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Research article

On the Gutman-Milovanović index and chemical applications

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Abstract: The determination of upper and lower bounds for topological indices in molecular graphs provides critical insights into the structural properties of chemical compounds. These bounds facilitate the estimation of the ranges of topological indices based on molecular structural parameters. This study presents novel inequalities for the Gutman-Milovanović index, which generalizes several significant indices such as the first and second Zagreb indices, the Randić index, the harmonic index, the geometric-arithmetic index, the general second Zagreb index, and the general sum-connectivity index. Moreover, we derive and characterize extremal graphs for many of these inequalities. Additionally, we explore the application of the Gutman-Milovanović index in modeling the physicochemical properties of 22 polycyclic aromatic hydrocarbons. Our results demonstrate that the topological index $M_{\alpha,\beta}$ provides accurate predictions for these properties, with R^2 values ranging from 0.9406 to 0.9983, indicating a strong correlation between the index and experimental data. The findings underscore the versatility of $M_{\alpha,\beta}$ in chemical applications.

Keywords: Gutman-Milovanović index; variable topological indices; general Zagreb indices; general sum-connectivity index; vertex-degree-based topological indices
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1. Introduction

A *topological index* is a single number, representing a chemical structure in graph-theoretical terms, which correlates with a molecular property. The concept of topological indices began with the work of Harold Wiener in the 1940s [42], particularly in relation to chemical graph theory. His Wiener index,

which quantifies the branching of a molecular structure by counting the sum of distances between all pairs of vertices in a graph, laid the groundwork for subsequent research.

Since then, numerous topological indices have been developed, each capturing different aspects of molecular structure and properties. Examples include the Zagreb indices and the Randić index, among many others. These indices are used to correlate structural features with various chemical properties, aiding in the prediction of physical and chemical behaviors of compounds. For additional approaches related to topological indices and their applications, see [1, 3, 28].

The first and second Zagreb indices, which we denote M_1 and M_2, respectively, are defined (see [18]) by

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

where $V(G)$ and $E(G)$ denote the set of vertices and edges of the graph G, respectively, and d_x denotes the degree (the number of neighbors) of the vertex x.

In [5, 23, 27] the *general first and second 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.

Note that M_1^α generalizes the first Zagreb index M_1, the inverse index $ID(G)$ [12], the forgotten index $F(G)$, etc.; also, M_2^α generalizes the Randić index, the second Zagreb index M_2, the modified Zagreb index [29], etc.

The concept of variable topological indices offers a flexible approach to characterizing molecular structures, especially when it comes to heteroatoms and the structural differences between acyclic and cyclic components in molecules like alkylcycloalkanes (see [32–34]). By allowing the variables to be optimized during regression analysis, the method aims to minimize the standard error of the estimate for a given property. This adaptability can lead to more accurate and reliable models for predicting molecular behavior and properties, making it a valuable tool in cheminformatics and molecular modeling.

The sum-connectivity index was introduced in [43]. It has been shown that it correlates well with the π-electronic energy of benzenoid hydrocarbons [24]. In [25] appear more applications of this index. This index was extended to the *general sum-connectivity index* in the paper [44], which is defined as

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

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

There are relationships between all these indices (see e.g. [13, 14]).

If α, β are arbitrary real numbers, the Gutman-Milovanović index is defined in [16] by

$$M_{\alpha,\beta}(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha (d_u + d_v)^\beta.$$

This index is a natural generalization of the first Zagreb, the general second Zagreb, and the general sum-connectivity indices.

Notice that $M_{0,1}$ is the first Zagreb index M_1, $M_{1,0}$ is the second Zagreb index M_2, $M_{-1/2,0}$ is the Randić index R, $2M_{1/2,-1}$ is the geometric-arithmetic index GA, $\frac{1}{2}M_{-1/2,1}$ is the arithmetic-geometric index AG, $M_{0,-1/2}$ is the sum-connectivity index χ, $2M_{0,-1}$ is the harmonic index H, $M_{\alpha,0}$ is the general second Zagreb index M_2^α, $M_{0,\beta}$ is the general sum-connectivity index χ_β, and $4M_{1,-2}$ is the harmonic-arithmetic index HA [2], etc. In all these examples we have $\alpha \neq \beta$, but we can also obtain known indices when $\alpha = \beta$: the third redefined Zagreb index (also called the second Gourava index) if $\alpha = \beta = 1$ (see [20]), the second hyper-Gourava index if $\alpha = \beta = 2$ (see [19]), and the Gourava product-connectivity index if $\alpha = \beta = 1/2$ (see [21]).

Note that the definition of $M_{\alpha,\beta}$ in [16] is slightly different, but it is equivalent to this one.

The purpose of this paper is to provide new inequalities for the Gutman-Milovanović index. Moreover, the characterization of extremal graphs with respect to many of these inequalities is obtained (by extremal graphs, we mean graphs for which the inequality is, in fact, an equality). Also, some applications are given to the study of the physicochemical properties of polycyclic aromatic hydrocarbons (PAHs). The physicochemical properties of these compounds studied are boiling point, entropy, acentric factor, octanol-water partition coefficient, Kovats retention index and enthalpy of formation.

One of the novelties of studying this index for all parameter values is that it allows obtaining results for many of the known indices in a unified way. On the other hand, this characteristic also introduces the main technical difficulty, since it is necessary to search for arguments that work for all parameter values.

2. Main inequalities

Given positive integers $\delta \leq \Delta$ and $a \in \mathbb{R}$, let us define the constants $c_a = c_a(\delta, \Delta)$ and $C_a = C_a(\delta, \Delta)$ as follows:

If $a \geq 0$, then

$$c_a = 2\delta^{2a+1}, \qquad C_a = 2\Delta^{2a+1}.$$

If $a \leq -1$, then

$$c_a = 2\Delta^{2a+1}, \qquad C_a = 2\delta^{2a+1}.$$

If $a = -1/2$, then

$$c_{-1/2} = 2, \qquad C_{-1/2} = \frac{\Delta + \delta}{\sqrt{\Delta\delta}}.$$

If $-1/2 < a < 0$ and $(a+1)\delta + a\Delta \geq 0$, then

$$c_a = 2\delta^{2a+1}, \qquad C_a = 2\Delta^{2a+1}.$$

If $-1/2 < a < 0$ and $(a+1)\delta + a\Delta < 0$, then

$$c_a = \min\left\{2\delta^{2a+1}, \frac{|a|^a}{(a+1)^{a+1}}\Delta^{2a+1}\right\},$$
$$C_a = \max\left\{(\Delta+\delta)(\Delta\delta)^a, 2\Delta^{2a+1}\right\}.$$

If $-1 < a < -1/2$ and $(a+1)\Delta + a\delta \leq 0$, then

$$c_a = 2\Delta^{2a+1}, \qquad C_a = 2\delta^{2a+1}.$$

If $-1 < a < -1/2$ and $(a+1)\Delta + a\delta > 0$, then

$$c_a = \min\left\{2\Delta^{2a+1}, \frac{|a|^a}{(a+1)^{a+1}}\,\delta^{2a+1}\right\},$$
$$C_a = \max\left\{(\Delta+\delta)(\Delta\delta)^a, 2\delta^{2a+1}\right\}.$$

Recall that a *biregular* graph is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ. We say that a graph is (Δ, δ)-*biregular* if we want to write explicitly the maximum and minimum degrees.

Proposition 2.1. *Let G be a graph with m edges, minimum degree δ, and maximum degree Δ, and $a \in \mathbb{R}$. Then,*

$$c_a m \le M_{a,1}(G) \le C_a m.$$

If c_a (respectively, C_a) is equal to $2\delta^{2a+1}$ or $2\Delta^{2a+1}$, then we have $M_{a,1}(G) = c_a m$ (respectively, $M_{a,1}(G) = C_a m$) for every regular graph G.

If c_a (respectively, C_a) is equal to $(\Delta\delta)^a(\Delta+\delta)$, then we have $M_{a,1}(G) = c_a m$ (respectively, $M_{a,1}(G) = C_a m$) for every biregular graph G.

Proof. We are going to compute the extremal values of the next function $\Lambda : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ of class C^∞ given by

$$\Lambda(x, y) = (x+y)(xy)^a = x^{a+1}y^a + x^a y^{a+1}.$$

We will prove that $c_a \le \Lambda(x, y) \le C_a$ for every $\delta \le x, y \le \Delta$, then $c_a \le (d_u + d_v)(d_u d_v)^a \le C_a$ for every edge $uv \in E(G)$, and so, $c_a m \le M_{a,1}(G) \le C_a m$.

Since c_a and C_a have different expressions depending on the values of a, it will be necessary to consider several cases in the proof depending on the values of a.

The partial derivatives of Λ are

$$\begin{aligned}\frac{\partial\Lambda}{\partial x}(x, y) &= (a+1)x^a y^a + a\,x^{a-1}y^{a+1}\\ &= x^{a-1}y^a((a+1)x + a\,y),\\ \frac{\partial\Lambda}{\partial y}(x, y) &= y^{a-1}x^a((a+1)y + a\,x).\end{aligned}$$

If $a \ge 0$, then $\partial\Lambda/\partial x, \partial\Lambda/\partial y > 0$ and so,

$$\begin{aligned}2\delta^{2a+1} = \Lambda(\delta, \delta) \le \Lambda(x, y) \le \Lambda(\Delta, \Delta) = 2\Delta^{2a+1},\\ c_a \le (d_u + d_v)(d_u d_v)^a \le C_a,\\ c_a m \le M_{a,1}(G) \le C_a m.\end{aligned}$$

If $a \le -1$, then $\partial\Lambda/\partial x, \partial\Lambda/\partial y < 0$ and so,

$$\begin{aligned}2\Delta^{2a+1} = \Lambda(\Delta, \Delta) \le \Lambda(x, y) \le \Lambda(\delta, \delta) = 2\delta^{2a+1},\\ c_a \le (d_u + d_v)(d_u d_v)^a \le C_a,\\ c_a m \le M_{a,1}(G) \le C_a m.\end{aligned}$$

If $a = -1/2$, then

$$\Lambda(x, y) = \frac{x + y}{\sqrt{xy}},$$

and it is well known that

$$c_{-1/2} = 2 \leq \frac{x + y}{\sqrt{xy}} \leq \frac{\Delta + \delta}{\sqrt{\Delta\delta}} = C_{-1/2},$$
$$c_{-1/2} \leq (d_u + d_v)(d_u d_v)^{-1/2} \leq C_{-1/2},$$
$$c_{-1/2}\, m \leq M_{-1/2,1}(G) \leq C_{-1/2}\, m.$$

We just need to consider the cases $-1/2 < a < 0$ and $-1 < a < -1/2$.

(A) Assume first $-1/2 < a < 0$. By symmetry, it suffices to study the function Λ on the set $A = \{(x, y) \in [\delta, \Delta] \times [\delta, \Delta] : x \geq y\}$. If (x_0, y_0) is a critical point of Λ, then $\nabla\Lambda(x_0, y_0) = 0$ and

$$(a + 1)x_0 + a y_0 = 0,$$
$$(a + 1)y_0 + a x_0 = 0.$$

Thus, we have $(x_0, y_0) = (0, 0) \notin A$. Since there are no critical points of Λ in A, the extremal values of Λ are attained on the boundary ∂A.

On the set $\{\delta \leq x = y \leq \Delta\} \subset \partial A$ one gets $\Lambda(x, x) = 2x^{2a+1}$. Since $2a + 1 > 0$, we have $2\delta^{2a+1} \leq \Lambda(x, x) \leq 2\Delta^{2a+1}$.

In order to deal with $[\delta, \Delta] \times \{\delta\} \subset \partial A$, let us consider the function $\gamma(x) = \Lambda(x, \delta)$. Thus, $\gamma'(x) = x^{a-1}\delta^a((a + 1)x + a\,\delta)$. Since $a + 1 > -a$, we have

$$\gamma'(x) > x^{a-1}\delta^a(-a\,x + a\,\delta) = -a\,x^{a-1}\delta^a(x - \delta) \geq 0.$$

Therefore,

$$2\delta^{2a+1} = \gamma(\delta) \leq \gamma(x) = \Lambda(x, \delta) \leq \gamma(\Delta) = (\Delta + \delta)(\Delta\delta)^a.$$

In order to deal with $\{\Delta\} \times [\delta, \Delta] \subset \partial A$, let us consider the function $\sigma(y) = \Lambda(\Delta, y)$. Thus, $\sigma'(y) = y^{a-1}\Delta^a((a + 1)y + a\,\Delta) = 0$ if and only if

$$y = \frac{-a}{a + 1}\,\Delta.$$

Note that $-1/2 < a < 0$ implies $a + 1 > -a$, and so,

$$0 < \frac{-a}{a + 1} < 1, \qquad \frac{-a}{a + 1}\,\Delta < \Delta.$$

(A.1) If $(a + 1)\delta + a\Delta \geq 0$, then $-a\Delta/(a + 1) \leq \delta$, and so,

$$0 \leq y^{a-1}\Delta^a((a + 1)\delta + a\,\Delta) < y^{a-1}\Delta^a((a + 1)y + a\,\Delta) = \sigma'(y),$$

if $y \in (\delta, \Delta]$. Hence,

$$(\Delta + \delta)(\Delta\delta)^a = \sigma(\delta) \leq \sigma(y) = \Lambda(\Delta, y) \leq \sigma(\Delta) = 2\Delta^{2a+1}.$$

Consequently,

$$2\delta^{2a+1} \le \Lambda(x,y) \le 2\Delta^{2a+1},$$
$$c_a \le (d_u + d_v)(d_u d_v)^a \le C_a,$$
$$c_a m \le M_{a,1}(G) \le C_a m.$$

(A.2) If $(a+1)\delta + a\Delta < 0$, then $\delta < -a\Delta/(a+1) < \Delta$. Since $2a+1 > 0$,

$$\sigma'(\delta) = \delta^{a-1}\Delta^a((a+1)\delta + a\,\Delta) < 0,$$
$$\sigma'(\Delta) = \Delta^{2a}(2a+1) > 0.$$

Since σ' has a single zero, we have

$$\sigma\Big(\frac{-a}{a+1}\,\Delta\Big) \le \sigma(y) = \Lambda(\Delta, y) \le \max\{\sigma(\delta), \sigma(\Delta)\},$$
$$\frac{|a|^a}{(a+1)^{a+1}}\,\Delta^{2a+1} \le \sigma(y) \le \max\Big\{(\Delta+\delta)(\Delta\delta)^a, 2\Delta^{2a+1}\Big\}.$$

Consequently,

$$\min\Big\{2\delta^{2a+1}, \frac{|a|^a}{(a+1)^{a+1}}\,\Delta^{2a+1}\Big\} \le \Lambda(x,y) \le \max\Big\{(\Delta+\delta)(\Delta\delta)^a, 2\Delta^{2a+1}\Big\},$$
$$c_a \le (d_u + d_v)(d_u d_v)^a \le C_a,$$
$$c_a m \le M_{a,1}(G) \le C_a m.$$

(B) Assume now $-1 < a < -1/2$. By symmetry, it suffices to study the function Λ on the set $B = \{(x,y) \in [\delta,\Delta]\times[\delta,\Delta] : y \ge x\}$. As in the previous case, the extremal values of Λ are attained on the boundary ∂B.

On the set $\{\delta \le x = y \le \Delta\} \subset \partial B$ one gets $\Lambda(x,x) = 2x^{2a+1}$. Since $2a+1 < 0$, we have $2\Delta^{2a+1} \le \Lambda(x,x) \le 2\delta^{2a+1}$.

In order to deal with $[\delta,\Delta]\times\{\Delta\} \subset \partial B$, let us consider the function $\eta(x) = \Lambda(x,\Delta)$. Thus, $\eta'(x) = x^{a-1}\Delta^a((a+1)x + a\,\Delta)$. Since $a+1 < -a$, we have

$$\eta'(x) < x^{a-1}\Delta^a(-a\,x + a\,\Delta) = a\,x^{a-1}\Delta^a(\Delta - x) \le 0.$$

Therefore,

$$2\Delta^{2a+1} = \eta(\Delta) \le \eta(x) = \Lambda(x,\Delta) \le \eta(\delta) = (\Delta+\delta)(\Delta\delta)^a.$$

In order to deal with $\{\delta\}\times[\delta,\Delta] \subset \partial B$, let us consider the function $\mu(y) = \Lambda(\delta, y)$. Thus, $\mu'(y) = y^{a-1}\delta^a((a+1)y + a\,\delta) = 0$ if and only if

$$y = \frac{-a}{a+1}\,\delta.$$

Note that $-1 < a < -1/2$ implies $a+1 < -a$, and so,

$$\frac{-a}{a+1} > 1, \qquad \frac{-a}{a+1}\,\delta > \delta.$$

(B.1) If $(a+1)\Delta + a\delta \le 0$, then $-a\delta/(a+1) \ge \Delta$, and so,

$$0 \ge y^{a-1}\delta^a((a+1)\Delta + a\delta) > y^{a-1}\delta^a((a+1)y + a\,\delta) = \mu'(y),$$

if $y \in [\delta, \Delta)$. Hence,

$$(\Delta + \delta)(\Delta\delta)^a = \mu(\Delta) \leq \mu(y) = \Lambda(\delta, y) \leq \mu(\delta) = 2\delta^{2a+1}.$$

Consequently,

$$\begin{aligned} 2\Delta^{2a+1} \leq \Lambda(x, y) \leq 2\delta^{2a+1}, \\ c_a \leq (d_u + d_v)(d_u d_v)^a \leq C_a, \\ c_a m \leq M_{a,1}(G) \leq C_a m. \end{aligned}$$

(B.2) If $(a + 1)\Delta + a\delta > 0$, then $\delta < -a\delta/(a + 1) < \Delta$. Since $2a + 1 < 0$,

$$\begin{aligned} \mu'(\delta) = \delta^{2a}(2a + 1) < 0, \\ \mu'(\Delta) = \Delta^{a-1}\delta^a((a + 1)\Delta + a\,\delta) > 0. \end{aligned}$$

Hence,

$$\begin{aligned} \mu\Big(\frac{-a}{a+1}\,\delta\Big) \leq \mu(y) = \Lambda(\delta, y) \leq \max\{\mu(\delta), \mu(\Delta)\}, \\ \frac{|a|^a}{(a+1)^{a+1}}\,\delta^{2a+1} \leq \mu(y) \leq \max\Big\{2\delta^{2a+1}, (\Delta + \delta)(\Delta\delta)^a\Big\}. \end{aligned}$$

Consequently,

$$\begin{aligned} \min\Big\{2\Delta^{2a+1}, \frac{|a|^a}{(a+1)^{a+1}}\,\delta^{2a+1}\Big\} \leq \Lambda(x, y) \leq \max\Big\{(\Delta + \delta)(\Delta\delta)^a, 2\delta^{2a+1}\Big\}, \\ c_a \leq (d_u + d_v)(d_u d_v)^a \leq C_a, \\ c_a m \leq M_{a,1}(G) \leq C_a m. \end{aligned}$$

If G is a regular graph, then $M_{a,1}(G) = 2\delta^{2a+1} = 2\Delta^{2a+1}$. Consequently, if c_a (respectively, C_a) is equal to $2\delta^{2a+1}$ or $2\Delta^{2a+1}$, then we have $M_{a,1}(G) = c_a m$ (respectively, $M_{a,1}(G) = C_a m$) for every regular graph G.

If G is a biregular graph, then $M_{a,1}(G) = (\Delta + \delta)(\Delta\delta)^a$. Consequently, if c_a (respectively, C_a) is equal to $(\Delta + \delta)(\Delta\delta)^a$, then we have $M_{a,1}(G) = c_a m$ (respectively, $M_{a,1}(G) = C_a m$) for every biregular graph G. □

Remark 2.2. *It is natural to wonder about equality in inequalities in Proposition 2.1 when the values of the constants are not equal to $2\delta^{2a+1}$, $2\Delta^{2a+1}$, or $(\Delta\delta)^a(\Delta + \delta)$. Although these inequalities are very good in these cases as well, equality is not achieved for any graph at almost every value of the parameter $a \in \mathbb{R}$, as the following example shows:*

Assume for instance (the other cases are similar) that $-1/2 < a < 0$, $(a + 1)\delta + a\Delta < 0$, as in Case (A.2), and

$$\frac{|a|^a}{(a+1)^{a+1}}\Delta^{2a+1} < 2\delta^{2a+1}.$$

Hence,

$$c_a = \frac{|a|^a}{(a+1)^{a+1}}\Delta^{2a+1}.$$

The argument in the proof of Proposition 2.1 provides that

$$c_a = \frac{|a|^a}{(a+1)^{a+1}}\Delta^{2a+1} = \Lambda\Big(\Delta, \frac{-a}{a+1}\,\Delta\Big).$$

And so, the equality $M_{a,1}(G) = c_a m$ is attained if and only if every edge in $E(G)$ has vertices with degrees Δ and $\frac{-a}{a+1}\Delta$. This can happen just if $k = \frac{-a}{a+1}\Delta$ is a positive integer, and then

$$\frac{k}{\Delta} = \frac{-a}{a+1} \qquad \Rightarrow \qquad ka + k = -a\Delta \qquad \Rightarrow \qquad a = \frac{-k}{k+\Delta} \in \mathbb{Q}.$$

Hence, for almost every value of a (when $a \in \mathbb{R} \setminus \mathbb{Q}$), there is no graph attaining the equality $M_{a,1}(G) = c_a m$.

Corollary 2.3. *Given $a \in \mathbb{R}$ and integers $1 \le \delta \le \Delta$, we have $c_a \le C_a$, and $c_a = C_a$ if and only if $\delta = \Delta$.*

Proof. Let $J = [\delta, \Delta] \times [\delta, \Delta]$ and let $\Lambda : J \to \mathbb{R}$ be the function defined as

$$\Lambda(x, y) = (x + y)(xy)^a.$$

Then the argument in the proof of Proposition 2.1 gives that

$$c_a = \min_{(x,y)\in J} \Lambda(x, y), \qquad C_a = \max_{(x,y)\in J} \Lambda(x, y).$$

The statement follows since Λ is not constant if $\delta < \Delta$. □

Given positive integers $\delta \le \Delta$ and $\alpha, \beta \in \mathbb{R}$, let us define the constants $c_{\alpha,\beta} = c_{\alpha,\beta}(\delta, \Delta)$ and $C_{\alpha,\beta} = C_{\alpha,\beta}(\delta, \Delta)$ as follows:

If $\beta > 0$, then

$$c_{\alpha,\beta} = c^{\beta}_{\alpha/\beta}, \qquad C_{\alpha,\beta} = C^{\beta}_{\alpha/\beta}.$$

If $\beta < 0$, then

$$c_{\alpha,\beta} = C^{\beta}_{\alpha/\beta}, \qquad C_{\alpha,\beta} = c^{\beta}_{\alpha/\beta}.$$

If $\beta = 0$ and $\alpha \ge 0$, then

$$c_{\alpha,0} = \delta^{2\alpha}, \qquad C_{\alpha,0} = \Delta^{2\alpha}.$$

If $\beta = 0$ and $\alpha < 0$, then

$$c_{\alpha,0} = \Delta^{2\alpha}, \qquad C_{\alpha,0} = \delta^{2\alpha}.$$

Theorem 2.4. *Let G be a graph with m edges, minimum degree δ, and maximum degree Δ, and $\alpha, \beta \in \mathbb{R}$. Then,*

$$c_{\alpha,\beta}\, m \le M_{\alpha,\beta}(G) \le C_{\alpha,\beta}\, m.$$

If $c_{\alpha,\beta}$ (respectively, $C_{\alpha,\beta}$) is equal to $2^{\beta}\delta^{2\alpha+\beta}$ or $2^{\beta}\Delta^{2\alpha+\beta}$, then we have $M_{\alpha,\beta}(G) = c_{\alpha,\beta}\, m$ (respectively, $M_{\alpha,\beta}(G) = C_{\alpha,\beta}\, m$) for every regular graph G.

If $c_{\alpha,\beta}$ (respectively, $C_{\alpha,\beta}$) is equal to $(\Delta\delta)^{\alpha}(\Delta + \delta)^{\beta}$, then we have $M_{\alpha,\beta}(G) = c_{\alpha,\beta}\, m$ (respectively, $M_{\alpha,\beta}(G) = C_{\alpha,\beta}\, m$) for every biregular graph G.

Proof. The argument in the proof of Proposition 2.1 implies that

$$c_a \le (xy)^a(x + y) \le C_a$$

for every $a \in \mathbb{R}$ and $\delta \le x, y \le \Delta$. Hence, if $\beta \ne 0$ and we take $a = \alpha/\beta$, we have

$$c_{\alpha/\beta} \le (xy)^{\alpha/\beta}(x + y) \le C_{\alpha/\beta}$$

for every $\delta \leq x, y \leq \Delta$.

If $\beta > 0$, then

$$c^{\beta}_{\alpha/\beta} \leq (xy)^{\alpha}(x+y)^{\beta} \leq C^{\beta}_{\alpha/\beta}$$

for every $\delta \leq x, y \leq \Delta$.

If $\beta < 0$, then

$$C^{\beta}_{\alpha/\beta} \leq (xy)^{\alpha}(x+y)^{\beta} \leq c^{\beta}_{\alpha/\beta}$$

for every $\delta \leq x, y \leq \Delta$.

If $\beta = 0$ and $\alpha \geq 0$, then

$$\delta^{2\alpha} \leq (xy)^{\alpha}(x+y)^{0} \leq \Delta^{2\alpha}$$

for every $\delta \leq x, y \leq \Delta$.

If $\beta = 0$ and $\alpha < 0$, then

$$\Delta^{2\alpha} \leq (xy)^{\alpha}(x+y)^{0} \leq \delta^{2\alpha}$$

for every $\delta \leq x, y \leq \Delta$.

Therefore, we have for every $\alpha, \beta \in \mathbb{R}$,

$$c_{\alpha,\beta} \leq (d_u d_v)^{\alpha}(d_u + d_v)^{\beta} \leq C_{\alpha,\beta}$$

for every $uv \in E(G)$, and so,

$$c_{\alpha,\beta}\, m \leq M_{\alpha,\beta}(G) \leq C_{\alpha,\beta}\, m.$$

The statements on the equalities follow from the argument in the proof of Proposition 2.1. □

The argument in the proof of Corollary 2.3 has the following consequence.

Corollary 2.5. *Given $\alpha, \beta \in \mathbb{R}$ and integers $1 \leq \delta \leq \Delta$, we have $c_{\alpha,\beta} \leq C_{\alpha,\beta}$; also, $c_{\alpha,\beta} = C_{\alpha,\beta}$ if and only if $\delta = \Delta$.*

The following inequality relating two $M_{\alpha,\beta}$ indices is direct.

Proposition 2.6. *Let G be a graph and $\alpha, \beta, \alpha', \beta' \in \mathbb{R}$ with $\alpha \leq \alpha'$ and $\beta \leq \beta'$. Then,*

$$M_{\alpha,\beta}(G) \leq M_{\alpha',\beta'}(G).$$

Theorem 2.4 allows us to prove the following inequality relating two $M_{\alpha,\beta}$ indices.

Theorem 2.7. *Let G be a graph with minimum degree δ, and maximum degree Δ, and $\alpha, \beta, \alpha', \beta' \in \mathbb{R}$. Then,*

$$c_{\alpha-\alpha',\beta-\beta'}\, M_{\alpha',\beta'}(G) \leq M_{\alpha,\beta}(G) \leq C_{\alpha-\alpha',\beta-\beta'}\, M_{\alpha',\beta'}(G).$$

Proof. The argument in the proof of Theorem 2.4 implies that

$$c_{\alpha-\alpha',\beta-\beta'} \leq (d_u d_v)^{\alpha-\alpha'}(d_u + d_v)^{\beta-\beta'} \leq C_{\alpha-\alpha',\beta-\beta'}$$

for every $uv \in E(G)$, and so,

$$c_{\alpha-\alpha',\beta-\beta'}(d_u d_v)^{\alpha'}(d_u + d_v)^{\beta'} \leq (d_u d_v)^{\alpha}(d_u + d_v)^{\beta} \leq C_{\alpha-\alpha',\beta-\beta'}(d_u d_v)^{\alpha'}(d_u + d_v)^{\beta'}$$

$$c_{\alpha-\alpha',\beta-\beta'}\, M_{\alpha',\beta'}(G) \leq M_{\alpha,\beta}(G) \leq C_{\alpha-\alpha',\beta-\beta'}\, M_{\alpha',\beta'}(G).$$

□

Recall that $M_2^{-1/2}$ is the Randić index R, $\chi_{-1/2}$ is the sum-connectivity index S, and $2\chi_{-1}$ is the harmonic index H. Thus, Theorem 2.7 has the following consequence.

Corollary 2.8. *Let G be a graph with minimum degree δ, maximum degree Δ, and $\alpha, \beta, \alpha', \beta' \in \mathbb{R}$. Then,*

$$\begin{aligned}
c_{\alpha-\alpha',\beta}\, M_2^{\alpha'}(G) \le M_{\alpha,\beta}(G) \le C_{\alpha-\alpha',\beta}\, M_2^{\alpha'}(G),\\
c_{\alpha,\beta-\beta'}\, \chi_{\beta'}(G) \le M_{\alpha,\beta}(G) \le C_{\alpha,\beta-\beta'}\, \chi_{\beta'}(G),\\
c_{\alpha-1,\beta}\, M_2(G) \le M_{\alpha,\beta}(G) \le C_{\alpha-1,\beta}\, M_2(G),\\
c_{\alpha+1/2,\beta}\, R(G) \le M_{\alpha,\beta}(G) \le C_{\alpha+1/2,\beta}\, R(G),\\
c_{\alpha,\beta-1}\, M_1(G) \le M_{\alpha,\beta}(G) \le C_{\alpha,\beta-1}\, M_1(G),\\
c_{\alpha,\beta+1/2}\, S(G) \le M_{\alpha,\beta}(G) \le C_{\alpha,\beta+1/2}\, S(G),\\
\frac{1}{2}\, c_{\alpha,\beta+1}\, H(G) \le M_{\alpha,\beta}(G) \le \frac{1}{2}\, C_{\alpha,\beta+1}\, H(G).
\end{aligned}$$

The *geometric-arithmetic* and the *arithmetic-geometric* indices are defined, respectively, as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \qquad AG(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$

The geometric-arithmetic index is a good predictor of the heat of formation of benzenoid hydrocarbons, and it has been extensively studied (see, e.g., [6–9, 35, 36]).

In [4, 10] (see also [37]), the *variable geometric-arithmetic* index was defined by

$$GA_a(G) = \sum_{uv\in E(G)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right)^a = 2^a M_{a/2,-a}(G).$$

Theorem 2.7 also has the following consequence.

Corollary 2.9. *Let G be a graph with minimum degree δ, maximum degree Δ, and $\alpha, \beta, a \in \mathbb{R}$. Then,*

$$2^{-a} c_{\alpha-a/2,\beta+a}\, GA_a(G) \le M_{\alpha,\beta}(G) \le 2^{-a} C_{\alpha-a/2,\beta+a}\, GA_a(G).$$

Corollary 2.9 has the following consequence for the geometric-arithmetic and the arithmetic-geometric indices.

Corollary 2.10. *Let G be a graph with minimum degree δ, maximum degree Δ, and $\alpha, \beta \in \mathbb{R}$. Then,*

$$\begin{aligned}
\frac{1}{2}\, c_{\alpha-1/2,\beta+1}\, GA(G) \le M_{\alpha,\beta}(G) \le \frac{1}{2}\, C_{\alpha-1/2,\beta+1}\, GA(G),\\
2\, c_{\alpha+1/2,\beta-1}\, AG(G) \le M_{\alpha,\beta}(G) \le 2\, C_{\alpha+1/2,\beta-1}\, AG(G).
\end{aligned}$$

In [40, 41], a family of Adriatic indices is introduced. An especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. Most of the indices showed good predictive properties on the testing sets provided by the International Academy of Mathematical Chemistry. Twenty of them were selected as good predictors. The *inverse sum indeg* index, ISI, is an Adriatic

index that was selected in [41] as a significant predictor of the total surface area of octane isomers. This index was defined by

$$ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v} = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = M_{1,-1}(G).$$

In the last years there has been an increasing interest in this index (see, e.g., [11, 15, 17, 30]).

Theorem 2.7 provides inequalities relating the inverse sum indeg and the Gutman-Milovanović indices.

Corollary 2.11. *Let G be a graph with minimum degree δ, maximum degree Δ, and $\alpha, \beta \in \mathbb{R}$. Then,*

$$c_{\alpha-1,\beta+1}\, ISI(G) \le M_{\alpha,\beta}(G) \le C_{\alpha-1,\beta+1}\, ISI(G).$$

3. Other inequalities

The following result is a useful and well-known inequality (see, e.g., [26, Lemma 3.4] for a proof of the statement of equality).

Lemma 3.1. *If $a_i, b_i \ge 0$ and $Mb_i \le a_i \le Nb_i$ for $1 \le i \le k$ and some positive constants M, N, then*

$$\Big(\sum_{i=1}^{k} a_i^2\Big)^{1/2}\Big(\sum_{i=1}^{k} b_i^2\Big)^{1/2} \le \frac{1}{2}\left(\sqrt{\frac{N}{M}} + \sqrt{\frac{M}{N}}\right)\sum_{i=1}^{k} a_i b_i.$$

If $a_i > 0$ for some $1 \le i \le k$, then the equality holds if and only if $M = N$ and $a_i = Mb_i = Nb_i$ for every $1 \le i \le k$.

Lemma 3.1 allows us to obtain the following result relating $M_{\alpha,\beta}$, the general second Zagreb index and the general sum-connectivity index.

Theorem 3.2. *Let G be a graph with minimum degree δ, maximum degree Δ, and $\alpha, \beta \in \mathbb{R}$. Then,*

$$M_{\alpha,\beta}(G)^2 \ge \frac{4}{\frac{C_{\alpha,-\beta}}{c_{\alpha,-\beta}} + \frac{c_{\alpha,-\beta}}{C_{\alpha,-\beta}} + 2} M_2^{2\alpha}(G)\chi_{2\beta}(G),$$

where $c_{\alpha,-\beta}, C_{\alpha,-\beta}$ are the constants in Theorem 2.4. The equality in the bound is attained if and only if G is regular.

Proof. The argument in the proof of Theorem 2.4 gives

$$c_{\alpha,\beta} \le (d_u d_v)^{\alpha}(d_u + d_v)^{\beta} \le C_{\alpha,\beta}$$

for every $\alpha, \beta \in \mathbb{R}$ and $uv \in E(G)$ and so, we have

$$c_{\alpha,-\beta} \le \frac{(d_u d_v)^{\alpha}}{(d_u + d_v)^{\beta}} \le C_{\alpha,-\beta}$$

for every $\alpha,\beta \in \mathbb{R}$ and $uv \in E(G)$. Hence, by applying Lemma 3.1, we obtain

$$\left(\sum_{uv\in E(G)} (d_u d_v)^{2\alpha}\right)\left(\sum_{uv\in E(G)} (d_u + d_v)^{2\beta}\right)$$
$$\leq \frac{1}{4}\left(\sqrt{\frac{C_{\alpha,-\beta}}{c_{\alpha,-\beta}}} + \sqrt{\frac{c_{\alpha,-\beta}}{C_{\alpha,-\beta}}}\right)^2 \left(\sum_{uv\in E(G)} (d_u d_v)^{\alpha}(d_u + d_v)^{\beta}\right)^2,$$
$$M_2^{2\alpha}(G)\chi_{2\beta}(G) \leq \frac{1}{4}\left(\frac{C_{\alpha,-\beta}}{c_{\alpha,-\beta}} + \frac{c_{\alpha,-\beta}}{C_{\alpha,-\beta}} + 2\right) M_{\alpha,\beta}(G)^2.$$

By Lemma 3.1, the equality in this bound is attained if and only if $C_{\alpha,-\beta} = c_{\alpha,-\beta}$; Corollary 2.5 gives that this happens if and only if $\delta = \Delta$, i.e., G is regular. □

The following results relate to the Gutman-Milovanović, the general second Zagreb and the general sum-connectivity indices.

Theorem 3.3. *Let G be a graph and $p, \alpha, \beta \in \mathbb{R}$ with $p > 1$. Then,*

$$M_{\alpha,\beta}(G) \leq \frac{1}{p} M_2^{p\alpha}(G) + \frac{p-1}{p}\chi_{p\beta/(p-1)}(G).$$

Proof. By applying Young's inequality, we obtain

$$\sum_{uv\in E(G)} (d_u d_v)^{\alpha}(d_u + d_v)^{\beta} \leq \frac{1}{p}\sum_{uv\in E(G)} (d_u d_v)^{p\alpha} + \frac{p-1}{p}\sum_{uv\in E(G)} (d_u + d_v)^{p\beta/(p-1)},$$
$$M_{\alpha,\beta}(G) \leq \frac{1}{p} M_2^{p\alpha}(G) + \frac{p-1}{p}\chi_{p\beta/(p-1)}(G).$$

□

Young's inequality is a very important result in analysis, since it is a key tool in the proof of Hölder's inequality. Its reverse inequality was given in [39] with Specht's ratio as follows:

$$S\left(\frac{x^p}{y^q}\right) xy \geq \frac{1}{p} x^p + \frac{1}{q} y^q, \tag{3.1}$$

where the Specht's ratio [38] is defined on $\mathbb{R}^+$ as

$$S(a) = \frac{a^{\frac{1}{a-1}}}{e \log a^{\frac{1}{a-1}}}.$$

In [31] appears the following version of (3.1) for n real numbers, improving Specht's ratio.

Theorem 3.4. *If $0 < a < 1$, $p_1, \ldots, p_n > 1$, and $x_1, \ldots, x_n \geq 0$ are real numbers such that $\frac{1}{p_1} + \cdots + \frac{1}{p_n} = 1$ and $a\, x_k^{p_k} \leq x_i^{p_i}$ for $1 \leq i, k \leq n$, then there exists a positive constant A, which just depends on $a, p_1, \ldots, p_n$, such that*

$$\frac{1}{p_1} x_1^{p_1} + \cdots + \frac{1}{p_n} x_n^{p_n} \leq A\, x_1 \cdots x_n. \tag{3.2}$$

In fact, if $\mathcal{P}_n$ denotes the group of permutations of $\{1,\dots,n\}$, then the best value of A is the maximum on the following finite set:

$$A = \max_{1\le m<n,\,\sigma\in\mathcal{P}_n} \Big(a + (1-a)\sum_{k=1}^{m}\frac{1}{p_{\sigma(k)}}\Big)a^{-1+\sum_{k=1}^{m}1/p_{\sigma(k)}}$$
$$\le \frac{a^{\frac{1}{a-1}}}{e\log a^{\frac{1}{a-1}}} = S(a)\,.$$

Corollary 3.5. *If $0<a<1$, $p,q>1$ and $x,y\ge 0$ are real numbers such that $\frac{1}{p}+\frac{1}{q}=1$ and $a\,x^p\le y^q$, $a\,y^q\le x^p$, then*

$$\frac{1}{p}\,x^p+\frac{1}{q}\,y^q\le A\,xy, \tag{3.3}$$

with

$$A=\max\Big\{\Big(a+(1-a)\frac{1}{p}\Big)a^{-1/q}\,,\,\Big(a+(1-a)\frac{1}{q}\Big)a^{-1/p}\Big\}\le S(a)\,.$$

Theorem 3.6. *Let G be a graph and $p,\alpha,\beta\in\mathbb{R}$ with $p>1$. Then,*

$$A_{\alpha,\beta,p}\,M_{\alpha,\beta}(G)\ge\frac{1}{p}\,M_2^{p\alpha}(G)+\frac{p-1}{p}\,\chi_{p\beta/(p-1)}(G),$$

where

$$a_{\alpha,\beta,p}:=\min\{c_{p\alpha,-p\beta/(p-1)}\,,\,c_{-p\alpha,p\beta/(p-1)}\},$$
$$A_{\alpha,\beta,p}:=\max\Big\{\frac{p\,a_{\alpha,\beta,p}+1-a_{\alpha,\beta,p}}{p}\,a_{\alpha,\beta,p}^{(1-p)/p}\,,\,\frac{a_{\alpha,\beta,p}+p-1}{p}\,a_{\alpha,\beta,p}^{-1/p}\Big\}$$
$$\le S(a_{\alpha,\beta,p}).$$

Proof. The argument in the proof of Theorem 2.4 gives

$$c_{p\alpha,-p\beta/(p-1)}\le\frac{(d_ud_v)^{p\alpha}}{(d_u+d_v)^{p\beta/(p-1)}}\,,$$
$$c_{-p\alpha,p\beta/(p-1)}\le\frac{(d_u+d_v)^{p\beta/(p-1)}}{(d_ud_v)^{p\alpha}}\,,$$

for every $uv\in E(G)$.

In order to apply Corollary 3.5, note that

$$A=\max\Big\{\Big(a+(1-a)\frac{1}{p}\Big)a^{-1/q}\,,\,\Big(a+(1-a)\frac{1}{q}\Big)a^{-1/p}\Big\}$$
$$=\max\Big\{\frac{pa+1-a}{p}\,a^{(1-p)/p}\,,\,\frac{a+p-1}{p}\,a^{-1/p}\Big\}\le S(a).$$

Taking into account the definitions of $a_{\alpha,\beta,p}$ and $A_{\alpha,\beta,p}$, Corollary 3.5 implies

$$A_{\alpha,\beta,p}\sum_{uv\in E(G)}(d_ud_v)^{\alpha}(d_u+d_v)^{\beta}\ge\frac{1}{p}\sum_{uv\in E(G)}(d_ud_v)^{p\alpha}+\frac{p-1}{p}\sum_{uv\in E(G)}(d_u+d_v)^{p\beta/(p-1)},$$
$$A_{\alpha,\beta,p}\,M_{\alpha,\beta}(G)\ge\frac{1}{p}\,M_2^{p\alpha}(G)+\frac{p-1}{p}\,\chi_{p\beta/(p-1)}(G).$$

□

4. Analysis of the predictive power of $M_{\alpha,\beta}$ for physicochemical properties of PAHs

In this section, we assess the predictive power of the topological index $M_{\alpha,\beta}$ in modeling the boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($\log P$), Kovats retention index (RI), and enthalpy of formation (ΔH_f) of 22 polycyclic aromatic hydrocarbons. The experimental data for these physicochemical properties were obtained from [22].

We first calculated the coefficient of determination (R^2) for each property between the experimental data and $M_{\alpha,\beta}$. The parameters α and β were varied systematically over a grid ranging from -20 to 20 with a step size of 0.1. Figure 1 shows grayscale maps of the R^2 values obtained from the variation of α and β, where darker regions indicate higher R^2 values. Subsequently, the optimal values of α and β that maximize R^2 in each case were identified; these are represented as red points in the same figure. The selection of the optimal combination is based on the pair of α and β that yields the maximum R^2 within the explored grid, ensuring the best linear relationship between $M_{\alpha,\beta}$ and the property. This systematic grid search guarantees comprehensive coverage of the parameter space, and the chosen step size balances computational feasibility with precision.

Once the optimal values of α and β are obtained, linear models of the form

$$\mathcal{P} = c_1 M_{\alpha,\beta} + c_2,$$

are constructed, where $\mathcal{P}$ represents the physicochemical property, and the coefficients c_1 and c_2 are determined using the linear regression method. After determining the linear models for each physicochemical property, the results are summarized as follows:

$$\begin{aligned} BP &= 11.072 \quad M_{-0.6,\,1.2} - 28.642, \\ S &= 26259 \quad M_{6.9,-13.4} + 53.611, \\ \omega &= 12.3447 \quad M_{5.8,-10.6} + 0.169, \\ \log P &= 0.2201 \quad M_{-0.1,\,0.3} + 0.344, \\ RI &= 10.8178 \quad M_{-0.6,\,1.2} - 54.59, \\ \Delta H_f &= 282.563 \quad M_{2.3,-4.5} + 37.322\,. \end{aligned} \tag{4.1}$$

The performance of these linear models was evaluated, and the results are presented in Figure 2, which shows the correlation between the predicted (red line) and experimental values (blue dots) for each physicochemical property.

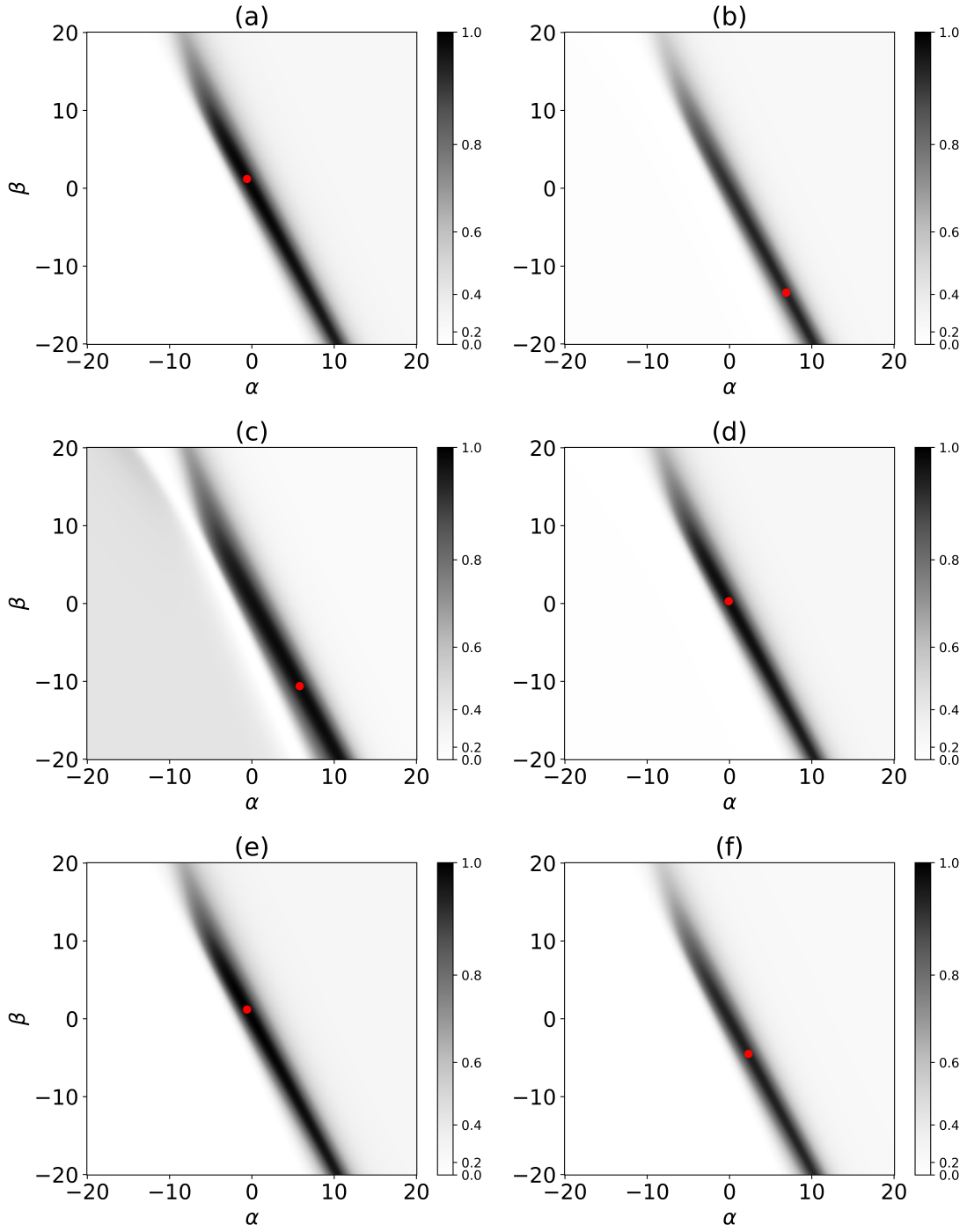

Figure 1. Greyscale maps of R^2 values obtained from the variation of α and β between $M_{\alpha,\beta}$ and the physicochemical properties of PAHs: (a) BP, (b) S, (c) ω, (d) $\log P$, (e) RI, and (f) ΔH_f. The red dot in each panel represents the optimal parameter combination, where R^2 reaches its maximum value.

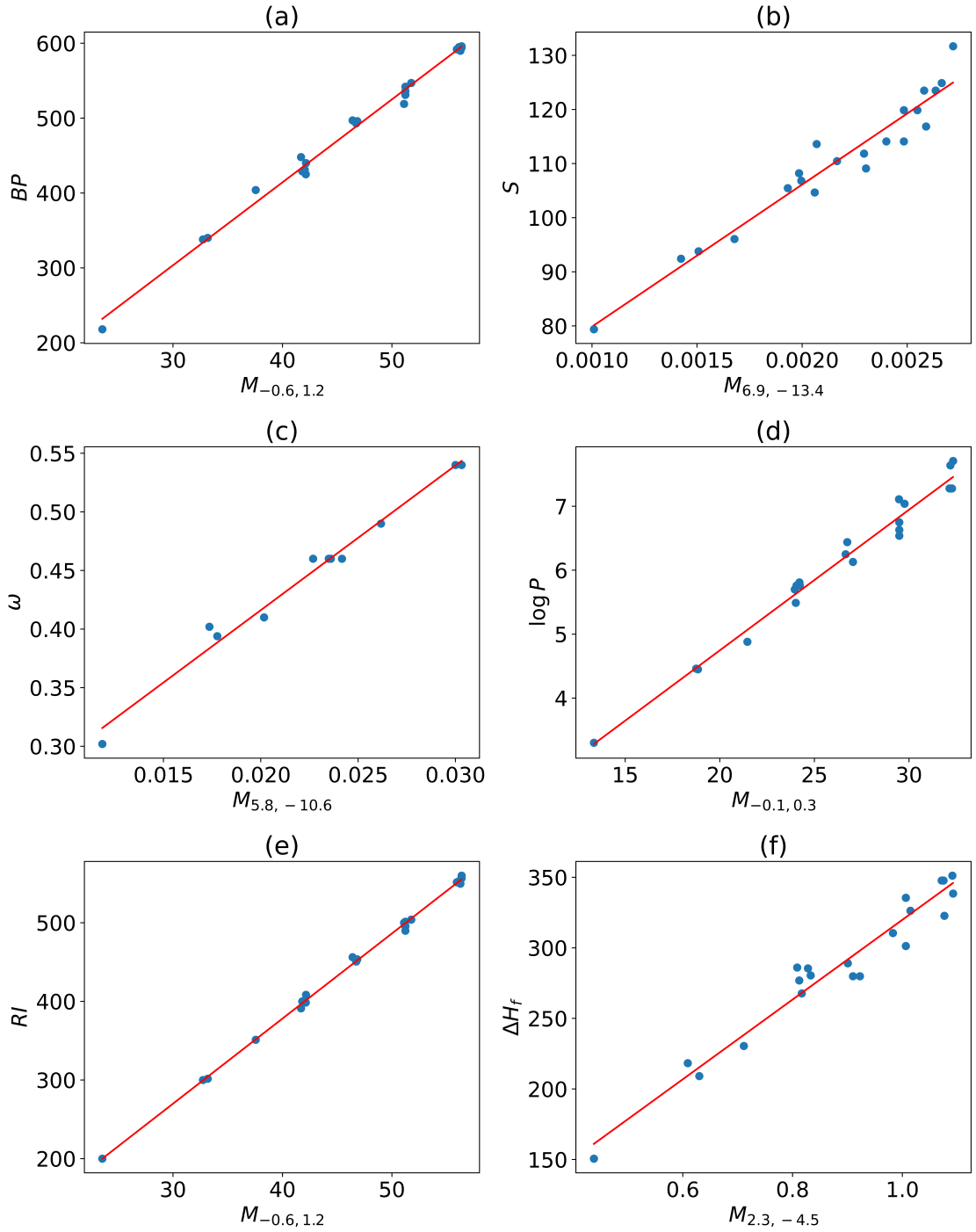

Figure 2. Scatter plot of $M_{\alpha,\beta}$ vs. the physicochemical properties of PAHs, for the values of α,β that maximize R^2. Red lines are the linear models of Eq (4.1), with the regression and statistical parameters resumed in Table 1.

Table 1. Parameters of the linear models of Eq (4.1). Here, c_1, c_2, R^2, SE, F, and SF are the slope, intercept, determination coefficient, standard error, F-test, and statistical significance, respectively.

Property $\mathcal{P}$	α	β	c_1	c_2	R^2	SE	F	SF
BP	−0.6	1.2	11.072	−28.642	0.9923	8.913	2565.3	1.36×10^{-22}
S	6.9	−13.4	26259	53.611	0.9406	3.08	316.6	9.9×10^{-14}
ω	5.8	−10.6	12.3447	0.169	0.9827	0.0095	511.3	3.1×10^{-9}
$\log P$	−0.1	0.3	0.2201	0.344	0.97853	0.172	911.4	3.7×10^{-18}
RI	2.1	−0.6	10.8178	−54.59	0.9983	4.12	11448	4.6×10^{-29}
ΔH_f	2.3	−4.5	282.563	37.322	0.946	12.22	351.7	3.7×10^{-14}

The analysis of the predictive power of the topological index $M_{\alpha,\beta}$ for modeling the physicochemical properties of polycyclic aromatic hydrocarbons reveals several key insights. The R^2 values obtained for the various properties, ranging from 0.9406 for entropy to 0.9983 for the Kovats retention index, indicate a generally strong correlation between the experimental data and the predictions derived from $M_{\alpha,\beta}$. This suggests that the topological index effectively captures the underlying structural variations in PAHs that influence these properties. Notably, the high R^2 value for BP and RI implies that $M_{\alpha,\beta}$ is particularly effective in modeling these properties, likely due to the sensitivity to molecular topology. Conversely, the relatively lower R^2 value for S and ΔH_f indicates a more complex relationship between molecular structure and these properties, which might require additional descriptors or interactions beyond those captured by $M_{\alpha,\beta}$ alone.

Furthermore, the optimal parameter combinations (α,β) vary significantly across different properties, highlighting the importance of parameter tuning for each specific property. This variability underscores the flexibility of the $M_{\alpha,\beta}$ index in adapting to different molecular interactions. However, as shown in Figure 1, the areas where the highest R^2 values are reached (darker areas) are similar across all properties. This suggests the possibility of identifying a combination of the parameters α and β that, while not optimal for each individual property, could provide a good overall fit for all the properties considered.

Building upon the insights gained in the previous analysis, we now explore the possibility of deriving a unified parameter combination (α^*,β^*) that achieves strong correlations collectively, ensuring a robust performance for all properties.

To identify (α^*,β^*), we evaluate the average of the R^2 values for all properties. The (α^*,β^*) combination is determined by maximizing this average over the same parameter grid used previously ($\alpha,\beta \in [-20, 20]$, with a step size of 0.1). In Figure 3 we show a greysacle map of the average values obtained from the variation of α and β across the grid.

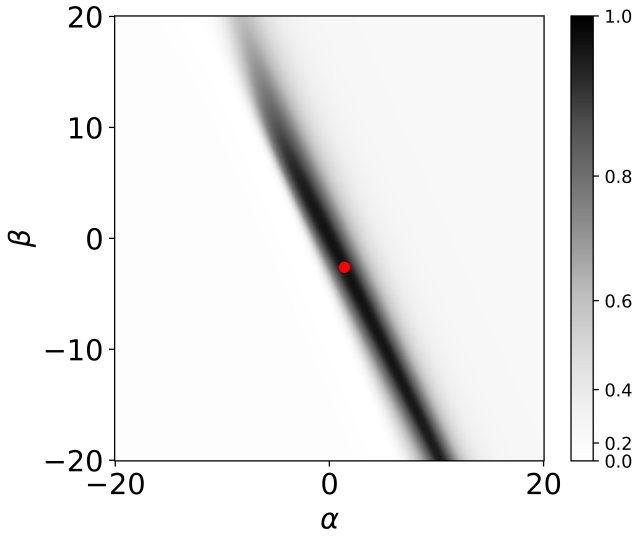

Figure 3. Greyscale map of the average of the R^2 values obtained from the variation of α and β. The red dot represents the optimal parameter combination, where the average reaches its maximum value.

From these calculations we obtain $(\alpha^*, \beta^*) = (1.4, -2.6)$ (red dot in Figure 3). With this combination of parameters, a linear model is proposed for each property.

$$\begin{aligned} BP &= 134.337 \quad M_{\alpha^*,\beta^*} - 15.58, \\ S &= 16.246 \quad M_{\alpha^*,\beta^*} + 50.754, \\ \omega &= 0.09 \quad M_{\alpha^*,\beta^*} + 0.153, \\ \log P &= 1.547 \quad M_{\alpha^*,\beta^*} + 0.44, \\ RI &= 131.26 \quad M_{\alpha^*,\beta^*} - 41.857, \\ \Delta H_f &= 68.245 \quad M_{\alpha^*,\beta^*} + 36.883. \end{aligned} \tag{4.2}$$

To assess the performance of the general model, we calculate the R^2 values for each property using (α^*, β^*) and compare them to the optimal R^2 values obtained for property-specific parameter combinations (see Table 2).

Table 2. Comparison of R^2 values for property-specific (α, β), generalized (α^*, β^*), and the unified model.

Property $\mathcal{P}$	Specific (α, β)	Generalized (α^*, β^*)	Unified Model
BP	0.9923	0.9888	0.9776
S	0.9406	0.9298	0.828
ω	0.9827	0.9766	0.8698
$\log P$	0.9785	0.9768	0.9679
RI	0.9983	0.9948	0.9901
ΔH_f	0.9462	0.9445	0.9382

The results in Table 2 demonstrate that the general parameter combination $(\alpha^*, \beta^*) = (1.4, -2.6)$ provides consistently high R^2 values across all physicochemical properties. While the $R^2(\alpha^*, \beta^*)$ values

are slightly lower than those achieved with property-specific parameter combinations, the differences are minimal (e.g., for RI, the difference is only 0.0035). This indicates that the models obtained from (α^*, β^*) capture the structural features relevant to all properties effectively, making it a robust alternative for predicting multiple properties.

Next, we aim to construct and evaluate a unified model using (α^*, β^*) to simultaneously predict all physicochemical properties. This approach will enable us to assess the practicality and effectiveness of a general model in capturing the structural factors influencing diverse properties. To ensure comparability across properties, each property is normalized to the range $[0, 1]$ using the transformation,

$$\mathcal{P}_{\text{norm}} = \frac{\mathcal{P} - \min(\mathcal{P})}{\max(\mathcal{P}) - \min(\mathcal{P})}.$$

This normalization removes scale differences and enables consistent evaluation of the generalized model. Then, the M_{α^*,β^*} index is calculated for each molecule using the general parameter combination (α^*, β^*). The normalized values of all properties are then combined into a single dataset. Thus, the general model takes the form

$$\mathcal{P}_{\text{norm}} = 0.3408 M_{\alpha^*,\beta^*} - 0.5888.$$

The performance of the unified model was evaluated by calculating the R^2 values for each property using the normalized data and comparing them to those from the property-specific models, as summarized in Table 2. The unified model achieves lower R^2 values overall, with the largest differences observed for S (0.828 vs. 0.9406) and ω (0.8698 vs. 0.9827). These results indicate that while the generalized model effectively captures overall trends, it struggles with some properties.

Finally, to place the predictive power of the topological index in context, we compare its performance against well-established indices commonly used in the modeling of physicochemical properties. The selected indices are the first Zagreb index M_1, the second Zagreb index M_2, the Randić index R, and the inverse degree index ID. In Table 3 we show the R^2 values calculated for each property and each index.

Table 3. Comparison of R^2 values for the $M_{\alpha,\beta}$ index and well-established indices (M_1, M_2, R, ID) across the evaluated physicochemical properties of PAHs.

Property	$M_{\alpha,\beta}$	M_1	M_2	R	ID
BP	0.9923	0.9666	0.8972	0.9575	0.8794
S	0.9406	0.887	0.8167	0.8916	0.7733
ω	0.9827	0.9662	0.937	0.9444	0.8745
$\log P$	0.9785	0.9541	0.8851	0.9401	0.8498
RI	0.9983	0.9729	0.9045	0.9641	0.8893
ΔH_f	0.9462	0.9031	0.8291	0.9198	0.8273

The results in Table 3 demonstrate that $M_{\alpha,\beta}$ consistently outperforms the other indices in terms of R^2 values across all properties. The most pronounced differences are observed for BP and S, where $M_{\alpha,\beta}$ shows a clear advantage. In contrast, for ω and $\log P$, the differences are smaller, with $M_{\alpha,\beta}$ performing comparably to the best alternative indices. Overall, $M_{\alpha,\beta}$ stands out as the most predictive and reliable index for modeling the physicochemical properties of PAHs.

5. Conclusions

In this study, we have derived novel inequalities for the Gutman-Milovanović index $M_{\alpha,\beta}$, which generalizes several important topological indices. By establishing new bounds based on the minimum and maximum degrees of graphs, we have deepened the understanding of the structural properties that influence this index. Additionally, we characterized extremal graphs that achieve these bounds, providing insights into their structural configurations and illustrating the scenarios where these inequalities are tight.

Our theoretical findings have direct implications for chemical graph theory. We demonstrated the applicability of the Gutman-Milovanović index in modeling the physicochemical properties of 22 polycyclic aromatic hydrocarbons. The high coefficients of determination R^2 values suggest a robust correlation between the index and experimental data, highlighting its effectiveness as a predictive tool in quantitative structure-property relationships (QSPR). The versatility of $M_{\alpha,\beta}$ in capturing complex molecular interactions indicates its potential for applications in chemical informatics, such as drug discovery and material science.

Future research could address the complexity of properties like entropy (S) and enthalpy of formation (ΔH_f) by integrating additional molecular descriptors, such as geometric-topological parameters or vertex distance and degree-based indices. Hybrid models combining $M_{\alpha,\beta}$ with these descriptors or non-linear techniques like machine learning could improve the predictions and uncover hidden structural patterns. Additionally, refining the parameter optimization for α and β could further enhance the predictive accuracy of the Gutman-Milovanović index. Extending these inequalities to other classes of graphs and assessing the applicability to a broader range of chemical compounds, such as heterocyclic compounds or large organic molecules, remain promising directions for future exploration. A more detailed analysis of the limitations encountered in generalizing this approach could also inform the development of more tailored predictive models.

Author contributions

All the authors contributed equally to this work. All the authors have agreed and given their consent for the publication of this research paper.

Use of Generative-AI tools declaration

The authors declare they have used Artificial Intelligence (AI) tools in the creation of this article.

Conflict of interest

Prof. Jose M. Rodriguez-Garcia is the Guest Editor of special issue "Graph theory and its applications, 2nd Edition" for AIMS Mathematics. Prof. Jose M. Rodriguez-Garcia was not involved in the editorial review and the decision to publish this article.

The authors confirm that the content of this article has no conflict of interest or competing interests.

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