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New bounds for variable topological indices and applications

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Abstract

One of the most important information related to molecular graphs is given by the determination (when possible) of upper and lower bounds for their corresponding topological indices. Such bounds allow to establish the approximate range of the topological indices in terms of molecular structural parameters. The purpose of this paper is to provide new inequalities relating several classes of variable topological indices including the first and second general Zagreb indices, the general sum-connectivity index, and the variable inverse sum deg index. Also, upper and lower bounds on the inverse degree in terms of the first general Zagreb are found. Moreover, the characterization of extremal graphs with respect to many of these inequalities is obtained. Finally, some applications are given.

Keywords General Zagreb indices · General sum-connectivity index · Variable inverse sum deg index · Inverse degree index · Converse Hölder inequality

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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. Those topological descriptors which correlate with some molecular property are called topological indices. It is a well known fact that the main application of topological indices focuses on the understanding of physicochemical properties of chemical compounds. Hundreds of topological indices have been introduced and its mathematical properties and chemical applications have been intensively studied, starting with the seminal work by H. Wiener [1], and more recently, we can mention the work [2] which includes some chemical applications in a similar way to the present work.

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 $5, 851, 000, 265, 625, 801, 806, 530$ (*cf.*, [3]). Therefore, modeling their physicochemical properties is crucial for predicting properties of currently unknown species. The main reason for using topological indices is to predict properties of molecular graphs. Therefore, given certain fixed parameters, a natural problem is to find, when possible, upper and lower bounds for such topological indices (see, e.g., [2] and the references therein).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Probably, among such descriptors, the best known is the Randić connectivity index (R) [4]. There are more than one thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [5–9] and the references therein). For many years, scientists have been trying to improve the predictive power of the Randić index. These efforts led to the introduction of a large number of new topological descriptors resembling the original Randić index. Two of the main successors of the latter are the first and second Zagreb indices, denoted by M_1 and M_2, respectively, and defined as

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

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. These indices have attracted increasing interest, see e.g., [10–13]. In particular, they are included in a number of programs used for the routine computation of topological indices.

The *inverse degree index* $ID(G)$ of a graph G is defined by

$$ID(G) = \sum_{u \in V(G)} \frac{1}{d_u} = \sum_{uv \in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2} \right) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2}.$$

The inverse degree index first attracted attention through numerous conjectures generated by the computer programme Graffiti [14]. Since then, its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, and Wiener index have been studied by several authors (see, e.g., [15–19]).

Miličević and Nikolić defined in [20] the *first and second variable Zagreb indices* as

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

with $\alpha \in \mathbb{R}$. In [21] and [22] the *first and second general Zagreb indices* are introduced as

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

respectively. It is clear that these indices are equivalent to the previous ones, since $^{\alpha}M_1(G) = M_1^{2\alpha}(G)$ and $^{\alpha}M_2(G) = M_2^{\alpha}(G)$. Furthermore, the first general Zagreb, $M_1^{\alpha}(G)$ also has the following representation

$$M_1^{\alpha}(G) = \sum_{uv \in E(G)} \left(d_u^{\alpha-1} + d_v^{\alpha-1} \right). \tag{1}$$

In what follows, $M_j^{\alpha}(G)$ will be used instead of $^{\alpha}M_j(G)$, for $j = 1, 2$, since the inequalities obtained in this paper become simpler with them.

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

The concept of the variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [23, 24]), but also to assess structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [25]). The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of an estimate for a studied property to be as small as possible.

In the paper of I. Gutman and J. Tosovic [26], 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 that the second general 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 second variable Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons [27]. Various properties and relations of these indices are discussed in several papers (see, e.g., [28–33]). The interested reader can find recent and interesting results involving several topological indices and their applications in [34–36].

The aim of this work is to provide new inequalities relating several classes of variable topological indices including the first and second general Zagreb indices, the general sum-connectivity index and the variable inverse sum deg index. Also, upper and lower bounds on the inverse degree in terms of the first general Zagreb are shown. Moreover, the characterization of extremal graphs with respect to many of such inequalities is obtained. Finally, some applications are given to the study of the physico-chemical properties of the octane isomers, in particular to the study of Entropy, Motor octane number, Standard enthalpy of vaporization and Acentric factor.

Throughout this paper, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) non-trivial (each vertex belongs to some edge) graph. Also, m and n will denote, respectively, the cardinality of the sets $E(G)$ and $V(G)$.

2 Main inequalities

The sum-connectivity index was proposed in [37]. It has been shown that this index correlates well with the π-electronic energy of benzenoid hydrocarbons [38]. More applications of the sum-connectivity index can be found in [39]. Recently, this concept was extended to the *general sum-connectivity index* in [40], which is defined by

$$\chi_a(G) = \sum_{uv \in E(G)} (d_u + d_v)^a .$$

Note that $\chi_{-1/2}$ is the sum-connectivity index, χ_1 is the first Zagreb index and χ_{-1} is half the harmonic index.

Let us start with the following elementary fact (see, for instance [41]).

Lemma 1 *If $f \in C^1[a, b]$ and $f' = g_1 g_2$ with $g_1, g_2 \in C[a, b]$, g_1 positive and g_2 non-increasing (resp. non-decreasing) on $[a, b]$, then f attains its minimum (resp. maximum) value on $[a, b]$ on the set $\{a, b\}$.*

The following result relates the general sum-connectivity and the first general Zagreb indices.

Theorem 2 *Let G be a graph with maximum degree Δ and minimum degree δ, and $a, b \in \mathbb{R}$.*

If $b \geq a$ and $b \geq 1$, then

$$2^{1-a} \delta^{b-a} \chi_a(G) \leq M_1^{b+1}(G) \leq \max \left\{ (\Delta + \delta)^{-a} \left(\Delta^b + \delta^b \right), 2^{1-a} \Delta^{b-a} \right\} \chi_a(G).$$

If $b \leq a$ and $b \leq 0$, then

$$2^{1-a} \Delta^{b-a} \chi_a(G) \leq M_1^{b+1}(G) \leq \max \left\{ 2^{1-a} \delta^{b-a}, (\Delta + \delta)^{-a} \left(\Delta^b + \delta^b \right) \right\} \chi_a(G).$$

Proof For each $\delta \le x, y \le \Delta$, define the function

$$\Gamma(x, y) = \frac{x^b + y^b}{(x+y)^a} = (x+y)^{-a}\left(x^b + y^b\right).$$

A computation gives

$$\begin{aligned}\frac{\partial \Gamma}{\partial x}(x, y) &= (x+y)^{-a-1}\left(-ax^b - ay^b + b(x+y)x^{b-1}\right)\\ &= (x+y)^{-a-1}\left(-ax^b + bx^b - ay^b + byx^{b-1}\right).\end{aligned} \tag{2}$$

Assume that $b \ge a$ and $b \ge 1$. By symmetry, we also can assume that $x \ge y$, then

$$\begin{aligned}\frac{\partial \Gamma}{\partial x}(x, y) &= (x+y)^{-a-1}\left(-ax^b + bx^b - ay^b + byx^{b-1}\right)\\ &\ge a(x+y)^{-a-1}\left(-x^b + x^b - y^b + yx^{b-1}\right)\\ &= a(x+y)^{-a-1}y\left(x^{b-1} - y^{b-1}\right) \ge 0.\end{aligned}$$

Hence, $\Gamma(y, y) \le \Gamma(x, y) \le \Gamma(\Delta, y)$.

Set

$$\Theta(y) = \Gamma(y, y) = (y+y)^{-a}\left(y^b + y^b\right) = 2^{1-a}y^{b-a}.$$

Since $b \ge a$, Θ is a non-decreasing function and

$$\Gamma(x, y) \ge \Gamma(y, y) = \Theta(y) \ge \Theta(\delta) = 2^{1-a}\delta^{b-a},$$

we get

$$d_u^b + d_v^b \ge 2^{1-a}\delta^{b-a}(d_u + d_v)^a,$$

for every $uv \in E(G)$. Hence, using the representation (1) for $M_1^{b+1}(G)$, we obtain

$$M_1^{b+1}(G) \ge 2^{1-a}\delta^{b-a}\,\chi_a(G).$$

Now, let

$$\Lambda(y) = \Gamma(\Delta, y) = (\Delta + y)^{-a}\left(\Delta^b + y^b\right)$$

on $[\delta, \Delta]$.

We have

$$\Lambda'(y) = (\Delta + y)^{-a-1}\left(-a\Delta^b + (b-a)y^b + \Delta b y^{b-1}\right).$$

Let us consider the function

$$\Psi(y) = -a\Delta^b + (b-a)y^b + \Delta b y^{b-1}$$

on $[\delta, \Delta]$. Since $b \ge a$ and $b \ge 1$, we have

$$\Psi'(y) = b(b-a)y^{b-1} + \Delta b(b-1)y^{b-2} \ge 0.$$

Consequently, Ψ is a non-decreasing function. Since $\Lambda'(y) = (\Delta + y)^{-a-1}\,\Psi(y)$, Lemma 1 gives

$$\begin{aligned}\Gamma(x, y) \le \Lambda(y) \le \max\{\Lambda(\delta),\ \Lambda(\Delta)\} &= \max\{\Gamma(\Delta, \delta),\ \Gamma(\Delta, \Delta)\}\\ &= \max\left\{(\Delta+\delta)^{-a}\left(\Delta^b + \delta^b\right),\ 2^{1-a}\Delta^{b-a}\right\}\end{aligned}$$

for every $y \in [\delta, \Delta]$.

Therefore,

$$\frac{x^b + y^b}{(x+y)^a} = \Gamma(x, y) \le \max\left\{(\Delta+\delta)^{-a}\left(\Delta^b + \delta^b\right),\ 2^{1-a}\Delta^{b-a}\right\},$$

and this last inequality implies that

$$d_u^b + d_v^b \le \max\left\{(\Delta+\delta)^{-a}\left(\Delta^b + \delta^b\right),\ 2^{1-a}\Delta^{b-a}\right\}(d_u + d_v)^a,$$

for every $uv \in E(G)$. Hence, it follows from (1) that

$$M_1^{b+1}(G) \le \max\left\{(\Delta+\delta)^{-a}\left(\Delta^b + \delta^b\right),\ 2^{1-a}\Delta^{b-a}\right\}\ \chi_a(G).$$

Now, assume that $b \le a$ and $b \le 0$. By symmetry, we can assume also that $x \le y$, then

$$\begin{aligned}\frac{\partial\Gamma}{\partial x}(x, y) &= (x+y)^{-a-1}\left(-ax^b + bx^b - ay^b + byx^{b-1}\right)\\ &\le a(x+y)^{-a-1}\left(-x^b + x^b - y^b + yx^{b-1}\right)\\ &= a(x+y)^{-a-1}y\left(x^{b-1} - y^{b-1}\right) \le 0.\end{aligned}$$

Hence, $\Gamma(y, y) \le \Gamma(x, y) \le \Gamma(\delta, y)$.

Consider the function

$$\Theta(y) = \Gamma(y, y) = (y+y)^{-a}\left(y^b + y^b\right) = 2^{1-a}y^{b-a}.$$

Since $b \le a$, Θ is a non-increasing function and

$$\Gamma(x, y) \ge \Gamma(y, y) = \Theta(y) \ge \Theta(\Delta) = 2^{1-a}\Delta^{b-a},$$

we get

$$d_u^b + d_v^b \geq 2^{1-a} \Delta^{b-a} (d_u + d_v)^a,$$

for every $uv \in E(G)$. Hence, using the representation (1) for $M_1^{b+1}(G)$, we obtain

$$M_1^{b+1}(G) \geq 2^{1-a} \Delta^{b-a} \chi_a(G).$$

Now, consider the function

$$\Lambda_1(y) = \Gamma(\delta, y) = (\delta + y)^{-a} \left(\delta^b + y^b\right)$$

on $[\delta, \Delta]$.

We have

$$\Lambda_1'(y) = (\delta + y)^{-a-1} \left(-a\delta^b + (b-a)y^b + \delta b y^{b-1}\right).$$

Let us consider the function

$$\Psi_1(y) = -a\delta^b + (b-a)y^b + \delta b y^{b-1}$$

on $[\delta, \Delta]$. Since $b \leq a$ and $b \leq 0$, we have

$$\Psi_1'(y) = b(b-a)y^{b-1} + \delta b(b-1)y^{b-2} \geq 0.$$

Consequently, Ψ_1 is a non-decreasing function. Since $\Lambda_1'(y) = (\delta + y)^{-a-1}\, \Psi_1(y)$, Lemma 1 gives

$$\begin{aligned}\Gamma(x, y) \leq \Lambda_1(y) &\leq \max\{\Lambda_1(\delta),\ \Lambda_1(\Delta)\} = \max\{\Gamma(\delta, \delta),\ \Gamma(\delta, \Delta)\} \\ &= \max\left\{2^{1-a}\delta^{b-a},\ (\Delta + \delta)^{-a}\left(\Delta^b + \delta^b\right)\right\}\end{aligned}$$

for every $y \in [\delta, \Delta]$.

Consequently,

$$\frac{x^b + y^b}{(x+y)^a} = \Gamma(x, y) \leq \max\left\{2^{1-a}\delta^{b-a},\ (\Delta + \delta)^{-a}\left(\Delta^b + \delta^b\right)\right\},$$

and this last inequality implies that

$$d_u^b + d_v^b \leq \max\left\{2^{1-a}\delta^{b-a},\ (\Delta + \delta)^{-a}\left(\Delta^b + \delta^b\right)\right\}(d_u + d_v)^a,$$

for every $uv \in E(G)$. Hence, it follows from (1) that

$$M_1^{b+1}(G) \leq \max\left\{2^{1-a}\delta^{b-a},\ (\Delta + \delta)^{-a}\left(\Delta^b + \delta^b\right)\right\} \chi_a(G).$$

This completes the proof of the theorem. □

The following proposition relates the first Zagreb and the inverse degree indices.

Proposition 3 *If G is a graph with m edges, then*

$$2\,ID(G) + M_2(G) \geq 4m.$$

Proof Since $x + 1/x \geq 2$ for every $x > 0$ and $2xy \leq x^2 + y^2$ for every $x, y \in \mathbb{R}$, we have

$$\begin{aligned}
\frac{d_u^2 + d_v^2}{d_u^2 d_v^2} + \frac{d_u^2 d_v^2}{d_u^2 + d_v^2} &\geq 2,\\
\sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2} + \sum_{uv \in E(G)} \frac{d_u^2 d_v^2}{d_u^2 + d_v^2} &\geq \sum_{uv \in E(G)} 2,\\
ID(G) + \sum_{uv \in E(G)} \frac{d_u^2 d_v^2}{2 d_u d_v} &\geq 2m,\\
2ID(G) + M_2(G) &\geq 4m.
\end{aligned}$$

□

We need the following converse Hölder inequality in [42, Theorem 3], which is interesting on its own. This result improves the inequality in [43, Theorem 2].

Theorem 4 *Let (X, μ) be a measure space, $f, g : X \to \mathbb{R}$ measurable functions, and $1 < p, q < \infty$ with $1/p + 1/q = 1$. If there exist positive constants a, b with $a|g|^q \leq |f|^p \leq b|g|^q$ μ-a.e., then:*

$$\|f\|_p \|g\|_q \leq K_p(a, b) \|fg\|_1, \tag{3}$$

with:

$$K_p(a,b) = \begin{cases} \dfrac{1}{p}\left(\dfrac{a}{b}\right)^{1/(2q)} + \dfrac{1}{q}\left(\dfrac{b}{a}\right)^{1/(2p)}, & \text{if } 1 < p < 2,\\[2ex] \dfrac{1}{p}\left(\dfrac{b}{a}\right)^{1/(2q)} + \dfrac{1}{q}\left(\dfrac{a}{b}\right)^{1/(2p)}, & \text{if } p \geq 2. \end{cases}$$

If these norms are finite, the equality in the bound is attained if and only if $a = b$ and $|f|^p = a|g|^q$ μ-a.e. or $f = g = 0$ μ-a.e.

Theorem 4 has the following consequence.

Corollary 5 *If* $1 < p, q < \infty$ *with* $1/p + 1/q = 1$, $x_j, y_j \geq 0$ *and* $ay_j^q \leq x_j^p \leq by_j^q$ *for* $1 \leq j \leq k$ *and some positive constants* a, b, *then:*

$$\left(\sum_{j=1}^{k} x_j^p\right)^{1/p} \left(\sum_{j=1}^{k} y_j^q\right)^{1/q} \leq K_p(a,b) \sum_{j=1}^{k} x_j y_j,$$

where $K_p(a,b)$ *is the constant in Theorem 4. If* $x_j > 0$ *for some* $1 \leq j \leq k$, *then the equality in the bound is attained if and only if* $a = b$ *and* $x_j^p = ay_j^q$ *for every* $1 \leq j \leq k$.

The next result relates several first general Zagreb indices. It generalizes [43, Theorem 2.12].

Theorem 6 *Let* G *be a nontrivial graph with* n *vertices, maximum degree* Δ *and minimum degree* δ, *and* $\alpha, p, q \in \mathbb{R}$ *with* $1/p + 1/q = 1$. *Then*

$$C_p(\delta,\Delta)\, n^{1/q} \left(M_1^{\alpha p}(G)\right)^{1/p} \leq M_1^{\alpha}(G) \leq n^{1/q} \left(M_1^{\alpha p}(G)\right)^{1/p}.$$

with:

$$C_p(\delta,\Delta) = \begin{cases} \dfrac{\left(\delta \Delta^{p/q}\right)^{\alpha/2}}{\frac{1}{p}\left(\delta^{\alpha}\right)^{p/2} + \frac{1}{q}\left(\Delta^{\alpha}\right)^{p/2}}, & \text{if } 1 < p < 2, \\[2ex] \dfrac{\left(\Delta \delta^{p/q}\right)^{\alpha/2}}{\frac{1}{p}\left(\Delta^{\alpha}\right)^{p/2} + \frac{1}{q}\left(\delta^{\alpha}\right)^{p/2}}, & \text{if } p \geq 2. \end{cases}$$

The lower bound is attained for every value of α *if* G *is regular. The upper bound is attained for some* $\alpha \neq 0$ *if and only if* G *is regular.*

Proof Applying Hölder inequality

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha} \leq \left(\sum_{u \in V(G)} d_u^{\alpha p}\right)^{1/p} \left(\sum_{u \in V(G)} 1\right)^{1/q} = n^{1/q} \left(M_1^{\alpha p}(G)\right)^{1/p}.$$

Note that

$$\begin{aligned} \delta^{\alpha} \leq d_u^{\alpha} \leq \Delta^{\alpha} \qquad & \text{if } \alpha \geq 0, \\ \Delta^{\alpha} \leq d_u^{\alpha} \leq \delta^{\alpha} \qquad & \text{if } \alpha \leq 0, \end{aligned}$$

In order to prove the other inequality we are going to use Corollary 5 with $a = \delta^{\alpha p}$ and $b = \Delta^{\alpha p}$.

$$M_1^\alpha(G) = \sum_{u\in V(G)} d_u^\alpha \geq \frac{\left(\sum_{u\in V(G)} d_u^{\alpha p}\right)^{1/p} \left(\sum_{u\in V(G)} 1\right)^{1/q}}{K_p(\delta^{\alpha p}, \Delta^{\alpha p})}$$
$$= C_p(\delta, \Delta)\, n^{1/q} \left(M_1^{\alpha p}(G)\right)^{1/p}.$$

For $\alpha \neq 0$, by Hölder inequality the upper bound is sharp if and only if the graph is regular. In this case $M_1^\alpha(G) = n\delta^\alpha = n\Delta^\alpha$ and both bounds coincide. □

The following result relates the inverse degree and the first general Zagreb indices.

Theorem 7 *If $\alpha \in \mathbb{R}$ and G is a non-trivial graph with n vertices, m edges, minimum degree δ and maximum degree Δ, then the following inequalities hold:*
(1) *if $\alpha < -1$, then*

$$ID(G)^{-\alpha} n^{-(\alpha+1)} \leq M_1^\alpha(G) \leq K_{-\alpha}^{-\alpha}\left(\Delta^\alpha, \delta^\alpha\right) ID(G)^{-\alpha} n^{-(\alpha+1)};$$

(2) *if $-1 < \alpha < 0$, then*

$$K_{-\frac{1}{\alpha}}^{-1}\left(\Delta^{-1}, \delta^{-1}\right) ID(G)^{-\alpha} n^{1+\alpha} \leq M_1^\alpha(G) \leq ID(G)^{-\alpha} n^{1+\alpha};$$

(3) *if $0 < \alpha < 1$, then*

$$K_{\frac{1}{\alpha}}^{-1}(\delta, \Delta)(2m)^\alpha n^{1-\alpha} \leq M_1^\alpha(G) \leq (2m)^\alpha n^{1-\alpha};$$

(4) *if $\alpha > 1$, then*

$$(2m)^\alpha n^{1-\alpha} \leq M_1^\alpha(G) \leq K_\alpha^\alpha(\delta^\alpha, \Delta^\alpha)(2m)^\alpha n^{1-\alpha},$$

where $K_p(a, b)$ is the constant in Theorem 4. Moreover, the equalities are attained if and only if G is regular. Also, for the three special cases, one gets

$$M_1^{-1}(G) = ID(G), \qquad M_1^0(G) = n, \qquad M_1^1(G) = 2m.$$

Proof For any graph G, the last three special cases are obtained straightforwardly by applying the definition of the first general Zagreb index. So, if $\alpha = -1$ one gets $M_1^{-1}(G) = ID(G)$; if $\alpha = 0$, then $M_1^0(G) = \sum_{u\in V(G)} d_u^0 = n$; and finally, if $\alpha = 1$, then $M_1^1(G) = \sum_{uv\in E(G)} \left(d_u^0 + d_v^0\right) = 2\,m$.

Now, for the case $\alpha > 1$, take $p = \alpha$ and $q = \alpha/(\alpha - 1)$. Then, Hölder's inequality gives

$$2m = M_1^1(G) = \sum_{u \in V(G)} d_u \leq \left(\sum_{u \in V(G)} d_u^\alpha \right)^{\frac{1}{\alpha}} \left(\sum_{u \in V(G)} 1^{\frac{\alpha}{\alpha-1}} \right)^{\frac{\alpha-1}{\alpha}} = M_1^\alpha(G)^{\frac{1}{\alpha}} n^{\frac{\alpha-1}{\alpha}}. \tag{4}$$

Next, the lower bound can be obtained applying Corollary 5 with $a = \delta^\alpha$ and $b = \Delta^\alpha$

$$2m = M_1^1(G) = \sum_{u \in V(G)} d_u \geq K_\alpha^{-1}(\delta^\alpha, \Delta^\alpha) \left(\sum_{u \in V(G)} d_u^\alpha \right)^{\frac{1}{\alpha}} \left(\sum_{u \in V(G)} 1^{\frac{\alpha}{\alpha-1}} \right)^{\frac{\alpha-1}{\alpha}} = K_\alpha^{-1}(\delta^\alpha, \Delta^\alpha) M_1^\alpha(G)^{\frac{1}{\alpha}} n^{\frac{\alpha-1}{\alpha}}. \tag{5}$$

Thus, Eqs. (4) and (5) give

$$(2m)^\alpha n^{1-\alpha} \leq M_1^\alpha(G) \leq K_\alpha^\alpha(\delta^\alpha, \Delta^\alpha)(2m)^\alpha n^{1-\alpha}.$$

The proofs of the remaining cases are similar choosing the appropriate values for the constants. Namely,

- if $\alpha < -1$, take $p = -\alpha$, $q = \alpha/(1 + \alpha)$, $a = \Delta^\alpha$ and $b = \delta^\alpha$;
- if $-1 < \alpha < 0$, take $p = -1/\alpha$, $q = 1/(1 + \alpha)$, $a = \Delta^{-1}$ and $b = \delta^{-1}$;
- if $0 < \alpha < 1$, take $p = 1/\alpha$, $q = 1/(1 - \alpha)$, $a = \delta$ and $b = \Delta$.

Note that for $\alpha \neq -1, 0, 1$, the tools used (Hölder inequality and Corollary 5) give that all inequalities are sharp if and only if the graph G is regular. □

The σ-*index* is defined in [44] as

$$\sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2.$$

Note that $\sigma(G) = F(G) - 2M_2(G)$.

Theorem 8 *Let G be a nontrivial graph with n vertices, maximum degree Δ and minimum degree δ. Then*

$$2M_2^{-1}(G) + \frac{\sigma(G)}{\Delta^4} \leq ID(G) \leq 2M_2^{-1}(G) + \frac{\sigma(G)}{\delta^4}$$

and the lower (respectively, upper) bound is attained if and only if G is regular.

Proof Note that

$$d_u^2 + d_v^2 = (d_u - d_v)^2 + 2d_u d_v,$$
$$\frac{1}{d_u^2} + \frac{1}{d_v^2} = \frac{2}{d_u d_v} + \frac{(d_u - d_v)^2}{d_u^2 d_v^2}.$$

Since $\delta^4 \leq d_u^2 d_v^2 \leq \Delta^4$, we deduce

$$\frac{1}{d_u^2} + \frac{1}{d_v^2} \leq \frac{2}{d_u d_v} + \frac{(d_u - d_v)^2}{\delta^4},$$
$$\frac{1}{d_u^2} + \frac{1}{d_v^2} \geq \frac{2}{d_u d_v} + \frac{(d_u - d_v)^2}{\Delta^4},$$

and the desired inequalities hold.

If the graph is regular, then the lower and upper bounds are the same, and both are equal to $ID(G)$. If the lower (respectively, upper) bound is attained, then $d_u = d_v = \Delta$ (respectively, $d_u = d_v = \delta$) for every $uv \in E(G)$ and so, G is regular. □

The following result relates the inverse degree index with the first Zagreb and the second general Zagreb indices.

Theorem 9 *Let G be a nontrivial graph with n vertices, maximum degree Δ and minimum degree δ. Then*

$$ID(G) \leq M_2^{-1}(G) - \delta^2 M_2^{-2}(G) + \frac{\delta}{\Delta^4} M_1(G)$$

and the bound is attained if and only if G is regular.

Proof Since $(d_u - d_v)^2 + (d_u - \delta)^2 + (d_v - \delta)^2 \geq 0$, we have

$$d_u^2 + d_v^2 + \delta^2 \geq \delta(d_u + d_v) + d_u d_v,$$
$$\frac{1}{d_u^2} + \frac{1}{d_v^2} + \frac{\delta^2}{d_u^2 d_v^2} \geq \frac{1}{d_u d_v} + \delta \frac{d_u + d_v}{d_u^2 d_v^2}.$$

Since $d_u^2 d_v^2 \leq \Delta^4$, we deduce

$$\frac{1}{d_u^2} + \frac{1}{d_v^2} + \frac{\delta^2}{d_u^2 d_v^2} \geq \frac{1}{d_u d_v} + \delta \frac{d_u + d_v}{\Delta^4},$$

and the inequality holds.

The bound is attained if and only if $d_u = d_v = \delta$ and $d_u = d_v = \Delta$ for every $uv \in E(G)$, i.e., if G is regular. □

In [45, 46] several degree-based topological indices called *adriatic indices* are introduced. The *inverse sum indeg* index ISI, defined by

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u\, d_v}{d_u + d_v},$$

is one of them. This index is one of the most predictive adriatic indices, associated with the total surface area of the isomers of octanes.

Also, this index has become one of the most studied from the mathematical point of view. We present here several inequalities relating the first variable Zagreb index with the *variable inverse sum deg index* defined, for each $a \in \mathbb{R}$, as

$$ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a}.$$

Note that ISD_{-1} is the inverse sum indeg index ISI.

The variable inverse sum deg index $ISD_{-1.950}$ is a good predictor of standard enthalpy of formation [47].

Theorem 10 *If G is a graph with m edges, and $a \in \mathbb{R}$, then*

$$ISD_a(G) + M_1^{a+1}(G) \geq \frac{5}{2}m, \qquad \text{if } a > 0, \tag{6}$$

$$ISD_a(G) + M_1^{a+1}(G) \geq 2m, \qquad \text{if } a < 0. \tag{7}$$

The equality in the first bound is attained if and only if G is a union of path graphs P_2.

Proof Recall that, for any function h,

$$\sum_{uv \in E(G)} \big(h(d_u) + h(d_v)\big) = \sum_{u \in V(G)} d_u h(d_u).$$

In particular,

$$\sum_{uv \in E(G)} \big(d_u^a + d_v^a\big) = \sum_{u \in V(G)} d_u^{a+1} = M_1^{a+1}(G).$$

The function $f(x) = x + 1/x$ is strictly decreasing on $(0, 1]$ and strictly increasing on $[1, \infty)$, and so, $f(x) \geq f(1) = 2$ for every $x > 0$. Hence,

$$\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq 2,$$

$$ISD_a(G) + M_1^{a+1}(G) \geq 2m.$$

If $a > 0$, then $d_u^a + d_v^a \geq 2$ and

$$\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq f(2) = \frac{5}{2},$$
$$ISD_a(G) + M_1^{a+1}(G) \geq \frac{5}{2}m.$$

The previous argument gives that the equality is attained if and only if $d_u = d_v = 1$ for every $uv \in E(G)$, i.e., G is a union of path graphs P_2. □

Proposition 11 *Let G be a graph with minimum degree $\delta > 1$ and m edges. If $a \leq -\log 2/\log \delta$, then*

$$ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.$$

and the equality is attained if and only if G is regular.

Proof Since $\delta > 1$ and $a \leq -\log 2/\log \delta < 0$, then $2\delta^a \leq 1$ and $d_u^a + d_v^a \leq 2\delta^a \leq 1$. Thus,

$$\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq f(2\delta^a) = 2\delta^a + \frac{1}{2\delta^a},$$
$$ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.$$

The equality holds if and only if $d_u^a + d_v^a = 2\delta^a$ for every $uv \in E(G)$, i.e., $d_u = d_v = \delta$ for every $uv \in E(G)$. That is, if and only if G is regular. □

3 Some applications: QSPR/QSAR models

In this section, the predictive power of the first general Zagreb index M_1^a will be investigated. For this purpose, experimental data on some physico-chemical properties of octane isomers are used. Namely,

- Entropy (S).
- Motor octane number (MON).
- Standard enthalpy of vaporization (DHVAP).
- Acentric factor (AcenFac).

Such experimental data are obtained from https://webbook.nist.gov. Later, they are processed with a self-developed program to calculate the absolute value of the Pearson's correlation coefficient ($|r|$) for values of $a \in [-5, 5]$ with a spacing of 0.01. The Fig. 1 show a plot of the results obtained for S, MON, DHVAP and AcenFac properties. The dashed vertical lines indicate the value of a that maximize $|r|$.

In the Fig. 2 we test linear regression models of the form:

$$\mathcal{P} = c_1\, M_1^a(G) + c_2\,, \tag{8}$$

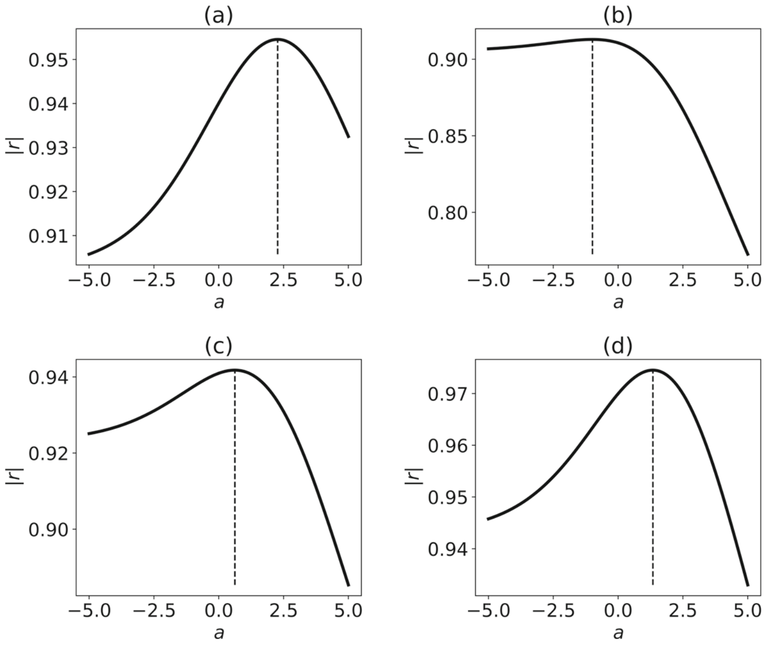

Fig. 1 Plots for S, MON, DHVAP and AcentFact

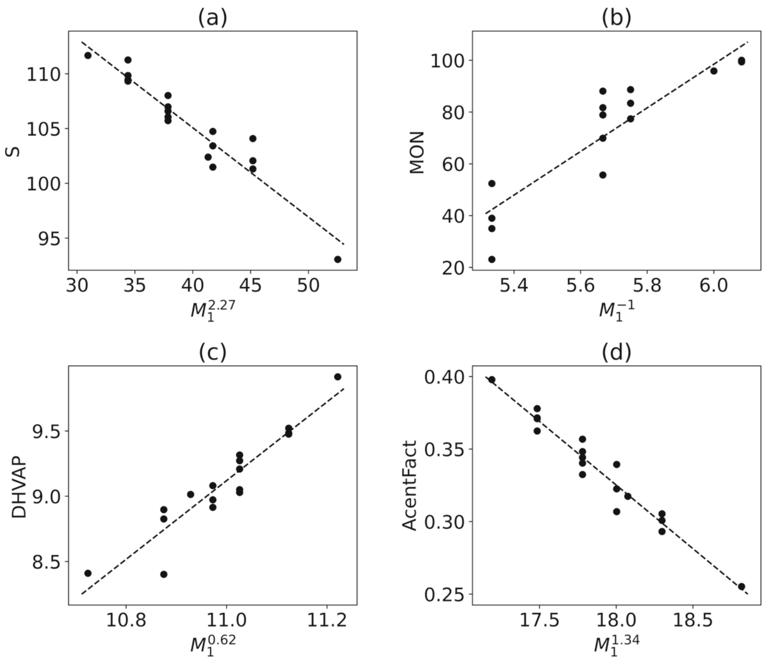

Fig. 2 Testing of linear regression models of the form (8)

Table 1 Regression and statistical parameters of linear QSPR models for S, MON, DHVAP and AcenFac

Property	a	r	c_1	c_2	SE	F	SF
S	2.27	−0.955	−0.815	137.675	1.309	164.1	7.94×10^{-10}
MON	−1	0.913	84.244	−406.982	9.791	70.07	8.05×10^{-7}
DHVAP	0.62	0.942	3.014	−24.037	0.125	125.5	5.52×10^{-9}
AcentFac	1.34	−0.975	−0.087	1.903	0.008	301.9	8.27×10^{-12}

where $\mathcal{P}$ is the S, MON, DHVAP or AcenFac property, and c_1, c_2 are constants. In the Table 1 we collect, respectively, the regression and statistical parameters of the linear QSPR models for the properties S, MON, DHVAP and AcenFac. See the dashed lines in the Fig. 1 given by Eq. (8).

$$
\begin{aligned}
S &= -0.815\, M_1^{2.270} + 137.675 \\
MON &= 84.244\, M_1^{-1} - 406.982 \\
DHVAP &= 3.014\, M_1^{0.62} - 24.037 \\
AcentFac &= -0.087\, M_1^{1.34} + 1.903
\end{aligned}
$$

A topological index is considered a good predictor for a property when the absolute value of the Pearson's correlation coefficient is greater than 0.9. From this analysis we can conclude that indices $M_1^{2.270}$, M_1^{-1}, $M_1^{0.62}$ and $M_1^{1.34}$ are good predictors, respectively, of the S, MON, DHVAP and AcenFac properties of the octane isomers. In particular, the index $M_1^{1.34}$ has $|r| = 0.975$.

4 Conclusion

The aim of our research was to determine novel inequalities relating several classes of variable topological indices, like the first and second general Zagreb indices, the general sum-connectivity index and the variable inverse sum deg index. It is worth noting that the results and methodology shown in this work allowed us to characterize extremal graphs with respect to many of such inequalities.

In addition, our analysis about the predictive power of the first general Zagreb index shows its applicability to the study of the physico-chemical properties of the octane isomers; in particular to the study of Entropy, Motor octane number, Standard enthalpy of vaporization and Acentric factor.

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Declarations

Conflict of interest The authors declare no competing interests..

Ethical approval Not applicable.

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