MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **82** (2019) 679-698

ISSN 0340 - 6253

A Unified Approach to Bounds for Topological Indices on Trees and Applications

Alvaro Martínez–Pérez[a], José M. Rodríguez[b]

[a]*Facultad de Ciencias Sociales, Universidad de Castilla-La Mancha, Avda. Real Fábrica de Seda, s/n. 45600 Talavera de la Reina, Toledo, Spain*
e-mail: alvaro.martinezperez@uclm.es

[b]*Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain*
e-mail: jomaro@math.uc3m.es

(Received March 19, 2019)

Abstract

The aim of this paper is to use a unified approach in order to obtain new inequalities for a large family of topological indices restricted to trees and to characterize the set of extremal trees with respect to them. Our main results provide upper and lower bounds for a large class of topological indices on trees, fixing or not the maximum degree or the number of pendant vertices. This class includes the variable first Zagreb, the multiplicative second Zagreb, the Narumi-Katayama and the sum lordeg indices. In particular, our results on the sum lordeg index partially solve an open problem on this index.

1 Introduction

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph. They play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [44]. The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v),$$

where $\{u,v\}$ runs over every pair of vertices in G.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) [33].

Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by M_1 and M_2, respectively, and introduced by Gutman et al. in [22] and [20]. They are defined as

$$M_1(G) = \sum_{u \in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. See the recent surveys on the Zagreb indices [1], [6] and [19] as well as [24], [25].

Along the paper, we will denote by m and n, the cardinality of the sets $E(G)$ and $V(G)$, respectively.

Miličević and Nikolić defined in [29] the *variable first and second Zagreb indices* as

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha}, \qquad M_2^{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha},$$

with $\alpha \in \mathbb{R}$.

Note that M_1^0 is n, M_1^1 is $2m$, M_1^2 is the first Zagreb index M_1, M_1^{-1} is the inverse index ID [14], M_1^3 is the forgotten index F, etc.; also, M_2^0 is m, $M_2^{-1/2}$ is the usual Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified second Zagreb index [31], etc.

The concept of variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [34], [35]), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [36]). The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a particular studied property is as small as possible.

In the paper of Gutman and Tošović [21], the correlation abilities of 20 vertex-degree-based topological indices occurring in the chemical literature were tested for the case of standard heats of formation and normal boiling points of octane isomers. It is remarkable to realize that the variable second Zagreb index M_2^α with exponent $\alpha = -1$ (and to a lesser extent with exponent $\alpha = -2$) performs significantly better than the Randić index ($R = M_2^{-1/2}$).

The variable second Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons [32]. Various properties and relations of these indices are discussed in several papers (see, e.g., [3], [27], [28], [37], [45], [46]).

The *sum lordeg index* is one of the Adriatic indices introduced in [41]. It is defined as

$$SL(G) = \sum_{u \in V(G)} d_u \sqrt{\log d_u}\,.$$

This index is interesting from an applied viewpoint since it is the best predictor of octanol-water partition coefficient for octane isomers [41], and so, it appears in numerical packages for the computation of topological indices [39]. For these reasons, in [42] is stated the open problem of find (sharp) lower and upper bounds for this index.

Recall that a main topic in the study of topological indices is to find bounds of the indices involving several parameters. The aim of this paper is to use a unified approach in order to obtain new inequalities for a large family of topological indices restricted to trees or graphs and to characterize the set of extremal trees or graphs with respect to them. Our main results provide upper and lower bounds for a large class of topological indices on trees or graphs, fixing or not the maximum degree or the number of pendant vertices. This class includes the variable first Zagreb, the multiplicative second Zagreb and the Narumi-Katayama indices. Also, our results can be applied to the sum lordeg index, and partially solve an open problem on this index (see Propositions 3.1 and 3.6, Remark 3.10 and Theorems 3.2, 3.5, 3.8 and 3.9).

A main tool of many proofs in this paper is the majorization method, which has already been successfully applied in several papers (see, e.g., [9], [15], [26]). An interesting fact is that although the majorization method requires to deal with convex (or concave) functions, our methods of proof allow to obtain inequalities also for the sum lordeg index, an interesting topological index involving a function which is neither convex nor concave.

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite connected simple (without multiple edges and loops) non-trivial ($E(G) \neq \emptyset$) graph. T denotes a tree, i.e., a graph without cycles. Note that the connectivity of G is not an important restriction, since any graph representing a molecule is connected.

2 Trees with a fixed number of pendant vertices

Given two n-tuples $\mathbf{x} = (x_1, \dots, x_n)$, $\mathbf{y} = (y_1, \dots, y_n)$ with $x_1 \geq x_2 \geq \cdots \geq x_n$ and $y_1 \geq y_2 \geq \cdots \geq y_n$, then $\mathbf{x}$ *majorizes* $\mathbf{y}$ (and we write $\mathbf{x} \succ \mathbf{y}$ or $\mathbf{y} \prec \mathbf{x}$) if

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i,$$

for $1 \leq k \leq n-1$ and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

A function $\Phi\colon \mathbb{R}^n \to \mathbb{R}$ is called *Schur-convex* if $\Phi(\mathbf{x}) \geq \Phi(\mathbf{y})$ for all $\mathbf{x} \succ \mathbf{y}$. Similarly, the function is *Schur-concave* if $\Phi(\mathbf{x}) \leq \Phi(\mathbf{y})$ for all $\mathbf{x} \succ \mathbf{y}$. We say that Φ is *strictly Schur-convex* (respectively, *strictly Schur-concave*) if $\Phi(\mathbf{x}) > \Phi(\mathbf{y})$ (respectively, $\Phi(\mathbf{x}) < \Phi(\mathbf{y})$) for all $\mathbf{x} \succ \mathbf{y}$ with $\mathbf{x} \neq \mathbf{y}$.

If

$$\Phi(\mathbf{x}) = \sum_{i=1}^{n} f(x_i),$$

where f is a convex (respectively, concave) function defined on a real interval, then Φ is Schur-convex (respectively, Schur-concave). If f is strictly convex (respectively, strictly concave), then Φ is strictly Schur-convex (respectively, strictly Schur-concave).

Thus,

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha},$$

is strictly Schur-convex if $\alpha \in (-\infty, 0) \cup (1, \infty)$ and strictly Schur-concave if $\alpha \in (0, 1)$.

A *pendant* vertex in a graph is a vertex with degree one. If the graph is a tree, a pendant vertex is also called a *leaf*.

Given $n \geq 3$ and $2 \leq p \leq n-1$, let $S_{n,p}$ be the set of n-tuples $\mathbf{x} = (x_1, x_2, \dots, x_{n-p}, 1, \dots, 1)$ with $x_i \in \mathbb{Z}^+$ such that $x_1 \geq x_2 \geq \cdots \geq x_{n-p} \geq 2$ and $\sum_{i=1}^{n-p} x_i = 2n - 2 - p$.

Remark 2.1. *Consider any tree T with n vertices $v_1, \dots, v_n$, ordered in such a way that if $\mathbf{x} = \mathbf{x}_T = (x_1, \dots, x_n)$ is the n-tuple where x_i is the degree of the vertex v_i, then $x_i \geq x_{i+1}$ for every $1 \leq i \leq n-1$. If T has p pendant vertices, one can check that $\mathbf{x}_T \in S_{n,p}$.*

Lemma 2.2. *Let $n \geq 3$ and $2 \leq p \leq n-1$. If $r = \left\lfloor \frac{n-2}{n-p} \right\rfloor$, $\mathbf{y} = (y_1, y_2, \dots, y_n)$ is such that*

- *$y_1 = p$,*
- *$y_j = 2$ for every $1 < j \leq n-p$,*
- *$y_j = 1$ for every $n-p < j \leq n$,*

and $\mathbf{z} = (z_1, z_2, \ldots, z_n)$ is such that

- *$z_j = r+2$ for every $1 \leq j \leq n-2-(n-p)r$,*
- *$z_j = r+1$ for every $n-2-(n-p)r < j \leq n-p$,*
- *$z_j = 1$ for every $n-p < j \leq n$,*

then $\mathbf{y}, \mathbf{z} \in S_{n,p}$ and

$$\mathbf{z} \prec \mathbf{x} \prec \mathbf{y}$$

for all $\mathbf{x} \in S_{n,p}$.

Proof. First of all note that $1 \leq r \leq n-2$: Since $p \leq n-1$, we have $r \leq n-2$. Since $p \geq 2$, we have $r \geq 1$.

Also, note that $0 \leq n-2-(n-p)r \leq n-p-1$.

We have

$$\sum_{j=1}^{n-p} y_j = p + 2(n-p-1) = 2n-2-p,$$

and so, $\mathbf{y} \in S_{n,p}$.

If $n-2-(n-p)r = 0$, then $r = \frac{n-2}{n-p} \in \mathbb{Z}$ and

$$\sum_{j=1}^{n-p} z_j = (r+1)(n-p) = \Big(\frac{n-2}{n-p} + 1\Big)(n-p) = 2n-2-p.$$

If $n-2-(n-p)r > 0$, then

$$\sum_{j=1}^{n-p} z_j = (r+2)(n-2-(n-p)r) + (r+1)(n-p-(n-2)+(n-p)r) = 2n-2-p.$$

Also, $r+1 \geq 2$ and so, $\mathbf{z} \in S_{n,p}$.

Seeking for a contradiction assume that

$$p + 2(k-1) = \sum_{i=1}^{k} y_i < \sum_{i=1}^{k} x_i,$$

for some $k < n-p$. Thus,

$$\sum_{i=1}^{n-p} x_i = \sum_{i=1}^{k} x_i + \sum_{i=k+1}^{n-p} x_i > \sum_{i=1}^{k} y_i + \sum_{i=k+1}^{n-p} 2 = \sum_{i=1}^{n-p} y_i = 2n-2-p,$$

leading to a contradiction. Hence, we have for every $k < n-p$,

$$p + 2(k-1) = \sum_{i=1}^{k} y_i \geq \sum_{i=1}^{k} x_i,$$

and so, $\mathbf{x} \prec \mathbf{y}$.

Seeking for a contradiction assume that

$$\sum_{i=k+1}^{n-p} z_i < \sum_{i=1}^{k} x_i$$

for some $k < n-p$. Thus, $z_{k+1} < x_{k+1}$.

If $k+1 > n-2-(n-p)r$, then $r+1 = z_{k+1} < x_{k+1}$ and so, $z_i \leq r+2 \leq x_{k+1} \leq x_i$ for every $1 \leq i \leq k$. Therefore,

$$2n-2-p = \sum_{i=1}^{n-p} z_i = \sum_{i=1}^{k} z_i + \sum_{i=k+1}^{n-p} z_i < \sum_{i=1}^{k} x_i + \sum_{i=k+1}^{n-p} x_i = \sum_{i=1}^{n-p} x_i,$$

a contradiction.

If $k+1 \leq n-2-(n-p)r$, then $r+2 = z_{k+1} < x_{k+1}$ and so, $z_i = r+2 \leq x_{k+1} \leq x_i$ for every $1 \leq i \leq k$. Therefore,

$$2n-2-p = \sum_{i=1}^{n-p} z_i = \sum_{i=1}^{k} z_i + \sum_{i=k+1}^{n-p} z_i < \sum_{i=1}^{k} x_i + \sum_{i=k+1}^{n-p} x_i = \sum_{i=1}^{n-p} x_i,$$

a contradiction.

Hence, we have for every $k < n-p$,

$$\sum_{i=k+1}^{n-p} z_i \geq \sum_{i=k+1}^{n-p} x_i,$$

$$\sum_{i=1}^{k} z_i = 2n-2-p - \sum_{i=k+1}^{n} z_i \leq 2n-2-p - \sum_{i=k+1}^{n} x_i = \sum_{i=1}^{k} x_i.$$

Thus, $\mathbf{z} \prec \mathbf{x}$. ∎

For a graph G and for any function $f : \{d_u : u \in V(G)\} \to \mathbb{R}$, let us define the index

$$I_f(G) = \sum_{u \in V(G)} f(d_u).$$

Besides, if f takes positive values, then we can define the index

$$II_f(G) = \prod_{u \in V(G)} f(d_u).$$

Lemma 2.2 has the following consequences. Along this section we will use the notation of r, $\mathbf{z}$ and $\mathbf{y}$ in Lemma 2.2.

Theorem 2.3. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $f : [1, \infty) \to \mathbb{R}$ is a convex function on $[2, \infty)$, then*

$$I_f(T) \geq (n - 2 - (n - p)r)f(r + 2) + ((n - p)(r + 1) - n + 2)f(r + 1) + pf(1),$$

$$I_f(T) \leq f(p) + (n - p - 1)f(2) + pf(1).$$

Moreover, if f is a strictly convex function, then the lower bound is attained if and only if the degree sequence of T is $\mathbf{z}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{y}$.

Proof. Let us define

$$S'_{n,p} = \big\{\mathbf{x} = (x_1, \dots, x_{n-p}) : (x_1, \dots, x_{n-p}, 1, \dots, 1) \in S_{n,p}\big\},$$

i.e., $S'_{n,p} = \Pi(S_{n,p})$, where $\Pi : \mathbb{R}^n \to \mathbb{R}^{n-p}$ is the canonical projection on the first $n - p$ variables. If $\mathbf{x} \in S'_{n,p}$, then $x_i \geq 2$ for every $1 \leq i \leq n - p$. It is clear that Lemma 2.2 can be formulated in terms of $S'_{n,p}$ instead of $S_{n,p}$. Note that

$$I_f(T) = pf(1) + I_f(T) - pf(1), \qquad I_f(T) - pf(1) = \sum_{u \in V(T),\, d_u \geq 2} f(d_u).$$

Since f is a convex function on $[2, \infty)$, Lemma 2.2, applied to $I_f(T) - pf(1)$, gives the result. ∎

Using the argument in the proof of Theorem 2.3, we can obtain, in a similar way, the following results.

Theorem 2.4. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $f : [1, \infty) \to \mathbb{R}$ is a concave function on $[2, \infty)$, then*

$$I_f(T) \geq f(p) + (n - p - 1)f(2) + pf(1),$$

$$I_f(T) \leq (n - 2 - (n - p)r)f(r + 2) + ((n - p)(r + 1) - n + 2)f(r + 1) + pf(1).$$

Moreover, if f is a strictly concave function, then the lower bound is attained if and only if the degree sequence of T is $\mathbf{y}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{z}$.

Since the logarithm is a strictly increasing function, a tree is extremal for $II_f(T)$ if and only if it is extremal for

$$\log II_f(T) = \sum_{u \in V(G)} \log f(d_u).$$

Thus, Lemma 2.2 implies the following results.

Theorem 2.5. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $f : [1, \infty) \to \mathbb{R}^+$ is a function such that $\log f$ is convex on $[2, \infty)$, then*

$$II_f(T) \geq f(r+2)^{n-2-(n-p)r} f(r+1)^{(n-p)(r+1)-n+2} f(1)^p,$$
$$II_f(T) \leq f(p) f(2)^{n-p-1} f(1)^p.$$

Moreover, if $\log f$ is a strictly convex function on $[2, \infty)$, then the lower bound is attained if and only if the degree sequence of T is $\mathbf{z}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{y}$.

Theorem 2.6. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $f : [1, \infty) \to \mathbb{R}^+$ is a function such that $\log f$ is concave on $[2, \infty)$, then*

$$II_f(T) \geq f(p) f(2)^{n-p-1} f(1)^p,$$
$$II_f(T) \leq f(r+2)^{n-2-(n-p)r} f(r+1)^{(n-p)(r+1)-n+2} f(1)^p.$$

Moreover, if $\log f$ is a strictly concave function on $[2, \infty)$, then the lower bound is attained if and only if the degree sequence of T is $\mathbf{y}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{z}$.

Since t^α is strictly convex if $\alpha \in (-\infty, 0) \cup (1, \infty)$ and strictly concave if $\alpha \in (0, 1)$, Theorems 2.3 and 2.4 imply, respectively, the following results.

Theorem 2.7. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $\alpha \in (-\infty, 0) \cup (1, \infty)$, then*

$$M_1^\alpha(T) \geq (n-2-(n-p)r)(r+2)^\alpha + ((n-p)(r+1)-n+2)(r+1)^\alpha + p,$$
$$M_1^\alpha(T) \leq p^\alpha + (n-p-1)2^\alpha + p.$$

Moreover, the lower bound is attained if and only if the degree sequence of T is $\mathbf{z}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{y}$.

Theorem 2.8. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, and $\alpha \in (0, 1)$, then*

$$M_1^\alpha(T) \geq p^\alpha + (n-p-1)2^\alpha + p,$$
$$M_1^\alpha(T) \leq (n-2-(n-p)r)(r+2)^\alpha + ((n-p)(r+1)-n+2)(r+1)^\alpha + p.$$

Moreover, the lower bound is attained if and only if the degree sequence of T is $\mathbf{y}$*, and the upper bound is attained if and only if the degree sequence of T is* $\mathbf{z}$*.*

The inequalities in Theorem 2.7 and 2.8 were proved in [26] with a different argument.

The *Narumi-Katayama index* is defined in [30] as

$$NK(G) = \prod_{u \in V(G)} d_u.$$

The *multiplicative second Zagreb index* or *modified Narumi-Katayama index*

$$NK^*(G) = \prod_{uv \in E(G)} d_u d_v = \prod_{u \in V(G)} d_u^{d_u}$$

was introduced in [23] and [16].

Since $t \log t$ is a strictly convex function and $\log t$ is a strictly concave function, Theorems 2.5 and 2.6 imply, respectively, the following results.

Theorem 2.9. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, then*

$$NK^*(T) \geq (r+2)^{(r+2)(n-2-(n-p)r)}(r+1)^{(r+1)((n-p)(r+1)-n+2)},$$
$$NK^*(T) \leq p^p 4^{n-p-1}.$$

Moreover, the lower bound is attained if and only if the degree sequence of T is $\mathbf{z}$*, and the upper bound is attained if and only if the degree sequence of T is* $\mathbf{y}$*.*

Theorem 2.10. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, then*

$$NK(T) \geq p\, 2^{n-p-1},$$
$$NK(T) \leq (r+2)^{n-2-(n-p)r}(r+1)^{(n-p)(r+1)-n+2}.$$

Moreover, the lower bound is attained if and only if the degree sequence of T is $\mathbf{y}$*, and the upper bound is attained if and only if the degree sequence of T is* $\mathbf{z}$*.*

The lower bounds in Theorems 2.9 and 2.10 were proved in [43] with different arguments.

3 Upper and lower bounds for the sum lordeg index

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5.85×10^{21} [40]. Hence, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species. The main reason for the use of topological indices is to obtain predictions of some property of certain molecules (see, e.g., [13], [17], [21], [36]). Therefore, given some fixed parameters, a natural problem is to find the graphs that minimize (or maximize) the value of a topological index (which correlates with a physico-chemical property) on the set of graphs (or trees) satisfying the restrictions given by the parameters (see, e.g., [2], [4], [5], [7], [8], [10], [11], [12], [18]).

In [42] is stated the open problem of finding (sharp) lower and upper bounds for the sum lordeg index. When the number of vertices is fixed, we solve here this open problem in the case of graphs, graphs with a fixed maximum degree Δ, trees and trees with a fixed number of pendant vertices. Also, we characterize the extremal graphs or trees. Recall that the sum lordeg index is the best predictor of octanol-water partition coefficient for octane isomers [41].

Proposition 3.1. *If G is a graph with n vertices, then*

$$SL(G) \le n(n-1)\sqrt{\log(n-1)}\,,$$

and the equality is attained if and only if G is the complete graph. If G is a minimal graph for SL, then G is a tree.

Besides, if G has maximum degree Δ and minimum degree δ, then

$$2m\sqrt{\log\delta} \le SL(G) \le 2m\sqrt{\log\Delta}\,, \qquad n\delta\sqrt{\log\delta} \le SL(G) \le n\Delta\sqrt{\log\Delta}\,,$$

and each equality is attained if and only if G is a regular graph.

Proof. The first inequality holds since $d_u \le n-1$ for every $u \in V(G)$ and $f(t) = t\sqrt{\log t}$ is an increasing function. The equality is attained if and only if $d_u = n-1$ for every $u \in V(G)$, i.e., G is the complete graph.

We have the two last inequalities since $f(t) = t\sqrt{\log t}$ is an increasing function and $\delta \le d_u \le \Delta$ for every $u \in V(G)$. This fact and

$$SL(G) = \sum_{u\in V(G)} d_u\sqrt{\log d_u} = \sum_{uv\in E(G)} \left(\sqrt{\log d_u} + \sqrt{\log d_v}\,\right)$$

give the other inequalities. It is clear that each equality is attained if and only if $d_u = \delta$ for every $u \in V(G)$ or $d_u = \Delta$ for every $u \in V(G)$, i.e., G is a regular graph.

Finally, assume that G is a minimal graph for SL, and that G is not a tree. Thus, there exists an edge $uv \in E(G)$ such that the graph $G \setminus uv$ (defined by $V(G \setminus uv) = V(G)$ and $E(G \setminus uv) = E(G) \setminus \{uv\}$) is connected. Since the degree of any $w \in V(G) \setminus \{u, v\}$ in $G \setminus uv$ is also d_w and the degree of u in $G \setminus uv$ is $d_u - 1$, we conclude $SL(G \setminus uv) < SL(G)$. By applying this argument a finite number of times we obtain a tree T with $SL(T) < SL(G)$. Hence, if G is a minimal graph for SL, it is a tree. ■

Since if G is a minimal graph for SL, then G is a tree by Proposition 3.1, it is interesting to study this index for trees.

The function $f(t) = t\sqrt{\log t}$ satisfies

$$\begin{aligned} f'(t) &= \frac{1}{2}\big(\log t\big)^{-1/2}\big(2\log t + 1\big), \\ f''(t) &= \frac{1}{4t}\big(\log t\big)^{-3/2}\big(2\log t - 1\big), \end{aligned}$$

and so, f is concave on $[1, e^{1/2}]$ and it is convex on $[e^{1/2}, \infty)$. Thus, f is not convex on $[1, \infty)$, but it is strictly convex on $[2, \infty)$, and Theorem 2.3 gives the following result.

Theorem 3.2. *If T is a tree with $n \geq 3$ vertices and p pendant vertices, then*
$SL(T) \geq (n-2-(n-p)r)(r+2)\sqrt{\log(r+2)} + ((n-p)(r+1)-n+2)(r+1)\sqrt{\log(r+1)}\,,$
$SL(T) \leq p\sqrt{\log p} + (n-p-1)2\sqrt{\log 2}\,.$
Moreover, the lower bound is attained if and only if the degree sequence of T is $\mathbf{z}$, and the upper bound is attained if and only if the degree sequence of T is $\mathbf{y}$.

By using Theorem 2.3 we can obtain also the following result.

Theorem 3.3. *If T is a tree with $n \geq 3$ vertices and $f : [1, \infty) \to \mathbb{R}$ is a convex function on $[2, \infty)$, then*

$$I_f(T) \leq \max\big\{f(2) + (n-3)f(2) + 2f(1),\ f(n-1) + (n-1)f(1)\big\}.$$

Proof. Since the number p of pendant vertices of a tree satisfies $2 \leq p \leq n-1$, Theorem 2.3 gives

$$I_f(T) \leq \max_{2 \leq p \leq n-1} \big(f(p) + (n-p-1)f(2) + pf(1)\big).$$

Let us consider the function $F : [2, n-1] \to \mathbb{R}$ given by $F(s) = f(s) + (n-s-1)f(2) + sf(1)$. Since f is a convex function on $[2, \infty)$ and $(n-s-1)f(2) + sf(1)$ is a polynomial of degree 1, F is convex on $[2, n-1]$ and so,

$$\max\big\{F(2),\ F(n-1)\big\} \leq \max_{2 \leq p \leq n-1} F(p) \leq \max_{s \in [2, n-1]} F(s) = \max\big\{F(2),\ F(n-1)\big\}.$$

Therefore,

$$\max_{2\le p\le n-1}\big(f(p)+(n-p-1)f(2)+pf(1)\big)=\max\big\{f(2)+(n-3)f(2)+2f(1),\ f(n-1)+(n-1)f(1)\big\},$$

and this finishes the proof. ■

The argument in the proof of Theorem 3.3 allows to prove the following result.

Theorem 3.4. *If T is a tree with $n \ge 3$ vertices and $f : [1,\infty) \to \mathbb{R}$ is a concave function on $[2,\infty)$, then*

$$I_f(T) \ge \min\big\{f(2)+(n-3)f(2)+2f(1),\ f(n-1)+(n-1)f(1)\big\}.$$

Theorem 3.3 allows to obtain another bound for the sum lordeg index.

Theorem 3.5. *Let T be a tree with $n \ge 3$ vertices.*

(1) *If $n < 10$, then*

$$SL(T) \le (n-2)2\sqrt{\log 2}\,,$$

and the equality is attained if and only if T is the path graph.

(2) *If $n \ge 10$, then*

$$SL(T) \le (n-1)\sqrt{\log(n-1)}\,,$$

and the equality is attained if and only if T is the star graph.

Proof. Theorem 3.3 gives

$$SL(T) \le \max\big\{(n-2)2\sqrt{\log 2}\,,\ (n-1)\sqrt{\log(n-1)}\ \big\},$$

Furthermore, the argument in the proof of Theorem 3.3 gives that if $(n-2)2\sqrt{\log 2} > (n-1)\sqrt{\log(n-1)}$, then the equality is attained if and only if T is the path graph, and that if $(n-2)2\sqrt{\log 2} < (n-1)\sqrt{\log(n-1)}$, then the equality is attained if and only if T is the star graph.

If $n=3$, then $T=P_3=S_3$ and the inequality is, in fact, an equality. Assume now $n \ge 4$.

Let us consider the functions

$$U(s)=\frac{s}{s-1}\sqrt{\log s}\,,\qquad V(s)=s-1-2\log s.$$

We have

$$U'(s)=\frac{\big(\log s\big)^{-1/2}}{2(s-1)^2}\big(s-1-2\log s\big)=\frac{\big(\log s\big)^{-1/2}}{2(s-1)^2}\,V(s).$$

Since $V' > 0$ on $(2,\infty)$, the function V is increasing on $(2,\infty)$. Since $V(4) > 0$, we have that $V(s) \ge V(4) > 0$ for every $s \in [4,\infty)$, and so, $U'(s) > 0$ for every $s \in [4,\infty)$. Since $U(9) > 2\sqrt{\log 2}$, we have $U(s) \ge U(9) > 2\sqrt{\log 2}$ for every $s \in [9,\infty)$, and so $(n-2)2\sqrt{\log 2} < (n-1)\sqrt{\log(n-1)}$ for every $n \ge 10$.

One can check that $(n-2)2\sqrt{\log 2} > (n-1)\sqrt{\log(n-1)}$ for $3 < n < 10$, and this finishes the proof. ■

Proposition 3.6. *Let G be a graph with $3 \le n \le 5$ vertices. Then*

$$SL(G) \ge (n-1)\sqrt{\log(n-1)}\,,$$

and the equality is attained if and only if G is the star graph.

Proof. By Proposition 3.1, if G is minimal, then G is a tree. Let T be a tree with n vertices. If $n=3$, then $T = P_3 = S_3$. If $n = 4$ it is immediate to check that either $T = S_4$ or $T = P_4$ and

$$3.1 \approx 3\sqrt{\log 3} = SL(S_4) < SL(P_4) = 4\sqrt{\log 2} \approx 3.3.$$

If $n=5$, then $T = S_5$ and $SL(T) = 4\sqrt{\log 4} \approx 4.7$, or $T = P_5$ and $SL(T) = 6\sqrt{\log 2} \approx 5.0$, or the degree sequence of T is $(3,2,1,1,1)$ and $SL(T) = 3\sqrt{\log 3} + 2\sqrt{\log 2} \approx 4.8$. ■

Lemma 3.7. *If $d \ge 6$,*

$$d\sqrt{\log d} > (d-1)\sqrt{\log(d-1)} + 2\sqrt{\log 2}\,,$$

and if $3 \le d \le 5$,

$$d\sqrt{\log d} < (d-1)\sqrt{\log(d-1)} + 2\sqrt{\log 2}\,.$$

Proof. Since $f(t) = t\sqrt{\log t}$ is convex on $[2,\infty)$,

$$(d+1)\sqrt{\log(d+1)} - d\sqrt{\log d} > d\sqrt{\log d} - (d-1)\sqrt{\log(d-1)}$$

for every $d \ge 3$. Thus, it suffices to check that

$$1.69 \approx 6\sqrt{\log 6} - 5\sqrt{\log 5} > 2\sqrt{\log 2} \approx 1.67,$$

and

$$1.67 \approx 2\sqrt{\log 2} > 5\sqrt{\log 5} - 4\sqrt{\log 4} \approx 1.63.$$

■

Let $n \geq 6$. If $r = \lceil \frac{n-2}{3} \rceil$ and $s = 3r - n + 2$, let us define $\mathbf{z} = (z_1, z_2, \dots, z_n)$ as

- $z_j = 4$ for every $1 \leq j \leq r - s$,
- $z_j = 3$ for every $r - s < j \leq r$,
- $z_j = 1$ for every $r < j \leq n$.

Note that $0 \leq s \leq 2 \leq r \leq n - 4$.

Theorem 3.8. *Let G be a graph with $n \geq 6$ vertices. If $r = \lceil \frac{n-2}{3} \rceil$ and $s = 3r - n + 2$, then*

$$SL(G) \geq 4(r-s)\sqrt{\log 4} + 3s\sqrt{\log 3}\,,$$

and the equality is attained if and only if G is a tree and its degree sequence is $\mathbf{z}$.

Proof. By Proposition 3.1, if G is minimal, then G is a tree. Suppose T is minimal for SL and has maximum degree Δ.

Claim 1: $\Delta \leq 5$. Suppose there is a vertex w with $deg(w) = d \geq 6$. Then consider any adjacent vertex v and any pendant vertex u in the connected component of $T \setminus \{wv\}$ containing w, and let

$$T' = \big(T \setminus \{wv\}\big) \cup \{uv\}.$$

Thus, in T', $deg_{T'}(w) = d - 1$, $deg_{T'}(u) = 2$ and, by Lemma 3.7,

$$SL(T) - SL(T') = d\sqrt{\log d} - (d-1)\sqrt{\log(d-1)} - 2\sqrt{\log 2} > 0,$$

leading to contradiction.

Claim 2: $\Delta \leq 4$. Suppose there is a vertex w with $deg(w) = 5$. Let v_1, v_2 be two vertices adjacent to w and u a pendant vertex in the connected component of $T \setminus \big(\{wv_1\} \cup \{wv_2\}\big)$ containing w, and let

$$T' = T \setminus \big(\{wv_1\} \cup \{wv_2\}\big) \cup \big(\{uv_1\} \cup \{uv_2\}\big).$$

Thus, in T', $deg_{T'}(w) = 3$, $deg_{T'}(u) = 3$ and

$$SL(T) - SL(T') = 5\sqrt{\log 5} - 6\sqrt{\log 3} > 0,$$

and we obtain a contradiction.

Claim 3: No vertex has degree 2. Suppose there is a vertex w with degree 2. Since $\sum_{u \in V(G),\, d_u > 1} (d_u - 1) = n - 2 \geq 4$, there exists a vertex v in T distinct from w with $deg(v) > 1$, and so, $2 \leq deg(v) \leq 4$.

- If $deg(v) = 2$, let u be the vertex adjacent to w such that w, v are in the same connected component of $T \setminus \{u\}$, and let
$$T' = \big(T \setminus \{wu\}\big) \cup \{uv\}.$$
Thus, in T', $deg_{T'}(w) = 1$, $deg_{T'}(v) = 3$ and
$$SL(T) - SL(T') = 4\sqrt{\log 2} - 3\sqrt{\log 3} > 0,$$
leading to contradiction.

- If $deg(v) = 3$, let u be the vertex adjacent to w such that w, v are in the same connected component of $T \setminus \{u\}$, and let
$$T' = \big(T \setminus \{wu\}\big) \cup \{uv\}.$$
Thus, in T', $deg_{T'}(w) = 1$, $deg_{T'}(v) = 4$ and
$$SL(T) - SL(T') = 2\sqrt{\log 2} + 3\sqrt{\log 3} - 4\sqrt{\log 4} > 0,$$
and we obtain a contradiction.

- If $deg(v) = 4$, let u be a vertex adjacent to v such that w, v are in the same connected component of $T \setminus \{u\}$ and let
$$T' = \big(T \setminus \{vu\}\big) \cup \{uw\}.$$
Thus, in T', $deg_{T'}(w) = 3$, $deg_{T'}(v) = 3$ and
$$SL(T) - SL(T') = 2\sqrt{\log 2} + 4\sqrt{\log 4} - 6\sqrt{\log 3} > 0,$$
leading to contradiction.

Claim 4: there are at most two vertices with degree 3. Suppose there exist three vertices v_1, v_2, v_3 with $deg(v_i) = 3$ for $1 \le i \le 3$. Hence, there is a vertex, let us assume it is v_1, with two adjacent vertices, u_1, u_2, for which v_1, v_2, v_3 are in the same connected component of $T \setminus \{u_j\}$ for $j = 1, 2$. Let
$$T' = T \setminus \big(\{v_1u_1\} \cup \{v_1u_2\}\big) \cup \big(\{v_2u_1\} \cup \{v_3u_2\}\big).$$
Thus, in T', $deg_{T'}(v_1) = 1$, $deg_{T'}(v_2) = 4$, $deg_{T'}(v_3) = 4$ and
$$SL(T) - SL(T') = 9\sqrt{\log 3} - 8\sqrt{\log 4} > 0,$$

and we obtain a contradiction.

Thus, from the claims above, for every vertex v with $d_v > 1$, we have either $d_v = 3$ or $d_v = 4$ with, at most, two vertices with degree 3. Since $\sum_{u\in V(G),\, d_u>1}(d_u - 1) = n - 2$, it follows that the degree sequence of T is necessarily $\mathbf{z}$. ■

Let $4 < \Delta < n - 2$. If $r = \lceil \frac{n-\Delta-1}{3} \rceil$ and $s = 3r - n + \Delta + 1$, let us define $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ as

- $a_1 = \Delta$,
- $a_j = 4$ for every $2 \le j \le r - s + 1$,
- $a_j = 3$ for every $r - s + 1 < j \le r + 1$,
- $a_j = 1$ for every $r + 1 < j \le n$.

Note that $0 \le s \le r \le n - 6$.

Theorem 3.9. *Let G be a graph with n vertices, maximum degree Δ and $4 < \Delta < n-2$. If $r = \lceil \frac{n-\Delta-1}{3} \rceil$ and $s = 3r - n + \Delta + 1$, then*

$$SL(G) \ge \Delta\sqrt{\log \Delta} + 4(r - s)\sqrt{\log 4} + 3s\sqrt{\log 3}\,,$$

and the equality is attained if and only if G is a tree and its degree sequence is $\mathbf{a}$.

Proof. First, let us see that if G is a minimal for SL in the class of graphs with maximum degree Δ, then G is a tree. Suppose $w \in G$ with $deg(w) = \Delta$. Then, if G is not a tree, there is an edge $uv \in E(G)$ (with $u \neq w \neq v$) such that $G' = G \setminus uv$ is connected. Hence, $SL(G') < SL(G)$ and $deg_{G'}(v) \le deg_{G'}(w) = \Delta$ for every $v \neq w$ leading to contradiction.

Now, the same claims from the proof of Theorem 3.8 imply that for every vertex $v \neq w$, $3 \le deg(v) \le 4$ and there are at most two vertices with degree 3. Therefore, the degree sequence of G is necessarily $\mathbf{a}$. ■

Remark 3.10. *Let G be a graph with n vertices and maximum degree $3 \le \Delta \le n - 2$.*

- *If $\Delta = n - 2$, then*

  $$SL(G) \ge \Delta\sqrt{\log \Delta} + 2\sqrt{\log 2}\,,$$

  and the equality is attained if and only if G is a tree and its degree sequence is $(\Delta, 2, 1, \ldots, 1)$.

- *If* $4 = \Delta < n-2$ *then, by Theorem 3.8,*

$$SL(G) \geq 4(r-s)\sqrt{\log 4} + 3s\sqrt{\log 3}\,,$$

and the equality is attained if and only if G *is a tree and its degree sequence is* $\mathbf{z}$.

- *If* $3 = \Delta < n-2$*, with the same argument from Claim 3 in the proof of Theorem 3.8, we conclude that there is at most one vertex with degree* 2*. Thus, let* $r = \left\lfloor \frac{n-2}{2} \right\rfloor$ *and* $s = n-2-2r$*, (note that* $0 \leq s \leq 1 < r \leq n-4$*) and let us define* $\mathbf{b} = (b_1, b_2, \dots, b_n)$ *as*

  - $b_j = 3$ *for every* $1 \leq j \leq r$,
  - $b_j = 2$ *for every* $r < j \leq r+s$,
  - $b_j = 1$ *for every* $r+s < j \leq n$.

Then,

$$SL(G) \geq 3r\sqrt{\log 3} + 2s\sqrt{\log 2}\,,$$

and the equality is attained if and only if G *is a tree and its degree sequence is* $\mathbf{b}$.

Acknowledgements: We would like to thank the referees for their careful reading of the manuscript and for helpful suggestions which have helped us to improve the presentation of the paper.

The firs author was partially supported by a grant from Ministerio de Ciencia, Innovación y Universidades (PGC2018-098321-B-I00), Spain; the second author was partially supported by two grants from Ministerio de Economía y Competitividad, Agencia Estatal de Investigación (AEI) and Fondo Europeo de Desarrollo Regional (FEDER) (MTM2016-78227-C2-1-P and MTM2017-90584-REDT), Spain.

References

[1] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.

[2] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalizations: Extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.

[3] V. Andova, M. Petruševski, Variable Zagreb indices and Karamata's inequality, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 685–690.

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

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

[6] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.

[7] R. Cruz, H. Giraldo, J. Rada, Extremal values of vertex–degree topological indices over hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 501–512.

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

[9] D. Dimitrov, A. Ali, On the extremal graphs with respect to the variable sum exdeg index, *Discr. Math. Lett.* **1** (2019) 42–48.

[10] Z. Du, B. Zhou, N. Trinajstić, Minimum general sum–connectivity index of unicyclic graphs, *J. Math. Chem.* **48** (2010) 697–703.

[11] Z. Du, B. Zhou, N. Trinajstić, Minimum sum–connectivity indices of trees and unicyclic graphs of a given matching number, *J. Math. Chem.* **47** (2010) 842–855.

[12] C. S. Edwards, The largest vertex degree sum for a triangle in a graph, *Bull. London Math. Soc.* **9** (1977) 203–208.

[13] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[14] S. Fajtlowicz, On conjectures of Graffiti–II, *Congr. Numer.* **60** (1987) 187–197.

[15] A. Ghalavand, A. R. Ashrafi, Extremal graphs with respect to variable sum exdeg index via majorization, *Appl. Math. Comput.* **303** (2017) 19–23.

[16] M. Ghorbani, M. Songhori, I. Gutman, Modified Narumi–Katayama index, *Kragujevac J. Sci.* **34** (2012) 57–64.

[17] I. Gutman, B. Furtula, Vertex–degree–based molecular structure descriptors of benzenoid systems and phenylenes, *J. Serb. Chem. Soc.* **77** (2012) 1031–1036.

[18] I. Gutman, B. Furtula, M. Ivanović, Notes on trees with minimal atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 467–482.

[19] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graphs Comb.* (2018) doi:10.1016/j.akcej.2018.05.002, in press.

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

[21] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex–degree–based topological indices, *J. Serb. Chem. Soc.* **78(6)** (2013) 805–810.

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

[23] A. Iranmanesh, M. A. Hosseinzadeh, I. Gutman, On multiplicative Zagreb indices of graphs, *Iranian J. Math. Chem.* **3(2)** (2012) 145–154.

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

[25] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac J. Math.* **35(1)** (2011) 173–182.

[26] S. Khalid, A. Ali, On the zeroth-order general Randić index, variable sum exdeg index and trees having vertices with prescribed degree, *Discrete Math. Algorithm. Appl.* **10** (2018) #1850015.

[27] X. Li and H. Zhao, Trees with the first three smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.

[28] M. Liu and B. Liu, Some properties of the first general Zagreb index, *Australas. J. Combin.* **47** (2010) 285–294.

[29] A. Miličević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (2004) 97–101.

[30] H. Narumi, M. Katayama, Simple topological index. A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Mem. Fac. Engin. Hokkaido Univ.* **16** (1984) 209–214.

[31] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.

[32] S. Nikolić, A. Miličević, N. Trinajstić, A. Jurić, On use of the variable Zagreb ${}^{\nu}M_2$ index in QSPR: boiling points of benzenoid hydrocarbons, *Molecules* **9** (2004) 1208–1221.

[33] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[34] M. Randić, Novel graph theoretical approach to heteroatoms in QSAR, *Chemometrics Intel. Lab. Syst.* **10** (1991) 213–227.

[35] M. Randić, On computation of optimal parameters for multivariate analysis of structure-property relationship, *J. Chem. Inf. Comput. Sci.* **31** (1991) 970–980.

[36] M. Randić, D. Plavšić, N. Lerš, Variable connectivity index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **41** (2001) 657–662.

[37] M. Singh, K. Ch. Das, S. Gupta, A. K. Madan, Refined variable Zagreb indices: highly discriminating topological descriptors for QSAR/QSPR, *Int. J. Chem. Model.* **6** (2014) 403–428.

[38] S. S. Tratch, M. I. Stankevich, N. S. Zefirov, Combinatorial models and algorithms in chemistry. The expanded Wiener numbers – A novel topological index, *J. Comput. Chem.* **11** (1990) 899–908.

[39] A. Vasilyev, D. Stevanović, MathChem: a Python package for calculating topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 657–680.

[40] M. Vöge, A. J. Guttmann, I. Jensen, On the number of benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **42** (2002) 456–466.

[41] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (2010) 243–260.

[42] D. Vukičević, Bond additive modeling 2. Mathematical properties of max-min rodeg index, *Croat. Chem. Acta* **83** (2010) 261–273.

[43] S. Wang, S. Ji, T. Muche, S. Hayat, Extremal structures of graphs with given connectivity or number of pendant vertices, *arXiv*:1711.09014v1

[44] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[45] S. Zhang, W. Wang, T. C. E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 579–592.

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