MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 17-100

ISSN 0340 - 6253

Bounds for Zagreb Indices

Bojana Borovićanin[1,*], **Kinkar Ch. Das**[2], **Boris Furtula**[1], **Ivan Gutman**[1]

[1] *Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia*
bojanab@kg.ac.rs , furtula@kg.ac.rs , gutman@kg.ac.rs

[2] *Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
kinkardas2003@gmail.com

(Received January 3, 2017)

Abstract

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let d_i be the degree of the vertex $v_i \in V(G)$. The first and second Zagreb indices, $M_1 = \sum_{v_i \in V(G)} d_i^2$ and $M_2 = \sum_{v_i v_j \in E(G)} d_i\, d_j$ are the oldest and most thoroughly investigated vertex–degree–based molecular structure descriptors. An unusually large number of lower and upper bounds for M_1 and M_2 have been established. We provide a survey of the most significant estimates of this kind, attempting to cover the existing literature up to the end of year 2016.

1 Introduction

Let G be a simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. 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 (= number of fist neighbors) of the vertex v_i. Throughout this paper, the vertex degrees are assumed to be ordered 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 G are denote by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively.

The first and the second Zagreb index are defined as

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

*Corresponding author

respectively.

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

$$M_1(G) = \sum_{v_iv_j \in E(G)} (d_i + d_j)\,.$$

The two Zagreb indices are the oldest vertex–degree–based molecular structure descriptors, invented in the 1970s [54, 55]. Details of their theory can be found in the recent reviews [13, 49] whereas data on their history in [50]. In this review, we focus our attention to a single aspect of the mathematical theory of Zagreb indices, namely on lower and upper bounds for M_1 and M_2. Inequalities between M_1 and M_2, as well as Nordhaus–Gaddum type relations are not considered here, and can be found elsewhere [13]. We also restrict our survey to the above defined Zagreb indices, and avoid to examine the related vertex–degree–based invariants, such as the multiplicative Zagreb indices, the general Zagreb indices, reformulated Zagreb indices, hyper–Zagreb index, Zagreb coindices, forgotten index and similar.

* * * * *

For considerations that follow we need a few more definitions.

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.,

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

2 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. [95] gave the following upper bound for the sum of the squares of vertex degrees

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

and de Caen [31] proved that

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

De Caen pointed out that the bounds (1) and (2) are incomparable. Das [21] proved that the equality in (2) holds if and only if G is a star or a complete graph or a complete graph with one isolated vertex.

Das [21], Zhou [114], and Liu et al. [75] established some new upper bounds for M_1.

Theorem 1. [21, 75] *Let G be a connected graph with n vertices and m edges. Then*

$$M_1(G) \leq m(m+1) \tag{3}$$

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

Theorem 2. [114] *Let G be a connected graph with n vertices and m edges. Then*

$$M_1(G) \leq n(2m - n + 1) \tag{4}$$

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 (4) is equal to (3). If $m \geq n$, then $m(m+1) \geq n(2m - n + 1)$ and thus the bound (4) is usually lower than the bound (3), as it was proven in [76].

Remark. If G is connected (n,m)-graph, then $m \leq \binom{n}{2}$, implying, as noted in [76], that

$$m \left(\frac{2m}{n-1} + n - 2 \right) \quad = \quad mn + 2m \left(\frac{m}{n-1} - 1 \right)$$

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

Thus, the bound (2) is usually finer than the bound (4).

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 [92] 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 [79], and later Aharoni [2], these problem were completely solved.

The graph formulation of these problems were first investigated by Ahlswede and Katona [3] 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).

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. [8]. Also, Olpp [89], 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).

In 1999, Peled et al. [91], and Byer [15], 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. [1]. 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 [1] and [100].

As it was proven by Peled et al. [91], 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 [81] $G = (V, E)$ 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. [3,8,89] *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 [15] and Peled et al. [91] it holds:

Theorem 4. [15,91] *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 [81], 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 4, there are at most six optimal partitions of graphs from $\mathcal{G}(n,m)$. Ábrego et al. [1] 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, the maximum value of M_1 equals to $S_{n,m}$ or $C_{n,m}$.

Theorem 5. [1] *Let n be a positive integer and m an integer such that $0 \le m \le \binom{n}{2}$. Let k, k', j, j' be the unique integers satisfying*

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

and

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

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 $k'+1 \le 2k'-j'-1 \le n-1$,*
3. $\pi_{1.3} = (n-1, n-2, \ldots, k'+1, 2, 1)$, *if $j' = 3$ and $n \ge 4$,*
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 $k+1 \le 2k-j-1 \le n-1$,*
6. $\pi_{2.3} = (k, k-1, \ldots, 3)$, *if $j = 3$ and $n \ge 4$.*

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 $S_{n,m} \ge C_{n,m}$, 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 $S_{n,m} \le C_{n,m}$, 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

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

and define the quadratic function

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

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 6. [1, 100] *Let n be a positive integer.*

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

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

$S_{n,m} \cong C_{n,m}$ *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

$$\begin{aligned} S_{n,m} &\geq C_{n,m} \qquad \text{for} \quad 0 \leq m \leq \frac{1}{2}\binom{n}{2} - R_0 \\ S_{n,m} &\leq C_{n,m} \qquad \text{for} \quad \frac{1}{2}\binom{n}{2} - R_0 \leq m \leq \frac{1}{2}\binom{n}{2} \\ S_{n,m} &\geq C_{n,m} \qquad \text{for} \quad \frac{1}{2}\binom{n}{2} \leq m \leq \frac{1}{2}\binom{n}{2} + R_0 \\ S_{n,m} &\leq C_{n,m} \qquad \text{for} \quad \frac{1}{2}\binom{n}{2} + R_0 \leq m \leq \binom{n}{2}. \end{aligned}$$

$S_{n,m} \cong C_{n,m}$ *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

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

$S_{n,m} \cong C_{n,m}$ *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 [87] obtained an upper bound for M_1, that is better than de Caen's (2), for the majority of graphs from $\mathcal{G}(n,m)$.

Theorem 7. [87] *For an integer n and $0 \le m \le \binom{n}{2}$, let*

$$F(n,m) = \begin{cases} 2m\sqrt{2m} & \text{if } n^2/4 \le m \\ (n^2-2m)\sqrt{n^2-2m} + 4mn - n^3 & \text{if } m < n^2/4 \,. \end{cases}$$

Then

$$F(n,m) - 4m \le \max\{S_{n,m}, C_{n,m}\} \le F(n,m)\,.$$

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 [19], 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 $n \ge 2$, $0 \le m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ and $\lceil \frac{n}{2} \rceil \le k \le n-1$ and let $m = qk + r$, where $0 \le r < k$. 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 8. [3] *For $0 \le m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ and $\lceil \frac{n}{2} \rceil \le k \le n-1$, 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 [19] for bipartite graphs with arbitrarily bipartition.

Theorem 9. [19] *Let n and m be two integers such that $n \ge 2$ and $0 \le m \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$. Let*

$$k_0 = \max\left\{k | m = kq + r \;,\; 0 \le r < k \;,\; \left\lceil \frac{n}{2} \right\rceil \le k \le n - q - sgn(r)\right\}. \tag{5}$$

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 [19].

Theorem 10. [19] *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 (5).

Zhang and Zhou [111] 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 11. [111]

(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 (5). *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

$$M_1 \geq \frac{4m^2}{n} \tag{6}$$

with equality if and only if the graph is regular. This bound was obtained several times in the literature [31, 64, 108] and it is close to the sharp lowest bound for M_1, determined in [21] and [48].

Theorem 12. [21, 48] *Let G be a simple (n,m)-graph. Then*

$$M_1 \geq 2m\left(\left\lfloor \frac{2m}{n} \right\rfloor + \left\lceil \frac{2m}{n} \right\rceil\right) - n\left\lfloor \frac{2m}{n} \right\rfloor \left\lceil \frac{2m}{n} \right\rceil \tag{7}$$

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. [19] 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 $x_i y_j$ 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 [19], a bipartite graph $B^s(n,m)$ with n vertices and m edges as follows.

If n is even, then $B^s(n,m) \cong B_{n,t} \cup \{x_i y_j | \, 1 \leq i \leq r/2\}$.

If n is odd and $nt \leq 2m < nt + t$, let

$$B^s(n,m) \cong B^s(n-1, m-t+1) \cup \Big\{x_i y_0 | (n+r-t+1)/2 + 1 \leq i \leq (n+r+t-1)/2\Big\}$$

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 $B^s(n,m) = B^s(n-1, m-t) \cup \{x_i y_0 | (r-t)/2 + 1 \leq i \leq (r+t)/2\}$, where the addition is taken modulo $(n-1)/2$.

Theorem 13. [19] *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 14. [19] *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 [101] 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 [88], for an (n,m)-graph G, the first three coefficients of its Laplacian polynomial are given by

$$q_0(G) = 1 \quad , \quad q_1(G) = -2m \quad , \quad q_2(G) = 2m^2 - m - \frac{1}{2}\sum_{i=1}^{n} d_i^2 \, .$$

The authors of [101,102] 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 $n = g + \ell - 1$.

$T_{\ell_1,\ell_2,\dots,\ell_k}$ denotes the starlike tree of order n with a vertex u of degree k satisfying $T_{\ell_1,\ell_2,\dots,\ell_k} - u = P_{\ell_1} \cup P_{\ell_2} \cup \ldots \cup P_{\ell_k}$, 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 $P^{a_1,a_2,\dots,a_t}_{z_1,z_2,\dots,z_t,\ell}$ is defined as a path of ℓ vertices with pendent paths of z_i edges joining at vertex a_i for $i = 1,2,\dots,t$, where $\{a_1,a_2,\dots,a_t\} \subseteq \{2,\dots,\ell-1\}$, $z_i \geq 1$ $(1 \leq i \leq t)$ and $n = \ell + \sum_{i=1}^{t} z_i$.

The sun-like graph $C^{a_1,a_2,\dots,a_t}_{z_1,z_2,\dots,z_t,g}$ is a cycle with girth g and with pendent paths of z_i edges joining at vertex a_i for $i = 1,2,\dots,t$, where $\{a_1,a_2,\dots,a_t\} \subseteq \{1,2,\dots,g\}$, $z_i \geq 1$ $(1 \leq i \leq t)$ 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 $M^{g}_{\ell_1,\ell_2,\ell_3}$ 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 $J^{g}_{\ell_1,\ell_2,\dots,\ell_k}$ we denote a jellyfish graph obtained from C_g and $T_{\ell_1,\ell_2,\dots,\ell_k}$, by identifying a vertex of C_g with the center of $T_{\ell_1,\ell_2,\dots,\ell_k}$, 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 $S^l_{\ell_1,\ell_2,\dots,\ell_k;h_1,h_2,\dots,h_s}$ is obtained by joining the centers of the graphs $T_{\ell_1,\ell_2,\dots,\ell_k}$ and $T_{h_1,h_2,\dots,h_s}$ with a path P_ℓ, where $\ell_i, h_j \geq 1$.

These graphs are depicted in Fig. 1.

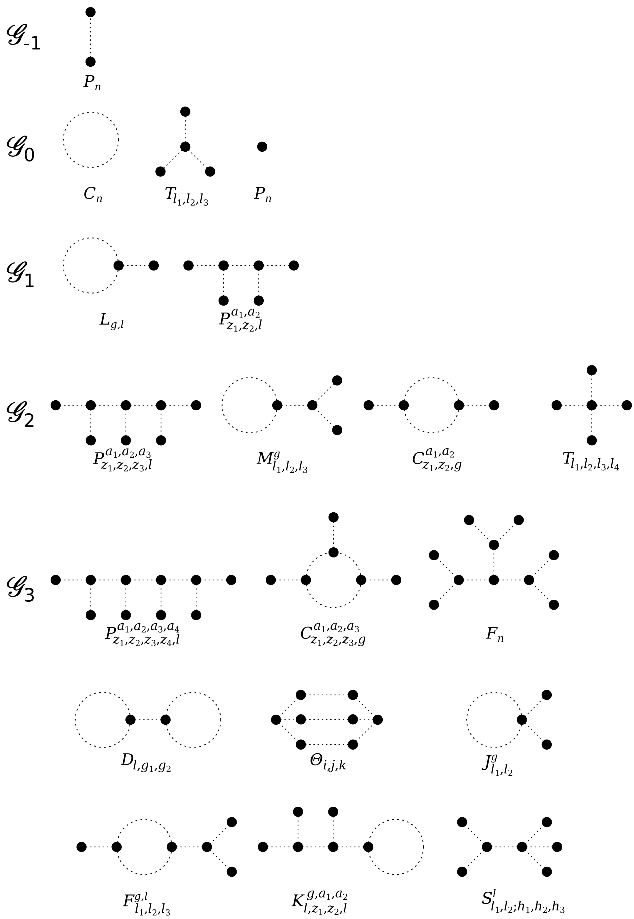

Fig. 1. The graphs occurring in Theorem 15.

Theorem 15. [101, 102] *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 [34, 51, 71, 103].

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 [101] suggested the following construction that can characterize all connected graphs in $\mathcal{G}_k$. Using this construction they generalized the result of Theorem 15.

Construction A. [101] 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 15.

Theorem 16. [101] *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 [34, 105]. 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 17. [34, 105] *Let G be a connected graph of order n with m edges $(n-1 \le m \le n+1)$. 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 [105]:

Theorem 18. [105] *Let G be a connected graph of order n with m $(= n+2)$ edges. Then*

$$M_1(G) \le n^2 - n + 24$$

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 $n+3 \le m \le 2n-4$, 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 19. [105] *Let G be a connected graph of order n with m edges, $n+3 \le m \le 2n-4$. Then*

$$M_1(G) \le n(n-1) + (m-n+1)(m-n+6)$$

with equality holding if and only if $G \cong N_{n,m}^{n-1,m-n+2}$.

3 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 (2) can be sharpened.

Theorem 20. [21] *Let G be a connected graph with n vertices, m edges and minimum degree δ. Then*

$$\sum_{1=1}^{n} d_i^2 \le 2mn - n(n-1)\delta + 2m(\delta - 1) \tag{8}$$

and the equality holds if and only if G is a star or a regular graph.

Theorem 21. [21] *Let G be a connected graph with n vertices, m edges and maximum degree Δ. Then*

$$M_1 \leq m\left(\frac{2m}{n-1}+n-2\right)-\Delta\left(\frac{4m}{n-1}-2m_1-\frac{n+1}{n-1}\Delta+n-1\right) \tag{9}$$

where m_1 is the average degree of the vertices adjacent to the highest degree vertex. Moreover, equality in (9) *holds if and only if G is a star or a complete graph or a graph consisting of isolated vertices.*

Das [21] suggested that in the case of trees, the upper bound (9) is always better than de Caen's bound (2).

Theorem 22. [114] *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. [30] determined an upper bound for M_1 in terms of n, m, and Δ.

Theorem 23. [30] *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 (2) are given in the following three theorems.

Theorem 24. [22] *Let G be a graph with n vertices, m edges, minimum degree δ, and maximum degree Δ. Then*

$$M_1 \leq m\left[\frac{2m}{n-1}+\frac{n-2}{n-1}\Delta+(\Delta-\delta)\left(1-\frac{\Delta}{n-1}\right)\right] \tag{10}$$

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 (10), it holds

$$M_1 \leq m \left[\frac{2m}{n-1} + (n-2) - \left[n - 2 - (\Delta - \delta) \right] \left(1 - \frac{\Delta}{n-1} \right) \right]$$

and since $1 - \Delta/(n-1) \geq 0$ and $n-2-(\Delta-\delta) \geq 0$ for connected or disconnected graphs, the upper bound (10) is always better than de Caen's bound (2), as proven in [22].

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 25. [20,22] *Let G be a graph with n vertices, m edges, minimum degree δ, and maximum degree Δ. Then*

$$M_1 \leq \frac{2m \left[2m + (n-1)(\Delta - \delta) \right]}{n + \Delta - \delta} \tag{11}$$

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 (11) *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 (11) is better than the bound (2), since the right–hand side of the inequality (11) is a monotonically increasing function of $\Delta - \delta$ and $\Delta - \delta \leq n - 2$.

In [22] Das also obtained the following upper bound on M_1.

Theorem 26. [22] *Let G be a graph with n vertices and m edges, minimum vertex degree δ and maximum vertex degree Δ. Then*

$$M_1 \leq 2m(\delta + \Delta) - n\delta\Delta \tag{12}$$

with equality if and only if G is a bidegreed graph, i.e., it has only two type of degrees, δ and Δ.

In [114], the above upper bound was improved by proving the following.

Theorem 27. [114] *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*

$$M_1 \leq 2m(\delta + \Delta) - n\delta\Delta + (\delta - k)(\Delta - k) \tag{13}$$

where k is an integer defined via

$$2m - n\delta \equiv k - \delta\,(mod\,(\Delta - \delta)) \quad , \quad \delta \leq k \leq \Delta - 1$$

i.e.,

$$k = 2m - \delta(n-1) - (\Delta - \delta) \left\lfloor \frac{2m - n\delta}{\Delta - \delta} \right\rfloor .$$

Equality in (13) *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 1. [114] *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 [63], the following inequality, stronger than (12), has been obtained.

Theorem 28. [63] *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*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta - (n - a - b)(\Delta - \delta - 1) \tag{14}$$

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 [38, 63, 76, 84, 85].

Theorem 29. [76] *Let G be a connected (n,m)-graph. Then*

$$M_1 \leq \max \left\{ m \left(\Delta + \delta - 1 + \frac{2m - \delta(n-1)}{\Delta} \right), m \left(\delta + 1 + \frac{2m - \delta(n-1)}{2} \right) \right\} \tag{15}$$

and the equality is attained, for example, by a star or a regular graph of order $n \geq 3$.

It was proven in [76] that for $n \geq 3$, the bound (15) is better than (3).

Theorem 30. [38, 63, 76] *Let G be connected (n,m)-graph. Then*

$$M_1(G) \leq \frac{2m^2}{n} + \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)\frac{m^2}{n} \tag{16}$$

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 [38,63,76], whereas the equality case was determined first in [76] and then corrected in [63]. As a simple corollary of the previous theorem, the following result was obtained.

Corollary 2. [63, 76] *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 (16) was improved in [84] in the following way.

Theorem 31. [84] *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*

$$M_1(G) \leq \frac{4m^2}{n}\left[1 + \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}}\right)^2 \beta(S)\right] \tag{17}$$

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 30.

As noted in [84], for each set $S \subset I_n$ it holds $\beta(S) \leq \frac{1}{4}$, implying that the inequality (17) is stronger than (16). Besides, by Theorem 31, the bounds from Corollary 2 were also improved:

Corollary 3. [84] *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 [38].

Theorem 32. [38] *Let G be a simple (n,m)-graph. Then*

$$M_1(G) \leq \frac{4m^2}{n} + \frac{n}{4}\,(\Delta - \delta)^2\,. \tag{18}$$

This bound is improved as follows.

Theorem 33. [59, 84, 85] *Let G be a connected (n,m)-graph. Then*

$$M_1(G) \leq \frac{1}{n}\left[\alpha(n)(\Delta-\delta)^2 + 4m^2\right] \tag{19}$$

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 [59], but the function $\alpha(n)$ was erroneously defined via $\lceil x \rceil$. The correct proof was given in [84, 85] and the equality case was characterized only in [84]. It can be easily seen [84] that the inequality (19) is stronger than the inequality (18) 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 [28].

Theorem 34. [28] *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*

$$M_1(G) \leq \frac{(2m-\Delta)^2}{n-1} + \Delta^2 + \frac{n-1}{4}(\Delta_2 - \delta)^2\,. \tag{20}$$

Equality holds in (20) 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 (20) was improved in the same paper.

Theorem 35. [28] *Let G be the same graph as in Theorem 34. Then*

$$M_1(G) \leq \Delta^2 + (\Delta_2 + \delta)(2m - \Delta) - (n-1)\Delta_2\,\delta\,. \tag{21}$$

Equality holds in (21) 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 [28], the bound (21) is always better than the bound (12). By [28], 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 [28] that the bound (21) is always better than the bound (20).

Some further estimations of the first Zagreb index were proposed in [29]. 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 36. [29] *Let G be a connected graph of order n with m edges. Then*

$$\frac{2m[2m - (\Delta-\nu)(n-1)]}{n+\nu-\Delta} \leq M_1(G) \leq \frac{2m[2m + (\mu-\delta)(n-1)]}{n+\mu-\delta}\,. \tag{22}$$

Equality on the left–hand side of (22) holds if and only if G is regular. The right–hand side equality holds in (22) if and only G is either regular graph or $G \cong CS(n,\alpha)$.

As noted in [29], Theorem 36 generalizes the previously obtained upper bound (11).

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 [24].

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

$$\Delta = t \quad , \quad d_i = 1\ ,\ i = t+1, t+2, \ldots, n\,.$$

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 37. [24] *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 [114,116,118] Zhou et al. determined upper bounds for M_1 of K_{r+1}-free graphs with n vertices, where $r \geq 2$.

Theorem 38. [114] *Let G be a triangle–free (n,m)-graph. Then*

$$M_1(G) \leq mn \tag{23}$$

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 [114]

$$M_1(G) \leq n \left\lfloor \frac{n^2}{4} \right\rfloor$$

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 [118]. 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 39. [118] *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 [57] proved that every r-regular Moore graph with diameter 2 must have $r \in \{2, 3, 7, 57\}$.

Theorem 40. [118] *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 [116] 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 41. [116] *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 [116] the following upper bound was obtained.

Theorem 42. [116] *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 [75], 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 43. [75] *Let G be an (n,m)-graph with diameter D. Then*

$$M_1(G) = n(n-1)^2 \quad \textit{if } D = 1$$

and

$$M_1(G) \leq m^2 - m(D-3) + (D-2) \quad \text{if } D > 1\,. \tag{24}$$

If $D = 2$, then equality in (24) holds if and only if either $G \cong K_{1,n-1}$ or $G \cong K_3$. If $D \geq 3$, then equality in (24) holds if and only if $G \cong P_{D+1}$.

Theorem 44. [75] *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 [67], 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 45. [67] *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 46. [67] *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 47. [67] *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 48. [106] *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 [86] derived an upper bound for M_1 in terms of n, m, and the number of triangles t.

Theorem 49. [86] *Let G be an (n,m)-graph with t triangles. Then,*

$$M_1(G) \leq mn + 3t\,. \tag{25}$$

As noted in [86], the equality in (25) 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 (23). Besides, for graphs with limited number of triangles, such as triangle–free graphs, the bound (25) is better than the de Caen's bound (2). Also, by [86], the bound (25) is better than Nikiforov' s bound (Theorem 7) for graphs with many edges.

By Theorem 49, the following corollary was obtained in [86].

Corollary 4. [86] *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 [86] 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 [42].

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 [86].

Theorem 50. [86] 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 51. [39] *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 52. [40] *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 [70] 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 [61] 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 53. [61, 70] 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 [61], 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 [61], 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 [61].

Theorem 54. [61] *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 55. [61] *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.

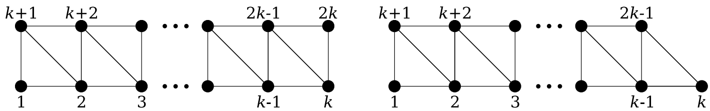

Fig. 2. The graph $P_{n,2}$ for $n = 2k$ and $2k-1$.

In thw paper [60], 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 56. [60] *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 $G \cong K_1 \vee P_{n-1}$.

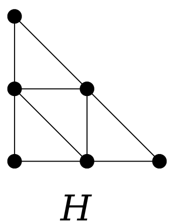

Fig. 3. The graph occurring in Theorem 56.

Theorem 57. [60] *Let G be conjugated maximal outerplanar graph on $2k$ vertices. Then*

$$32k - 38 \leq M_1(G) \leq 4k^2 + 14k - 18\,. \tag{26}$$

The left equality holds if and only if $G \cong P_{2k,2}$. If $k \neq 3$, then the right equality holds in (26) *if and only if $G \cong K_1 \vee P_{2k-1}$. If $k = 3$, then the right equality holds in* (26) *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 56 and 57 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 [35]. For example, outerplanar graphs are series–parallel.

Theorem 58. [115] *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 [104]. 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 59. [104] *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 [21, 30] obtained the following lower bounds for M_1 which are better than (6).

Theorem 60. [21] *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 61. [30] *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 [84] proposed a new lower bound for M_1 better than (6). The conclusion related to the equality case was wrong in [84] and it was eventually corrected in [82], and the equality case additionally corrected in [25].

Theorem 62. [25, 82, 84] *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 [25], the following strengthening of Theorem 62 was achieved:

Theorem 63. [25] *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 [82], the following lower bounds for M_1, better than (6), were also obtained.

Theorem 64. [82] *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 5. [82] *With the assumptions as in Theorem 64, 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 [60].

Theorem 65. [60] *Let G be maximal outerplanar graph on n vertices. Then*

$$M_1(G) \geq 16n - 38 \tag{27}$$

and the equality holds if and only if $G \cong P_{n,2}$.

In the paper [104], a sharp lower bound for M_1 of n-vertex graphs with a given clique number has been determined.

Theorem 66. [104] *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 $\frac{1}{n}\sum_{v \in V(G)} \alpha(v)$, [32].

In the paper [86], 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 67. [86] *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 [38] 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 $G \cong P_3$.

4 Second Zagreb index

We first consider upper bounds for M_2.

Let G be an (n,m)-graph. Bollobás and Erdős [9] 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 68. [9] *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 [34, 105].

Theorem 69. [34, 105] *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 [105]:

Theorem 70. [105] *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 [105]:

Theorem 71. [105] *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 [105] gave the following conjecture:

Conjecture 6. *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 [10] proved the following:

Theorem 72. [10] *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 [114, 116, 118], results concerning upper bounds for the second Zagreb index of K_{r+1}-free graphs, $r \geq 2$, were obtained.

Theorem 73. [114] *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 [114]

$$M_2(G) \leq \left\lfloor \frac{n^2}{4} \right\rfloor^2$$

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 74. [118]

(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 3 (in Theorem 39).

(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 75. [116] *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 76. [116] *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 [65], 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 [65], 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 77. [65] *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 78. [65] *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 79. [118] *(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 39) 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 [117], 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 27). Fonseca and Stevanović [44] proved the analogous upper bound on M_2 for general values of n, m, δ, and Δ.

Theorem 80. [44] *Let G be a graph with n vertices, m edges, the minimum vertex degree δ and maximum vertex degree $\Delta > \delta + 1$. Then*

$$\begin{aligned} M_2 \;\leq\; & \frac{1}{2}\Big[(2m-k)(\Delta^2 + \Delta\delta + \delta^2) - (n-1)\Delta\delta(\Delta+\delta)\Big] \\ & + \begin{cases} k\delta(k - \frac{\delta}{2}) & \text{if } \; k \leq (\Delta+\delta)/2 \\ k\Delta(k - \frac{\Delta}{2}) & \text{if } \; k > (\Delta+\delta)/2 \end{cases} \end{aligned} \tag{28}$$

where k is an integer defined via

$$2m - n\delta \equiv k - \delta\,(mod\,(\Delta - \delta)) \quad , \quad \delta \leq k \leq \Delta - 1$$

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 (28) *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 (28) 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 27 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 [44].

The appearance of disconnected multigraphs as extremal graphs for the second Zagreb index may be avoided in the case of trees (see Theorem 97).

In the papers [28, 30], Das et al. established some upper and lower bounds on $M_2(G)$ in terms of n, m, δ, Δ, and Δ_2.

Theorem 81. [28] *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 82. [30] *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)

$$\begin{aligned} M_2(G) &\le 2m^2 - (n-1)m\delta \\ &+ \frac{1}{2}(\delta-1)\left[(n+1)m - \Delta(n-\Delta) + \frac{2(m-\Delta)^2}{n-2}\right] \end{aligned}$$

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 83. [106] *Let G be a triangle– and quadrangle–free connected graph with n vertices, m edges and radius r. Then, $M_2(G) \le m(n+1-r)$ 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 [39].

Theorem 84. [39] *Let G be a connected graph with $n \ge 4$ vertices and matching number β, $2 \le \beta \le \lfloor n/2 \rfloor$. 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*

$$M_2(G) \le \frac{1}{2}n(n-1)^3$$

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

(2) If $c < \beta \le \lfloor n/2 \rfloor - 1$, *then*

$$M_2(G) \le n^2 + 4n\beta^2 - 6n\beta - 20\beta^3 + 8\beta^4 + 14\beta^2 - \beta$$

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*

$$M_2(G) \le n^2 + 4nc^2 - 6nc - 20c^3 + 8c^4 + 14c^2 - c = \frac{1}{2}c(n-1)(1-c-2c^2-n+3cn)$$

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 $2 \le \beta < c$, *then*

$$M_2(G) \le \frac{1}{2}\beta(n-1)(1-\beta-2\beta^2-n+3\beta n)$$

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

In [40] and [41], 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 85. [40,41] *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 [70] 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 86. [70] *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. [60] 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 87. [60] *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 88. [60] *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 87 and 88. 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 [115].

Theorem 89. [115] *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 90. [115] *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 [104] 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 91. [104] *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.

5 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 (2) and (7) are significantly simplified and thus, the following result is straightforward.

Theorem 92. [51] *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 (15) from [76], the first four trees from the class $\mathcal{T}(n)$ of trees on n vertices whose M_1 is maximum were determined.

Theorem 93. [76] *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.*

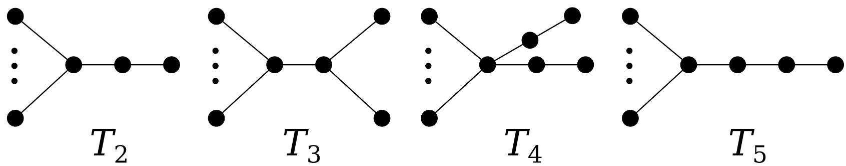

Fig. 4. The trees occurring in Theorem 93.

In [26], the trees with maximal and minimal value of the second Zagreb index are obtained as follows.

Theorem 94. [26] *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. [27] obtained the following upper bound on $M_1(T)$ in terms of n and Δ:

Theorem 95. [27] *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 [24], 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

$$\Delta = t \quad , \quad d_i = 1\,,\; i = t, t+1, \ldots, n\,.$$

Theorem 96. [24] *Let T be a tree of order n with irregularity index t and maximum degree Δ. Then*

$$M_1(T) \leq \left[n - 3 - \frac{t(t-3)}{2} \right] \Delta^2 - (t-1)(t-2)\Delta + \frac{1}{3}\,(t^3 - 3t^2 + 2t + 6)$$

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 [97] it was noted that each even number, except 4 and 8 is the first Zagreb index of a caterpillar.

From Theorem 27, 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 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 [80]. As in [80], 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,

$$M_1(T) \leq \begin{cases} 6n - 10 & \text{if } n \equiv 2 \pmod 3 \\ 6n - 12 & \text{otherwise} \end{cases}$$

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 [44].

Theorem 97. [44] *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

$$k \equiv n - 1 (mod\,(\Delta - 1))\,, \ 1 \leq k \leq \Delta - 1$$

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 [80].

$$M_2(T) \leq \begin{cases} 8n - 24 & \text{if } n \equiv 2 \pmod 3 \\ 8n - 26 & \text{otherwise} \end{cases}$$

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 [99] we need the following notations. Denote by m_{ij} $(1 \leq i, j \leq \Delta)$ 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 98. [99] *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) $m_{ij} = \min\left\{ n_i - \sum\limits_{k=j+1}^{\Delta} m_{ik}\ ,\ j n_j - \sum\limits_{k=i+1}^{j} m_{kj} - \sum\limits_{k=j}^{\Delta} m_{jk} \right\}$ *for each* $1 \leq i < j \leq \Delta$;

3) $m_{ii} = n_i - \sum\limits_{k=i+1}^{\Delta} m_{ik}$ *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 $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is called to be a *majorization* [83]. 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 [77] 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

$$\sum_{i=1}^{n} d_i = 2(n-1)\,. \tag{29}$$

In order to present the main results of the paper [77], 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 [112], 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 [77] used the method of [112] 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.

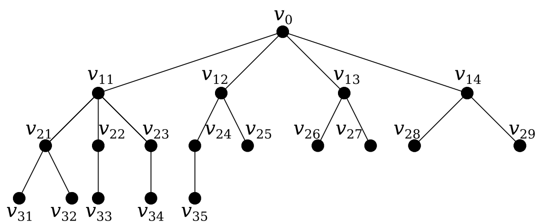

Fig. 5. The BFS-tree T_1^* with degree sequence $(4, 4, \underbrace{3, \ldots, 3}_{4}, 2, 2, 2, \underbrace{1, 1, \ldots, 1}_{10})$.

Theorem 99. [112] *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 [77] can be stated as follows.

Theorem 100. [77] *Given a tree degree sequence π, the BFS-tree T^* has the maximum second Zagreb index in $\Gamma(\pi)$.*

Hence, by Theorems 99 and 100, 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 [77].

Theorem 101. [77] *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 101, 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 102. [77] *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 Alekstić Lampert [12]. 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 [12] that $1 \leq k \leq n/2 - 1$.

Theorem 103. [12] *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 104. [12] *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 105. [12] *Let $T \in \mathcal{T}_{n,k}$, where $1 \le k \le n/2 - 1$. Then*

$$M_2(T) \le (k-1)\Delta^2 + 2p(\Delta-1)^2 + \mu(\Delta+\mu-1) + \Delta(n-k-(\Delta-1)p-\mu)$$

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

$$(\underbrace{\Delta,\dots,\Delta}_{k}, \underbrace{\Delta-1,\dots,\Delta-1}_{p}, \mu, \underbrace{1,\dots,1}_{n-k-p-1}) .$$

(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 106. [12] *Let $T \in \mathcal{T}_{n,k}$, where $1 \le k \le n/2 - 1$. Then*

$$M_2(T) \ge \begin{cases} 3k+4n-10, & \text{if } n \ge 3k+1 \\ 6k+3n-9, & \text{if } n < 3k+1 . \end{cases}$$

The equality holds if and only if the following three conditions are satisfied.

(i) The tree T has the vertex degree sequence $(\underbrace{3,\dots,3}_{k}, \underbrace{2,\dots,2}_{n-2k-2}, \underbrace{1,\dots,1}_{k+2})$.

(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 [45] 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 107. [45, 52] *Let T be a tree with $n_1 \geq 2$ pendent vertices and first Zagreb index M_1.*

(a) If n_1 is even, then $M_1(T) \geq 9n_1 - 16$ with equality if and only if all non-pendent vertices of T are of degree 4.

(b) If n_1 is odd, then $M_1(T) \geq 9n_1 - 15$, 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 107 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 108. [53] *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 [45, 47]. The corresponding optimal trees were determined, too.

As in [17, 45], 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 109. [45, 47] *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 [46]. 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 [11, 73], 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 [73], 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 110. [73] *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 111. [11] *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 112. [11] *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 [11], 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 [11].

In the paper [29], 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 113. [29] *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 [98], 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).

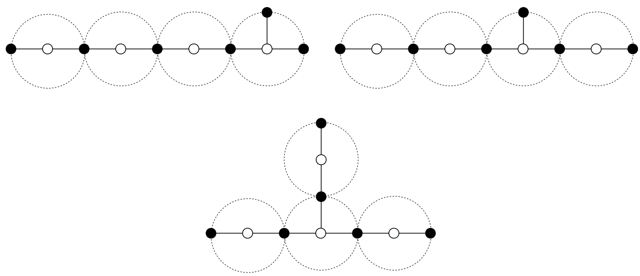

Fig. 6. Three non-isomorphic trees with $n = 10\,, \alpha = 6$ and minimum value of $M_1 = 36\,.$

The following holds:

Theorem 114. [98] *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 [98], 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 [12], 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 [90] 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. [43] that equality holds only for C_4 and for graphs of the form $H \circ K_1$, for some H.

Theorem 115. [12] *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 [12] 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 116. [12] *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 117. [12] *Let T be a tree on n vertices with domination number γ, where $\frac{n}{3} \leq \gamma \leq \frac{n}{2}$. Then,*

$$M_1(T) \geq \begin{cases} 4n - 6 & \text{if } \gamma = \left\lceil \frac{n}{3} \right\rceil \\ 2n + 6\gamma = 10 & \text{if } \frac{n+3}{3} \leq \gamma \leq \frac{n}{2} \end{cases}$$

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 [62], and independently Li and Zhao [69] and Sun and Chen [94], 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.

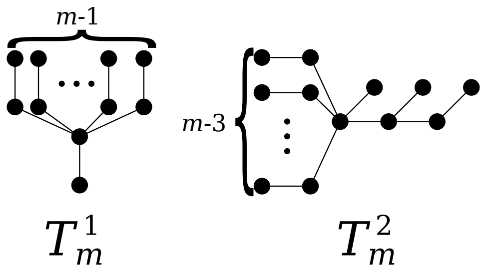

Fig. 7. The trees occurring in Theorem 118.

Theorem 118. [62, 69, 94]

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 [37] 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 [4], 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.

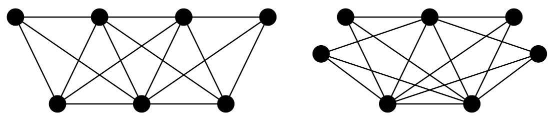

Fig. 8. The 3-path and 3-star with 7 vertices.

The first and second Zagreb indices of k-paths and k-stars have been calculated in [37].

Theorem 119. [37] *Let P_n^k be the k-path on $n \geq k+3$ vertices. Then*

$$M_1(P_n^k) = 2nk(n-2) - \frac{1}{3}n(n-1)(n-2) - \frac{1}{3}k(k+1)(2k-5)$$

$$\text{for } \ k+3 \leq n \leq 2k \ \text{ and } \ k \geq 3$$

$$M_1(P_n^k) = 4nk^2 - \frac{1}{3}k(10k-1)(k+1) \quad \text{for } \ n \geq \max(4, 2k+1)\,.$$

Theorem 120. [37] *Let P_n^k be the k-path on $n \geq k+3$ vertices. Then*

$$M_2(P_n^k) = \frac{1}{2}(k^4 + 9k^3 + 12k^2 - 8k + 2), \quad n = k+3$$

$$M_2(P_n^k) = \frac{1}{24}((10-4k)n^3 - n^4 + (54k^2 - 18k - 23)n^2$$

$$
\begin{aligned}
& - \quad (44k^3+66k^2-54k-14)n+7k^4+38k^3+5k^2-26k) \\
& \quad\quad \textit{for } \ k+4 \le n \le 2k \\
M_2(P_n^k) &= \frac{1}{24}(n^4-(12k+6)n^3+(54k^2+54k+11)n^2 \\
& - \quad (12k^3+162k^2+66k+6)n-(25k^4-70k^3-109k^2-14k)) \\
& \quad\quad \textit{for } \ 2k+1 \le n \le 3k-1 \\
M_2(P_n^k) &= \frac{1}{24}(48nk^3-53k^4-46k^3+5k^2-2k) \quad \textit{for } \ n \ge \max(5,3k)\,.
\end{aligned}
$$

Theorem 121. [37] *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 122. [37] *Let T_n^k be a k-tree on $n \geq k$ vertices. Then*

$$M_1(P_n^k) \le M_1(T_n^k) \le M_1(S_{k,n-k})$$

and

$$M_2(P_n^k) \le M_2(T_n^k) \le M_2(S_{k,n-k})$$

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 [26,51] (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 [60], who determined sharp upper and lower bounds for M_1- and M_2-values of maximal outerplanar graphs.

In the recent paper [36], for a given tree T, a finite sequence of trees $\{T_i\}_0^k$ was constructed, such that $T_0 \cong P_n$ and $T_k \cong S_n$, and T belongs to this sequences. Conditions were established in [36], under which $M_1(T_{i-1}) \leq M_1(T_i)$ and $M_2(T_{i-1}) \leq M_2(T_i)$ hold for $i = 1, 2, \ldots, k$.

6 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 [110] 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 [76] using a different approach.

Theorem 123. [76, 110] *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.*

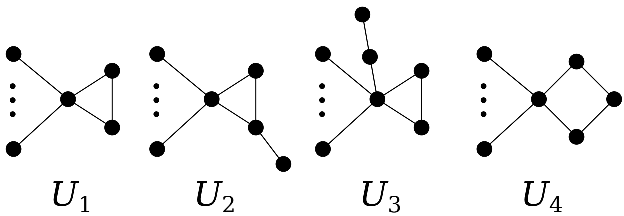

Fig. 9. The graphs occurring in Theorem 123.

Theorem 124. [110] *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 [107].

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

$$\begin{aligned}
\mathcal{U}^*_{n,0} &= \{C_n\} \\
\mathcal{U}^*_{n,k} &= \{C_q(p_1, p_2, \ldots, p_k) : p_i \geq 2, 1 \leq i \leq k, q \geq 3\} \quad , \quad k \geq 1 \\
U^n_k &= C_3(1, 1, \ldots, 1, \underbrace{2, 2, \ldots, 2}_{n-k-3})
\end{aligned}$$

see Fig. 10. Obviously, $\mathcal{U}^*_{n,k} \subseteq \mathcal{U}_{n,k}$ and $U^n_k \in \mathcal{U}_{n,k}$.

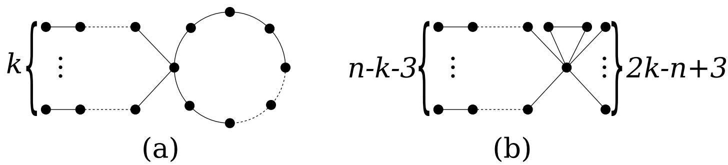

Fig. 10. (a) An element of $\mathcal{U}^*_{n,k}$, and (b) the graph U^n_k . These graphs are mentioned in Theorem 125.

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.

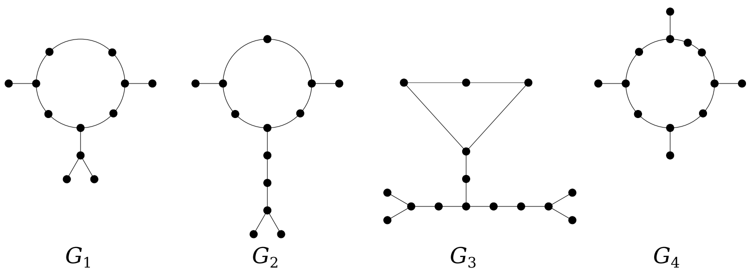

Fig. 11. For graphs belonging to the set $\mathcal{U}^+_{13,4}$. These graphs are mentioned in Theorem 126.

Theorem 125. [107] *Let $G \in \mathcal{U}_{n,k}$, $0 \leq k \leq n-3$. Then*

$$M_2(G) \leq \begin{cases} 4n + 2k(k+1) & \text{if } n \geq 2k+3 \\ \\ 4n + (n-1)k, & \text{if } n \leq 2k+2\,. \end{cases}$$

Equalities hold if and only if $G \in \mathcal{U}^*_{n,k}$, for $n \geq 2k+3$, and $G \cong U^n_k$, for $n \leq 2k+2$.

Theorem 126. [107] *Let $G \in \mathcal{U}_{n,k}$, $0 \leq k \leq n-3$. Then*

$$M_2(G) \geq 4n + 3k$$

and the equality holds if and only if $n \geq 3k$ 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 $0 \leq k \leq n-3$. The functions $\varphi(n,k)$ and $\phi(n,k)$ increase strictly monotonically in $0 \leq k \leq n-3$ [107]. As the set of all unicyclic graphs with n vertices is $\bigcup_{k=0}^{n-3} \mathcal{U}_{n,k}$, by Theorems 125 and 126, U^n_{n-3} and C_n have the maximum and the minimum second Zagreb index among all unicyclic graphs with n vertices [107].

In the paper [78], 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 $c \geq 0$, then

$$\sum_{i=1}^{n} d_i = 2(n+c-1) \quad , \quad d_1 \geq d_2 \geq c+1\,. \tag{30}$$

We now present the construction of the graph $G^* \in \Gamma(\pi)$ as in [77, 78, 109, 112].

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

$$\begin{aligned} N(v_2) &= \{v_1, v_3, \ldots, v_{c+2}, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-c}\} \\ N(v_3) &= \{v_1, v_2, v_{d_1+d_2-c+1}, \ldots, v_{d_1+d_2+d_3-c-2}\} \\ &\ \ \cdots \\ N(v_{c+2}) &= \{v_1, v_2, v_{(\sum_{i=1}^{c+1} d_i)-3c+3}, \ldots, v_{(\sum_{i=1}^{c+2} d_i)-3c}\}\,. \end{aligned}$$

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 [109], 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 100. 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 (30)). 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 127. [78] *If $d_n = 1$, then U^* achieves the maximum second Zagreb index in the class of unicyclic graph with degree sequence π.*

Remark. [78] 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 [78].

In addition, it is proven in [78], 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 127, the result from [107], which is concerned with unicyclic graphs with n vertices and k pendent vertices whose second Zagreb index is maximum is reproven in [78]. 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 [78].

Theorem 128. [78] *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.*

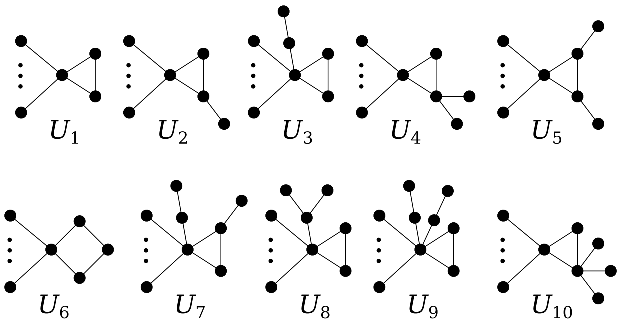

Fig. 12. The unicyclic graphs $U_1, U_2, \ldots, U_{10}$ occurring in Theorem 128.

In the paper [98], 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 $\overline{S} = V \setminus S$ 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).

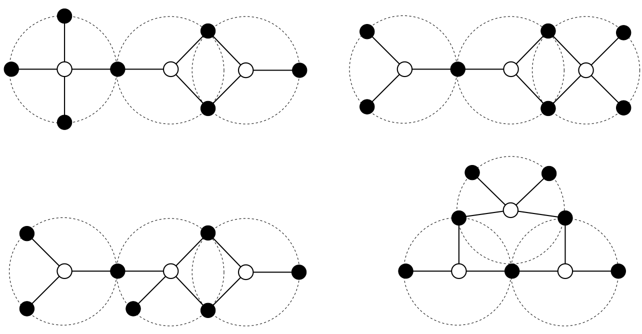

Fig. 13. Four non-isomorphic unicyclic graphs with $n = 10\,, \alpha = 7$ and minimum value of $M_1 = 50\,.$

Theorem 129. [98] *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 [62] 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).

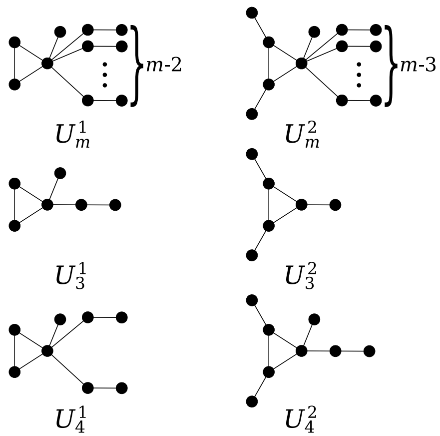

Fig. 14. The graphs occurring in Theorem 130.

Theorem 130. [62]

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 [58] 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 131. [58] *Let G be a connected unicyclic graph of order n with maximum degree Δ and cycle length k $(3 \le k \le n-\Delta+2)$. Then*

$$M_1(G) \ge \Delta(\Delta-3)+4n+2$$

with equality if and only if $G \in \mathcal{B}_n(k,\Delta)$.

Let B_n^k $(k \le n)$ 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 $C_{n,\Delta}^k$ $(\Delta \ge 4)$, 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 $D_{n,\Delta}^k$ $(\Delta \ge 4)$, 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 $\Delta+k \le n+2$. 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 $\Delta+k \ge n$ 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 [58], Horoldagva and Das obtained the following lower bound on $M_2(G)$ and characterize extremal graphs when $\Delta+k<n$.

Theorem 132. [58] *Let G be a connected unicyclic graph of order n with maximum degree Δ and cycle length k $(\Delta+k<n)$. Then*

$$M_2(G) \ge \begin{cases} \Delta(\Delta-3)+4n+6 & \text{if } \Delta \ge 5 \\ 4n+10 & \text{if } \Delta = 4 \\ 4n+4 & \text{if } \Delta = 3 \end{cases} \tag{31}$$

where Δ is the maximum degree in G. Moreover, the equalities hold in (31) 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 [113] 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 [34,113], 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 $\mathcal{B}^i_{n,k}$ 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 $i = 1,2,3$.

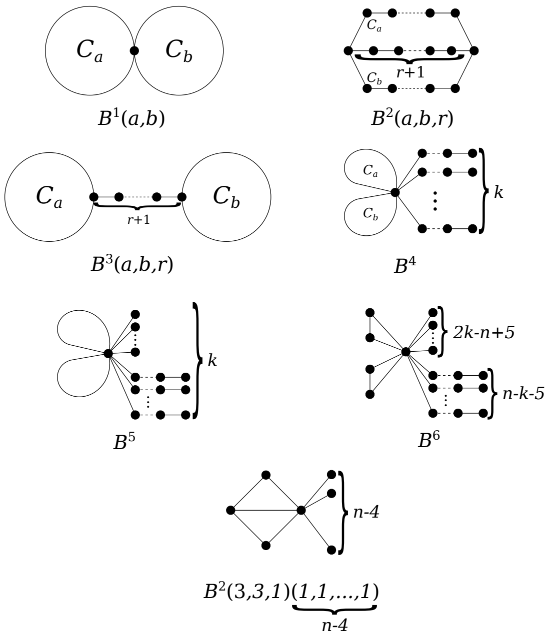

Fig. 15. The different types of bicyclic graphs.

Denote by $B^i(a,b)(p_1,p_2,\ldots,p_k)$, $i = 1,2,3$, $k \geq 1$, 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 133. [113] *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 134. [113] *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 135. [113] *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*

$$M_1(G) \geq \begin{cases} 4n + 2k + 10 & \text{if } n \geq 2k+2 \\ (-d^2-d+3)n + (d^2+3d+2)k + (4d+10) & \text{if } n \leq 2k+1 \,. \end{cases} \tag{32}$$

Equalities in (32) hold if and only if $G \in \mathcal{B}^{++}_{n,k}$.

Theorem 136. [113] *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 133 and 134, Zhao and Li [113] deduced that if $0 \le k \le n-5$, 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 [113]

$$G \cong B^2(3,3,1)(\underbrace{1,\dots,1}_{n-4}) \ , \ \text{and} \ \ M_1(G) = n^2 - n + 14 \ , \ M_2(G) = n^2 + 2n + 9 \, .$$

Hence, the graph $B^2(3,3,1)(\underbrace{1,\dots,1}_{n-4})$, 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 [34]. The same result concerning bicyclic graphs with maximal M_1 was obtained independently in [16] using a different approach.

Also, it was easy to deduce [113] 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 [34] 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 [109] and some results that generalize the main results of the papers [77,78] 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 137. [109] *Let $\pi = (d_1, d_2, \dots, d_n)$ 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 $c \ge 0$,

(ii) $d_1 \ge d_2 \ge c+1$,

(iii) $d_3 \ge d_4 = d_5 = \cdots = d_{c+2}$, for $c \ge 1$,

(iv) $d_n = 1$,

then the graph G^*, constructed as described in the explanation of Theorem 127, is an optimal graph in $\Gamma(\pi)$, i.e., for any graph $G \in \Gamma(\pi)$, $M_2(G) \le M_2(G^*)$.

The previous theorem implies the results of Theorems 100 and 127. Also, the corresponding result for bicyclic graphs was obtained. A bicyclic graph has the so-called bicyclic degree sequence π which satisfies the condition (30) for $c = 2$. We will use the notation from [113], 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 138. [109] *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 100), is an optimal graph in the set $\mathcal{B}_\pi$.

Remark. [109] 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 [109].

Besides, in paper [109], it was proven:

Theorem 139. [109] *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 138 (parts (3) and (4)) the results of Theorem 134, concerned with bicyclic graphs with n vertices and k pendent vertices whose second Zagreb index is maximum are reproved.

Recall that Goubko (see Theorem 107) determined the lower bound for M_1 of trees with a given number of pendent vertices. This result was extended in [53] to any connected graph with a given number of pendents and fixed cyclomatic number.

Theorem 140. [53] *Let G be a connected graph with k pendent vertices and cyclomatic number c. Then,*

$$M_1(G) \geq 9k+16(c-1)\,. \tag{33}$$

Equality in (33) *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 108, and the result for unicyclic graphs is stated below.

Theorem 141. [53] *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 141, exist for any value of n and k, provided $n \geq 3$ and $k \geq 0$.

Besides, in [53], the result from [113] were reproved, with some additional conditions proposed. In fact, it was shown in [53] 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 135).

In the paper [96], 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 [113]. 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 142. [96] *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 [68] determined sharp upper bounds for M_1 and M_2 of bicyclic graphs with perfect matchings. Besides, in [68], 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.

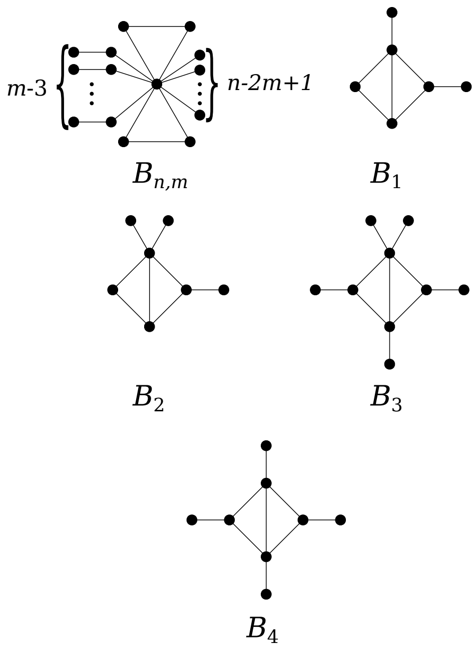

Fig. 16. Bicyclic graphs playing role in Theorems 143 and 144.

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 143. [68] *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 [68], $B_{6,3}$ 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 144. [68] *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 [68], $B_{7,3}$ 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 [33], 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 $E(G) = \{v_1 v_i, v_2 v_j : 2 \leq i \leq 5, 3 \leq j \leq 5\}$ 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.

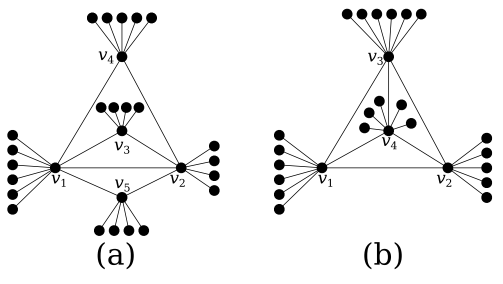

Fig. 17. (a) The graph $q_n(n_1, n_2, n_3, n_4, n_5)$; (b) The graph $K_n(n_1, n_2, n_3, n_4)$.

It was concluded in [33] 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 145. [33]

(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 [56], 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 $n_i \geq 1$, $1 \leq i \leq 6$.

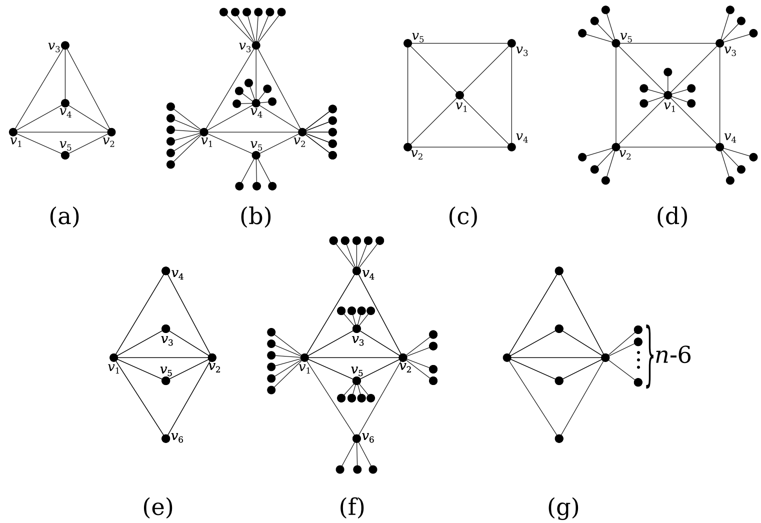

Fig. 18. (a) F_5; (b) $F_n(n_1, n_2, n_3, n_4, n_5)$; (c) W_5; (d) $W_n(n_1, n_2, n_3, n_4, n_5)$; (e) $Q(6, 3, 3, 3, 3)$ (f) $Q_n(n_1, n_2, n_3, n_4, n_5, n_6)$; (g) $Q_n(n-5, 1, 1, 1, 1, 1)$.

By considering tetracyclic graphs with a few non-pendent vertices, the authors came to the following conclusions.

Theorem 146. [56] *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 147. *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 148. [56] *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 [66], 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 149. [66] *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.

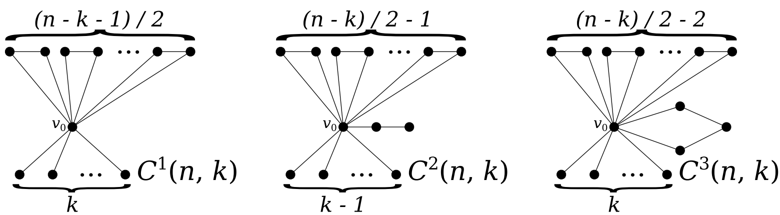

Fig. 19. Cacti occurring in Theorem 149.

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 150. [66] *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.

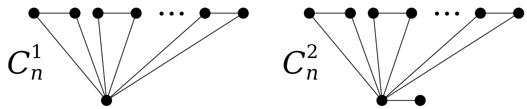

Fig. 20. Cacti occurring in Theorem 150.

Theorem 151. [66] *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 [66], 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 152. [66] *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 [34], [7], and [6] which provide a unified approach to the largest and smallest Zagreb indices of trees and cyclic graphs. In the paper [34], Deng introduced some transformations that increase (decrease) the Zagreb indices. First, we present two transformations from [34] 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.

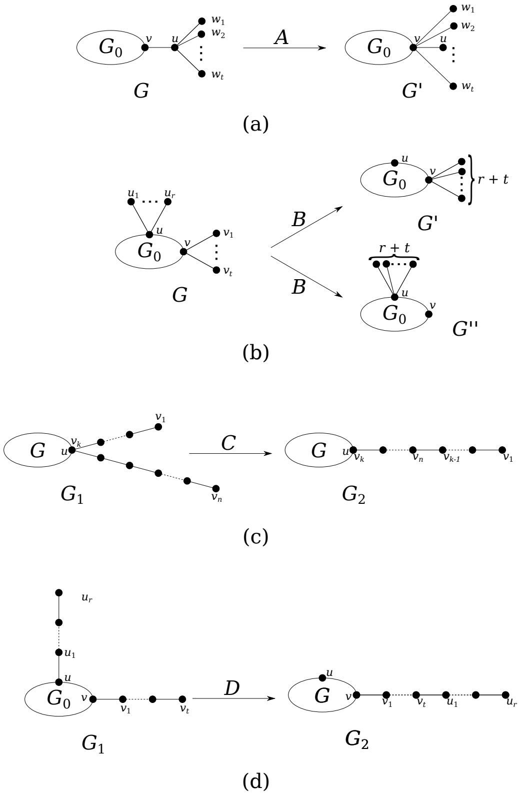

Fig. 21. The transformations A, B, C, and D.

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

$$G' \quad = \quad G - \{uu_1, uu_2, \ldots, uu_r\} + \{vu_1, vu_2, \ldots, vu_r\}$$

$$G'' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$$

see Fig. 21.

It has been proven in [34], 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 [34], 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 [26, 51], concerning extremal trees with maximal values of Zagreb indices were reproven. Also, Deng [34] obtained the corresponding results for unicyclic and bicyclic graphs with maximal Zagreb indices and in such a way some previously known results from [76, 107, 110] were reproven.

Deng [34] 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 $v_1v_2 \ldots v_n$, $1 < k < n$. 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 $u_0u_1 \ldots u_r$ and identifying v with the vertex v_0 of a path $v_0v_1 \ldots v_t$. Graph G_2 is obtained from G_1 by deleting uu_1 and adding v_tu_1 (see Fig. 21).

It was proven in [34], 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 153. [34] *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 [34], and in such a way some earlier known results for trees and unicyclic graphs have been confirmed [26,51,76,110] and new results on extremal bicyclic graphs with minimal Zagreb indices, presented in the previous discussions, have been obtained.

In the papers [6,7] 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 [83]. In fact, in the class of c-cyclic graphs, Bianchi et al. [6,7] were interested in finding graphs associated to the maximal (minimal) degree sequence with respect to the majorization order. Before we present the results of [6,7], 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 [6]. In such a way, some existing results mentioned previously [33,51,56,76,78,110,113] for $0 \leq c \leq 4$ 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 145). Thus we present here only the lower bounds arising from considerations in the paper [6].

(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 $n \geq 5$, 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 $M_1 \geq 4n + 20$.

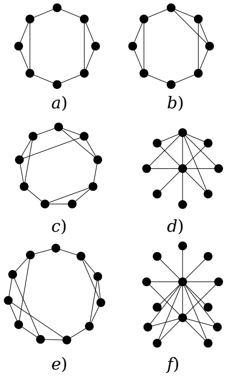

Fig. 22. Tricyclic and higher-cyclic graphs with minimal M_1, according to [6].

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 146.

(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 $52 \leq M_1 \leq 54$.

(ii) For $n \geq 6$ 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 $M_1 \geq 4n + 30$.

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 [6], 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 [6] 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 [7] 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 [83]. 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 [28, 107, 113].

References

[1] B. M. Abrego, S. Fernández–Merchant, M. G. Neubauer, W. Watkins, Sum of squares of degrees in a graph, *J. Inequal. Pure Appl. Math.* **10** (2009) #64.

[2] R. Aharoni, A problem of rearragements in $(0, 1)$-matrices, *Discr. Math.* **30** (1980) 191–200.

[3] R. Ahlswede, G. O. H. Katona, Graphs with maximal number of adjacent pairs of edges, *Acta Math. Acad. Sci. Hung.* **32** (1978) 97–120.

[4] L. W. Beineke, R. E. Pipet, The number of labeled k-dimensional trees, *J. Comb. Theory* **6** (1969) 200–205.

[5] L. W. Beineke, R. J. Wilson, *Topics in Algebraic Graph Theory*, Cambridge Univ. Press, New York, 2004.

[6] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, New bounds of degree–based topological indices for some classes of c-cyclic graphs, *Discr. Appl. Math.* **184** (2015) 62–75.

[7] M. Bianchi, A. Cornaro, A. Torriero, Majorization under constraints and bounds of the second Zagreb index, *Math. Ineq. Appl.* **16** (2013) 329–347.

[8] F. Boesch, R. Brigham, S. Burr, R. Dutton, R. Tindell, Maximizing the sum of squares of the degrees of a graph, Technical report, *Stevens Inst. Techn.*, Hoboken (1990).

[9] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[10] B. Bollobás, P. Erdős, A. Sarkar, Extremal graphs for weights, *Discr. Math.* **200** (1999) 5–19.

[11] B. Borovićanin, On the extremal Zagreb indices of trees with given number of segments or given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 55–79.

[12] B. Borovićanin, T. Aleksić Lampert, On the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 81–96.

[13] B. Borovićanin, B. Furtula, K. C. Das, I. Gutman, Zagreb indices: bounds and extremal graphs, in: I. Gutman, B. Furtula, K. C. Das, I. Ž. Milovanović, E. I. Milovanović, *Bounds in Chemical Graph Theory – Basics*, Univ. Kragujevac, Kragujevac, 2017, pp. 67–153.

[14] B. Borovićanin, B. Furtula, On extremal Zagreb indices of trees with given domination number, *Appl. Math. Comput.* **279** (2016) 208–218.

[15] O. D. Byer, Two path extremal graphs and an application to a Ramsey–type problem, *Discr. Math.* **196** (1999) 51–64.

[16] S. Chen, H. Deng, Extremal $(n, n+1)$-graphs with respected to zeroth-order general Randić index, *J. Math. Chem.* **42** (2007) 555–564.

[17] S. Chen, W. Liu, Extremal Zagreb indices of graphs with a given number of cut edges, *Graphs Comb.* **30** (2014) 109–118.

[18] S. Chen, F. Xia, Ordering unicyclic graphs with respect to Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 663–673.

[19] T. C. E. Cheng, Y. Guo, S. Zhang, Y. Du, Extreme values of the sum of squares of degrees of bipartite graphs, *Discr. Math.* **309** (2009) 1557–1564.

[20] S. M. Cioabă, Sums of powers of the degrees of a graph, *Discr. Math.* **306** (2006) 1959–1964.

[21] K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.

[22] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.

[23] K. C. Das, On comparing Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 433–440.

[24] K. C. Das, N. Akgunes, M. Togan, A. Yurttas, I. N. Cangul, A. S. Cevik, On the first Zagreb index and multiplicative Zagreb coindices of graphs, *An. St. Univ. Ovidius Constanta* **24** (2016) 153–176.

[25] K. C. Das, B. Borovićanin, I. Gutman, Remark on the first Zagreb index of graphs, forthcoming.

[26] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[27] K. C. Das, I. Gutman, B. Horoldagva, Comparing Zagreb indices and coindices of trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 189–198.

[28] K. C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices, *J. Math. Chem.* **46** (2009) 514–521.

[29] K. C. Das, K. Xu, I. Gutman, On Zagreb and Harary indices, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 301–314.

[30] K. C. Das, K. Xu, J. Nam, Zagreb indices of graphs, *Front. Math. China* **10** (2015) 567–582.

[31] D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discr. Math.* **185** (1998) 245–248.

[32] E. De LaViña, B. Waller, Spanning trees with many leaves and average distance, *El. J. Comb.* **15** (2008) 1–16.

[33] T. Dehghan–Zadeh, H. Hua, A. R. Ashrafi, N. Habibi, Extremal tri-cyclic graphs with respect to the first and second Zagreb indices, *Note Math.* **33** (2013) 107–121.

[34] H. Deng, A unified approach to the extremal Zagreb indices of trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[35] R. J. Duffin, Topology of series–parallel networks, *J. Math. Anal. Appl.* **10** (1965) 303–318.

[36] J. Estes, E. Nicholson, B. Wei, Partial orderings of trees according to Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 649–657.

[37] J. Estes, B. Wei, Sharp bounds of the Zagreb indices of k-trees, *J. Comb. Optim.* **27** (2014) 271–291.

[38] G. H. Fath–Tabar, Old and new Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 79–84.

[39] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* **23** (2010) 943–948.

[40] Y. Feng, X. Hu, S. Li, On the extremal Zagreb indices of graphs with cut edges, *Acta Appl. Math.* **110** (2010) 667–684.

[41] Y. Feng, X. Hu, S. Li, Erratum to: On the extremal Zagreb indices of graphs with cut edges, *Acta Appl. Math.* **110** (2010) 685–685.

[42] L. M. Fernandes, L. Gouveia, Minimal spanning trees with a constraint on the number of leaves, *Eur. J. Oper. Res.* **104** (1998) 250–261.

[43] J. F. Fink, L. F. Kinch, J. Roberts, On graphs having domination number half their order, *Period. Math. Hung.* **16** (1985) 287–293.

[44] C. M. da Fonseca, D. Stevanović, Further properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 655–668.

[45] M. Goubko, Minimizing degree–based topological indices for trees with given number of pendent vertices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 33–46.

[46] M. Goubko, I. Gutman, Degree–based topological indices: Optimal trees with given number of pendents, *Appl. Math. Comput.* **240** (2014) 387–398.

[47] M. Goubko, T. Réti, Note on minimizing degree–based topological indices of trees with given number of pendent vertices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 633–639.

[48] I. Gutman, Graphs with smallest sum of squares of vertex degrees, *Kragujevac J. Math.* **25** (2003) 51–54.

[49] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[50] I. Gutman, On the origin of two degree–based topological indices, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **146** (2014) 39–52.

[51] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[52] I. Gutman, M. Goubko, Trees with fixed number of pendent vertices with minimal first Zagreb index, *Bull. Int. Math. Virt. Inst.* **3** (2013) 161–164.

[53] I. Gutman, M. K. Jamil, N. Akhter, Graphs with fixed number of pendent vertices and minimal first Zagreb index, *Trans. Comb.* **4**(1) (2015) 43–48.

[54] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[55] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[56] N. Habibi, T. Dehghan–Zadeh, A. R. Ashrafi, Extremal tetracyclic graphs with respect to the first and second Zagreb indices, *Trans. Comb.* **5**(4) (2016) 35–55.

[57] A. J. Hoffman, R. R. Singleton, On Moore graphs with diameters 2 and 3, *IBM J. Res. Develop.* **4** (1960) 497–504.

[58] B. Horoldagva, K. C. Das, Sharp lower bounds for the Zagreb indices of unicyclic graphs, *Turk. J. Math.* **39** (2015) 595–603.

[59] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 97–101.

[60] A. Hou, S. Li, L. Song, B. Wei, Sharp bounds for Zagreb indices of maximal outerplanar graphs, *J. Comb. Optim.* **22** (2011) 252–269.

[61] H. Hua, Zagreb M_1 index, independence number and connectivity in graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 45–56.

[62] Z. Huang, H. Deng, On Zagreb indices of trees and unicyclic graphs with perfect matchings, in: I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008, pp. 235–250.

[63] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac J. Math.* **35** (2011) 173–182.

[64] A. Ilić, D. Stevanović, On comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 681–687.

[65] R. Lang, X. Deng, H. Lu, Bipartite grphs with the maximal value of the second Zagreb index, *Bull. Malays. Math. Sci. Soc.* **36**(1) (2103) 1–6.

[66] S. Li, H. Yang, Q. Zhao, Sharp bounds on Zagreb indices of cacti with k pendent vertices, *Filomat* **26** (2012) 1189–1200.

[67] S. Li, M. Zhang, Sharp upper bounds for Zagreb indices of bipartite graphs with a given diameter, *Appl. Math. Lett.* **24** (2011) 131–137.

[68] S. Li, Q. Zhao, Sharp upper bounds on Zagreb indices of bicyclic graphs with a given matching number, *Math. Comput. Model.* **54** (2011) 2869–2879.

[69] S. Li, Q. Zhao, On acyclic and unicyclic conjugated graphs with maximum Zagreb indices, *Util. Math.* **86** (2011) 115–128.

[70] S. Li, H. Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most k, *Appl. Math. Lett.* **23** (2010) 128–132.

[71] X. Li, Z. Li, L. Wang, The inverse problem for some topological indices in combinatorial chemistry, *J. Comput. Biol.* **10** (2003) 47–55.

[72] H. Lin, On the Wiener index of trees with given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 301–310.

[73] H. Lin, On segments, vertices of degree two and the first Zagreb index of trees, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 825–834.

[74] B. Liu, I. Gutman, Estimating the Zagreb and the general Randić indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 617–632.

[75] B. Liu, I. Gutman, Upper bounds for Zagreb indices of connected graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 439–446.

[76] M. Liu, B. Liu, New sharp upper bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 689–698.

[77] M. Liu, B. Liu, The second Zagreb indices and Wiener polarity indices of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 439–450.

[78] M. Liu, B. Liu, The second Zagreb indices of unicyclic graphs with given degree sequences, *Discr. Appl. Math.* **167** (2014) 217–221.

[79] M. Katz, Rearrangements of $(0,1)$-matrices, *Israel J. Math* **9** (1971) 13–15.

[80] Ž. Kovijanić Vukićević, G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iran. J. Math. Chem* **5**(1) (2014) 19–29.

[81] N. V. R. Mahadaev, U. N. Peled, *Threshold Graphs and Related Topics*, North–Holland, Amsterdam, 1995.

[82] T. Mansour, M. A. Rostami, E. Suresh, G. B. A. Xavier, New sharp lower bounds for the first Zagreb index, *Sci. Publ. State Univ. Novi Pazar, Ser. A, Appl. Math. Inform. Mech.* **8**(1) (2016) 11–19.

[83] A. W. Marshall, I. Olkin, *Inequalities: Theory of Majorization and its Applications*, Academic Press, London, 1979.

[84] E. I. Milovanović, I. Ž. Milovanović, Sharp bounds for the first Zagreb index and first Zagreb coindex, *Miskolc Math. Notes* **16** (2015) 1017–1024.

[85] I. Ž. Milovanović, E. I. Milovanović, Correcting a paper on first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 693–695.

[86] M. J. Morgan, S. Mukwembi, Bounds on the first Zagreb index, with applications in: I. Gutman (Ed.), *Topics in Chemical Graph Theory*, Univ. Kragujevac, Kragujevac, 2014, 215–228.

[87] V. Nikiforov, The sum of squares of degrees: Sharp asymptotics, *Discr. Math.* **307** (2007) 3187–3193.

[88] C. S. Oliveira, N. M. M. de Abreu, S. Jurkiewicz, The characteristic polynomial of the Laplacian of graphs in $(a;b)$-linear classes, *Lin. Algebra Appl.* **356** (2002) 113–121.

[89] D. Ollp, A conjecture of Goodman and the multiplicities of graphs, *Australas. J. Comb.* **14** (1996) 267–282.

[90] O. Ore, *Theory of Graphs*, Am. Math. Soc., Providence, 1962.

[91] U. N. Peled, R. Petreschi, A. Sterbini, (n,e)-graphs with maximum sum of squares of degrees, *J. Graph. Theory* **31** (1999) 283–295.

[92] R. Schwarz, Rearragements of square matrices with non-negative elements, *Duke Math. J.* **31** (1964) 45–62.

[93] D. Stevanović, *Mathematical Properties of Zagreb Indices*, Akademska misao, Beograd, 2014 (in Serbian).

[94] L. Sun, R. Chen, The second Zagreb index of acyclic conjugated molecules, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 57–64.

[95] L. A. Székely, L. H. Clark, R. C. Entringer, An equality for degree sequences, *Discr. Math.* **103** (1992) 293–300.

[96] R. M. Tache, On degree–based topological indices for bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 99–116.

[97] M. Tavakoli, F. Rahbarnia, Note on properties of first Zagreb index of graphs, *Iran. J. Math. Chem.* **3**(1) (2012) 1–5.

[98] A. Vasilyev, R. Darda, D. Stevanović, Trees of given order and independence number with minimal first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 775–782.

[99] D. Vukičević, S. M. Rajtmajer, N. Trinajstić, Trees with maximal second zagreb index and prescribed number of vertices of given degree, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 65–70.

[100] S. Wagner, H. Wang, On a problem of Ahlswede and Katona, *Studia Sci. Math. Hung.* **46** (2009) 423–435.

[101] J. F. Wang, F. Belardo, A lower bound for the first Zagreb index and its application, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 35–56.

[102] J. F. Wang, F. Belardo, Q. L. Zhang, Signless Laplacian spectral characterization of line graphs of T-shape trees, *Lin. Multilin. Algebra* **62** (2014) 1529–1545.

[103] F. L. Xia, S. B. Chen, Ordering unicyclic graphs with respect to Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 663–673.

[104] K. Xu, The Zagreb indices of graphs with a given clique number, *Appl. Math. Lett.* **24** (2011) 1026–1030.

[105] K. Xu, K. C. Das, S. Balachandran, Maximizing the Zagreb indices of (n, m)-graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654.

[106] S. Yamaguchi, Estimating the Zagreb indices and the spectral radius of triangle– and quadrangle–free connected graphs, *Chem. Phys. Lett.* **458** (2008) 396–398.

[107] Z. Yan, H. Liu, H. Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, *J. Math. Chem.* **42** (2006) 565–574.

[108] Y. S. Yoon, J. K. Kim, A relationship between bounds on the sum of squares of degrees of a graph, *J. Appl. Math. Comput.* **21** (2006) 233–238.

[109] W. G. Yuan, X. D. Zhang, The second Zagreb indices of graphs with given degree sequence, *Discr. Appl. Math.* **185** (2015) 230–238.

[110] S. Zhang, H. Zhang, Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 427–438.

[111] S. Zhang, C. Zhou, Bipartite graphs with the maximum sum of squares of degrees, *Acta Math. Appl. Sin.* **30** (2014) 1–6.

[112] X. D. Zhang, The Laplacian spectral radii of trees with degree sequences, *Discr. Math.* **308** (2008) 3143–3150.

[113] Q. Zhao, S. Li, Sharp bounds for the Zagreb indices of bicyclic graphs with k pendent vertices, *Discr. Appl. Math.* **158** (2010) 1953–1962.

[114] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.

[115] B. Zhou, Upper bounds for the Zagreb indices and the spectral radius of series–parallel graphs, *Int. J. Quantum. Chem.* **107** (2007) 875–878.

[116] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.

[117] B. Zhou, I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.

[118] B. Zhou, D. Stevanović, A note on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 571–578.