

since $\frac{4}{i+j} - \frac{1}{j}$ is a decreasing function on $j \in (i, n-i]$. Hence,

$$\begin{aligned} H(G) &\ge \frac{n}{2} + \frac{1}{2} \sum_{\delta \le i < j \le n-\delta} \Big(\frac{4}{n} - \frac{n}{i(n-i)}\Big) m_{i,j} \\ &\ge \frac{n}{2} + \frac{1}{2} \sum_{\delta \le i < j \le n-\delta} \Big(\frac{4}{n} - \frac{n}{\delta(n-\delta)}\Big) m_{i,j} \\ &= \frac{n}{2} - \frac{m}{2} \frac{(n-2\delta)^2}{n\delta(n-\delta)} \ge \frac{n}{2} - \frac{k(n-k)}{2} \frac{(n-2\delta)^2}{n\delta(n-\delta)} \\ &\ge \frac{n}{2} - \frac{k(n-k)}{2} \frac{(n-2k)^2}{nk(n-k)} = \frac{2k(n-k)}{n}. \end{aligned}$$

In this inequality chain equality holds throughout if and only if $m = k(n-k) = m_{k,n-k}$, which is equivalent to $G \cong K_{k,n-k}$. ∎

Theorem 3.10. *[95, Theorem 3.1] Let G be a triangle-free graph with $n \ge 4$ vertices and minimum degree $\delta \ge 2$. Then*

$$H(G) \ge 4 - \frac{8}{n}$$

with equality if and only if $G \cong K_{2,n-2}$.

A vertex in a graph is said to be a *pendent vertex* if it has degree one. An edge in a graph is said to be a *pendent edge* if it is incident to a pendent vertex.

For each $3 \leq k \leq n$, let C_k^n be the graph with n vertices obtained from a cycle C_k by attaching $n-k$ pendent vertices to exactly one vertex of C_k.

Theorem 3.11. *[102, Theorem 2.4] Let G be a connected graph with n vertices and girth $g(G) \geq k \geq 3$. Then*

$$H(G) \geq 1 + \frac{k}{2} + \frac{4}{n-k+4} - \frac{6}{n-k+3}$$

with equality if and only if $G \cong C_k^n$.

We have several lower bounds of the harmonic index involving the number of the pendent vertices.

Theorem 3.12. *[97, Theorem 2.4] Let G be a nontrivial connected graph with n vertices, m edges and p pendent vertices. Then*

$$H(G) \geq \frac{p}{n-1} + \frac{m-p}{(n-1-\frac{p}{2})^2}.$$

Proof. Since $0 < \frac{1}{d(u)}, \frac{1}{d(v)} \leq 1$, we have for each edge $uv \in E(G)$,

$$\frac{2}{d(u)+d(v)} \geq \frac{\frac{1}{d(u)} + \frac{1}{d(v)}}{d(u)+d(v)} = \frac{1}{d(u)d(v)}.$$

For each pendent edge uv, we clearly have

$$\frac{1}{d(u)d(v)} \geq \frac{1}{n-1}.$$

If uv is a non-pendent edge, then $d(u)+d(v) \leq 2(n-1)-p$, since any pendent vertex is adjacent to at most one of u and v. So

$$d(u)d(v) \leq \left(\frac{d(u)+d(v)}{2}\right)^2 \leq \left(n-1-\frac{p}{2}\right)^2,$$

and

$$H(G) \geq \frac{p}{n-1} + \frac{m-p}{(n-1-\frac{p}{2})^2}.$$

■

Remark 3.13. *If $n-1-\frac{p}{2} = 0$, then $p = m$ and the inequality in Theorem 3.12 is*

$$H(G) \geq \frac{p}{n-1}.$$

Furthermore, since $p = m$ and G is connected, we have $G \cong S_{m+1}$ and

$$H(G) = H(S_{m+1}) = \frac{2m}{m+1} = \frac{2(n-1)}{n}.$$

The argument in the proof of Theorem 3.12, using the inequalities $d(u)+d(v) \leq \Delta + 1$ for any pendent edge uv, and $d(u)+d(v) \leq 2(n-1)-p$ for any non-pendent edge uv, gives the following improvement.

Corollary 3.8. *Let G be a nontrivial connected graph with n vertices, m edges, p pendent vertices $(m > p)$ and maximum degree Δ. Then*

$$H(G) \geq \frac{2p}{\Delta + 1} + \frac{m - p}{n - 1 - \frac{p}{2}}.$$

By using the inequality $d(u) + d(v) \leq 2\Delta$ for any non-pendent edge uv, we obtain the following result.

Corollary 3.9. *[59, Theorem 2.1] Let G be a nontrivial connected graph with m edges, p pendent vertices and maximum degree Δ. Then*

$$H(G) \geq \frac{2p}{\Delta + 1} + \frac{m - p}{\Delta}.$$

Let us denote by $S_{n,p}$ the tree obtained by attaching $p - 1$ pendent vertices to an end vertex of the path graph P_{n-p+1}.

Theorem 3.14. *[62, Theorem 8] Let T be a tree with n vertices and p pendent vertices, where $2 \leq p \leq n - 2$. Then*

$$H(T) \geq \frac{2}{p + 2} - \frac{4}{p + 1} + \frac{n - p}{2} + \frac{5}{3}$$

with equality if and only if $T \cong S_{n,p}$.

Corollary 3.10. *[62, Corollary 10] Among all trees with n vertices, the minimum harmonic index is attained uniquely by the star graph S_n.*

Theorem 3.14 can be improved for molecular trees.

Let us introduce two classes of molecular trees with n vertices and p pendent vertices. Denote by $\mathcal{L}_e(n,p)$ for even p with $6 \leq p \leq \lfloor (n+3)/2 \rfloor$ the set of those trees that are composed of $(p-2)/2$ star graphs S_5, which are connected by paths whose lengths may be zero. Denote by $\mathcal{L}_l(n,p)$ for odd p with $9 \leq p \leq \lfloor (n+2)/2 \rfloor$ the set of those trees that are composed of $(p-3)/2$ star graphs S_5 and a star graph S_4, which are connected by paths whose lengths may be zero, and the unique star S_4 is connected to three stars S_5.

Theorem 3.15. *[62, Theorem 11] Let T be a molecular tree with n vertices and $p \geq 5$ pendent vertices. Then*

$$H(T) \geq \frac{n}{2} - \frac{4p}{15} + \frac{1}{6}$$

with equality if and only if $T \in \mathcal{L}_e(n,p)$ for even p with $6 \leq p \leq \lfloor (n+3)/2 \rfloor$. Moreover, if p is odd and $9 \leq p \leq \lfloor (n+2)/2 \rfloor$, then

$$H(T) \geq \frac{n}{2} - \frac{4p}{15} + \frac{1}{5}$$

with equality if and only if $T \in \mathcal{L}_l(n,p)$.

Theorem 3.16. *[62, Theorem 13] Let T be a molecular tree with n vertices and $p \geq 2$ pendent vertices. Then*

$$H(T) \leq \frac{n}{2} - \frac{p}{12}$$

with equality if and only if $T \cong P_n$.

Let us denote by S_n^+ the unicyclic graph obtained from the star S_n by adding an edge joining two pendent vertices. The bicyclic graph S_n^1 is obtained from S_n by adding a path of length 2 joining three pendent vertices. Finally, denote by S_n^2 the bicyclic graph obtained from S_n by adding two edges joining two different pairs of pendent vertices.

Theorem 3.17. *[52, Theorem 4] [100, Theorem 1] Let G be a connected unicyclic graph with $n \geq 3$ vertices. Then*

$$H(G) \geq \frac{5}{2} - \frac{2(n+3)}{n(n+1)}$$

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

Theorem 3.18. *[52, Theorem 5] [109, Theorem 3.1] Let G be a connected bicyclic graph with $n \geq 4$ vertices. Then*

$$H(G) \geq \frac{14}{5} - \frac{2n^2 + 14n + 16}{n(n+1)(n+2)}$$

with equality if and only if $G \cong S_n^1$.

Two different edges in a graph G are called *independent* if they are not adjacent. A *matching* of G is a set of mutually independent edges in G. The largest matching is called a *maximum matching*. The *matching number* of G is the cardinality of a maximum matching of G. If M is a matching of G, then M is called the *μ-matching* of G if M contains exactly μ edges of G. A vertex $v \in G$ is said to be *M-saturated* if it is incident with an edge of M. The matching M of G is called a *perfect matching* if all vertices of G are M-saturated.

Let $T^0(n, \mu)$ be a tree with n vertices obtained from a 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 clear that $T^0(n, \mu)$ has a μ-matching.

Theorem 3.19. *[66, Theorem 3.1] Let T be a tree with $n = 2\mu$ vertices and a perfect matching. Then*

$$H(T) \geq \frac{2}{\mu+1} + \frac{2(\mu-1)}{\mu+2} + \frac{2(\mu-1)}{3}$$

with equality if and only if $T \cong T^0(2\mu, \mu)$.

Theorem 3.20. *[66, Theorem 3.2] Let T be a tree with n vertices and a μ-matching, where $n > 2\mu$. Then*

$$H(T) \geq \frac{2(n-2\mu+1)}{n-\mu+1} + \frac{2(\mu-1)}{n-\mu+2} + \frac{2(\mu-1)}{3}$$

with equality if and only if $T \cong T^0(n, \mu)$.

A subset $S \subset V(G)$ 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. The *domination number* of G is defined as the minimum cardinality of dominating sets of G.

Theorem 3.21. *[58, Theorem 3.3] Let T be a tree with n vertices and domination number γ. Then*

$$H(T) \geq \frac{2(n-2\gamma+1)}{n-\gamma+1} + \frac{2(\gamma-1)}{n-\gamma+2} + \frac{2(\gamma-1)}{3}$$

with equality if and only if $T \cong T^0(n, \gamma)$.

Let $L^*_{n,3}$ be the unicyclic graph with n vertices obtained by attaching $n-4$ and one pendent vertices to two adjacent vertices u, v of a triangle, respectively. For each $4 \leq k \leq n-2$, let $L^*_{n,k}$ be the set of unicyclic graphs with n vertices obtained by attaching $n-k-1$ and one pendent vertices to two non-adjacent vertices u, v of the cycle graph C_k, respectively.

Theorem 3.22. *[103, Theorem 2.3] Let $G \ncong L_{n,k}$ be a unicyclic graph with $n \geq 5$ vertices and girth k, where $3 \leq k \leq n$.*

(1) *If $k = 3$, then*

$$H(G) \geq \frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$$

with equality if and only if $G \cong L^*_{n,3}$.

(2) *If $4 \leq k \leq n-2$, then*

$$H(G) \geq \frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}$$

with equality if and only if $G \in L^*_{n,k}$.

Theorem 3.23. *[82, Corollary 9] Let G be a nontrivial connected graph with n vertices and m edges. Then*

$$\frac{m}{n-1} \leq H(G) \leq m.$$

The lower bound is attained if and only if $G \cong K_n$. The upper bound is attained if and only if $G \cong K_2$.

Proof. Since for any edge $uv \in E(G)$ we have $2 \leq d(u) + d(v) \leq 2n-2$, we have

$$\frac{1}{2n-2} \leq \frac{1}{d(u)+d(v)} \leq \frac{1}{2}.$$

Hence,

$$\sum_{uv \in E(G)} \frac{1}{n-1} \leq \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)} \leq \sum_{uv \in E(G)} 1,$$

and

$$\frac{m}{n-1} \leq H(G) \leq m.$$

Furthermore, the lower and upper bounds are attained if and only if $G \cong K_n$ and $G \cong K_2$, respectively.

■

Theorem 3.24. *[82, Theorem 17] Let G be a connected graph with n vertices and maximum degree $\Delta \geq 2$. Then*

$$H(G) \geq \frac{2n\Delta}{(\Delta+1)^2}$$

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

Denote by $\lfloor t \rfloor$ (respectively, $\lceil t \rceil$) the lower (respectively, upper) integer part of the real number t.

Proposition 3.25. *[82, Corollary 13] Let G be a complete bipartite graph with $n \geq 4$ vertices and m edges. Then*

$$\frac{2(n-1)}{n} \leq H(G) = \frac{2m}{n} \leq \frac{2}{n}\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil.$$

The lower bound is attained if and only if $G \cong K_{1,n-1} \cong S_n$. The upper bound is attained if and only if $G \cong K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Proof. Since G is a complete bipartite graph, we have $d(u)+d(v)=n$ for any $uv \in E(G)$. Thus,

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)} = \frac{2m}{n}.$$

The complete bipartite graph G that has the minimum value of edges is $K_{1,n-1}$ and the complete bipartite graph that has the maximum value of edges is $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. Hence,

$$\frac{2(n-1)}{n} \leq H(G) \leq \frac{2}{n}\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil.$$

■

Recall that a nontrivial connected graph with maximum degree at most four is a molecular graph representing hydrocarbons. If G is a molecular graph with n vertices and m edges, then

$$n-1 \leq m \leq 2n.$$

Theorem 3.26. *[82, Theorem 14] If G is a molecular graph with $n \geq 3$ vertices and m edges, then*

$$\frac{3m+4n}{20} \leq H(G) \leq \frac{m+2n}{6}. \tag{6}$$

The lower bound is attained if and only if G has only vertices of degree one and four, and the upper bound is attained if and only if G is either a path or a cycle.

We present another result that studies how the harmonic index behaves when the graph is subject to perturbations. In fact, it deals with the behavior of the harmonic index if we remove a vertex of minimal degree. We use $N_G(v)$ to denote the neighborhood of vertex $v \in V$, and $N_G^2(v)$ to denote the set of vertices at distance 2 of $v \in V$.

Lemma 3.27. *[24, Lemma 1] Let $\delta \leq d(i), d(j)$ and $d(i), d(j) \geq 2$. Then*

$$\frac{1}{(d(i)-1)(\delta+d(i))} + \frac{1}{(d(j)-1)(\delta+d(j))} \geq \frac{2}{d(i)+d(j)-2} - \frac{2}{d(i)+d(j)}.$$

Lemma 3.28. *[24, Lemma 2] Let $\delta \leq d(p)$ and $d(i) \geq 2$. Then*

$$\frac{1}{(d(i)-1)(\delta+d(i))} \geq \frac{1}{d(i)+d(p)-1} - \frac{1}{d(i)+d(p)}.$$

Theorem 3.29. *[24, Theorem 3] Let G be a nontrivial graph with minimum degree $\delta \geq 1$ and $v \in V(G)$ with degree δ. Then*

$$H(G) \geq H(G-v).$$

Proof. Removal of a vertex v with $d(v) = \delta$ and of all edges incident with v entails reduction by 1 of both end-degrees of all edges $ij \in E(G)$ both vertices of which are adjacent to v, and reduction by 1 of the first end-degree of all edges $ip \in E(G)$ for which the first vertex is adjacent to v and the second one at distance 2 from v. Let $d'(i) = d_{G-v}(i)$ be the degree of vertex i in $G - v$.

We can assume that $d(i) \geq 2$ for every $i \in N_G(v)$, since otherwise $\delta = 1$ and the connected component of v in G has just an edge.

$$\begin{aligned}
&H(G) - H(G-v) \\
&\quad = \sum_{pq \in E(G)} \frac{2}{d(p)+d(q)} - \sum_{pq \in E(G-v)} \frac{2}{d'(p)+d'(q)} \\
&\quad = \sum_{i \in N_G(v)} \frac{2}{\delta + d(i)} + \sum_{ij \in E(G) | i,j \in N_G(v)} \left(\frac{2}{d(i)+d(j)} - \frac{2}{d(i)+d(j)-2} \right) \\
&\qquad\quad + \sum_{ip \in E(G) | i \in N_G(v), p \in N_G^2(v)} \left(\frac{2}{d(i)+d(p)} - \frac{2}{d(i)+d(p)-1} \right).
\end{aligned}$$

Note that

$$\begin{aligned}
\sum_{i \in N_G(v)} \frac{2}{\delta + d(i)} &= \sum_{i \in N_G(v)} \sum_{p \in N_G(i) \setminus \{v\}} \frac{2}{(d(i)-1)(\delta+d(i))} \\
&= \sum_{i \in N_G(v)} \sum_{p \in N_G^2(v) \cap N_G(i)} \frac{2}{(d(i)-1)(\delta+d(i))} \\
&\quad + \sum_{ij \in E(G) | i,j \in N_G(v)} \left(\frac{2}{(d(i)-1)(\delta+d(i))} + \frac{2}{(d(j)-1)(\delta+d(j))} \right).
\end{aligned}$$

Hence

$$\begin{aligned}
&H(G) - H(G-v) \\
&= \sum_{i \in N_G(v)} \sum_{p \in N_G^2(v) \cap N_G(i)} \left(\frac{2}{(d(i)-1)(\delta+d(i))} + \frac{2}{d(i)+d(p)} - \frac{2}{d(i)+d(p)-1} \right) \\
&\quad + \sum_{ij \in E(G) | i,j \in N_G(v)} \left(\frac{2}{(d(i)-1)(\delta+d(i))} + \frac{2}{(d(j)-1)(\delta+d(j))} \right. \\
&\qquad\qquad \left. + \frac{2}{d(i)+d(j)} - \frac{2}{d(i)+d(j)-2} \right)
\end{aligned}$$

and $H(G) - H(G-v) \geq 0$ from Lemmas 3.27 and 3.28. ■

Theorem 3.29 can be used in order to prove the following result. Recall that we denote the chromatic number of a graph G by $\chi^*(G)$.

Theorem 3.30. *[24, Theorem 4] Let G be a nontrivial graph. Then*

$$H(G) \geq \frac{1}{2}\chi^*(G).$$

with equality if and only if G is a complete graph possibly with some additional isolated vertices.

For a vertex u in a connected nontrivial graph G, let us define the $eccentricity$ of u as

$$ecc_G(u) = \max\{d_G(u, v) \mid v \in V(G)\},$$

where d_G denotes the distance in G. The *radius* $r(G)$ of G is defined as

$$r(G) = \min\{ecc_G(u) \mid u \in V(G)\}.$$

Theorem 3.31. *[97, Theorem 2.3] Let G be a nontrivial connected graph with n vertices and m edges. Then*

$$H(G) \geq \frac{m}{n - r(G)}.$$

Furthermore, the equality is attained for the complete graph K_n.

Proof. Note that for each vertex $u \in V(G)$, we have $d(u) \leq n - ecc_G(u)$. Thus, for each edge $uv \in E(G)$,

$$\begin{aligned} \frac{2}{d(u)+d(v)} &\geq \frac{2}{2n - ecc_G(u) - ecc_G(v)} \geq \frac{1}{n - r(G)}, \\ H(G) &\geq \frac{m}{n - r(G)}. \end{aligned}$$

It is easily seen that the complete graph K_n attains the equality. ■

The study of Gromov hyperbolic graphs is a subject of increasing interest, both in pure and applied mathematics (see, e.g., [7], [9], [68] and the references cited therein). We say that a graph G is t-*hyperbolic* ($t \geq 0$) if any side of every geodesic triangle in G is contained in the t-neighborhood of the union of the other two sides. We define the *hyperbolicity constant* $\delta(G)$ of G as the infimum of the constants $t \geq 0$ such that G is t-hyperbolic. We consider that every edge has length 1.

The following inequality relates the harmonic index with the hyperbolicity constant $\delta(G)$.

Theorem 3.32. *Let G be a nontrivial graph that is not a tree. Then*

$$H(G) \geq \frac{4\delta(G) - 1}{2\delta(G)}.$$

Furthermore, if G is a triangle-free graph with minimum degree greater or equal to $k \geq 1$, then

$$H(G) \geq \frac{k(4\delta(G) - k)}{2\delta(G)}$$

with equality if and only if $k = 2$ and $G \cong C_4$.

Proof. Theorem 3.5 gives
$$H(G) \geq \frac{2(n-1)}{n}.$$
It is well-known that if G is not a tree, then $\delta(G) > 0$. Since the function $f(x) = \frac{2(x-1)}{x}$ is increasing in $(0, \infty)$, and $\delta(G) \leq \frac{n}{4}$ by [68, Theorem 30], we have $n \geq 4\delta(G) > 0$ and
$$H(G) \geq \frac{2(n-1)}{n} \geq \frac{2(4\delta(G)-1)}{4\delta(G)}.$$
By using Theorem 3.9 instead of Theorem 3.5, the previous argument gives
$$H(G) \geq \frac{k(4\delta(G)-k)}{2\delta(G)}$$
with equality if and only if $G \cong K_{k,n-k}$ and $\delta(G) = \frac{n}{4}$. If $G \cong K_{k,n-k}$ is not a tree (i.e., if $k \geq 2$), then [81, Thoerem 10] gives $\delta(K_{k,n-k}) = 1$. Since $n \geq 2k$, we have the equality if and only if $G \cong K_{k,n-k}$, $n = 4$ and $k \geq 2$, i.e., $G \cong K_{2,2} \cong C_4$. ■

One can think that perhaps it is possible to obtain an upper bound for $H(G)$ in terms of $\delta(G)$, i.e., the inequality
$$H(G) \leq \Psi\big(\delta(G)\big),$$
for every graph G and some function Ψ. However, this is not possible, as the following example shows. For each integer $d \geq 3$ consider two copies A_d and B_d of the path graph with (ordered) vertices $a_1, \dots, a_d$ and $b_1, \dots, b_d$, respectively. Let G_d be the graph obtained from A_d and B_d by connecting with an edge the vertices a_i and b_i for every $i \in \{1, \dots, d\}$. One can check that $\delta(G) = \frac{3}{2}$ for every $d \geq 3$. However, $\lim_{d\to\infty} H(G_d) = \infty$.

We relate now the harmonic index of a graph with its girth.

Theorem 3.33. *[94, Theorem 3] Let G be a connected graph with $n \geq 3$ vertices and girth $g(G)$. Then*
$$H(G) + g(G) \geq \frac{11}{2} - \frac{6}{n} + \frac{4}{n+1}, \qquad H(G)g(G) \geq \frac{15}{2} - \frac{18}{n} + \frac{12}{n+1}$$
with equalities if and only if $G \cong S_n^+$.

Theorem 3.34. *[102, Theorem 2.6] Let G be a connected graph with n vertices and girth $g(G) \geq k \geq 3$. Then*
$$1 + \frac{3k}{2} - \frac{6}{n-k+3} + \frac{4}{n+1} \leq H(G) + g(G) \leq \frac{3n}{2}$$
and
$$k\Big(1 + \frac{k}{2} - \frac{6}{n-k+3} + \frac{4}{n+1}\Big) \leq H(G)g(G) \leq \frac{n^2}{2}.$$
The lower bounds are attained if and only if $G \cong C_k^n$, and the upper bounds are attained if and only if $G \cong C_n$.

Theorem 3.35. *[102, Theorem 2.7] Let G be a connected graph with n vertices and girth $g(G) \geq k \geq 3$. Then*

$$-\frac{n}{2} \leq H(G) - g(G) \leq \frac{n}{2} - k, \quad \frac{1}{2} \leq \frac{H(G)}{g(G)} \leq \frac{n}{2k}.$$

The lower bounds are attained if and only if $G \cong C_n$, and the upper bounds are attained if and only if G is a regular graph with $g(G) = k$.

Next, we relate the harmonic index of a graph with its diameter. Theorem 3.1 allows to deduce the following result.

Theorem 3.36. *[60, Theorem 2.2] Let G be a connected graph with $n \geq 4$ vertices and diameter $D(G)$. Then*

$$H(G) - D(G) \leq \frac{n}{2} - 1, \qquad \frac{H(G)}{D(G)} \leq \frac{n}{2}$$

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

Theorem 3.37. *[60, Theorem 2.5] Let T be a connected tree with $n \geq 4$ vertices and diameter $D(T)$. Then*

$$H(T) - D(T) \geq \frac{5}{6} - \frac{n}{2}, \qquad \frac{H(T)}{D(T)} \geq \frac{1}{2} + \frac{1}{3(n-1)}$$

with equality if and only if $T \cong P_n$.

The inequalities in Theorem 3.37 can be improved for unicyclic graphs.

Let $\mathcal{C}$ be a set of graphs obtained from C_4 by attaching one pendant edge and a path of length $n-5$ to two diametrically nonadjacent vertices of C_4. For each $n \geq 7$, we have exactly one graph in this set.

Theorem 3.38. *[3, Theorem 3.1] Let G be a unicyclic graph with $n \geq 7$ vertices and diameter $D(G)$. Then*

$$H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}$$

with equality if $G \in \mathcal{C}$.

Let $U_{n,l}^{x,y}$ be a unicyclic graph obtained from a cycle C_l by attaching two paths P_x and P_y to two diametrically opposite vertices of C_l such that $n = l + x + y$.

Theorem 3.39. *[4, Theorem 3.1] Let G be a unicyclic graph with $n \geq 7$ vertices and diameter $D(G)$. Then*

$$\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$$

with equality if and only if $G \cong U_{n,4}^{1,n-5}$.

3.1 Harmonic index of graph operations

Caporossi et al. [10] showed that among all graphs with n vertices, the graphs containing no isolated vertices, in which all connected components are regular, have the maximum value $\frac{n}{2}$ for the Randić index. By Theorem 2.1, we know that these graphs are also the extremal graphs with the maximum harmonic index. This implies the following NordhausGaddumtype results for the harmonic index.

The complement $\overline{G}$ of a graph G is the graph whose vertex set is $V(G)$ and $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$ for $u, v \in V(G)$.

Theorem 3.40. *[105, Theorem 3.2] Let G be a graph with n vertices, then*

$$\frac{n}{2} \leq H(G) + H(\overline{G}) \leq n.$$

The lower bound is attained if and only if $G \cong K_n$ or $\overline{G} \cong K_n$, and the upper bound is attained if and only if G is a k-regular graph with $1 \leq k \leq n-2$.

Proof. Let us denote by m and $\overline{m}$ the number of edges in G and $\overline{G}$, respectively. Then

$$\begin{aligned} H(G) + H(\overline{G}) &= \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)} + \sum_{uv \in E(\overline{G})} \frac{2}{(n-1-d(u)) + (n-1-d(v))} \\ &\geq \sum_{uv \in E(G)} \frac{2}{2n-2} + \sum_{uv \in E(\overline{G})} \frac{2}{2n-2} \\ &= \frac{1}{n-1}(m+\overline{m}) = \frac{1}{n-1} \cdot \frac{n(n-1)}{2} = \frac{n}{2}, \end{aligned}$$

with equality if and only if either $d(u) = d(v) = n-1$ for every edge uv of G or $E(G) = \emptyset$, i.e., $G \cong K_n$ or $\overline{G} \cong K_n$.

In order to prove the upper bound, Theorem 2.1 gives

$$H(G) + H(\overline{G}) \leq R(G) + R(\overline{G}) \leq \frac{n}{2} + \frac{n}{2} = n,$$

with equalities if and only if both G and $\overline{G}$ contain no isolated vertices (i.e., $1 \leq \delta(G) \leq \Delta(G) \leq n-2$) and all connected components of G and $\overline{G}$ are regular.

Let us prove that G is a regular graph.

Seeking for a contradiction assume that there exist $u, v \in V(G)$ with $d(u) \neq d(v)$. Thus, u and v are contained in two different connected components of G, and hence $uv \in E(\overline{G})$. Hence, u and v lie in the same component of $\overline{G}$. Since each connected component of $\overline{G}$ is regular, we have $n-1-d(u) = n-1-d(v)$, a contradiction. This finishes the proof. ■

In [84], some bounds for the harmonic index of the join, corona product, Cartesian product, composition and symmetric difference of graphs are obtained.

It is well-known that the *composition* $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph with vertex set $V(G_1) \times V(G_2)$ and (u_i, v_j) is adjacent with (u_k, v_l) whenever u_i is adjacent with u_k, or $u_i = u_k$ and v_j is adjacent with v_l.

Theorem 3.41. *[84, Theorem 2.1] Let G_1 and G_2 be two connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$H(G_1[G_2]) \leq \frac{1}{(1+n_2)^2}\Big(\frac{n_1}{2}ABC(G_2) + n_1R(G_2) + n_1n_2m_2 \\ + \frac{n_2^3}{2}ABC(G_1) + n_2^3R(G_1) + n_2^2m_1\Big).$$

Recall that 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 $(u_i, v_j)(u_k, v_l)$ is an edge of $G_1 \times G_2$ if $u_i = u_k$ and $v_jv_l \in E(G_2)$, or $u_iu_k \in E(G_1)$ and $v_j = v_l$.

Theorem 3.42. *[84, Theorem 2.2] Let G_1 and G_2 be two connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$H(G_1 \times G_2) \leq \frac{1}{8}\big(n_1ABC(G_2) + 2n_1R(G_2) + 2n_1m_2 \\ + n_2ABC(G_1) + 2n_2R(G_1) + 2n_2m_1\big).$$

Let G_1 and G_2 be two graphs we define the *corona product* $G_1 \circ G_2$ as the graph obtained by taking $|V(G_1)|$ copies of G_2 and joining each vertex of the *i*-th copy with vertex $v_i \in V(G_1)$.

One can check that

$$|V(G_1 \circ G_2)| = |V(G_1)|\,(1 + |V(G_2)|)$$
$$|E(G_1 \circ G_2)| = |E(G_1)| + |V(G_1)|\,(|V(G_2)| + |E(G_2)|).$$

Theorem 3.43. *[84, Theorem 2.3] For $i \in \{1, 2\}$, let G_i be a graph with n_i vertices, m_i edges, minimum degree δ_i and maximum degree Δ_i. Then*

$$H(G_1 \circ G_2) \geq \frac{m_1}{\Delta_1 + n_2} + \frac{m_2n_1}{\Delta_2 + 1} + \frac{2n_1n_2}{\Delta_1 + \Delta_2 + n_2 + 1},$$
$$H(G_1 \circ G_2) \leq \frac{m_1}{\delta_1 + n_2} + \frac{m_2n_1}{\delta_2 + 1} + \frac{2n_1n_2}{\delta_1 + \delta_2 + n_2 + 1}.$$

Proof. The edges of $G_1 \circ G_2$ are partitioned into three subsets E_1, E_2 and E_3 as follows

$$E_1 = \{e \in E(G_1 \circ G_2), e \in E(G_1)\},$$
$$E_2 = \{e \in E(G_1 \circ G_2), e \in E(G_{2i})\ i = 1, 2 \ldots, |V(G_1)|\},$$
$$E_3 = \{e \in E(G_1 \circ G_2), e = uv, u \in V(G_{2i}),\ i = 1, 2, \ldots, |V(G_1)|\ \ and\ \ v \in V(G_1)\}.$$

If u is a vertex of $G_1 \circ G_2$, then

$$d_{G_1 \circ G_2}(u) = \begin{cases} d_{G_1}(u) + |V(G_2)| & if \quad u \in V(G_1) \\ d_{G_2}(u) + 1 & if \quad u \in V(G_2). \end{cases}$$

Let $G_1 = (V_i, E_i), i \in \{1, 2\}$ and $G_1 \circ G_2 = (V, E)$. Thus,

$$H(G_1 \circ G_2) = \sum_{uv \in E(G_1 \circ G_2)} \frac{2}{d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)} \\ = Q_1 + Q_2 + Q_3,$$

with

$$\begin{aligned}
Q_1 &= \sum_{uv\in E_1} \frac{2}{d_{G_1}(u)+n_2+d_{G_1}(v)+n_2} \\
&\geq \frac{2m_1}{\Delta_1+n_2+\Delta_1+n_2} = \frac{m_1}{\Delta_1+n_2}, \\
Q_2 &= n_1 \sum_{uv\in E_2} \frac{2}{d_{G_2}(u)+1+d_{G_2}(v)+1} \\
&\geq \frac{2n_1m_2}{\Delta_2+1+\Delta_2+1} = \frac{n_1m_2}{\Delta_2+1}, \\
Q_3 &= \sum_{uv\in E_3, u\in V_1, v\in V_2} \frac{2}{d_{G_1}(u)+n_2+d_{G_2}(v)+1} \\
&\geq \frac{2n_1n_2}{\Delta_1+\Delta_2+n_2+1}.
\end{aligned}$$

Thus,

$$H(G_1\circ G_2) \geq \frac{m_1}{\Delta_1+n_2} + \frac{m_2n_1}{\Delta_2+1} + \frac{2n_1n_2}{\Delta_1+\Delta_2+n_2+1}.$$

We deduce the upper bound in a similar way. ■

The *join* G_1+G_2 of two graphs G_1 and G_2 is defined as the graph obtained from disjoined graphs G_1 and G_2 by taking one copy of G_1 and one copy of G_2 and joining by an edge each vertex of G_1 with each vertex of G_2.

Theorem 3.44. *[84, Theorem 2.4] Let G_1 and G_2 be two connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$H(G_1+G_2) \geq \frac{2}{m_1+2n_2+1}R(G_1) + \frac{2}{m_2+2n_1+1}R(G_2) + \frac{n_1n_2}{n_1+n_2-1}.$$

Proof. Let $V(G_1)=\{u_1,u_2,\ldots,u_{n_1}\}$ and $V(G_2)=\{v_1,v_2,\ldots,v_{n_2}\}$. If $u\in V(G_1+G_2)$, then

$$d_{G_1+G_2}(u) = \begin{cases} d_{G_1}(u)+|V(G_2)| & if \quad u\in V(G_1) \\ d_{G_2}(u)+|V(G_1)| & if \quad u\in V(G_2). \end{cases}$$

Hence,

$$\begin{aligned}
H(G_1+G_2) &= \sum_{uv\in E(G_1+G_2)} \frac{2}{d_{G_1+G_2}(u)+d_{G_1+G_2}(v)} \\
&= \sum_{uv\in E(G_1)} \frac{2}{d_{G_1}(u)+n_2+d_{G_1}(v)+n_2} \\
&\quad + \sum_{uv\in E(G_2)} \frac{2}{d_{G_2}(u)+n_1+d_{G_2}(v)+n_1} \\
&\quad + \sum_{u\in V(G_1), v\in V(G_2)} \frac{2}{d_{G_1}(u)+n_2+d_{G_2}(v)+n_1} \\
&= A_1+A_2+A_3,
\end{aligned}$$

where A_i denotes the i-th sum.

For each $uv \in E(G)$, we have $d_G(u) + d_G(v) \leq |E(G)| + 1$ with equality if and only if every other edge of G is adjacent to the edge uv. Also, $1 \leq \sqrt{d(u)d(v)}$, and the equality holds if and only if $d(u) = d(v) = 1$. Hence,

$$\begin{aligned} A_1 &\geq \sum_{uv \in E(G_1)} \frac{2}{|E(G_1)| + 1 + 2n_2} \frac{1}{\sqrt{d(u)d(v)}} \\ &= \frac{2}{m_1 + 1 + 2n_2} R(G_1). \end{aligned}$$

Similarly,

$$A_2 \geq \frac{2}{m_2 + 1 + 2n_1} R(G_2).$$

Since for any graph G with n vertices we have $d(w) \leq n - 1$ for any $w \in V(G)$, we deduce

$$\begin{aligned} A_3 &= \sum_{u \in V(G_1), v \in V(G_2)} \frac{2}{d_{G_1}(u) + n_2 + d_{G_2}(v) + n_1} \\ &\geq \sum_{u \in V(G_1), v \in V(G_2)} \frac{2}{n_1 - 1 + n_2 + n_2 - 1 + n_1} \\ &= \frac{n_1 n_2}{n_1 + n_2 - 1}. \end{aligned}$$

Thus,

$$H(G_1 + G_2) \geq \frac{2}{m_1 + 2n_2 + 1} R(G_1) + \frac{2}{m_2 + 2n_1 + 1} R(G_2) + \frac{n_1 n_2}{n_1 + n_2 - 1}.$$

■

Finally, we define the *symmetric difference* $G_1 \oplus G_2$ of two graphs G_1 and G_2 as the graph with vertex set $V(G_1) \times V(G_2)$ and $E(G_1 \oplus G_2) = \{(u_1, u_2)(v_1, v_2) \mid u_1v_1 \in E(G_1)$ or $u_2v_2 \in E(G_2)$ but not both$\}$.

Theorem 3.45. *[84, Theorem 2.5] For $i \in \{1, 2\}$, let G_i be a graph with n_i vertices, m_i edges and diameter $D(G_i)$. Then*

$$H(G_1 \oplus G_2) \geq \frac{n_2^2 m_1 + n_1^2 m_2 - 4m_1 m_2}{n_2(n_1 - D(G_1)) + n_1(n_2 - D(G_2)) - 2(n_1 - D(G_1))(n_2 - D(G_2))}.$$

3.2 Harmonic polynomial of a graph

The characterization of any graph by a polynomial is one of the open important problems in graph theory. In recent years there have been many works on graph polynomials (see, e.g., [2, 11, 12, 83, 91]). The research in this area has been largely driven by the advantages offered by the use of computers: it is simpler to represent a graph by a polynomial (a vector with dimension $O(n)$) than by the adjacency matrix (an $n \times n$ matrix). Some parameters of a graph allow to define polynomials related to a graph. Although several polynomials are interesting since they compress information about the graphs structure, unfortunately, the well-known polynomials do not solve this problem since there are often non-isomorphic graphs with the same polynomial.

In this subsection we introduce the harmonic polynomial of a graph and we present explicit formulas for this polynomial for several families of graphs. The harmonic polynomial of a graph G is defined in [54] as

$$H(G,x) = \sum_{uv \in E(G)} 2x^{d(u)+d(v)-1}.$$

Note that the harmonic index $H(G)$ can be obtained by integrating this polynomial:

$$H(G) = \int_0^1 H(G,x)\,dx.$$

Proposition 3.46. *[54, Proposition 1] If G is a k-regular graph with n vertices and m edges, then*

$$H(G,x) = 2mx^{2k-1}, \qquad H(G) = \frac{n}{2}.$$

Proof. Since G is k-regular graph, so for every edge in G we have $x^{d(u)+d(v)-1} = x^{2k-1}$ and hence,

$$H(G,x) = 2mx^{2k-1}.$$

Since $2m = nk$ for every k-regular graph, the previous equality gives $H(G) = \int_0^1 H(G,x)\,dx = \frac{n}{2}$. ■

Proposition 3.46 has the following consequences on the graphs: K_n (the complete graph with n vertices), C_n (the cycle with n vertices), Π_n (the n-sided prism), A_n (the n-sided antiprism) and Q_n (the n-dimensional hypercube).

Corollary 3.11. *[54, Proposition 2] We have*

$$\begin{aligned} H(K_n,x) &= n(n-1)x^{2n-3}, \\ H(C_n,x) &= 2nx^3, \\ H(\Pi_n,x) &= 6nx^5, \\ H(A_n,x) &= 8nx^7, \\ H(Q_n,x) &= n2^n x^{2n-1}. \end{aligned}$$

Proposition 3.47. *[54, Proposition 4-5] Let K_{n_1,n_2} be a complete bipartite graph with n_1+n_2 vertices. For $n_1, n_2 \geq 1$, we have*

$$H(K_{n_1,n_2},x) = 2n_1n_2x^{n_1+n_2-1}.$$

In particular, if $S_n = K_{n-1,1}$ denotes the star graph with $n \geq 2$ vertices, then

$$H(S_n,x) = 2(n-1)x^{n-1}.$$

In the following results, we compute the harmonic polynomial of other well-known families of graphs.

Proposition 3.48. *[54, Proposition 7] Let P_n be the path graph with n vertices. Then*

$$H(P_n,x) = 4x^2 + 2(n-3)x^3.$$

Proposition 3.49. *Let W_n be the wheel graph with $n \geq 4$ vertices. Then*

$$H(W_n, x) = 2(n-1)(x^{n+1} + x^5)$$

and

$$H(W_n) = \frac{2(n-1)}{n+2} + \frac{n-1}{3}.$$

Proposition 3.50. *Let S_{n_1,n_2} be a double star graph. For $n_1, n_2 \geq 1$, we have*

$$H(S_{n_1,n_2}, x) = 2n_1 x^{n_1+1} + 2n_2 x^{n_2+1} + 2x^{n_1+n_2+1}$$

and

$$H(S_{n_1,n_2}) = \frac{2n_1}{n_1+2} + \frac{2n_2}{n_2+2} + \frac{2}{n_1+n_2+2}.$$

Moreover, in [54], the lower and upper bounds for harmonic index of caterpillars with diameter four are computed.

At the light of the results on harmonic polynomials we asked the following question: How many graphs can be characterized by their harmonic polynomial? Another fundamental problem is to obtain properties of harmonic polynomials and their coefficients.

4. Generalization of the harmonic index

In this final section, we show some important inequalities on a generalization of the harmonic index known as general sum connectivity index. In particular, we relate these indices to other well-known topological indices.

With motivation from the first Zagreb, harmonic and sum-connectivity indices, the *general sum-connectivity index* $\chi_\alpha(G)$ is defined by Zhou and Trinajstić in [108], as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^\alpha,$$

with $\alpha \in \mathbb{R}$.

Note that $\chi_1(G)$ is the first Zagreb index $M_1(G)$, $2\chi_{-1}(G)$ is the harmonic index $H(G)$, $\chi_{-1/2}(G)$ is the sum-connectivity index $\chi(G)$, etc.

4.1 Inequalities for the general sum–connectivity index

For molecular graphs, in [14] appear efficient formulas for calculating the general sum-connectivity index of benzenoid systems and their phenylenes.

The following inequalities for the harmonic index are known: $H(G) \leq n/2$ and for $n \geq 3$, $\frac{2(n-1)}{n} \leq H(G)$. The corollary of the next result generalizes these inequalities for $\chi_\alpha(G)$.

Theorem 4.1. *[80, Theorem 2.3] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} 2^{\alpha-1}\Delta^{\alpha-1}M_1(G) \le \chi_\alpha(G) \le 2^{\alpha-1}\delta^{\alpha-1}M_1(G), \qquad & \textit{if } \alpha < 1, \\ 2^{\alpha-1}\delta^{\alpha-1}M_1(G) \le \chi_\alpha(G) \le 2^{\alpha-1}\Delta^{\alpha-1}M_1(G), \qquad & \textit{if } \alpha \ge 1, \end{aligned}$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is regular.

Corollary 4.1. *[80, Corollary 2.4] Let G be a nontrivial connected graph with n vertices, m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} 2^{\alpha+1}\Delta^{\alpha-1}\frac{m^2}{n} \le \chi_\alpha(G) \le 2^{\alpha}\delta^{\alpha-1}\Delta m, \qquad & \textit{if } \alpha < 1, \\ 2^{\alpha+1}\delta^{\alpha-1}\frac{m^2}{n} \le \chi_\alpha(G) \le 2^{\alpha}\Delta^{\alpha} m, \qquad & \textit{if } \alpha \ge 1, \end{aligned}$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is regular.

Proof. Since $4m^2/n \le M_1(G)$ (see [34]) and $M_1(G) \le 2m\Delta$, Theorem 4.1 gives the inequalities.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $\chi_\alpha(G)$. If some equality holds for some $\alpha \neq 1$, then some equality holds in Theorem 4.1 and G is regular. ∎

Recall that a *biregular* graph is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ. If there are n_1 vertices with degree δ and n_2 vertices with degree Δ, then $m = \delta n_1 = \Delta n_2$ and we deduce $\Delta\delta n = \big(\Delta + \delta\big)m$. Note that a regular graph is biregular if and only if it is bipartite.

Next, we present several inequalities relating general sum connectivity indices with different parameters.

Theorem 4.2. *[80, Theorem 2.7] Let G be a nontrivial connected graph with m edges, $\alpha \in \mathbb{R}$ and $\beta > 0$. Then*

$$\chi_\alpha(G) \ge m^{1+1/\beta}\chi_{-\alpha\beta}(G)^{-1/\beta},$$

and the equality is attained for some values $\alpha \neq 0$ and β if and only if G is regular or biregular.

Proof. Since $f(x) = x^{-\beta}$ is a convex function in $\mathbb{R}_+$ for each $\beta > 0$, Lemma 2.16 gives

$$\begin{aligned} \left(\frac{m}{\sum_{uv\in E(G)}(d(u)+d(v))^\alpha}\right)^\beta &\le \frac{1}{m}\sum_{uv\in E(G)}(d(u)+d(v))^{-\alpha\beta}, \\ \frac{m}{\chi_\alpha(G)} &\le \frac{1}{m^{1/\beta}}\,\chi_{-\alpha\beta}(G)^{1/\beta}. \end{aligned}$$

Assume that $\alpha \neq 0$. Since $f(x) = x^{-\beta}$ is a strictly convex function, the equality is attained if and only if $d(u) + d(v)$ is constant for every $uv \in E(G)$, and this is equivalent to the following: for each vertex $u \in V(G)$, every neighbor of u has the same degree. Since G is connected, this holds if and only if G is regular or biregular. ∎

Next, we prove nonlinear relations between $\chi_\alpha(G)$, $\chi_{\alpha+\beta}(G)$ and $\chi_{\alpha-\beta}(G)$ which allow to obtain a family of linear inequalities (see Corollary 4.3).

Theorem 4.3. *[80, Theorem 2.8] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha, \beta \in \mathbb{R}$. Then*

$$c_{\alpha,\beta} \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)} \le \chi_\alpha(G) \le \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)}\,,$$

with

$$c_{\alpha,\beta} := \min\left\{ \frac{2(\Delta\delta)^{\beta/2}}{\Delta^\beta + \delta^\beta}\,,\, \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha + \delta^\alpha} \right\} = \begin{cases} \frac{2(\Delta\delta)^{\beta/2}}{\Delta^\beta+\delta^\beta}\,, & \text{if } |\alpha| < |\beta|, \\ \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\,, & \text{if } |\alpha| \ge |\beta|. \end{cases}$$

The lower bound is attained for every values of α, β if G is regular. The upper bound is attained for some values of α, β with $\beta \neq 0$ if and only if G is regular or biregular.

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned}
\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^\alpha &= \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{(\alpha+\beta)/2+(\alpha-\beta)/2} \\
&\le \Big(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha+\beta} \Big)^{1/2} \Big(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha-\beta} \Big)^{1/2} \\
&= \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)}\,.
\end{aligned}$$

Since

$$\begin{array}{ll}
\big(2\delta\big)^{(\alpha+\beta)/2} \le \big(d(u)+d(v)\big)^{(\alpha+\beta)/2} \le \big(2\Delta\big)^{(\alpha+\beta)/2} & \text{if } \alpha+\beta \ge 0, \\
\big(2\Delta\big)^{(\alpha+\beta)/2} \le \big(d(u)+d(v)\big)^{(\alpha+\beta)/2} \le \big(2\delta\big)^{(\alpha+\beta)/2} & \text{if } \alpha+\beta \le 0, \\
\big(2\delta\big)^{(\alpha-\beta)/2} \le \big(d(u)+d(v)\big)^{(\alpha-\beta)/2} \le \big(2\Delta\big)^{(\alpha-\beta)/2} & \text{if } \alpha-\beta \ge 0, \\
\big(2\Delta\big)^{(\alpha-\beta)/2} \le \big(d(u)+d(v)\big)^{(\alpha-\beta)/2} \le \big(2\delta\big)^{(\alpha-\beta)/2} & \text{if } \alpha-\beta \le 0,
\end{array}$$

Lemma 2.5 gives, if $(\alpha+\beta)(\alpha-\beta) \ge 0$ (i.e., $|\alpha| \ge |\beta|$),

$$\begin{aligned}
\chi_\alpha(G) &= \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^\alpha \\
&\ge \frac{\Big(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha+\beta} \Big)^{1/2} \Big(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha-\beta} \Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\alpha/2} + \big(\frac{\delta}{\Delta}\big)^{\alpha/2} \Big)} \\
&= \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha} \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)} \\
&= c_{\alpha,\beta} \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)}
\end{aligned}$$

and, if $(\alpha+\beta)(\alpha-\beta) < 0$ (i.e., $|\alpha| < |\beta|$), then

$$\chi_\alpha(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^\alpha$$

$$
\begin{aligned}
&\geq \frac{\left(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha+\beta}\right)^{1/2} \left(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha-\beta}\right)^{1/2}}{\frac{1}{2}\left(\left(\frac{\Delta}{\delta}\right)^{\beta/2} + \left(\frac{\delta}{\Delta}\right)^{\beta/2}\right)} \\
&= \frac{2(\Delta\delta)^{\beta/2}}{\Delta^{\beta}+\delta^{\beta}} \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)} \\
&= c_{\alpha,\beta} \sqrt{\chi_{\alpha+\beta}(G)\chi_{\alpha-\beta}(G)}.
\end{aligned}
$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $\chi_\alpha(G)$. If G is biregular, then $\chi_t(G) = (\Delta+\delta)^t m$ and the upper bound is attained. If the upper bound is attained for some values of α, β, then $\big(d(u)+d(v)\big)^{(\alpha+\beta)/2} / \big(d(u)+d(v)\big)^{(\alpha-\beta)/2} = \big(d(u)+d(v)\big)^{\beta}$ is constant for every $uv \in E(G)$. If $\beta \neq 0$, then $d(u)+d(v)$ is constant for every $uv \in E(G)$; hence, for each vertex $u \in V(G)$, every neighbor of u has the same degree, and thus G is regular or biregular. (Note that the upper bound is $\chi_\alpha(G) \leq \chi_\alpha(G)$ if $\beta = 0$.) ■

Theorem 4.3 with $\beta = \alpha$ has the following consequence.

Corollary 4.2. *[80, Corollary 2.9] Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$
\frac{2(\Delta\delta)^{\alpha/2}}{\Delta^{\alpha}+\delta^{\alpha}} \sqrt{m\chi_{2\alpha}(G)} \leq \chi_\alpha(G) \leq \sqrt{m\chi_{2\alpha}(G)}\,.
$$

The lower bound is attained for every value of α if G is regular. The upper bound is attained for some $\alpha \neq 0$ if and only if G is regular or biregular.

Theorem 4.3 and the inequality $\sqrt{ab} \leq \frac{s}{2}a + \frac{1}{2s}b$ (for $a, b \geq 0$ and $s > 0$) give the following family of linear inequalities.

Corollary 4.3. *[80, Corollary 2.10] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, $s > 0$ and $\alpha, \beta \in \mathbb{R}$. Then*

$$
\chi_\alpha(G) \leq \frac{s}{2}\,\chi_{\alpha+\beta}(G) + \frac{1}{2s}\,\chi_{\alpha-\beta}(G),
$$

Theorem 4.4. *[80, Theorem 2.12] Let G be a nontrivial connected graph with m edges, maximum degree Δ and $2\Delta \leq m-1$. We have for any integer $\alpha \geq 1$*

$$
\chi_\alpha(G) \leq (m-1)^{\alpha-1}\chi_{\frac{1}{\alpha}}(G)^{\alpha}.
$$

The following results relate $\chi_\alpha(G)$ with $M_1(G)$ and $M_2(G)$.

Theorem 4.5. *[80, Theorem 2.13] Let G be a nontrivial connected graph with m edges and minimum degree δ, and $0 < \alpha \leq 1$. Then*

$$
\chi_\alpha(G) \leq \delta^{\alpha} m + \alpha\delta^{\alpha-2} M_2(G).
$$

Proof. We have

$$\begin{aligned}
&(d(u)-\delta)(d(v)-\delta) \geq 0,\\
&d(u)d(v)+\delta^2 \geq \delta\big(d(u)+d(v)\big),\\
&\big(\delta^{-2}d(u)d(v)+1\big)^{\alpha} \geq \delta^{-\alpha}\big(d(u)+d(v)\big)^{\alpha}.
\end{aligned}$$

Bernoulli inequality $(1+x)^{\alpha} \leq 1+\alpha x$ for $x \geq -1$ gives

$$\delta^{-\alpha}\big(d(u)+d(v)\big)^{\alpha} \leq \big(\delta^{-2}d(u)d(v)+1\big)^{\alpha} \leq 1+\alpha\delta^{-2}d(u)d(v),$$

$$\delta^{-\alpha}\chi_{\alpha}(G) \leq m+\alpha\delta^{-2}M_2(G).$$

■

Theorem 4.6. *[108, Proposition 1] Let G be a graph with $m \geq 1$ edges. If $0<\alpha<1$, then $\chi_{\alpha}(G) \leq M_1^{\alpha}(G)m^{1-\alpha}$, and if $\alpha<0$ or $\alpha>1$, then $\chi_{\alpha}(G) \geq M_1^{\alpha}(G)m^{1-\alpha}$, and either equality holds if and only if $d(u)+d(v)$ is a constant for any edge $uv \in E(G)$.*

Proof. If $0<\alpha<1$, then $-x^{\alpha}$ for $x>0$ is strictly convex, and thus:

$$\begin{aligned}
\Big(\frac{M_1(G)}{m}\Big)^{\alpha} &= \Big(\frac{1}{m}\sum_{uv\in E(G)}(d(u)+d(v))\Big)^{\alpha}\\
&\geq \frac{1}{m}\sum_{uv\in E(G)}\big(d(u)+d(v)\big)^{\alpha} = \frac{1}{m}\chi_{\alpha}(G),
\end{aligned}$$

i.e., $\chi_{\alpha}(G) \leq M_1^{\alpha}(G)m^{1-\alpha}$, with equality if and only if $d(u)+d(v)$ is a constant for any $uv \in E(G)$. Similarly, if $\alpha<0$ or $\alpha>1$, then x^{α} for $x>0$ is strictly convex, and thus $\chi_{\alpha}(G) \geq M_1^{\alpha}(G)m^{1-\alpha}$, with equality if and only if $d(u)+d(v)$ is a constant for any $uv \in E(G)$. ■

Theorem 4.7. *[80, Theorem 2.14] Let G be a nontrivial connected graph with m edges, and $\alpha \geq 1$. Then*

$$m+\alpha M_1(G) \leq \big(\chi_{\alpha}(G)^{1/\alpha}+m^{1/\alpha}\big)^{\alpha}.$$

The *forgotten topological index* is defined as $F(G)=\sum_{u\in V(G)} d(u)^3$ (see [38]).

Theorem 4.8. *[80, Theorem 2.15] Let G be a nontrivial connected graph with n vertices, m edges, maximum degree Δ and minimum degree δ. Then*

$$\begin{aligned}
&\chi_2(G)=F(G)+2M_2(G),\\
&\chi_2(G) \geq \max\Big\{4M_2(G),\ \frac{M_1(G)^2}{2m}+2M_2(G),\ \frac{M_1(G)^2}{m}\Big\} \geq \delta M_1(G)+2M_2(G),\\
&\chi_2(G) \leq \min\big\{4M_2(G)+m(n-2),\ \Delta M_1(G)+2M_2(G)\big\}.
\end{aligned}$$

4.2 Trees, unicyclic and bicyclic graphs

Let T_n be the tree obtained by attaching $\frac{n-1}{2}$ paths on two vertices to a common vertex for odd n, and obtained by attaching a path on three vertices and $\frac{n-4}{2}$ paths on two vertices to a common vertex for even n, where $n \geq 4$.

Theorem 4.9. *[33, Theorem 1] Let T be a tree with $n \geq 4$ vertices and $\alpha < \alpha_0$, where $\alpha_0 = -4.3586\ldots$ is the unique root of the equation $\frac{4^\alpha - 5^\alpha}{5^\alpha - 6^\alpha} = 3$. Then*

$$\chi_\alpha(T) \leq \begin{cases} \frac{n-1}{2}\left(3^\alpha + \frac{(n+3)^\alpha}{2^\alpha}\right), & \text{if } n \text{ is odd,} \\ \frac{n-2}{2}\left(3^\alpha + \frac{(n+2)^\alpha}{2^\alpha}\right) + 4^\alpha, & \text{if } n \text{ is even,} \end{cases}$$

with equality if and only if $T \cong T_n$.

See [33] for more information on general sum-connectivity index of trees.

Lemma 4.10. *[86, Lemma 2.3] For every $-1 \leq \alpha < 0$ and $x > 1$ we have*

$$x^\alpha - (x-1)^\alpha \geq \frac{-x^\alpha}{x-1},$$

and the equality holds if $\alpha = -1$.

Proposition 4.11. *[86, Lemma 3.1] Let uv be an edge of a graph G such that $d(u) + d(v)$ is minimum. If $-1 \leq \alpha < 0$, then*

$$\chi_\alpha(G - uv) < \chi_\alpha(G).$$

Proof. Suppose that $d(u) = p$, $d(v) = q$, $N(u) = v, x_1, ..., x_{p-1}$ and $N(v) = u, y_1, ..., y_{q-1}$, $p, q \geq 1$. By the hypothesis we have $p + d(x_i) \geq p + q$ for $i = 1, ..., p-1$ and $q + d(y_j) \geq p + q$ for $j = 1, ..., q-1$. By Lemma 4.10 we can write

$$\begin{aligned} \chi_\alpha(G) - \chi_\alpha(G - uv) &= (d(u) + d(v))^\alpha + \sum_{i=1}^{p-1} \left[(p + d(x_i))^\alpha - (p + d(x_i) - 1))^\alpha\right] \\ &+ \sum_{j=1}^{q-1} \left[(q + d(y_j))^\alpha - (q + d(y_j) - 1))^\alpha\right] \\ &\geq (d(u) + d(v))^\alpha - \sum_{i=1}^{p-1} \frac{(p + d(x_i))^\alpha}{p + d(x_i) - 1} - \sum_{j=1}^{q-1} \frac{(q + d(y_j))^\alpha}{q + d(y_j) - 1}. \end{aligned}$$

We have

$$\begin{aligned} (p + d(x_i))^\alpha &\leq (p+q)^\alpha, \\ p + d(x_i) - 1 &\geq p + q - 1, \\ \frac{(p + d(x_i))^\alpha}{p + d(x_i) - 1} &\leq \frac{(p+q)^\alpha}{p+q-1}. \end{aligned}$$

A similar argument gives

$$\frac{(q + d(y_j))^\alpha}{q + d(y_j) - 1} \leq \frac{(p+q)^\alpha}{p+q-1}.$$

Hence,

$$\begin{aligned} &\chi_\alpha(G) - \chi_\alpha(G - uv) \\ &\quad \geq (p+q)^\alpha - (p-1)\frac{(p+q)^\alpha}{p+q-1} - (q-1)\frac{(p+q)^\alpha}{p+q-1} = \frac{(p+q)^\alpha}{p+q-1} > 0. \end{aligned}$$

■

Theorem 4.12. *[86, Theorem 3.2] Let G be a graph with $n \geq 3$ vertices and maximum degree $\delta \geq 2$. If $-1 \leq \alpha < \alpha_0$, then*

$$\chi_\alpha(G) \geq 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha$$

with equality if and only if $G \cong K_2 + \overline{K_{n-2}}$.

Proposition 4.13. *[108, Proposition 4] Let G be a triangle-free graph with n vertices and $m \geq 1$ edges. If $\alpha > 0$, then $\chi_\alpha(G) \leq mn^\alpha$, with equality if and only if G is a complete bipartite graph. If $\alpha < 0$, then the above inequality on $\chi_\alpha(G)$ is reversed.*

Denote by $S_{n,p}$ the tree with p pendant vertices formed by attaching $p-1$ pendant vertices to an endvertex of the path P_{n-p+1}. In particular $S_{n,2} = P_n$ and $S_{n,n-1} = K_{1,n-1}$. Minimum value of $\chi_\alpha(T)$ for trees of given diameter $D(G)$ and $-1 \leq \alpha < 0$ has been deduced in [87] using graph transformations:

Theorem 4.14. *[87, Theorem 3.1] For $-1 \leq \alpha < 0$, in the set of trees T with $n \geq 3$ vertices and diameter $2 \leq D(G) \leq n-1$, $\chi_\alpha(T)$ is minimum if and only if $T \cong S_{n,n-D(G)+1}$.*

Another important result is the following.

Theorem 4.15. *[87, Theorem 3.4] Let T be a tree with $n \geq 5$ vertices and p pendant vertices, where $3 \leq p \leq n-2$, and $-1 \leq \alpha < 0$. Then*

$$\chi_\alpha(T) \geq (p-1)(p+1)^\alpha + (p+2)^\alpha + 3^\alpha + (n-p-2)4^\alpha$$

with equality if and only if $T \cong S_{n.p}$.

For $n \geq 3$ and $0 \leq k \leq n-3$, let $C_{n-k,k}$ denote the unicyclic graph with n vertices consisting of a cycle C_{n-k} and k pendant edges attached to a unique vertex of C_{n-k}.

Theorem 4.16. *[88, Theorem 3.1] Let G be a connected unicyclic graph with $n \geq 3$ vertices and k pendant vertices $(0 \leq k \leq n-3)$. If $-1 \leq \alpha < 0$, then*

$$\chi_\alpha(T) \geq k(k+3)^\alpha + 2(k+4)^\alpha + (n-k-2)4^\alpha$$

with equality if and only if $G \cong C_{n-k,k}$.

We have a similar result for bicyclic graphs.

Theorem 4.17. *[1, Theorem 3.7] For $-1 \leq \alpha < 0$, in the set of connected bicyclic graphs with $n \geq 4$ vertices, the minimum general sum-connectivity index is reached only by the graph consisting of two triangles with a common edge and $n-4$ pendant vertices adjacent to a vertex of degree three of this graph.*

4.3 Further results on general sum–connectivity index

Recall that the *variable Zagreb index* (also called *general Randić index*) is defined in [69] as

$$Z_\alpha(G) = \sum_{uv\in E(G)} \big(d(u)d(v)\big)^\alpha,$$

with $\alpha \in \mathbb{R}\setminus\{0\}$. The variable Zagreb index was used in the structure-boiling point modeling of benzenoid hydrocarbons. Note that $Z_{-1/2}(G)$ is the usual Randić index, $Z_1(G)$ is the second Zagreb index $M_2(G)$, $Z_{-1}(G)$ is the modified Zagreb index [71], etc.

We have several inequalities relating $\chi_\alpha(G)$ with the variable Zagreb index.

Theorem 4.18. *[80, Theorem 2.16] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha,\beta\in\mathbb{R}$. Then*

$$k_{\alpha,\beta}\Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} \le \chi_\alpha(G) \le 2^\alpha\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\,, \quad \text{if } \alpha<0,$$
$$k_{\alpha,\beta}\,2^\alpha\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} \le \chi_\alpha(G) \le \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\,, \quad \text{if } \alpha\ge 0,$$

with

$$k_{\alpha,\beta} := \begin{cases} \frac{2(\Delta\delta)^{(2\beta-\alpha)/2}}{\Delta^{2\beta-\alpha}+\delta^{2\beta-\alpha}}\,, & \text{if } \beta(\alpha-\beta)<0,\\ \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\,, & \text{if } \beta(\alpha-\beta)\ge 0. \end{cases}$$

Each one of the three first inequalities is attained for some values of α,β with $\alpha\neq 0$ if and only if G is regular. The last inequality is attained for some values of α,β with $\alpha\neq 0$ if and only if G is regular or biregular.

Proof. By Lemma 2.15, we have

$$2\sqrt{d(u)d(v)} \le d(u)d(v) \le \frac{\Delta+\delta}{\sqrt{\Delta\delta}}\sqrt{d(u)d(v)}\,.$$

If $\alpha\ge 0$, then

$$2^\alpha\big(d(u)d(v)\big)^{\alpha/2} \le \big(d(u)+d(v)\big)^\alpha \le \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha\big(d(u)d(v)\big)^{\alpha/2}.$$

If $\alpha<0$, then

$$\Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha\big(d(u)d(v)\big)^{\alpha/2} \le \big(d(u)+d(v)\big)^\alpha \le 2^\alpha\big(d(u)d(v)\big)^{\alpha/2}.$$

Cauchy-Schwarz inequality gives

$$\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{\alpha/2} = \sum_{uv\in E(G)}\big(d(u)d(v)\big)^{\beta/2+(\alpha-\beta)/2}$$
$$\le \Big(\sum_{uv\in E(G)}\big(d(u)d(v)\big)^\beta\Big)^{1/2}\Big(\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{\alpha-\beta}\Big)^{1/2} = \sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\,.$$

Since

$$\begin{aligned}
\delta^\beta \le \big(d(u)d(v)\big)^{\beta/2} \le \Delta^\beta \qquad & \text{if } \beta > 0,\\
\Delta^\beta \le \big(d(u)d(v)\big)^{\beta/2} \le \delta^\beta \qquad & \text{if } \beta < 0,\\
\delta^{\alpha-\beta} \le \big(d(u)d(v)\big)^{(\alpha-\beta)/2} \le \Delta^{\alpha-\beta} \qquad & \text{if } \alpha-\beta \ge 0,\\
\Delta^{\alpha-\beta} \le \big(d(u)d(v)\big)^{(\alpha-\beta)/2} \le \delta^{\alpha-\beta} \qquad & \text{if } \alpha-\beta < 0,
\end{aligned}$$

Lemma 2.5 gives, if $\beta(\alpha-\beta) \ge 0$,

$$\begin{aligned}
\sum_{uv\in E(G)} & \big(d(u)d(v)\big)^{\alpha/2}\\
&\ge \frac{\Big(\sum_{uv\in E(G)} \big(d(u)d(v)\big)^{\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d(u)d(v)\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\alpha/2} + \big(\frac{\delta}{\Delta}\big)^{\alpha/2}\Big)}\\
&= \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\\
&= k_{\alpha,\beta}\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)},
\end{aligned}$$

and, if $\beta(\alpha-\beta) < 0$, then

$$\begin{aligned}
\sum_{uv\in E(G)} & \big(d(u)d(v)\big)^{\alpha/2}\\
&\ge \frac{\Big(\sum_{uv\in E(G)} \big(d(u)d(v)\big)^{\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d(u)d(v)\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{(2\beta-\alpha)/2} + \big(\frac{\delta}{\Delta}\big)^{(2\beta-\alpha)/2}\Big)}\\
&= \frac{2(\Delta\delta)^{(2\beta-\alpha)/2}}{\Delta^{2\beta-\alpha}+\delta^{2\beta-\alpha}}\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\\
&= k_{\alpha,\beta}\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}.
\end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $\chi_\alpha(G)$.

If the second or the third inequality is attained for some values of α, β with $\alpha \neq 0$, then $2\sqrt{d(u)d(v)} = d(u) + d(v)$ for every $uv \in E(G)$, and Lemma 2.15 gives $d(u) = d(v)$ for every $uv \in E(G)$; since G is connected, G is regular.

Assume now that the first or the last inequality is attained for some values of α, β with $\alpha \neq 0$. Thus, $d(u) + d(v) = \frac{\Delta+\delta}{\sqrt{\Delta\delta}}\sqrt{d(u)d(v)}$ for every $uv \in E(G)$. By Lemma 2.15, this holds if and only if every edge joins a vertex of degree δ with a vertex of degree Δ, and this is equivalent to the following: for each vertex $u \in V(G)$, we have $d(u) \in \{\delta, \Delta\}$, if $d(u) = \delta$ then every neighbor of u has degree Δ, and if $d(u) = \Delta$ then every neighbor of u has degree δ. Since G is connected, this holds if and only if G is regular or biregular.

If G is regular or biregular, then $\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} = \sqrt{(\Delta\delta)^\beta m(\Delta\delta)^{\alpha-\beta}m} = (\Delta\delta)^{\alpha/2}m$ and $\chi_\alpha(G) = (\Delta+\delta)^\alpha m$. Hence, the last inequality is attained. If $\alpha \neq 0$, then the first inequality is attained if and only if $k_{\alpha,\beta} = 1$, and this holds if and only $\Delta = \delta$ by Lemma 2.15, i.e., G is regular. ■

We have the following consequence.

Corollary 4.4. *[80, Corollary 2.17] Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\frac{2(\Delta+\delta)^\alpha}{\Delta^\alpha+\delta^\alpha} Z_{\alpha/2}(G) \le \chi_\alpha(G) \le 2^\alpha Z_{\alpha/2}(G), \qquad \text{if } \alpha < 0,$$
$$\frac{2^{\alpha+1}(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha} Z_{\alpha/2}(G) \le \chi_\alpha(G) \le \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha Z_{\alpha/2}(G), \qquad \text{if } \alpha \ge 0.$$

Each one of the three first inequalities is attained for some value of $\alpha \neq 0$ if and only if G is regular. The last inequality is attained for some value of $\alpha \neq 0$ if and only if G is regular or biregular.

In [85] appears the following result.

Lemma 4.19. *[85, Lemma 3] Let h be the function $h(x,y) = \frac{2xy}{x+y}$ with $\delta \le x, y \le \Delta$. Then $\delta \le h(x,y) \le \Delta$. Furthermore, the lower (respectively, upper) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).*

Theorem 4.20. *[80, Theorem 2.19] Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\frac{2^\alpha m^2}{\delta^\alpha Z_{-\alpha}(G)} \le \chi_\alpha(G) \le \frac{\Delta^{3\alpha/2}+\delta^{3\alpha/2}}{\Delta^{7\alpha/4}\delta^{3\alpha/4}} \frac{2^{\alpha-1}m^2}{Z_{-\alpha}(G)}, \qquad \text{if } \alpha < 0,$$
$$\frac{2^\alpha m^2}{\Delta^\alpha Z_{-\alpha}(G)} \le \chi_\alpha(G) \le \frac{\Delta^{3\alpha/2}+\delta^{3\alpha/2}}{\Delta^{3\alpha/4}\delta^{7\alpha/4}} \frac{2^{\alpha-1}m^2}{Z_{-\alpha}(G)}, \qquad \text{if } \alpha \ge 0,$$

and each inequality is attained for some value of $\alpha \neq 0$ if and only if G is regular.

Proof. By Lemma 4.19, we have

$$\Big(\frac{2}{\Delta}\Big)^{\alpha/2} \le \frac{\big(d(u)+d(v)\big)^{\alpha/2}}{\big(d(u)d(v)\big)^{\alpha/2}} \le \Big(\frac{2}{\delta}\Big)^{\alpha/2}, \qquad \text{if } \alpha \ge 0,$$
$$\Big(\frac{2}{\delta}\Big)^{\alpha/2} \le \frac{\big(d(u)+d(v)\big)^{\alpha/2}}{\big(d(u)d(v)\big)^{\alpha/2}} \le \Big(\frac{2}{\Delta}\Big)^{\alpha/2}, \qquad \text{if } \alpha < 0.$$

Cauchy-Schwarz inequality gives

$$\left(\sum_{uv\in E(G)} \frac{\big(d(u)+d(v)\big)^{\alpha/2}}{\big(d(u)d(v)\big)^{\alpha/2}}\right)^2 \le \Big(\sum_{uv\in E(G)} \big(d(u)+d(v)\big)^\alpha\Big)\Big(\sum_{uv\in E(G)} \big(d(u)d(v)\big)^{-\alpha}\Big)$$
$$= \chi_\alpha(G) Z_{-\alpha}(G).$$

These inequalities provide the lower bounds.

Since

$$(2\delta)^{\alpha/2} \le \big(d(u)+d(v)\big)^{\alpha/2} \le (2\Delta)^{\alpha/2}, \Delta^{-\alpha} \le \big(d(u)d(v)\big)^{-\alpha/2} \le \delta^{-\alpha}, \quad \text{if } \alpha \ge 0,$$
$$(2\Delta)^{\alpha/2} \le \big(d(u)+d(v)\big)^{\alpha/2} \le (2\delta)^{\alpha/2}, \delta^{-\alpha} \le \big(d(u)d(v)\big)^{-\alpha/2} \le \Delta^{-\alpha}, \quad \text{if } \alpha < 0,$$

Lemma 2.5 gives in both cases

$$\begin{aligned}\left(\sum_{uv\in E(G)}\frac{\big(d(u)+d(v)\big)^{\alpha/2}}{\big(d(u)d(v)\big)^{\alpha/2}}\right)^2 &\geq \frac{\Big(\sum_{uv\in E(G)}\big(d(u)+d(v)\big)^{\alpha}\Big)\Big(\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{-\alpha}\Big)}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{3\alpha/4}+\big(\frac{\delta}{\Delta}\big)^{3\alpha/4}\Big)}\\ &= \frac{2(\Delta\delta)^{3\alpha/4}}{\Delta^{3\alpha/2}+\delta^{3\alpha/2}}\,\chi_\alpha(G)Z_{-\alpha}(G),\end{aligned}$$

and this gives the upper bounds.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $\chi_\alpha(G)$. If some bound is attained for some value of $\alpha \neq 0$, then Lemma 4.19 gives $d(u) = d(v) = \delta$ for every $uv \in E(G)$ or $d(u) = d(v) = \Delta$ for every $uv \in E(G)$; hence, G is regular. ∎

Theorem 4.21. *[80, Theorem 2.20] Let G be a nontrivial connected graph with n vertices, and $\alpha > 1$. Then*

$$n^\alpha \leq \chi_\alpha(G)Z_{\frac{-\alpha}{\alpha-1}}(G)^{\alpha-1},$$

and the equality is attained for some value of $\alpha > 1$ if and only if G is regular or biregular.

Proof. Recall that $\sum_{uv\in E(G)}\big(f(d(u))+f(d(v))\big)=\sum_{u\in V(G)}d(u)d(v)$. Hence,

$$n=\sum_{u\in V(G)}\frac{d(u)}{d(u)}=\sum_{uv\in E(G)}\Big(\frac{1}{d(u)}+\frac{1}{d(v)}\Big)=\sum_{uv\in E(G)}\frac{d(u)+d(v)}{d(u)d(v)}.$$

Since $\alpha > 1$, Hölder inequality gives

$$\begin{aligned} n &\leq \Big(\sum_{uv\in E(G)}\big(d(u)+d(v)\big)^\alpha\Big)^{\frac{1}{\alpha}}\Big(\sum_{uv\in E(G)}\big(d(u)d(v)\big)^{\frac{-\alpha}{\alpha-1}}\Big)^{\frac{\alpha-1}{\alpha}}\\ &= \chi_\alpha(G)^{\frac{1}{\alpha}}Z_{\frac{-\alpha}{\alpha-1}}(G)^{\frac{\alpha-1}{\alpha}}.\end{aligned}$$

If G is regular or biregular, then $\Delta\delta n = \big(\Delta+\delta\big)m$, $\chi_\alpha(G) = (\Delta+\delta)^\alpha m$, $Z_{\frac{-\alpha}{\alpha-1}}(G) = (\Delta\delta)^{\frac{-\alpha}{\alpha-1}}m$, and the equality is attained.

If the equality is attained for some value of $\alpha > 1$, then $\big(d(u)d(v)\big)^{\frac{-\alpha}{\alpha-1}}/\big(d(u)+d(v)\big)^\alpha$ is constant for every $uv \in E(G)$, i.e., $d(u)d(v)\big(d(u)+d(v)\big)^{\alpha-1}$ is constant for every $uv \in E(G)$. Since the function $F(t) = d(u)t\big(d(u)+t\big)^{\alpha-1}$ is increasing when $t \in [1,\infty)$, we have the following: for each vertex $u \in V(G)$, every neighbor v of u has the same degree, and the degree of every neighbor of v is $d(u)$. Since G is connected, G is regular or biregular. ∎

We have the following consequence, that improves the lower bound in Theorem 4.20 when $\alpha = 2$, since $2m \leq \Delta n$.

Corollary 4.5. *[80, Corollary 2.21] Let G be a nontrivial connected graph with n vertices. Then*

$$n^2 \leq \chi_2(G) Z_{-2}(G),$$

and the equality is attained if and only if G is regular or biregular.

We need the following result.

Lemma 4.22. *[108, Proposition 2] Let G be a graph with $n \geq 2$ vertices. If $0 < \alpha < 1$, then $\chi_\alpha(G) \geq M_1(G)^\alpha$ with equality if and only if $G \cong K_2 \cup \overline{K_{n-2}}$ or $G \cong \overline{K_n}$, and if $\alpha < 0$, then $\chi_\alpha(G) \leq 2^{\alpha-1} n(n-1)$ with equality if and only if $G \cong K_2$.*

Zhou and Trinajstić [108] showed a result for the general sum-connectivity index of Nordhaus-Gaddum type.

Theorem 4.23. *[108, Proposition 5] Let G be a graph with $n \geq 2$ vertices.*

If $\alpha > 0$, then

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \leq 2^{\alpha-1} n(n-1)^{\alpha+1}$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$,

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \geq 2^{-1} n(n-1)^{\alpha+1} \qquad \text{for } \alpha \geq 1,$$

with equality if and only if G is a regular graph of degree $\frac{n-1}{2}$, and

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) > 2^{-\alpha} n^\alpha (n-1)^{2\alpha} \qquad \text{for } 0 < \alpha < 1.$$

If $\alpha < 0$, then

$$2^{\alpha-1} n(n-1)^{\alpha+1} \leq \chi_\alpha(G) + \chi_\alpha(\overline{G}) < 2^\alpha n(n-1)$$

with left equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$,

Proof. Let m and $\overline{m}$ be respectively the numbers of edges of G and $\overline{G}$. Thus, $m + \overline{m} = \frac{n(n-1)}{2}$. If $\alpha > 0$, then

$$\begin{aligned}\chi_\alpha(G) + \chi_\alpha(\overline{G}) &= \sum_{uv \in E(G)} \big(d_G(u) + d_G(v)\big)^\alpha + \sum_{uv \in E(\overline{G})} \big(d_{\overline{G}}(u) + d_{\overline{G}}(v)\big)^\alpha \\ &\leq m(2n-2)^\alpha + \overline{m}(2n-2)^\alpha = (m + \overline{m})(2n-2)^\alpha = 2^{\alpha-1} n(n-1)^{\alpha+1}\end{aligned}$$

with equality if and only if either $d(u) = d(v) = n-1$ for every edge $uv \in E(G)$ or $E(G) = \emptyset$, i.e., $G \cong K_n$ or $G \cong \overline{K_n}$.

Similarly, if $\alpha < 0$, then

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \geq 2^{\alpha-1} n(n-1)^{\alpha+1}$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

It is easily seen that

$$\begin{aligned}\chi_1(G) + \chi_1(\overline{G}) &= \sum_{u \in V(G)} \big(d_G(u)^2 + d_{\overline{G}}(u)^2\big) \\ &\geq \sum_{u \in V(G)} \frac{\big(d_G(u) + d_{\overline{G}}(u)\big)^2}{2} = \frac{n(n-1)^2}{2}\end{aligned}$$

with equality if and only if $d_G(u) = d_{\overline{G}}(u)$ for all $u \in V(G)$, i.e., G is a regular graph of degree $\frac{n-1}{2}$. If $\alpha > 1$, then x^α is strictly convex and thus

$$\begin{aligned}
&\chi_\alpha(G) + \chi_\alpha(\overline{G}) \\
&\quad \geq (m+\overline{m}) \left(\frac{\sum_{uv\in E(G)}(d_G(u)+d_G(v)) + \sum_{uv\in E(\overline{G})}(d_{\overline{G}}(u)+d_{\overline{G}}(v))}{m+\overline{m}} \right)^\alpha \\
&\quad = (m+\overline{m})^{1-\alpha} \left(\chi_1(G) + \chi_1(\overline{G})\right)^\alpha \\
&\quad \geq \left(\frac{n(n-1)}{2}\right)^{1-\alpha} \left(\frac{n(n-1)^2}{2}\right)^\alpha \\
&\quad = 2^{-1} n(n-1)^{\alpha+1}
\end{aligned}$$

with equality if and only if G is a regular graph of degree $\frac{n-1}{2}$. If $0 < \alpha < 1$, then

$$\begin{aligned}
\chi_\alpha(G) + \chi_\alpha(\overline{G}) &\geq \left(\sum_{uv\in E(G)} (d_G(u)+d_G(v)) + \sum_{uv\in E(\overline{G})} (d_{\overline{G}}(u)+d_{\overline{G}}(v)) \right)^\alpha \\
&= \left(\chi_1(G) + \chi_1(\overline{G})\right)^\alpha \geq \left(\frac{n(n-1)^2}{2}\right)^\alpha = 2^{-\alpha} n^\alpha (n-1)^{2\alpha}.
\end{aligned}$$

Since a graph G with $|E(G) \cup E(\overline{G})| \leq 1$ is not possible to be a regular graph of degree $\frac{n-1}{2}$ for $n \geq 2$, we have

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) > 2^{-\alpha} n^\alpha (n-1)^{2\alpha}.$$

If $\alpha < 0$, then by Lemma 4.22,

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) < 2^{\alpha-1} n(n-1) + 2^{\alpha-1} n(n-1) = 2^\alpha n(n-1).$$

The proof is now completed. ■

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Bounds of the Wiener Polarity Index

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Abstract

The Wiener polarity index $W_p(G)$ of a graph G, proposed by Wiener in 1947, is the number of unordered pairs of vertices $\{u, v\}$ of G such that the distance between u and v is 3. We survey some recent development on bounding the Wiener polarity index and related results.

Contents

1. Introduction

In theoretical chemistry molecular structure descriptors are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [24]. There exist several types of such indices, especially those based on vertex and edge distances. One of the best known such indices is the Wiener index, defined as the sum of distances between all pairs of vertices of the molecular graph [15]:

$$W(G) = \sum_{u,v \in V(G)} d(u,\ v).$$

The Wiener index was introduced by Wiener [49] in 1947. It has since become one of the best known chemical indices. For more results on the Wiener index, we refer the readers to the survey paper [15] written by Dobrynin, Entringer and Gutman.

Wiener also introduced another index for acyclic molecules, called the *Wiener polarity index* and defined as

$$W_p(G) := |\{\{u,v\}|d(u,v) = 3, u,v \in V(G)\}|.$$

Wiener [49] used a linear formula of W and W_P to calculate the boiling points t_B of the paraffins, *i.e.,* $t_B = aW + bW_p + c$, where a, b and c are constants for a given isomeric group. Like $W(G)$, the Wiener polarity index received much attention from biochemical point of view. Through the Wiener polarity index, the authors of [37] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya presented a physical-chemical interpretation of $W_P(G)$ in [26]. In recent years there has been more studies on the mathematical properties of this index. In 2009, Du, Li and Shi [17] described a linear time algorithm APT for computing the Wiener polarity index of trees, and characterized the trees maximizing the Wiener polarity index among all trees of given order. The extremal Wiener polarity index of (chemical) trees with given different parameters (e.g. order, diameter, maximum degree, the number of pendants, etc.) were studied in [17, 18, 20, 36, 38]. The unicyclic graphs minimizing (resp. maximizing) the Wiener polarity index among all unicyclic graphs of order n were given in [29]. There are also extremal results on some other graphs, such as fullerenes, hexagonal systems, lattices and cactus graphs [10, 11, 13, 19].

We aim to report some of the most recent results on bounding the Wiener polarity index. In the next section we present the necessary background information. Section 3 discusses bounds of the Wiener polarity index for trees and trees with certain restrictions. In Section 4 we consider the unicyclic graphs and the extremal problem with respect to the Wiener polarity index. Section 5 presents some results on the Wiener polarity index of graph products and the Nordhaus-Gaddum-type inequality. In Section 6, we discuss representing and bounding the Wiener polarity index in terms of other graph invariants such as the Wiener index, hyper-Wiener index, first Zagreb index, second Zagreb index, etc.. Last but not least, we briefly discuss the generalization of the Wiener polarity index and related extremal problems in Section 7.

2. Preliminaries

We follow [4] for general graph theoretical notations and terminologies. For a graph G, let $V(G)$, $E(G)$, $|G|$, $e(G)$, and $\overline{G}$ denote the set of vertices, the set of edges, the order, the size and the complement of G, respectively. The set of neighbors of a vertex v in G is denoted by $N_G(v)$ or simply $N(v)$. The *degree* $d_G(v) = d(v)$ of a vertex v is the number of edges adjacent to v. A vertex of degree 1 is a pendent vertex. We let $\delta(G) := min\{d(v)|v \in V\}$ denote the *minimum degree* of G, and let $\Delta(G) := max\{d(v)|v \in V\}$ denote its *maximum degree*. The minimum length of a cycle in a graph G is the *girth* $g(G)$ of G. The *distance* $d_G(u,\ v)$ in G of two vertices $u,\ v$ is the length of a shortest $u - v$ path in G; if no such path exists, we set $d(u, v) := \infty$. The greatest distance between any two vertices in G is the *diameter* of G, denoted by $diam(G)$.

An acyclic graph is called a *forest*. A connected forest is called a *tree*. The pendant vertices in a tree are its *leaves*. A *unicyclic graph* is a connected graph containing exactly one cycle. It is easily to see that $|V(G)| = |E(G)|$ for any unicyclic graph G. A graph is called *k-cyclic* if $|E(G)| = |V(G)| - 1 + k$, where $k \geq 2$. Let $K_{1,n-1}$, C_n and P_n be the star, cycle and path of order n, respectively. A "hanging tree" on vertex v in G, denoted by $T[v]$, is a pendant subtree rooted at v.

It is easy to see that $W_P(G) = \sum_{i=1}^{t} W_p(G_i)$ if $G_1, G_2, \cdots, G_t$ (where $t \geq 2$) are the connected components of a graph G. So it suffices to consider the Wiener polarity index of connected graphs. We first present some operations that decrease or increase the Wiener polarity index of connected graphs. Although we are not going to present any proofs in this survey, it is worth pointing out that these operations pay crucial roles in the proofs of most of the extremal results.

Let $\mathrm{T}(n)$ denote the set of trees on n vertices. Let $T \in \mathrm{T}(n)$ be a tree with $diam(T) = k \geq 4$. Suppose that $P(T) = v_0v_1v_2 \cdots v_k$ is a longest path of T. Let $T \circledast v_0$ denote the tree obtained from T by removing the edge v_0v_1 and adding a new edge v_0v_3. This operation, shown in Figure 1, is called a *maximization operation* as it only increases the Wiener polarity index.

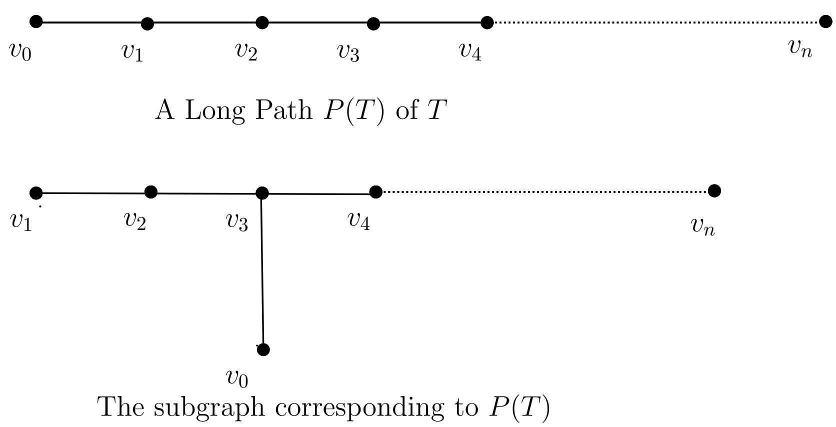

Figure 1. Maximization operation of a tree T.

Theorem 2.1. *[17] Let $T = (V, E)$ be a tree and $P(T) = v_0v_1v_2 \cdots v_k$ be a longest path of T with $k \geq 4$. Then*

i) $W_p(T) < W_p(T \circledast v_0)$ if $diam(T) \geq 5$;

ii) $W_p(T) \leq W_p(T \circledast v_0)$ if $diam(T) = 4$.

Next we introduce the transformation "Sigma" on unicyclic graphs that only increases the Wiener polarity index:

Let $T[v_i]$ denote a hanging tree on vertex v_i of a unicyclic graph U with $g(U) \geq 4$, where $v_i \in V(C)$ and $C = v_1 v_2 \cdots v_g v_1$ is the cycle of U. Among all hanging trees, suppose $P_l = v_i u_1 \cdots u_l$ is one of the longest path from the root v_i to a leaf u_l of the hang tree $T[v_i]$. If $l \geq 2$, then after removing the edge $v_i u_1$ from U, we obtain a unicyclic graph A and a tree B such that $v_i \in A$ and $u_1 \in B$. Let U^* denote the unicyclic graph obtained from A and B by identifying u_1 and $v_{i+1(mod\ g)}$ and adding a new leaf w_1 adjacent to v_i (see Figure 2).

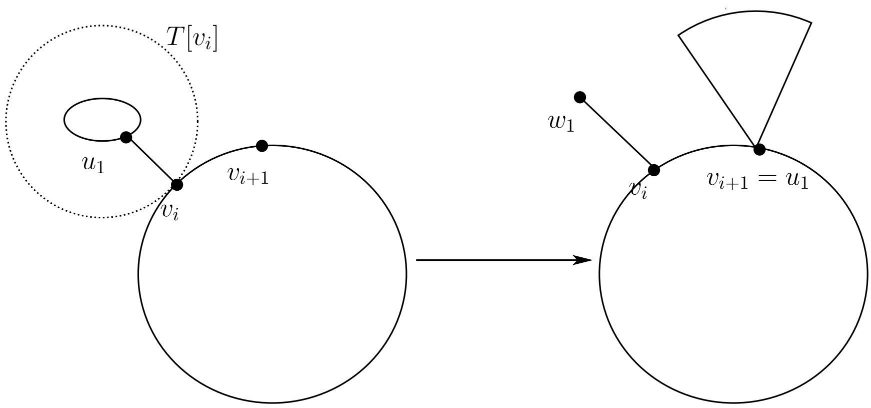

Figure 2. The transformation “Sigma”.

Theorem 2.2. *[30] Let U be a unicyclic graph with $g(U) \geq 4$ and U^* be the unicyclic graph obtained from U by applying transformation Sigma. If $g(U) \geq 5$, then*

$$W_p(U) < W_p(U^*),$$

If $g(U) = 4$, then

$$W_p(U) \leq (W_p(U^*).$$

The “Edge rotation”, as described below, also only incrases the Wiener polarity index. Let $C_g = v_1 v_2 \cdots v_g$ be the cycle of a unicyclic graph $C_g(k_1, \cdots, k_g)$ with $g(U) \geq 4$. Here k_i is the number of pendant edges at vertex v_i, and every edge not on the cycle is a pendant edge. Without loss of generality, let v_1 and v_3 be the two vertices such that $d(v_1) + d(v_3) = max\{d(v_i) + d(v_{i+2})\}$, where $i = 1, 2, \cdots, g\ (mod\ g)$. We can construct a new graph $C_g(k_1, k_2 + k_i, k_3, \cdots, k_{i-1}, 0, k_{i+1}, \cdots, k_g)$ by removing k_i pendant vertices from v_i and reattaching them to v_2 as shown in Figure 3 ($4 \leq i \leq g$).

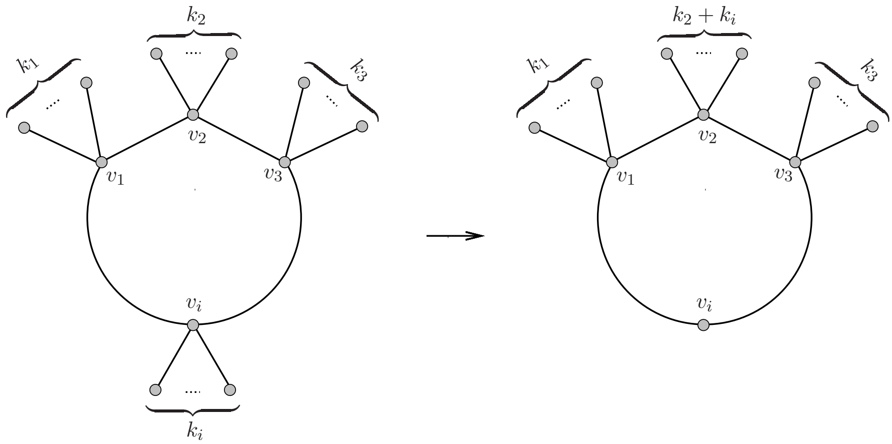

Figure 3. Edge rotation.

Theorem 2.3. *[30] Let $g \geq 4$, then*

$$W_p(C_g(k_1, k_2, \cdots, k_g) \leq W_p(C_g(k_1, k_2 + k_i, \cdots, k_g).$$

3. Bounds for the Wiener polarity index of trees

We start with the following formula of the Wiener polarity index of a tree.

Lemma 3.1. *[17] Let $T = (V, E)$ be a tree, then $W_p(T) = \sum\limits_{uv \in E} (d_T(u) - 1)(d_T(v) - 1)$.*

We now define some specific trees. Let $\mathrm{T}(n)$ denote the set of the trees on n vertices. Let $\mathrm{T}_3(n) := \{T \in \mathrm{T}(n) | diam(T) = 3, W_p(T) = \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil\}$, and $\mathrm{T}_4(n) := \{T(k_1, k_2, k_3, l_1, \cdots, l_m) \in \mathrm{T}(n) | m + k_2 + 1 = \lfloor \frac{n-2}{2} \rfloor$ or $\lceil \frac{n-2}{2} \rceil\}$. Here $T(k_1, k_2, k_3, l_1, \cdots, l_m)$ is a tree with diameter 4 as in Figure 4, with $k_i \geq 0$ ($i = 1, 2, 3$), $m \geq 1$, $1 \leq j \leq m$, and $k_1 + k_2 + k_3 + l_1 + \cdots + l_m = n - 5 - m$.

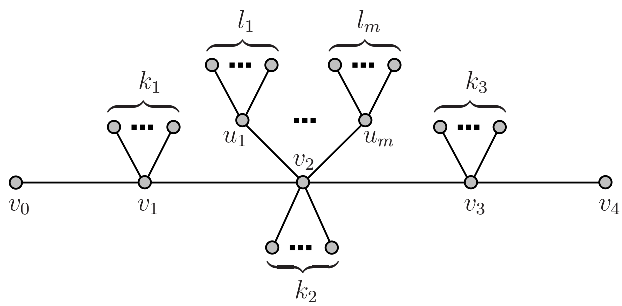

Figure 4. The tree $T(k_1, k_2, k_3, l_1, \cdots, l_m)$.

Theorem 3.1. *[17] A tree T of order n has Wiener polarity index*

$$W_p \leq \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$$

with equality if and only if $T \in \mathrm{T}_3(n) \cup \mathrm{T}_4(n)$.

It is obvious that the Wiener polarity index of a star is zero. So it is natural to leave the star out when we consider the minimum Wiener polarity index. A *general double star* $P(k; a, b)$ is a tree obtained from a path $P_k = v_0 v_1 \cdots v_k$ ($k \geq 3$) by attaching a pendent vertices and b pendent vertices to the vertices v_1 and v_k, respectively. Such structures have been shown to minimize the Wiener polarity index.

Theorem 3.2. *[38] Suppose that $T \in \mathrm{T}(n) \backslash \{K_{1,n-1}\}$, then*

$$W_p(T) \geq n - 3$$

with equality if and only if $T \cong P(k; n-k-b, b)$, where $k \geq 3$, $n-k \geq b \geq 0$.

Besides bounding the Wiener polarity index among general trees, it is of interest to consider more specific classes of trees under various constraints. To introduce such work we present some more definitions. A *chemical graph* is a graph with maximum degree no more than 4. In general, let T_n^{Δ} be the set of all trees with n vertices and maximum degree Δ. For a positive integer p and nonnegative integers $n_1,\ n_2$, let $S^p_{n_1,n_2}$ be a tree obtained from a path $v_1 v_2 \cdots v_p$ by attaching n_1 and n_2 pendant edges to the vertices v_1 and v_p, respectively. Let $V^{(\Delta)}(T) = \{v \in V(T) | d_T(v) = \Delta\}$, $N^{(\Delta)}(T) = \cup_{u \in V^{(\Delta)}(T)} N_T(u)$, $h = n - (\Delta + 1)$ and $T_0 = S_{\Delta+1}$, construct T_i from T_{i-1} by attaching a vertex to one vertex of $N^{(\Delta)}(T_{i-1}) \backslash V^{(\Delta)}(T_{i-1})$ for $i = 1, 2, \cdots, h$. The set of all possible T_h after h steps is denoted by $T^{n,\Delta}_{max}$.

Deng et al. obtained the maximum Wiener polarity index among chemical trees on n vertices.

Theorem 3.3. *[14] Let T be a chemical tree of order n (≥ 7), then*

$$W_p(T) \leq 3(n-5)$$

with equality if and only if $T \in T^{n,4}_{max}$.

This result was generalized to the following theorem, which determines the maximum and minimum Wiener polarity indices in T^{Δ}_n. Here $S(n-\Delta+1-l; \Delta-1, l)$ is a tree obtained from a path $P_{n-\Delta+1-l} = v_1 v_2 \cdots v_{n-\Delta+1-l}$ by attaching $\Delta - 1$ pendant vertices to v_1 and a pendant vertex to v_k.

Theorem 3.4. *[36] Let $T \in \mathrm{T}_n^{\Delta}$, where $3 \leq \Delta \leq n-3$. Then*

$$n - 3 \leq W_P(T) \leq (n - \Delta - 1)(\Delta - 1).$$

The left equality holds if and only if $T \cong S(n-\Delta+1-l; \Delta-1, l)$ where $0 \leq l \leq min\{\Delta-1, n-\Delta-2\}$, while the right equality holds if and only if $T \in T^{n,\Delta}_{max}$.

Let $\mathrm{T}(n, d)$ be the set of trees of order n with diameter d. It is easy to see that $W_p(G) = 0$ if $diam(G) \leq 2$. For $3 \leq diam(G) \leq n-1$, we have the following theorems.

Theorem 3.5. *[20] Let $T \in \mathrm{T}(n,d)$, where $3 \leq d \leq n-1$. Then*

$$W_p(T) \geq n-3$$

with equality if and only if: $T \cong S(d-2; n+2-d-t, t)$, where $n+2-d-t \geq t \geq 1$, if $d > 3$; and $T \cong P(3; n-4, 0)$, if $d = 3$.

Theorem 3.6. *[20] Let $T \in \mathrm{T}(n,d)$, where $5 \leq d \leq n-1$. Then*

$$W_p(T) \leq \lfloor \frac{n-d-1}{2} \rfloor \lceil \frac{n-d-1}{2} \rceil + 2n-d-4.$$

Moreover, the equality holds if and only if $T \cong T(n,d; 0, \cdots, 0, x_i, x_{i+1}, x_{i+2}, 0, \cdots, 0)$, where $2 \leq i \leq d-4$, $x_i \geq 0$, $x_{i+2} \geq 0$ and $x_{i+1} = \lfloor \frac{n-d-1}{2} \rfloor$or$\lceil \frac{n-d-1}{2} \rceil$. Here $T(n,d; 0, \cdots, 0, x_i, x_{i+1}, x_{i+2}, 0, \cdots, 0)$ is obtained from a path $P_d = v_0 v_1 \cdots v_d$ by attaching x_i ,x_{i+1} and x_{i+2} pendent vertices to the vertices v_i, v_{i+1} and v_{i+2}, respectively.

Note that when $d = 3$ or 4, Theorem 3.1 implies that $W_p(T) = \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$ if and only if $T \in \mathrm{T}_3(n) \cup \mathrm{T}_4(n)$. Tang and Deng [47] characterized the trees with the first three smallest Wiener polarity indices in $T(n,d)$.

Let $\mathcal{T}(n,k)$ be the set of trees of order n with k pendant vertices. It is easy to see that $T(n,2) = \{P_n\}$ with $W_p(P_n) = n-3$, and $T(n, n-1) = \{S_n\}$ with $W_p(S_n) = 0$. For $3 \leq k \leq n-2$, we have the following theorems with $\mathcal{T}_{n,n-2} = \{S(n_1, n_2) | n_1 + n_2 = n, n_1 \geq n_2 \geq 2\}$. Here $S(n_1, n_2)$ is the graph obtained from joining the centers of S_{n_1} and S_{n_2} by an edge, also called a double-star.

Theorem 3.7. *[18, 36] If $T \in \mathcal{T}_{n,n-2}$, then*

$$n-3 \leq W_p(T) \leq \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$$

where the left equality holds if and only if $T \cong S(n-2, 2)$, and the right equality holds if and only if $T \cong S(\lceil \frac{n-2}{2} \rceil + 1, \lfloor \frac{n-2}{2} \rfloor + 1)$.

Theorem 3.8. *[36] Let $T \in \mathcal{T}(n,k)$, where $3 \leq k \leq n-3$. Then*

$$W_p(T) \geq n-3$$

with equality if and only if $T \cong S(n-k; n_1, k-n_1)$, where $0 \leq n_1 \leq k-n_1$.

Theorem 3.9. *[18] Let $T \in \mathcal{T}(n,k)$, where $k+2 \leq n \leq 2k$ and $n \geq 4$. Then*

$$W_p \leq \lfloor \frac{n-2}{2} \rfloor \lceil \frac{n-2}{2} \rceil$$

with equality if and only if $T \cong T(k_1, k_2, k_3, l_1, \cdots, l_s)$ where $k_2 = k+1-\lfloor \frac{n-2}{2} \rfloor$(or $\lceil \frac{n-2}{2} \rceil$), or $T \cong S(\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)$.

Theorem 3.10. *[18] Let $T \in \mathcal{T}(n,k)$. If $n \geq 2k+1$, then*

$$W_p(T) \leq k^2 - 3k + n - 1$$

with equality if and only if T is a starlike tree of order n in which the lengths of all pendant chains are at least 2.

Deng et al. also identified the maximum Wiener polarity index of chemical trees with n vertices and k pendent vertices [19].

Furthermore, in [50], Wang et al. consider the smallest and the largest Wiener polarity index among all Hückel trees on $2n$ vertices and characterize the corresponding extremal graphs. Recently, in [35], Lei et al. studied trees with a given degree sequence, and characterized the extremal graphs attaining the maximum and minimum values of the Wiener polarity index, respectively. In [3], Ashrafi et al. presented an ordering of chemical trees of order n with respect to the Wiener polarity index.

4. Bounds for the Wiener polarity index of unicyclic graphs

Moving our attention to the unicyclic graphs, we first present a formula of the Wiener polarity index.

Lemma 4.1. *[38] Let $U = (V,E)$ be a unicyclic graph and let C denote the unique cycle of U. If $g(U) = 3$ with $V(C) = \{v_1, v_2, v_3\}$, then*

$$W_p(U) = \sum_{uv \in E} (d_U(u)-1)(d_U(v)-1) + 9 - 2d_U(v_1) - 2d_U(v_2) - 2d_U(v_3).$$

If $g(U) = 4$ and $V(C) = \{v_1, v_2, v_3, v_4\}$, then

$$W_p(U) = \sum_{uv \in E} (d_U(u)-1)(d_U(v)-1) + 4 - d_U(v_1) - d_U(v_2) - d_U(v_3) - d_U(v_4).$$

If $g(U) \geq 5$, then

$$W_p(U) = \begin{cases} \sum\limits_{uv \in E} (d_U(u)-1)(d_U(v)-1) - 5, & \text{if } g(U) = 5; \\ \sum\limits_{uv \in E} (d_U(u)-1)(d_U(v)-1) - 3, & \text{if } g(U) = 6; \\ \sum\limits_{uv \in E} (d_U(u)-1)(d_U(v)-1), & \text{if } g(U) \geq 7. \end{cases}$$

First we have the following bounds.

Theorem 4.1. *[30] Let U be a unicyclic chemical graph with $n(\geq 5)$ vertices. Then*

$$n - 3 \leq W_p(U) \leq 3(n+4).$$

Theorem 4.2. *[30] Let U be a unicyclic graph of order $n \geq 11$. Then*

$$W_p(U) \leq W_p(U_3)$$

with equality if and only if $U \cong U_3$. Here U_3 denotes the "caterpillar cycle" $C_3(k_1, k_2, k_3)$ with $|k_i - k_j| \leq 1$ $(i,j = 1,2,3)$ of order n.

Now for unicyclic graphs with a given girth:

- Let U_1 be the unicyclic graph obtained from $K_{1,n-1}$ by adding one edge between two pendant vertices of $K_{1,n-1}$.
- Let U_2 be the unicyclic graph obtained form a $C_3 = v_0v_1v_2$ by attaching $n-4$ pendent vertices and one pendent vertex to the vertices v_0 and v_2, respectively.
- Let C^j_{g,l_1,l_2} be a unicyclic graph obtained from C_g by attaching l_1 and l_2 pendant vertices to u_i and u_{i+j} respectively, where $i, j \in \{1, \cdots, g \pmod g\}$.
- Let $\mathbb{U}(n,g)$ be the set of unicyclic graphs of order n with girth g.
- Let $C_g(P_{n-g})$ be the unicyclic graph on n vertices formed by attaching a path P_{n-g} to one vertex of C_g.
- Let $C^1_{n,g}$ be the unicyclic graph obtained from a cycle C_g by attaching a path P_{n-g-1} to a vertex u_0 of C_g, and one pendent vertex to another vertex v_0 of C_g.

Theorem 4.3. *[29] For $n \geq 9$ we have*
(1) $\mathbb{U}(n,n) = \{C_n\}$, and $W_p(C_n) = n$;
(2) $\mathbb{U}(n,n-1) = \{C_{n,n-1}\}$, and $W_p(C_{n,n-1}) = n+1$;
(3) $\mathbb{U}(n,n-2) = \{C_{n-2}(P_2), C_{n,n-2}, C^j_{n-2,1,1}$, and $W_p(C^1_{n-2,1,1}) = n+3 > n+2 = W_p(C_{n-2}(P_2)) = W_P(C_{n,n-2}) = W_p(C^j_{n-2,1,1})$, where $1 \leq j \leq \lfloor \frac{n-2}{2} \rfloor$.

For smaller values of g we define the following special graph in $\mathbb{U}(n,g)$.

- Let $C(v_0, \cdots, v_t; p)$ denote a comet, which is a tree obtained from a path $v_0v_1 \cdots v_t$ by attaching p vertices to the vertex v_t, where $t, p \geq 1$.
- Let $C_g \bigodot C(v_0, \cdots, v_t; n-t-g)$ be a unicyclic graph obtained from a cycle C_g and $C(v_0, \cdots, v_t; n-t-g)$ by identifying a vertex of C_g and v_0.

Theorem 4.4. *[29] Let $U \in \mathbb{U}(n,g)$, where $5 \leq g \leq n-3$. Then*

$$W_p(U) \geq n+2 \ (resp.\ n-1, n-3)$$

if $g \geq 7$ (resp. g= 6,5), with equalities if and only if $U \cong C_g \bigodot C(v_0, \cdots, v_t; n-t-g)$ with $t \geq 2, n-t-g \geq 1$.

Theorem 4.5. *[38] Suppose $n \geq 7$. If $U \in \mathbb{U}(n,3) \backslash \{U_1\}$, then*

$$W_p(U) \geq n-4$$

with equality if and only if $U \cong U_2$. If $U \in \mathbb{U}(n,4)$, then

$$W_p(U) \geq n-4$$

with equality if and only if $U \cong C_{n,4}$ or $C^2_{4,l,n-4-l}$, where $1 \leq l \leq n-5$.

As for maximizing the Wiener polarity index, we have the following.

Theorem 4.6. *[29] Let $U \in \mathbb{U}(n,g)$, where $5 \le g \le n-3$. Then*

$$W_p(U) \le \lfloor \frac{n-g}{2} \rfloor \lceil \frac{n-g}{2} \rceil + \begin{cases} 2n-10, & \text{if } g(U)=5; \\ 2n-9, & \text{if } g(U)=6; \\ 2n-g, & \text{if } g(U) \ge 7. \end{cases}$$

with equality if and only if $U \cong C_g(k_1,k_2,k_3,0,\cdots,0)$, where $k_1,k_2,k_3 \ge 0$, $\sum_{i=1}^{3} k_i = n-g$, and $k_2 = \lfloor \frac{n-g}{2} \rfloor (or \lceil \frac{n-g}{2} \rceil)$.

Let $C_4(k_1,k_2,k_3,0) \bigotimes (t)$ denote the unicyclic graph obtained from attaching t pendant edges to any pendant vertices of $N_{C_4(k_1,k_2,k_3,0)}(v_2)$, where $k_1,k_2,k_3 \ge 0$ and $t \ge 1$.

Theorem 4.7. *[29] Let $U \in \mathbb{U}(n,4)$. Then*

$$W_p(U) \le \lfloor \frac{n-4}{2} \rfloor \lceil \frac{n-4}{2} \rceil + n - 4$$

with equality if and only if $U \cong C_4(k_1,k_2,k_3,k_4)$, where $k_1,k_2,k_3,k_4 \ge 0$ and $n-4-k_1-k_3 = k_2+k_4 = \lfloor \frac{n-4}{2} \rfloor or \lceil \frac{n-4}{2} \rceil$, or $U \cong C_4(k_1,k_2,k_3,0) \bigotimes (t)$, where $k_1,k_2,k_3,k_4 \ge 0$, $t \ge 1$ and $n-4-k_1-k_3 = k_2+k_4 = \lfloor \frac{n-4}{2} \rfloor or \lceil \frac{n-4}{2} \rceil$.

Theorem 4.8. *[29] Let $U \in \mathbb{U}(n,3)$, where $n \ge 11$. Then*

$$W_p(U) \le \begin{cases} \frac{1}{3}(n-3)^2, & \text{if } n = 0 \pmod 3; \\ \frac{1}{3}(n-2)(n-4), & \text{if } n \ne 0 \pmod 3. \end{cases}$$

where equality if and only if $U \cong U_3$.

Let $\mathcal{U}_{n,k}$ be the set of unicyclic graphs on n vertices with k pendent vertices. The next result determines the minimum Wiener polarity index in $\mathcal{U}_{n,k}$ for any k.

Theorem 4.9. *[29] For $n \ge 9$ we have*

(1) $\mathcal{U}_{n,0} = \{C_n\}$, and $W_p(U) = n$;

(2) $\mathcal{U}_{n,1} = \{C_g(P_{n-g}\}$ $(n \ge g \ge 3)$, where $W_p(C_{n-1}(P_1)) = n+1$, and $W_p(C_g(P_{n-g})) = n+2$ for $g \le n-2$;

(3) Let $U \in \mathcal{U}_{n,n-3}$. Then $W_p(U) \ge 0$ with equality if and only if $U \cong U_1$.

(4) Let $U \in \mathcal{U}_{n,n-4}$. Then $W_P(U) \ge n-4$ with equality if and only if $U \cong C_{n,4}$ or $C^2_{4,l,n-4-l}$, where $1 \le l \le n-5$.

(5) If $2 \le k \le n-5$ and $U \in \mathcal{U}_{n,k}$, then $W_p(U) \ge n-3$.

It is worth noting that, for $2 \le k \le n-5$, the extremal unicyclic graphs of Theorem 4.9 were also characterized in [29]. Now let $\mathcal{U}_n^{\Delta}$ be the set of unicyclic graphs on n vertices with maximum degree Δ. Clearly, $2 \le \Delta \le n-1$. It is easy to see that $\mathcal{U}_n^2 = \{C_n\}$ and $\mathcal{U}_n^{n-1} = \{U_1\}$. For $3 \le \Delta \le n-2$, we have the following theorem.

Theorem 4.10. *[29] Let $U \in \mathcal{U}_n^{\Delta}$ and $n \geq 7$.*
(1) If $3 \leq \Delta < \lceil \frac{n}{2} \rceil$, then $W_p(U) \geq n-3$.
(2) If $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, then $W_p(U) \geq n-4$ with equality if and only if $U \cong C^1_{3,n-4,1}$ or $C_{n,4}$ if $\Delta = n-2$, and $U \cong C^2_{4,\Delta-2,n-2-\Delta}$ if $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-3$.

Since $W_p(C_n) = n$ and $W_p(U_1) = 0$ for $n \geq 7$, Theorem 4.10 determines the minimum Wiener polarity index in $\mathcal{U}_n^{\Delta}$ for arbitrary Δ. The extremal unicyclic graphs for $3 \leq \Delta < \lceil \frac{n}{2} \rceil$ of Theorem 4.10 were also characterized in [29]. Next let $\mathcal{U}(n,d)$ be the set of unicyclic graphs with order n and diameter d. For $d \geq 3$, we first introduce the following graphs:

- Let $U_3(s,t)$ $(s+t = n-d-3)$ be a unicyclic graph, obtained from a path $P = v_0v_1\cdots v_d$ of length d by adding s pendant vertices to v_1, t pendant vertices to v_{d-1}, and identifying a vertex of a triangle with v_1 or v_{d-1}.

- Denote the unicyclic graph $U_3(a_1,\ a_2,\ a_3)$ with $|a_i - a_j| \leq 1$ $(i,j \in \{1,2,3\})$ of order n and diameter d by U_3^*, and the unicyclic graph $U_3'(a_1', a_2', a_3')$ with $|a_i' - a_j'| \leq 1$ $(i,j \in \{1,2,3\})$ of order n and diameter d by U_3^{**}.

- In general let U^* denote the unicyclic graph (among the graphs under consideration) with maximum Wiener polarity index.

Theorem 4.11. *[41] Let U be unicyclic graph in $\mathcal{U}(n,d)$ $(d \geq 3)$, then*
(1) If $d = 3$, then $W_p(U) \geq n-3$ with equality if and only if $U \cong U_3(0,t)$ $(t = n-6)$.
(2) If $d = 4$, then $W_p(U) \geq n-3$ with equality if and only if $U \cong U_3(s,t)$ $(s+t = n-7)$.
(3) If $d \geq 5$, then $W_p(U) \geq n-3$ with equality if and only if $U \cong U_3(s,t)$ $(s+t = n-d-3), U_4(n-d-2,0), U_5(n-d-3,0)$.

Theorem 4.12. *[41] Let U be a unicyclic graph in $\mathcal{U}(n,d)$ $(d \geq 4, n \geq d+8)$, and U^*denote the unicyclic graph with the maximum Wiener polarity index.*
(1) If $d = 4$, then $U^* \cong U_3'(a_1,a_2,a_3)$ with $|a_1+1-a_i| \leq 1$ $(i = 2,3)$, $|a_2 - a_3| \leq 1$, and

$$W_p(U^*) = \begin{cases} \frac{(n-6)(n-1)}{3} + 3, & \text{if } a_1+a_2+a_3 = 0 \pmod 3; \\ \frac{n(n-7)}{3} + 5, & \text{if } a_1+a_2+a_3 = 1 \pmod 3; \\ \frac{(n-8)(n+1)}{3} + 8, & \text{if } a_1+a_2+a_3 = 2 \pmod 3. \end{cases}$$

(2) If $d \geq 5$, then $U^* \cong U_3^{**}$, and

$$W_p(U^*) = \begin{cases} \frac{(n-d-2)(n-d+4)}{3} + d, & \text{if } a_1+a_2+a_3 = 0 \pmod 3; \\ \frac{(n-d-3)(n-d+5)}{3} + d+2, & \text{if } a_1+a_2+a_3 = 1 \pmod 3; \\ \frac{(n-d-4)(n-d+6)}{3} + d+5, & \text{if } a_1+a_2+a_3 = 2 \pmod 3. \end{cases}$$

In [45], the authors also determined the minimum Wiener polarity index of unicyclic graphs and characterized the extremal graphs. In [50], the following theorem was shown by Wang el al..

Theorem 4.13. *[50] Let U be a unicyclic Hückel graph of $2n$ vertices, where $n \geq 4$. Then*

$$2n - 7 \leq W_p(U) \leq 4n + 4.$$

For further results on the Wiener polarity index of other classes of graph, one may see [43] (bicyclic graphs), [13] (cactus graphs), [10] (fullerenes and hexagonal systems), [11] (various lattices), and [28,31] (some chemical structures).

5. Graph products and the Nordhaus-Gaddum-type inequalities

Various products of graphs often appear in the study of chemical graphs. Examining the Wiener polarity index of graph products is an important step towards bounding it for these graphs. First we introduce several different products of graphs.

The *Cartesian product* of two graphs G and H, denoted by $G\Box H$, is defined on the Cartesian product $V(G)\times V(H)$ of the vertex sets of G and H. The edge set $E(G\Box H)$ is the set of all pairs $((u,x),\ (v,y))$ of vertices for which either $u = v$ and $xy \in E(H)$ or $uv \in E(G)$ and $x = y$, where $u, v \in V(G)$ and $x, y \in V(H)$.

The *strong product* $G \boxtimes H$ of G and H is defined on the Cartesian product of the vertex sets of G and H. Two distinct vertices (u,x) and (v,y) of $G \boxtimes H$ are adjacent with respect to the strong product if

$$u = v \text{ and } xy \in E(H),\ \text{or } uv \in E(G) \text{ and } x = y,\ \text{or } uv \in E(G) \text{ and } xy \in E(H).$$

The vertex set of the *direct product* $G \times H$ (G and H are called the factors of $G \times H$) of two graphs is $V(G) \times V(H)$. Two vertices $(u,x), (v,y)$ are adjacent if both $uv \in E(G)$ and $xy \in E(H)$.

The *lexicographic product* $G \circ H$ of two graphs G and H is defined on $V(G \circ H) = V(G) \times V(H)$. Two vertices (u,x), (v,y) of $G \circ H$ are adjacent whenever $uv \in E(G)$, or $u = v$ and $xy \in E(H)$. Note that the lexicographic product $G \circ H$ can be obtained from G by substituting a copy H_v of H for every vertex v of G and joining all vertices of H_v with all vertices of H_u if $uv \in E(G)$.

For a given connected graph G, we define $W_2(G) := |\{\{u,v\} \mid d(u,v) = 2, u,v \in V(G)\}|$, which is the number of unordered pairs of vertices $\{u,v\}$ of G such that $d_G(u,v) = 2$. For a given graph $W_2(G)$ can be computed in polynomial time. In the following theorems we denote by $m(G)$ and $n(G)$ the number of edges and vertices of G.

Theorem 5.1. *[42] Let G and H be two non-trivial connected graphs, then*

$$W_p(G\Box H) = W_p(G)V(H) + W_p(H)V(G) + 2W_2(G)m(H) + 2W_2(H)m(G).$$

Theorem 5.2. *[42] Let G and H be two non-trivial connected graphs, then*

$$\begin{aligned} W_p(G \boxtimes H) =& W_p(G)[2W_p(H) + 2W_2(H) + 2m(H) + n(H)] \\ &+ W_p(H)[2W_2(G) + 2m(G) + n(G)]. \end{aligned}$$

Theorem 5.3. *[42] Let G and H be two non-trivial connected graphs and at least one of them is non-bipartite, then*

$$W_p(G \times H) = 2W_p(G)W_p(H) + 2W_p(H)m(G) + 2W_p(G)m(H).$$

Theorem 5.4. *[42] Let G and H be two non-trivial connected graphs, then*

$$W_p(G \circ H) = W_p(G)(n(H))^2.$$

The Cartesian product $G\square H$ and strong product $G \boxtimes H$ were also considered in [23], along with some other graph operations.

Let G and H be simple connected graphs. The join $G+H$, symmetric difference $G \triangle H$, disjunction $G \vee H$, composition $G[H]$ are defined as follows:

(1) $V(G+H) = V(G) \cup V(H)$, $E(G+H) = E(G) + E(H) + \{uv|u \in V(G), v \in V(H)\}$;

(2) $V(G \triangle H) = V(G)\square V(H)$, $E(G \triangle H) = \{(a,b)(c,d)|ac \in E(G)$ or $bd \in E(H)$ not both$\}$;

(3) $E(G \vee H) = \{(a,b)(c,d)|ac \in E(G)\text{or}bd \in E(H)\}$;

(4) $E(G[H]) = \{(a,b)(c,d)|ac \in E(G)$ or $a = c$ and $bd \in E(H)\}$.

Theorem 5.5. *[23] Let $G_1, G_2, \cdots, G_k$ be connected graphs, then*

$$W_p(G_1[G_2[\cdots[G_k]\cdots]]) = W_p(G_1)\prod_{i=2}^{k}|V(G_i)|.$$

Note that the Wiener polarity index of join $G+H$, symmetric difference $G \triangle H$ and the disjunction $G \vee H$ are zero.

When bounding a graph invariant another important direction of study is to consider the Nordhaus-Gaddum-type results. Denote by G^* the graph of order $n \geq 5$ obtained from joining $n-4$ vertices to each internal vertex of the path P_4 such that $V(G^*) \setminus V(P_4)$ is a clique. Let $S^*_{p,q}$ be a graph containing a double star $S_{p,q}$, such that any two vertices both in $V(S_p)$ or both in $V(S_q)$ may be adjacent. From the definition of the Wiener polarity index, we easily obtain that

$$W_P(G^*) = 1, \quad W_P(\overline{G^*}) = 1$$

and

$$W_P(S^*_{p,q}) = (p-1)(q-1), \;\; W_p(\overline{S^*_{p,q}}) = 1.$$

Theorem 5.6. *[51] Let G be a graph of order $n \geq 4$, and $\overline{G}$ be its complement. If $diam(G) = 3$ and $diam(\overline{G}) = 3$, then*

$$2 \leq W_p(G) + W_p(\overline{G}) \leq \lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil - n + 2.$$

Moreover, the lower bound is achieved if and only if $G \cong P_4$ or G is isomorphic to some G^*; the upper bound is achieved if and only if G is isomorphic to $S^*_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$ or $\overline{G}$ is isomorphic to $S^*_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$.

A better lower bound was given by Hua et al. [27].

Theorem 5.7. *[27] Let G be a connected graph with a connected complement $\overline{G}$. Then* $d + \overline{d} - 4 \leq W_p(G) + W_p(\overline{G}) \leq \frac{n(n-1)(n-2)^2}{2} + 2m^2 + (n - \frac{3}{2})[\frac{2(m-\Delta)^2}{n-2} - \Delta(n-\Delta)] -$

$$\frac{m}{2}(4n^2 - 19n + 17) - 2[\Delta^2 + \frac{(2m-\Delta)^2 + \frac{2(n-2)(\Delta_2-\delta)^2}{(n-1)^2}}{n-1}],$$

where d and $\overline{d}$ are the diameter of G and $\overline{G}$, Δ, Δ_2 and δ are the maximum degree, the second maximum degree and the minimum degree in G, respectively. Moreover, the low bound holds if and only if $G \cong P_n$ or $G \cong G^*$.

In addition, Zhang and Hu provided the Nordhaus-Gaddum-type inequality of the Wiener polarity index for trees in [51].

6. Bounds in terms of other indices

First we recall some of the best known chemical indices. The *Wiener index* $W(G)$ is defined as [26]

$$W(G) = \sum_{(u,v)\subseteq E(G)} d(u,v)$$

and the *hyper-Wiener index* $WW(G)$ is defined as [44]

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{(u,v)\subseteq E(G)} d^2(u,v).$$

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as [25]

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

In terms of representing or bounding the Wiener polarity index with these graph invariants, we have the following.

Theorem 6.1. *[38] Let G be a graph with order n and size m, then*

$$W_p(G) = M_2(G) - M_1(G) + m$$

with equality if and only if G is a tree or $g(G) \geq 7$.

Theorem 6.2. *[38] If G is a triangle- and quadrangle-free connected graph, whose order is n and size is m, then*

$$W_p(G) \geq 2n(n-1) - m - M_1(G) - W(G)$$

with equality if and only if $diam(G) \leq 4$.

Theorem 6.3. *[38] If G is a triangle- and quadrangle-free connected graph, whose order is n and size is m, then*

$$W_p(G) \geq \frac{5}{4}n(n-1) - \frac{1}{2}m - \frac{7}{8}M_1(G) - \frac{1}{4}WW(G)$$

with equality if and only if $diam(G) \leq 4$.

In [27], Hua also presented a result on the Wiener polarity index and the first Zagreb index, involving the independence number.

Theorem 6.4. *[27] Let G be a connected triangle-free graph of order n and size m with independence number $\alpha(G)$. Then*

$$W_P(G) < \frac{1}{3}[\frac{n(n-1)}{2}\alpha(G) + m - M_1(G)].$$

The *Hosoya index* of a graph, denoted by $Z(G)$, is defined to be the total number of matchings, that is,

$$Z(G) = \sum_{k\geq 0} m(G;k),$$

where $m(G;k)$ is the number of k-matchings in G for $k \geq 1$, and $m(G;0) = 1$.

Theorem 6.5. *[27] Let G be a connected graph of order n and size m. Then*

$$W_p(G) \leq Z(G) - 1 - m$$

with equality if and only if $G \cong C_3$ or S_n or a double-star.

Theorem 6.6. *[27] Let G be a connected graph of size m. Then $W_p(G) = Z(G) - m - 2$ if and only if $G \cong P_5$ or G_1, where G_1 is constructed from attaching a pendant edge to C_3.*

There are also some studies on the relation between the Wiener polarity index and the Wiener index of specific classes of graphs [9].

Theorem 6.7. *[9] If G is a connected graph, then $W_p(G) \leq \frac{n(n-1)}{2} - \frac{1}{2}M_1(G)$ with equality if and only if $d(G) = 3$.*

Theorem 6.8. *[9] $W(G) \leq 2n(n-1) - W_p(G) - M_1(G) - m$ with equality if and only if $diam(G) \leq 4$.*

In the following theorem we let $L(T)$ be the line graph of a tree T and denote by $d(T,k)$ the number of unordered pairs of vertices u and v of T such that $d_T(u,v) = k$.

Theorem 6.9. *[9] For a tree T:*
(1) $W_p(L(T)) = d(T,4)$;
(2) $W_p(T) + W_p(L(T)) \leq \frac{n(n-1)}{2}$ with equality if and only if $diam(T) \leq 4$;
(3) $W(T) \leq 4W_p(L(T)) + 3W_p(T) + M_1(T) - m$ with equality if and only if $diam(T) \leq 4$.

Theorem 6.10. *[9] If T is a tree, then $W(T) \leq \frac{1}{2}(5n-2)(n-1) - 2W_p(T) - 3W_p(L(T)) - \frac{3}{2}M_1$ with equality if and only if $diam(T) \leq 5$.*

In [9,35], the relations between the Wiener polarity index and $M_1,\ M_2$ are also considered for various graphs.

7. Generalizations of the Wiener polarity index

For $k \geq 1$, the generalized Wiener polarity index is defined as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is k [46]. This is denoted by

$$W_{P_k}(G) = \frac{1}{2} \sum_{v \in V(G)} d_k(v) = |\{(u, v)|d(u, v) = k, u, v \in V\}|$$

where $d_k(u)$ is the number of vertices at distance k from the vertex u. Along the same line, a generalization of the Zagreb indices can be defined as

$$M_k(T) = \sum_{d(u,v)=k-1} d(u)d(v)$$

for $k \geq 3$. First we have the following representation of the generalized Wiener polarity index.

Theorem 7.1. *For a tree T and integer $k \geq 3$, we have*

$$W_k(T) = (-1)^k \left(\frac{k-1}{2} M_1(T) + \sum_{i=2}^{k-1} (-1)^{i+1} (k-i) M_i(T) - (n-1) \right).$$

In [48], Tyomkyn and Uzzell independently introduced the same concept, where they considered it as a new Turán-type problem on distances of graphs. It is a generalization of the problem studied by Bollobás and Tyomkyn in [8]: determining the maximum number of paths with length k in a tree T on n vertices. More generally, the problem of computing the number of subgraphs is still a high-profile problem in the field of extremal graph theory [1, 2, 21]. Bollobás et al. studied the case of path with a given length [5–8]. In [6], it is shown that if $10 \leq \binom{k}{2} \leq m < \binom{k+1}{2}$, then the number of paths of length three in graph G of size m is at most $2m(m-k)(k-2)/k$. In [7], the maximum number of paths of length four of graph G of size m, denoted by $p_4(m)$, is determined.

Theorem 7.2. *[7] If m is sufficiently large then*

$$p_4(m) = p_4(G_m) = \begin{cases} \frac{m^3}{8} - \frac{3m^2}{4} + m, & \text{if } m \text{ is even;} \\ \frac{m^3}{8} - \frac{7m^2}{8} + \frac{15m}{8} - \frac{9}{8}, & \text{if } m \text{ is odd.} \end{cases}$$

and G_m is the unique extremal graph. Here G_m is the complete bipartite graph $K(\frac{m}{2}, 2)$ if m is even; or the complete bipartite graph $K(\frac{m-1}{2}, 2)$ if m is odd.

Furthermore, in [8], Bollobás and Tyomkyn determined the maximum number of paths of length k in a tree T on n vertices. Inspired by this work, similar natural question can be asked for the generalized Wiener polarity index:

Question. For a graph G on n vertices, what is the maximum possible number of pairs of vertices at distance k?

For $k = 2$, the following is known.

Theorem 7.3. *[40] Let G be a graph on n vertices with no three vertices pairwise at distance 2. If there exists a vertex $v \in V(G)$ whose neighbors are covered by at most two cliques, then G has at most $(n-1)^2/4+1$ pairs of vertices at distance 2.*

Corollary 7.1. *[40] Let G be a quasi-line graph on n vertices, which has no three vertices pairwise at distance 2. Then G has at most $(n-1)^2/4+1$ pairs of vertices at distance 2.*

For a graph G, let G_k be the graph with vertex set $V(G)$ and $\{x, y\} \in E(G_k)$ if and only if x and y are at distance k in G. We call G_k the *distance-k graph*. Adjacent vertices x and y in G_k are called *k-neighbors*. We call $d_{G_k}(x)$ the *k-degree* of x and say that a graph G is k-isomorphic to a graph H if G_k is isomorphic to H. Our question naturally turns into finding the maximum size of G_k, denoted by $e(G_k)$ in the following theorems.

Theorem 7.4. *[8,46] If G is a tree on n vertices, then $e(G_k)$ is maximized when G is a t-broom. If k is odd, then $t=2$. If k is even, then t is within 1 of*

$$\frac{1}{4}+\sqrt{\frac{1}{16}+\frac{n-1}{k-2}}.$$

Theorem 7.5. *[48] There is a constant k_0 and a function $n_0 : N \to N$ such that for all $k \geq k_0$, all $n \geq n_0(k)$ and all graphs G of order n with no three vertices pairwise at distance k, we have*

$$e(G_k) \leq (n-k+1)^2/4$$

with equality if and only if G is k-isomorphic to the double broom.

In the end we list some problems posted in [48]:

Conjecture 7.1. *[48] Let $k \geq 3$ and $t \geq 2$, there is a function $h_2 : N \times N \to N$ such that: if $n \geq h_2(k,t)$, then $e(G_k)$ is maximized over all G with $|G| = n$ and $\omega(G_k) \leq t$ when G is k-isomorphic to a t-broom for some t.*

Conjecture 7.2. *[48] Let $k \geq 3$, there exists $h = h(k)$ such that: if $n \geq h(k)$, then $e(G_k)$ is maximized over all G with $|G| = n$ when G is k-isomorphic to a t-broom for some t.*

Conjecture 7.3. *[48] Let $k \geq 3$ and $t \geq 2$, there is a function $h_2 : N \times N \to N$ such that: if $n \geq h_2(k,t)$, then $e(G_k)$ is maximized over all G with $|G| = n$ and $\omega(G_k) \leq t$ when G is k-isomorphic to a t-broom for some t.*

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