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General Hyperbolic Sombor Index: Theory and Applications

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Abstract. The hyperbolic Sombor index has attracted considerable attention from both theoretical and applied perspectives. In this work we study the general hyperbolic Sombor index HSO_a, obtaining optimal upper and lower bounds for HSO_a in terms of well-known indices such as the forgotten index, harmonic index, inverse degree index, max-min deg index, modified Sombor index, first Banhatti–Sombor index, diminished Sombor index, general second Zagreb index, general sum-connectivity index, and general elliptic Sombor index. Moreover, the paper presents extremal results for connected graphs, trees, and unicyclic graphs, identifying structures that maximize or minimize the index under various constraints. Furthermore, we show the applicability of the general hyperbolic Sombor index HSO_a as a structural descriptor in a quantitative structure–property relationship framework for polychlorinated biphenyls, where the parameter a is optimized for each physicochemical property. This analysis demonstrates that an appropriate choice of a provides high predictive power for several properties, yielding strong linear correlations between the general hyperbolic Sombor index and experimental data.

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1. Introduction

A topological descriptor is a numerical invariant that represents a chemical structure through its molecular graph and plays a fundamental role in mathematical chemistry, particularly in QSPR and QSAR studies. Topological descriptors that exhibit correlation with molecular properties are known as topological indices. Since the seminal work of Wiener [1], hundreds of such indices have been introduced to capture structural features relevant to physicochemical behavior.

Over the years, a wide variety of topological indices have been proposed to encode different aspects of molecular structure, including branching, cyclicity, distance distribution, and degree heterogeneity. Classical examples include distance-based indices and degree-based indices, such as the Randić connectivity index [2]. Further developments in distance-based descriptors led to highly discriminating indices, such as the Balaban and hyper-Wiener indices [3, 4].

Many of these descriptors have been extensively investigated from both theoretical and applied perspectives [5–16], particularly in relation to QSPR and QSAR modeling, where their ability to capture structural information relevant to physicochemical properties has been systematically assessed.

Topological indices based on end-vertex degrees of edges have been studied for more than five decades. Among the most prominent examples are the Randić connectivity index and the first and second Zagreb indices, defined by Gutman and Trinajstić [6] 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 d_u denotes the degree of vertex u.

Recently, new degree-based indices constructed using geometric considerations have attracted considerable attention. In this context, the harmonic index and its generalizations have been shown to possess rich mathematical structure and tight extremal bounds [17]. More recently, the Sombor index [18] and the elliptic Sombor index [19] have been introduced and shown to exhibit strong discriminative and predictive capabilities [8, 19]. Motivated by these developments, the hyperbolic Sombor index [20] was proposed as a further refinement incorporating a hyperbolic weighting scheme.

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}\,, \qquad ESO(G) = \sum_{uv \in E(G)} (d_u + d_v)\sqrt{d_u^2 + d_v^2}\,.$$

For recent results on the Sombor index and the elliptic Sombor index we refer to [18, 21–29]. Both indices were conceived using geometric considerations and have shown good predictive potential [8, 19].

Also based on geometric considerations, the *hyperbolic Sombor index* HSO [20] is defined as

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\,,$$

where the endpoints of each edge are labeled so that $d_u \leq d_v$. Equivalently,

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{\min\{d_u, d_v\}}.$$

This index introduces a hyperbolic weighting scheme that emphasizes the interplay between low and high-degree vertices, potentially capturing structural asymmetries more effectively than its predecessors. Reference [20] discusses key properties of this index, including predictive power, structural sensitivity, and degeneracy.

If $a \in \mathbb{R}$, the *general hyperbolic Sombor index* is defined in [30] as

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

The central aim of this work is to establish optimal bounds for the general hyperbolic Sombor index in terms of other well-known indices, including the forgotten index, harmonic index, inverse degree index, max-min deg index, modified Sombor index, first Banhatti-Sombor index, diminished Sombor index, general second Zagreb index, general sum-connectivity index, and general elliptic Sombor index. The results are framed in terms of graph parameters such as maximum and minimum degree, size, and regularity conditions, thereby linking the index to fundamental graph-theoretic properties.

Moreover, the paper explores extremal problems associated with HSO_a, identifying graph structures that maximize or minimize this index under various constraints. These optimization results shed light on the structural features that drive the index to its extremes.

Furthermore, we show the applicability of the general hyperbolic Sombor index $HSO_a(G)$ in a QSPR setting for polychlorinated biphenyls (PCBs), where the parameter a is systematically explored and, for each physicochemical property, an optimal value a^* is selected by maximizing the coefficient of determination R^2. This procedure reveals that the predictive capability of the index strongly depends on the choice of a and leads to high explanatory power for several properties, with multiple cases exhibiting very strong linear associations between $HSO_{a^*}(G)$ and the corresponding experimental data.

2. Optimal inequalities

Throughout this section, whenever an edge $uv \in E(G)$ is considered, we assume without loss of generality that $d_u \leq d_v$, so that $\min\{d_u, d_v\} = d_u$.

A general index that encompasses most Sombor-type indices is the first $(\alpha, \beta) - KA$ *index* of G, introduced in [31] as

$$KA_{\alpha,\beta}(G) = KA^1_{\alpha,\beta}(G) = \sum_{uv \in E(G)} \left(d_u^\alpha + d_v^\alpha\right)^\beta, \tag{1}$$

with $\alpha, \beta \in \mathbb{R}$. Note that $SO(G) = KA_{2,1/2}(G)$, the modified Sombor index is $SO^m(G) = KA_{2,-1/2}(G)$, the first Banhatti-Sombor index is $BSO(G) = KA_{-2,1/2}(G)$, and the general Sombor index is $SO_\alpha(G) = KA_{\alpha,1/\alpha}(G)$. Also, $KA_{1,\beta}(G)$ equals the general sum-connectivity index. For more information about this index, see, e.g., [32] and the references therein.

In order to obtain relations between HSO_a and $KA_{2,-a/2}$ we need the following classical result, which provides a converse of the Cauchy-Schwarz inequality (see, e.g., [33, Lemma 5] for a proof of the equality statement).

Lemma 1. *If $a_i, b_i \geq 0$ and $\omega b_i \leq a_i \leq \Omega b_i$ for $1 \leq i \leq n$, then*

$$\Big(\sum_{i=1}^{n} a_i^2\Big)\Big(\sum_{i=1}^{n} b_i^2\Big) \leq \frac{(\Omega+\omega)^2}{4\Omega\,\omega}\Big(\sum_{i=1}^{n} a_i b_i\Big)^2.$$

If $a_i > 0$ for some $1 \leq i \leq n$, then the equality holds if and only if $\omega = \Omega$ and $a_i = \omega b_i$ for every $1 \leq i \leq n$.

Theorem 1. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ, and $a > 0$. Then*

$$\frac{m^2}{\Delta^a\, KA_{2,-a/2}(G)} \leq HSO_a(G) \leq \frac{\big((\Delta^2+\delta^2)^{a/2} + 2^{\,a/2}\,\delta^a\big)^2\, m^2}{2^{2+a/2}\delta^{2a}(\Delta^2+\delta^2)^{a/2}\, KA_{2,-a/2}(G)}\,.$$

The equality holds in each bound if G is a regular graph.

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned}
\left(\sum_{uv\in E(G)} 1\right)^2 &= \left(\sum_{uv\in E(G)} \left(\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)^{1/2} \left(\left(\frac{d_u}{\sqrt{d_u^2+d_v^2}}\right)^a\right)^{1/2}\right)^2 \\
&\leq \left(\sum_{uv\in E(G)} \left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)\left(\sum_{uv\in E(G)} \left(\frac{d_u}{\sqrt{d_u^2+d_v^2}}\right)^a\right) \\
&\leq \left(\sum_{uv\in E(G)} \left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)\left(\sum_{uv\in E(G)} \left(\frac{\Delta}{\sqrt{d_u^2+d_v^2}}\right)^a\right).
\end{aligned}$$

If $d_u \leq d_v$, then

$$m^2 \leq HSO_a(G)\,\Delta^a\, KA_{2,-a/2}(G).$$

Since

$$2^{\,a/2} \leq \frac{\left(\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)^{1/2}}{\left(\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)^{1/2}} = \left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a \leq \left(\frac{\sqrt{\Delta^2+\delta^2}}{\delta}\right)^a,$$

Lemma 1 gives

$$\frac{\left((\Delta^2+\delta^2)^{a/2}+2^{\,a/2}\,\delta^a\right)^2}{2^{2+a/2}\delta^{2a}\delta^{-a}(\Delta^2+\delta^2)^{a/2}}\left(\sum_{uv\in E(G)}1\right)^2=\left(\sum_{uv\in E(G)}\left(\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)^{1/2}\left(\left(\frac{d_u}{\sqrt{d_u^2+d_v^2}}\right)^a\right)^{1/2}\right)^2$$
$$\geq\left(\sum_{uv\in E(G)}\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)\left(\sum_{uv\in E(G)}\left(\frac{d_u}{\sqrt{d_u^2+d_v^2}}\right)^a\right)$$
$$\geq\left(\sum_{uv\in E(G)}\left(\frac{\sqrt{d_u^2+d_v^2}}{d_u}\right)^a\right)\left(\sum_{uv\in E(G)}\left(\frac{\delta}{\sqrt{d_u^2+d_v^2}}\right)^a\right)$$

and so,

$$\frac{\left((\Delta^2+\delta^2)^{a/2}+2^{\,a/2}\,\delta^a\right)^2 m^2}{2^{2+a/2}\delta^a(\Delta^2+\delta^2)^{a/2}}\geq HSO_a(G)\,\delta^a\,KA_{2,-a/2}(G).$$

The equality holds in each bound if G is a regular graph, since

$$HSO_a(G)=2^{a/2}\,m,$$
$$KA_{2,-a/2}(G)=2^{-a/2}\delta^{-a}\,m,$$
$$\frac{m^2}{\Delta^a\,KA_{2,-a/2}(G)}=\frac{m^2}{\delta^a\,2^{-a/2}\delta^{-a}\,m}=2^{a/2}\,m,$$
$$\frac{\left((\Delta^2+\delta^2)^{a/2}+2^{\,a/2}\,\delta^a\right)^2 m^2}{2^{2+a/2}\delta^{2a}(\Delta^2+\delta^2)^{a/2}\,KA_{2,-a/2}(G)}=\frac{\left(2^{\,a/2}\,\delta^a+2^{\,a/2}\,\delta^a\right)^2 m^2}{2^{2+a/2}\delta^{2a}\,2^{\,a/2}\,\delta^a\,2^{-a/2}\delta^{-a}\,m}=2^{a/2}\,m.$$

The *modified Sombor index* of G was proposed in [34] as

$$SO^m(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u^2+d_v^2}}\,.$$

Theorem 1 has the following direct consequence relating the hyperbolic Sombor and the modified Sombor indices.

Corollary 1. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$\frac{m^2}{\Delta\,SO^m(G)}\leq HSO(G)\leq\frac{\left(\sqrt{\Delta^2+\delta^2}+\sqrt{2}\,\delta\right)^2 m^2}{4\sqrt{2}\,\delta^2\sqrt{\Delta^2+\delta^2}\,SO^m(G)}\,.$$

The following result relates the general hyperbolic Sombor index and $KA_{-2,a}$.

Theorem 2. *Let G be a graph with maximum degree Δ and minimum degree δ.*
(1) *If $a>0$, then*

$$2^{-a/2}\,\delta^{2a}\,KA_{-2,a}(G)\leq HSO_a(G)\leq 2^{-a/2}\,\Delta^{2a}\,KA_{-2,a}(G).$$

(2) *If $a < 0$, then*

$$2^{-a/2}\,\Delta^{2a}\,KA_{-2,a}(G) \leq HSO_a(G) \leq 2^{-a/2}\,\delta^{2a}\,KA_{-2,a}(G).$$

The equality holds in each bound if and only if G is a regular graph.

Proof. Define

$$D := \left\{(x,y) \in [\delta,\Delta]^2 : x \leq y\right\},$$

and consider the function $f : D \to \mathbb{R}$ given by

$$f(x,y) := \frac{\sqrt{x^2+y^2}}{\dfrac{x}{\dfrac{x^2+y^2}{x^2y^2}}} = xy^2\left(x^2+y^2\right)^{-1/2}.$$

We have

$$\begin{aligned}\frac{\partial f}{\partial x}(x,y) &= y^2\left(x^2+y^2\right)^{-1/2} - \frac{1}{2}\,2x\left(x^2+y^2\right)^{-3/2}xy^2\\ &= y^2\left(x^2+y^2\right)^{-3/2}\left(x^2+y^2-x^2\right)\\ &= y^4\left(x^2+y^2\right)^{-3/2} > 0\end{aligned}$$

and so, f is strictly increasing in x. Also,

$$\begin{aligned}\frac{\partial f}{\partial y}(x,y) &= 2xy\left(x^2+y^2\right)^{-1/2} - \frac{1}{2}\,2y\left(x^2+y^2\right)^{-3/2}xy^2\\ &= xy\left(x^2+y^2\right)^{-3/2}\left(2x^2+2y^2-y^2\right)\\ &= xy\left(x^2+y^2\right)^{-3/2}\left(2x^2+y^2\right) > 0\end{aligned}$$

and so, f is strictly increasing in y. Hence,

$$f(x,y) \leq f(\Delta,\Delta) = 2^{-1/2}\Delta^2,$$

and this upper bound is attained if and only if $x = y = \Delta$. Also,

$$f(x,y) \geq f(\delta,\delta) = 2^{-1/2}\,\delta^2,$$

and this lower bound is attained if and only if $x = y = \delta$. Consequently,

$$\begin{aligned}2^{-1/2}\,\delta^2\left(d_u^{-2}+d_v^{-2}\right) = 2^{-1/2}\,\delta^2\,\frac{d_u^2+d_v^2}{d_u^2d_v^2} &\leq \frac{\sqrt{d_u^2+d_v^2}}{d_u}\\ &\leq 2^{-1/2}\Delta^2\,\frac{d_u^2+d_v^2}{d_u^2d_v^2} = 2^{-1/2}\Delta^2\left(d_u^{-2}+d_v^{-2}\right).\end{aligned}$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

The equality holds in the bounds involving δ (respectively, Δ) if and only if $d_u = d_v = \delta$ (respectively, $d_u = d_v = \Delta$) for every $uv \in E(G)$, and this holds if and only if G is a regular graph.

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 [35]. Since then its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, and Wiener index, has been studied by several authors (see, e.g., [36–43]).

The following direct consequence of Theorem 2 relates the hyperbolic Sombor index and the inverse degree index.

Corollary 2. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$2^{-1/2} \, \delta^2 \, ID(G) \leq HSO(G) \leq 2^{-1/2} \Delta^2 \, ID(G).$$

The equality holds in each bound if and only if G is a regular graph.

The following result relates the general hyperbolic Sombor index and $KA_{-2,a/2}$.

Theorem 3. *Let G be a graph with maximum degree Δ and minimum degree δ.*
(1) *If $a > 0$, then*

$$\delta^a \, KA_{-2,a/2}(G) \leq HSO_a(G) \leq \Delta^a \, KA_{-2,a/2}(G).$$

The equality holds in the lower bound if and only if G is a regular graph. The equality holds in the upper bound if and only if every edge of G is incident to a vertex with degree Δ.
(2) *If $a < 0$, then*

$$\Delta^a \, KA_{-2,a/2}(G) \leq HSO_a(G) \leq \delta^a \, KA_{-2,a/2}(G).$$

The equality holds in the upper bound if and only if G is a regular graph. The equality holds in the lower bound if and only if every edge of G is incident to a vertex with degree Δ.

Proof. If $d_u \leq d_v$, then

$$\delta \left(d_u^{-2} + d_v^{-2} \right)^{1/2} \leq \frac{\sqrt{d_u^2 + d_v^2}}{d_u} = d_v \, \frac{\sqrt{d_u^2 + d_v^2}}{d_u d_v} \leq \Delta \left(d_u^{-2} + d_v^{-2} \right)^{1/2} .$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

The above argument implies that the equality in each bound involving δ holds if and only if $\delta \leq d_u \leq d_v = \delta$ (i.e., $d_u = d_v = \delta$) for every $uv \in E(G)$, and this holds if and only if G is a regular graph.

Also, the equality in each bound involving Δ holds if and only if $d_u \leq d_v = \Delta$ for every $uv \in E(G)$, and this holds if and only if every edge of G is incident to a vertex with degree Δ.

The *first Banhatti-Sombor index* [44] is defined by

$$BSO(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}}\,.$$

The following consequence of Theorem 3 relates the hyperbolic Sombor and the first Banhatti-Sombor indices.

Corollary 3. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$\delta\, BSO(G) \leq HSO(G) \leq \Delta\, BSO(G).$$

The equality holds in the lower bound if and only if G is a regular graph. The equality holds in the upper bound if and only if every edge of G is incident to a vertex with degree Δ.

The following result relates the general hyperbolic Sombor index and $KA_{2,a}$.

Theorem 4. *Let G be a graph with maximum degree Δ and minimum degree δ.*
(1) *If $a > 0$, then*

$$2^{-a/2}\,\Delta^{-2a}\,KA_{2,a}(G) \leq HSO_a(G) \leq 2^{-a/2}\,\delta^{-2a}\,KA_{2,a}(G).$$

(2) *If $a < 0$, then*

$$2^{-a/2}\,\delta^{-2a}\,KA_{2,a}(G) \leq HSO_a(G) \leq 2^{-a/2}\,\Delta^{-2a}\,KA_{2,a}(G).$$

The equality holds in each bound if and only if G is a regular graph.

Proof. If $d_u \leq d_v$, then

$$\frac{d_u^2 + d_v^2}{\sqrt{2}\,\Delta^2} \leq \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\,\frac{\sqrt{d_u^2 + d_v^2}}{\sqrt{d_u^2 + d_v^2}} \leq \frac{d_u^2 + d_v^2}{\sqrt{2}\,\delta^2}\,.$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

The above argument implies that the equality in the bounds involving Δ (respectively, δ) holds if and only if $d_u = d_v = \Delta$ (respectively, $d_u = d_v = \delta$) for every $uv \in E(G)$, and this holds if and only if G is a regular graph.

In the same paper in which the Zagreb indices were introduced, the *forgotten topological index* (or *F-index*) was defined as

$$F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2).$$

Both the forgotten topological index and the first Zagreb index were used in formulas for the total π-electron energy [6] as measures of the branching of the carbon-atom skeleton of the underlying molecule. However, the F-index received little attention until Furtula and Gutman [45] established some of its basic properties and showed that its predictive ability is comparable to that of the first Zagreb index. For entropy and the acentric factor, both indices yield correlation coefficients greater than 0.95. They also showed that the F-index can provide accurate predictions of the logarithm of the octanol–water partition coefficient. Additional bounds for the forgotten index can be found in [46].

The following direct consequence of Theorem 4 relates the hyperbolic Sombor and the forgotten indices.

Corollary 4. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$2^{-1/2}\,\Delta^{-2}\,F(G) \leq HSO(G) \leq 2^{-1/2}\,\delta^{-2}\,F(G).$$

The equality holds in each bound if and only if G is a regular graph.

The following lower bound for the hyperbolic Sombor index also involves the number of edges of the graph.

Proposition 1. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$\left(\sqrt{1+\frac{\Delta^2}{\delta^2}}+\sqrt{2}\right) HSO(G) \geq \frac{1}{\Delta^2}\,F(G) + \sqrt{2}\sqrt{1+\frac{\Delta^2}{\delta^2}}\;m.$$

The equality holds for every regular graph.

Proof. Let us consider the strictly increasing function $\sqrt{1+t^2}$ on the interval $[1, \Delta/\delta]$. We have

$$\left(\sqrt{1+t^2}-\sqrt{2}\right)\left(\sqrt{1+\frac{\Delta^2}{\delta^2}}-\sqrt{1+t^2}\right) \geq 0,$$

$$\left(\sqrt{1+\frac{\Delta^2}{\delta^2}}+\sqrt{2}\right)\sqrt{1+t^2} \geq 1+t^2+\sqrt{2}\sqrt{1+\frac{\Delta^2}{\delta^2}}\,.$$

If $d_u \leq d_v$ and $t = d_v/d_u$, then

$$\begin{aligned}\left(\sqrt{1+\frac{\Delta^2}{\delta^2}}+\sqrt{2}\right)\frac{\sqrt{d_u^2+d_v^2}}{d_u} &\geq \frac{d_u^2+d_v^2}{d_u^2}+\sqrt{2}\sqrt{1+\frac{\Delta^2}{\delta^2}} \\ &\geq \frac{d_u^2+d_v^2}{\Delta^2}+\sqrt{2}\sqrt{1+\frac{\Delta^2}{\delta^2}}\,.\end{aligned}$$

If we add the term corresponding to each edge, we obtain the desired bound.

Assume that G is a regular graph. Therefore,

$$\left(\sqrt{1+\frac{\Delta^2}{\delta^2}}+\sqrt{2}\right) HSO(G) = \left(\sqrt{2}+\sqrt{2}\right)\sqrt{2}\, m = 4m,$$

$$\frac{1}{\Delta^2}\, F(G) + \sqrt{2}\sqrt{1+\frac{\Delta^2}{\delta^2}}\, m = \frac{1}{\Delta^2}\, 2\Delta^2 m + \sqrt{2}\,\sqrt{2}\, m = 4m.$$

The *max-min deg index* is one of the Adriatic indices introduced in [47]. It is defined as

$$MD(G) = \sum_{uv\in E(G)} \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}\,.$$

This index is interesting from an applied viewpoint since it is a good predictor of density for octane isomers [47].

The following result relates the hyperbolic Sombor and the max-min deg indices.

Theorem 5. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$\frac{1}{\sqrt{2}}\, MD(G) + \frac{m}{\sqrt{2}} \le HSO(G) \le MD(G) + \left(\sqrt{2}-1\right) m.$$

The equality holds in each bound if and only if each connected component of G is a regular graph.

Proof. Consider the function

$$f(t) = \sqrt{1+t^2} - t - \sqrt{2} + 1$$

for every $t \ge 1$. We have

$$f'(t) = \frac{t}{\sqrt{1+t^2}} - 1 < 0$$

and so, $f(t) \le f(1) = 0$, i.e.,

$$\sqrt{1+t^2} \le t + \sqrt{2} - 1$$

for every $t \ge 1$, and the equality holds if and only if $t = 1$, since f is strictly decreasing. Also,

$$\sqrt{1+t^2} \ge \frac{1+t}{\sqrt{2}}$$

for every $t \ge 0$, and the equality holds if and only if $t = 1$.

If $d_u \le d_v$, then

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

If we add the term corresponding to each edge, we obtain the desired bounds.

The above argument implies that the equality in each bound holds if and only if $d_u = d_v$ for every $uv \in E(G)$, and this holds if and only if each connected component of G is a regular graph.

The sum-connectivity index χ was introduced in [48]. It has been shown that it correlates well with the π-electronic energy of benzenoid hydrocarbons [49]. Further applications of χ can be found in [7]. This index was extended to the *general sum-connectivity index* in the paper [50], that 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. See [46, 51] for some studies on this index.

The bounds involving $2^{3a/2}\delta^a$ appear in [30]; the remaining bounds improve those obtained in [30].

Recall that a graph with maximum degree Δ and minimum degree $\delta < \Delta$ is *biregular* if it is a bipartite graph for which every vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ.

Theorem 6. *Let G be a graph with maximum degree Δ and minimum degree δ.*

(1) *If $a > 0$, then*

$$2^{3a/2}\,\delta^a\,\chi_{-a}(G) \le HSO_a(G) \le \delta^{-a}(\Delta+\delta)^a(\Delta^2+\delta^2)^{a/2}\,\chi_{-a}(G).$$

The equality holds in the lower bound if and only if G is a regular graph, and in the upper bound if and only if G is either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

(2) *If $a < 0$, then*

$$\delta^{-a}(\Delta+\delta)^a(\Delta^2+\delta^2)^{a/2}\,\chi_{-a}(G) \le HSO_a(G) \le 2^{3a/2}\,\delta^a\,\chi_{-a}(G).$$

The equality holds in the upper bound if and only if G is a regular graph, and in the lower bound if and only if G is either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

Proof. Define

$$D := \left\{(x,y) \in [\delta,\Delta]^2 : x \le y\right\},$$

and consider the function $f : D \to \mathbb{R}$ given by

$$f(x,y) := \frac{(x^2+y^2)(x+y)^2}{x^2}.$$

It is clear that f is strictly increasing in y. Also,

$$\begin{aligned}
\frac{\partial f}{\partial x}(x,y) &= \frac{(2x(x+y)^2 + 2(x^2+y^2)(x+y))x^2 - (x^2+y^2)(x+y)^2 2x}{x^4} \\
&= \frac{2(x+y)}{x^3}\big((x(x+y)+x^2+y^2)x - (x^2+y^2)(x+y)\big) \\
&= \frac{2(x+y)}{x^3}\big(x^3 - y^3\big) < 0
\end{aligned}$$

for every $x < y$ and so, f is strictly decreasing in x on D. Hence,

$$f(x,y) \leq f(\delta,y) \leq f(\delta,\Delta) = \delta^{-2}(\Delta^2+\delta^2)(\Delta+\delta)^2,$$

and this upper bound is attained if and only if $x = \delta$ and $y = \Delta$. Also,

$$f(x,y) \geq f(y,y) = 8y^2 \geq 8\delta^2,$$

and this lower bound is attained if and only if $x = y = \delta$. Consequently,

$$8\delta^2 \leq \frac{(x^2+y^2)(x+y)^2}{x^2} \leq \delta^{-2}(\Delta^2+\delta^2)(\Delta+\delta)^2,$$

$$8\delta^2(x+y)^{-2} \leq \frac{x^2+y^2}{x^2} \leq \delta^{-2}(\Delta^2+\delta^2)(\Delta+\delta)^2(x+y)^{-2},$$

$$2^{3/2}\delta(d_u+d_v)^{-1} \leq \frac{\sqrt{d_u^2+d_v^2}}{d_u} \leq \delta^{-1}(\Delta^2+\delta^2)^{1/2}(\Delta+\delta)(d_u+d_v)^{-1}.$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

If $a > 0$ (respectively, $a < 0$), the equality holds in the lower (respectively, upper) bound if and only if $d_u = d_v = \delta$ for every $uv \in E(G)$, and this holds if and only if G is a regular graph. The equality holds in the upper (respectively, lower) bound if and only if $d_u = \delta$ and $d_v = \Delta$ for every $uv \in E(G)$, and this holds if and only if G is either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

Theorem 6 has the following consequence relating hyperbolic Sombor and harmonic indices.

Corollary 5. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$2^{1/2}\,\delta\,H(G) \leq HSO(G) \leq (2\delta)^{-1}(\Delta+\delta)(\Delta^2+\delta^2)^{1/2}\,H(G).$$

The equality holds in the lower bound if and only if G is a regular graph, and in the upper bound if and only if G is either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

The *general elliptic Sombor index* ESO_a is defined for $a \in \mathbb{R}$ in [27] as

$$ESO_a(G) = \sum_{uv \in E(G)} (d_u+d_v)^a \left(d_u^2+d_v^2\right)^{a/2}.$$

The following result relates the general hyperbolic and the general elliptic Sombor indices.

Theorem 7. *Let G be a graph with maximum degree Δ and minimum degree δ, and $a \in \mathbb{R}$.*

(1) *If $a > 0$, then*

$$2^{-a}\,\Delta^{-2a}\,ESO_a(G) \leq HSO_a(G) \leq 2^{-a}\,\delta^{-2a}\,ESO_a(G).$$

(2) *If $a < 0$, then*

$$2^{-a}\,\delta^{-2a}\,ESO_a(G) \leq HSO_a(G) \leq 2^{-a}\,\Delta^{-2a}\,ESO_a(G).$$

The equality holds in each bound if and only if G is a regular graph.

Proof. If $d_u \leq d_v$, then

$$\frac{(d_u+d_v)\sqrt{d_u^2+d_v^2}}{2\Delta^2} \leq \frac{\sqrt{d_u^2+d_v^2}}{d_u}\,\frac{d_u+d_v}{d_u+d_v} \leq \frac{(d_u+d_v)\sqrt{d_u^2+d_v^2}}{2\delta^2}\,.$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

The above argument implies that the equality holds in the bounds involving Δ (respectively, δ) if and only if $d_u = d_v = \Delta$ (respectively, $d_u = d_v = \delta$) for every $uv \in E(G)$, and this holds if and only if G is a regular graph.

Miličević and Nikolić defined in [52] the *general first and second Zagreb indices* as

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

respectively, with $a \in \mathbb{R}$. Note that M_1^1 is $2m$, M_1^2 is the first Zagreb index M_1, M_1^{-1} is the inverse index $ID(G)$ [35], M_1^3 is the forgotten index $F(G)$, etc.; also, $M_2^{-1/2}$ is the usual Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified Zagreb index [53], etc. Note that it is interesting to study M_1^α for $\alpha \neq 0, 1$, and M_2^α for $\alpha \neq 0$, since if G has n vertices and m vertices, then $M_1^0(G) = n$, $M_1^1(G) = 2m$ and $M_2^0(G) = m$.

The following result relates the general hyperbolic Sombor and the general second Zagreb indices.

Theorem 8. *Let G be a graph with maximum degree Δ and minimum degree δ, and $a \in \mathbb{R}$.*
(1) *If $a > 0$, then*

$$2^{a/2}\,\Delta^{-2a}\,M_2^a(G) \leq HSO_a(G) \leq 2^{a/2}\,\delta^{-2a}\,M_2^a(G).$$

(2) *If $a < 0$, then*

$$2^{a/2}\,\delta^{-2a}\,M_2^a(G) \leq HSO_a(G) \leq 2^{a/2}\,\Delta^{-2a}\,M_2^a(G).$$

The equality holds in each bound if and only if G is a regular graph.

Proof. Define

$$D := \left\{(x,y) \in [\delta,\Delta]^2 : x \leq y\right\},$$

and consider the function $f : D \to \mathbb{R}$ given by

$$g(x,y) := \frac{xy}{\frac{\sqrt{x^2+y^2}}{x}} = x^2 y\left(x^2+y^2\right)^{-1/2}.$$

The argument in the proof of Theorem 2 gives that f is strictly increasing in each variable on D. Then,

$$g(x,y) \leq g(\Delta,\Delta) = 2^{-1/2}\Delta^2,$$

and this upper bound is attained if and only if $x = y = \Delta$; also

$$g(x, y) \geq g(\delta, \delta) = 2^{-1/2}\, \delta^2,$$

and this lower bound is attained if and only if $x = y = \delta$. Consequently,

$$2^{-1/2}\, \delta^2\, \frac{\sqrt{d_u^2 + d_v^2}}{d_u} \leq d_u d_v \leq 2^{-1/2} \Delta^2\, \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\,.$$

If we take the power a and add the term corresponding to each edge, we obtain the desired bounds.

The previous argument shows that the equality holds in the bounds involving Δ (respectively, δ) if and only if $d_u = d_v = \Delta$ (respectively, $d_u = d_v = \delta$) for every $uv \in E(G)$, and this holds if and only if G is a regular graph.

The *diminished Sombor index* of a graph G is defined as

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

Although DSO was introduced as early as in 2021 [54], its properties have not been studied until now [55], where its chemical applicability is shown in the study of the properties of octanes.

The following result relates the hyperbolic Sombor and the diminished Sombor indices.

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

$$2\, DSO(G) \leq HSO(G) \leq \left(1 + \frac{\Delta}{\delta}\right) DSO(G).$$

The equality holds in the lower bound if and only if each connected component of G is a regular graph. The equality holds in the upper bound if and only if G is a either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

Proof. If $d_u \leq d_v$, then

$$2\, \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} \leq \frac{\sqrt{d_u^2 + d_v^2}}{d_u} = \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\, \frac{d_u + d_v}{d_u + d_v} \leq \left(1 + \frac{\Delta}{\delta}\right) \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v}\,.$$

If we add the term corresponding to each edge, we obtain the desired bounds.

The above argument implies that the equality in the lower bound holds if and only if $2d_u = d_u + d_v$ for every $uv \in E(G)$, i.e. $d_u = d_v$ for every $uv \in E(G)$, and this holds if and only if each connected component of G is a regular graph.

The equality in the upper bound holds if and only if $d_u = \delta$ and $d_v = \Delta$ for every $uv \in E(G)$, and this holds if and only if G is a either a regular (when $\Delta = \delta$) or a biregular (when $\Delta > \delta$) graph.

We finish this section by relating the hyperbolic Sombor index with another geometric parameter of a graph.

The study of Gromov hyperbolicity on graphs is a subject of increasing interest, both in pure and applied mathematics (see, e.g., [56–65] and the references therein). A graph is said to be *t-hyperbolic*, with $t \geq 0$, if any side in every geodesic triangle is contained in the t-neighborhood of the union of the other two sides. Define the *hyperbolicity constant* $\delta_0(G)$ of the graph G as the infimum of the constants $t \geq 0$ such that G is t-hyperbolic. We emphasize that $\delta_0(G)$ denotes the hyperbolicity constant, whereas δ denotes the minimum degree of G. In order to compute distances in graphs, every edge is assumed to have length 1.

The following inequality relates the hyperbolic Sombor index with the hyperbolicity constant $\delta_0(G)$.

Theorem 10. *Let G be a graph and $a > 0$. Then*

$$HSO_a(G) \geq 2^{2+a/2}\, \delta_0(G).$$

Proof. Let m be the cardinality of the set $E(G)$. We know that $HSO_a(G) \geq 2^{a/2} m$.

By [66, Theorem 19], we have $\delta_0(G) \leq m/4$ and so, $m \geq 4\delta_0(G)$. Hence, the desired inequality holds.

3. Optimization results for connected graphs

The optimization problems for this index have an obstacle: even if $a = 1$, to add an edge can increase or decrease the value of the hyperbolic Sombor index, as the following example shows: Consider the graph G_0 obtained by removing an edge from K_4, the complete graph with 4 vertices. By removing an appropriate edge from G_0 we obtain C_4, the cycle graph with 4 vertices. However,

$$\begin{aligned} HSO(G_0) &= \sqrt{2} + 2\sqrt{13} \approx 8.62, \\ HSO(K_4) &= 6\sqrt{2} \approx 8.49, \\ HSO(C_4) &= 4\sqrt{2} \approx 5.66, \end{aligned}$$

and therefore, $HSO(G_0) > HSO(K_4)$ and $HSO(G_0) > HSO(C_4)$.

We need the following technical result.

Lemma 2. *Let $0 < a \leq b$, $\alpha > 0$ and let $g : [a, b] \to \mathbb{R}$ be the function defined as*

$$g(t) = \left(1 + \frac{b^2}{t^2}\right)^{\alpha} + \left(1 + \frac{t^2}{a^2}\right)^{\alpha}.$$

Then

$$g(t) \leq \max\{g(a), g(b)\}$$

for every $t \in [a, b]$.

Proof. It suffices to consider the case $a < b$. We have

$$g'(t) = -2\,\alpha\,b^2 t^{-3}\left(1+\frac{b^2}{t^2}\right)^{\alpha-1} + \frac{2\,\alpha}{a^2}\,t\left(1+\frac{t^2}{a^2}\right)^{\alpha-1}.$$

Since

$$\begin{aligned} g'(a) &= -2\,\alpha\,b^2 a^{-3}\left(1+\frac{b^2}{a^2}\right)^{\alpha-1} + \frac{2\,\alpha}{a^2}\,a\left(1+\frac{a^2}{a^2}\right)^{\alpha-1} \\ &= \frac{2\,\alpha}{a}\left(2^{\alpha-1} - \frac{b^2}{a^2}\left(1+\frac{b^2}{a^2}\right)^{\alpha-1}\right), \end{aligned}$$

we trivially have $g'(a) < 0$ if $\alpha \geq 1$. Assume now that $0 < \alpha < 1$. Thus, $\frac{1}{1-\alpha} > 1$ and

$$\begin{aligned} 1+\frac{b^2}{a^2} &< 2\left(\frac{b^2}{a^2}\right)^{\frac{1}{1-\alpha}}, \\ \left(1+\frac{b^2}{a^2}\right)^{1-\alpha} &< \frac{b^2}{a^2}\,2^{1-\alpha}, \\ g'(a) &= \frac{2\,\alpha}{a}\left(2^{\alpha-1} - \frac{b^2}{a^2}\left(1+\frac{b^2}{a^2}\right)^{\alpha-1}\right) < 0\,, \end{aligned}$$

also when $0 < \alpha < 1$.

Hence, it suffices to prove that g' has at most one zero on $(0,\infty)$. (If g' does not have zeros on (a,b), then g is decreasing on (a,b) and its maximum is attained at a; if g' has one zero t_0 on (a,b), then g is decreasing on (a,t_0) and increasing on (t_0,b), or g is decreasing on (a,b), and the conclusion holds in both cases.) We have the equivalences

$$\begin{aligned} g'(t) = -2\,\alpha\,b^2 t^{-3}\left(1+\frac{b^2}{t^2}\right)^{\alpha-1} + \frac{2\,\alpha}{a^2}\,t\left(1+\frac{t^2}{a^2}\right)^{\alpha-1} &= 0\,, \\ t^4\left(1+\frac{t^2}{a^2}\right)^{\alpha-1} &= a^2b^2\left(1+\frac{b^2}{t^2}\right)^{\alpha-1}, \\ t^4\left(\frac{t^2(t^2+a^2)}{a^2(t^2+b^2)}\right)^{\alpha-1} &= a^2b^2. \end{aligned}$$

If $\alpha \geq 1$, then the function

$$t^4\left(\frac{t^2(t^2+a^2)}{a^2(t^2+b^2)}\right)^{\alpha-1}$$

is increasing on $(0,\infty)$ and so, the proof is finished. Assume now that $0 < \alpha < 1$. Thus, $g'(t) = 0$ is equivalent to

$$\begin{aligned} t^{\frac{2\alpha+2}{\alpha-1}}\,\frac{t^2+a^2}{t^2+b^2} &= a^2(ab)^{\frac{2}{\alpha-1}}, \\ t^{\frac{2\alpha+2}{1-\alpha}}\,\frac{t^2+b^2}{t^2+a^2} &= a^{-2}(ab)^{\frac{2}{1-\alpha}}. \end{aligned}$$

If we make the change of variable $x = t^2$, then it suffices to show that the function

$$h(x) = x^\beta \, \frac{x + b^2}{x + a^2}, \qquad \text{with } \beta = \frac{1+\alpha}{1-\alpha} > 1,$$

is increasing on $(0, \infty)$. We have

$$\begin{aligned} h'(x) &= \beta x^{\beta-1} \, \frac{x + b^2}{x + a^2} + x^\beta \, \frac{x + a^2 - (x + b^2)}{(x + a^2)^2} \\ &= \frac{x^{\beta-1}}{(x + a^2)^2} \left(\beta(x + b^2)(x + a^2) - x(b^2 - a^2)\right) \\ &> \frac{x^{\beta-1}}{(x + a^2)^2} \left((x + b^2)(x + a^2) - x(b^2 - a^2)\right), \end{aligned}$$

and so, if suffices to prove that

$$\begin{aligned} (x + b^2)(x + a^2) - x(b^2 - a^2) > 0, \\ x^2 + 2a^2x + a^2b^2 > 0, \end{aligned}$$

for every $x > 0$, and this is direct.

For each $n \geq 3$, let S_n^* be the unicyclic graph obtained from the star graph S_n with n vertices by adding an edge connecting two vertices of degree 1.

Proposition 2. *Let G be a connected graph with m edges such that is not a tree and there is no vertex with degree $m - 1$, and $a \geq 1$. Then*

$$HSO_a(G) < HSO_a(S_m^*) = (m-3)\left(1 + (m-1)^2\right)^{a/2} + 2\left(1 + \frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2}.$$

Proof. Since G is not a tree, we have $m \geq 3$. If $m = 3$, then $G = C_3 = S_3^*$ and every vertex has degree $2 = m - 1$. Hence, we can assume that $m \geq 4$.

Since there is no vertex with degree $m - 1$, every vertex has degree at most $m - 2$. Since G is not a tree, there exists a cycle C in G.

Case 1. Assume that the cycle C has length greater than 3.

Each edge in the cycle contributes to $HSO_a(G)$ at most

$$\left(1 + \frac{(m-2)^2}{4}\right)^{a/2}.$$

The contribution of each other edge is at most

$$\left(1 + (m-2)^2\right)^{a/2}.$$

Since C has at least 4 edges, we obtain

$$HSO_a(G) \leq 4\left(1 + \frac{(m-2)^2}{4}\right)^{a/2} + (m-4)\left(1 + (m-2)^2\right)^{a/2}.$$

We have

$$HSO_a(S_m^*) = (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2}.$$

Note that $m^2-2m+2 \geq m^2-4m+8$ for $m \geq 4$ implies

$$\frac{1+(m-1)^2}{1+\frac{(m-2)^2}{4}} \geq 4,$$

and since $a \geq 1$, we have

$$\left(\frac{1+(m-1)^2}{1+\frac{(m-2)^2}{4}}\right)^{a/2} \geq \left(\frac{1+(m-1)^2}{1+\frac{(m-2)^2}{4}}\right)^{1/2} \geq 2\,,$$

$$2\left(1+\frac{(m-2)^2}{4}\right)^{a/2} \leq \left(1+(m-1)^2\right)^{a/2}.$$

Hence,

$$\begin{aligned}
HSO_a(G) &\leq 4\left(1+\frac{(m-2)^2}{4}\right)^{a/2} + (m-4)\left(1+(m-2)^2\right)^{a/2} \\
&\leq 2\left(1+\frac{(m-2)^2}{4}\right)^{a/2} + \left(1+(m-1)^2\right)^{a/2} + (m-4)\left(1+(m-2)^2\right)^{a/2} \\
&\leq (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} \\
&< (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2} \\
&= HSO_a(S_m^*).
\end{aligned}$$

Case 2. Assume now that the cycle C has length 3.

Let $u, v, w \in V(G)$ be the vertices in C, with $2 \leq d_u \leq d_v \leq d_w \leq m-2$. We have

$$\begin{aligned}
HSO_a(G) &\leq \left(1+\frac{d_w^2}{d_u^2}\right)^{a/2} + \left(1+\frac{d_w^2}{d_v^2}\right)^{a/2} + \left(1+\frac{d_v^2}{d_u^2}\right)^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2} \\
&\leq \left(1+\frac{(m-2)^2}{4}\right)^{a/2} + \left(1+\frac{(m-2)^2}{d_v^2}\right)^{a/2} + \left(1+\frac{d_v^2}{4}\right)^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2}.
\end{aligned}$$

Consider the function

$$g(t) = \left(1+\frac{(m-2)^2}{t^2}\right)^{a/2} + \left(1+\frac{t^2}{4}\right)^{a/2}$$

on the interval $[2, m-2]$ (recall that $m \geq 4$). By Lemma 2,

$$\begin{aligned} g(t) &\leq \max\{g(2), g(m-2)\} \\ &= \max\left\{\left(1+\frac{(m-2)^2}{4}\right)^{a/2} + 2^{a/2},\ 2^{a/2} + \left(1+\frac{(m-2)^2}{4}\right)^{a/2}\right\} \\ &= 2^{a/2} + \left(1+\frac{(m-2)^2}{4}\right)^{a/2} \end{aligned}$$

for every $t \in [2, m-2]$. Thus,

$$\begin{aligned} HSO_a(G) &\leq \left(1+\frac{(m-2)^2}{4}\right)^{a/2} + \left(1+\frac{(m-2)^2}{d_v^2}\right)^{a/2} + \left(1+\frac{d_v^2}{4}\right)^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2} \\ &\leq 2\left(1+\frac{(m-2)^2}{4}\right)^{a/2} + 2^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2} \\ &< (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2} \\ &= HSO_a(S_m^*). \end{aligned}$$

Thus, the result follows.

Proposition 2 allows to obtain this known result [30].

Corollary 6. *Let G be a unicyclic connected graph with m edges, and $a \geq 1$. Then*

$$HSO_a(G) \leq (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2}.$$

The equality holds if and only if $G = S_m^*$.

Proof. Denote by n the cardinality of the set of the vertices $V(G)$. Since G is a unicyclic connected graph, we have $n = m$.

If there is no vertex with degree $m-1 = n-1$, then Proposition 2 gives $HSO_a(G) < HSO_a(S_m^*)$.

If there is a vertex with degree $m-1 = n-1$, then $G = S_m^*$.

Theorem 11. *Let G be a connected graph with m edges that it is not a tree, and $a \geq 1$. Then*

$$HSO_a(G) \leq (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2}.$$

The equality holds if and only if $G = S_m^*$.

Proof. If G is a unicyclic graph, then Corollary 6 gives the result.

Assume now that G has at least two cycles. If n denotes the cardinality of the set of the vertices $V(G)$, then $m \geq n+1$. Since $m-1 \geq n$, there is no vertex with degree $m-1$, and Proposition 2 finishes the proof.

Finally, we obtain a valid result for values of a less than 1.

Theorem 12. *Let G be a connected graph with m edges and a cycle C with odd length without vertices of degree $m-1$, and $a > 0$. Then*

$$HSO_a(G) < HSO_a(S_m^*) = (m-3)\left(1+(m-1)^2\right)^{a/2} + 2\left(1+\frac{(m-1)^2}{4}\right)^{a/2} + 2^{a/2}.$$

Proof. Let $C = \{v_1, \ldots, v_k\}$ be a cycle in G with odd k without vertices of degree $m-1$. We are going to prove that there exists $1 \leq i \leq k$ with $d_{v_{i-1}} \leq d_{v_i} \leq d_{v_{i+1}}$ or $d_{v_{i-1}} \geq d_{v_i} \geq d_{v_{i+1}}$ (if $v_0 = v_k$ and $v_{k+1} = v_1$).

Let us assume that neither $d_{v_0} \leq d_{v_1} \leq d_{v_2}$ nor $d_{v_0} \geq d_{v_1} \geq d_{v_2}$ happens. We can assume that $d_{v_1} < d_{v_0}, d_{v_2}$, since the case $d_{v_1} > d_{v_0}, d_{v_2}$ is similar. If $d_{v_2} \leq d_{v_3}$, then $i = 2$; otherwise, $d_{v_2} > d_{v_3}$. If $d_{v_3} \geq d_{v_4}$, then $i = 3$; otherwise, $d_{v_3} < d_{v_4}$. Since k is odd, we obtain the desired i by iterating this process.

Let $u, v, w \in V(G)$ be consecutive vertices in C with $2 \leq d_u \leq d_v \leq d_w \leq m-2$. We have

$$\begin{aligned} HSO_a(G) &\leq \left(1+\frac{d_w^2}{d_u^2}\right)^{a/2} + \left(1+\frac{d_w^2}{d_v^2}\right)^{a/2} + \left(1+\frac{d_v^2}{d_u^2}\right)^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2} \\ &\leq \left(1+\frac{(m-2)^2}{4}\right)^{a/2} + \left(1+\frac{(m-2)^2}{d_v^2}\right)^{a/2} + \\ &\qquad + \left(1+\frac{d_v^2}{4}\right)^{a/2} + (m-3)\left(1+(m-2)^2\right)^{a/2} \end{aligned}$$

and so, the argument in the proof of Case 2 in Proposition 2 (which works for $a > 0$) gives the result.

4. Application to the study of physicochemical properties of PCBs

In this section, we investigate the performance of the topological index $HSO_a(G)$ as a structural descriptor within a quantitative structure–property relationship (QSPR) framework for polychlorinated biphenyls (PCBs). The data set comprises 209 congeners for which several physicochemical properties have been reported experimentally [67, 68]. The properties considered are melting point (MP), relative retention time (RRT), octanol–water partition coefficient ($\log P$), total surface area (TSA), Henry's law constant ($\log H$), aqueous solubility ($\log S_w$), water activity coefficient ($\log Y_w$), and relative enthalpy of formation (dHf). Due to incomplete experimental coverage, the statistical analysis is performed independently for each property. This approach ensures that all available data are used while avoiding biases introduced by uneven sample sizes.

The index $HSO_a(G)$ depends on a real-valued parameter a, which modulates the contribution of vertex degrees to the overall topological descriptor. Rather than prescribing a fixed value of a, we explore its influence on the quality of linear structure–property relationships. For each physicochemical property, the coefficient of determination R^2 is evaluated as a function of $a \in [-4, 4]$ with a 0.01 resolution. The optimal value a^* is then defined as the value that maximizes R^2 for the corresponding property. The resulting dependence of R^2 on a is summarized in Figure 1.

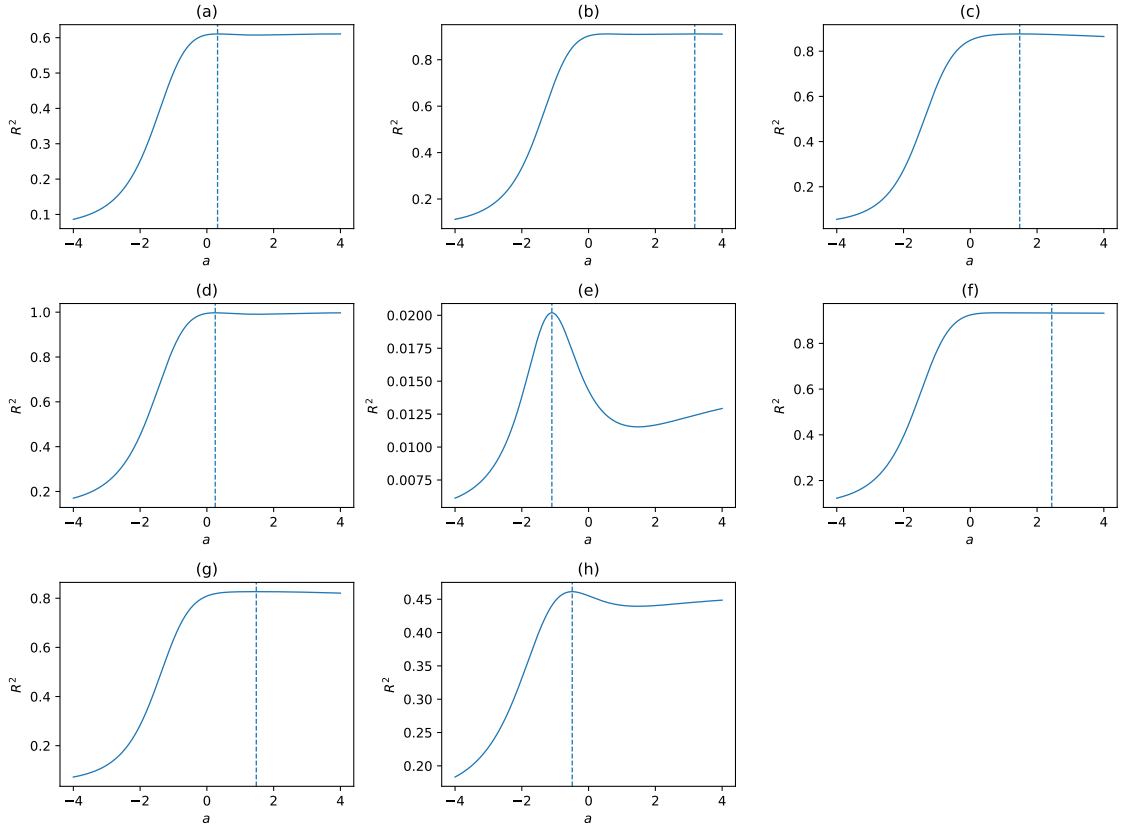

Figure 1: Dependence of the coefficient of determination (R^2) on the parameter a for the index $HSO_a(G)$. Each panel corresponds to a different physicochemical property of PCBs: (a) MP, (b) RRT, (c) $\log P$, (d) TSA, (e) $\log H$, (f) $\log S_w$, (g) $\log Y_w$, and (h) dHf. The vertical dashed line indicates the value a^* at which R^2 is maximized for each property.

Once the optimal parameter a^* has been identified for each property, linear regression models of the form

$$P = c_1\, HSO_{a^*}(G) + c_2$$

are constructed, where P denotes the experimental property value and (c_1, c_2) are regression coefficients estimated by ordinary least squares (OLS). The quality of each model is assessed using the Pearson correlation coefficient r, the coefficient of determination R^2, the standard error of the estimate, and the Fisher F-statistic with its associated significance

level.

Scatter plots of P versus $HSO_{a^*}(G)$, together with the corresponding regression lines, are shown in Figure 2. These plots provide a direct visual comparison of the linear behaviour observed across different properties. The estimated regression parameters and statistical indicators are reported in Table 1.

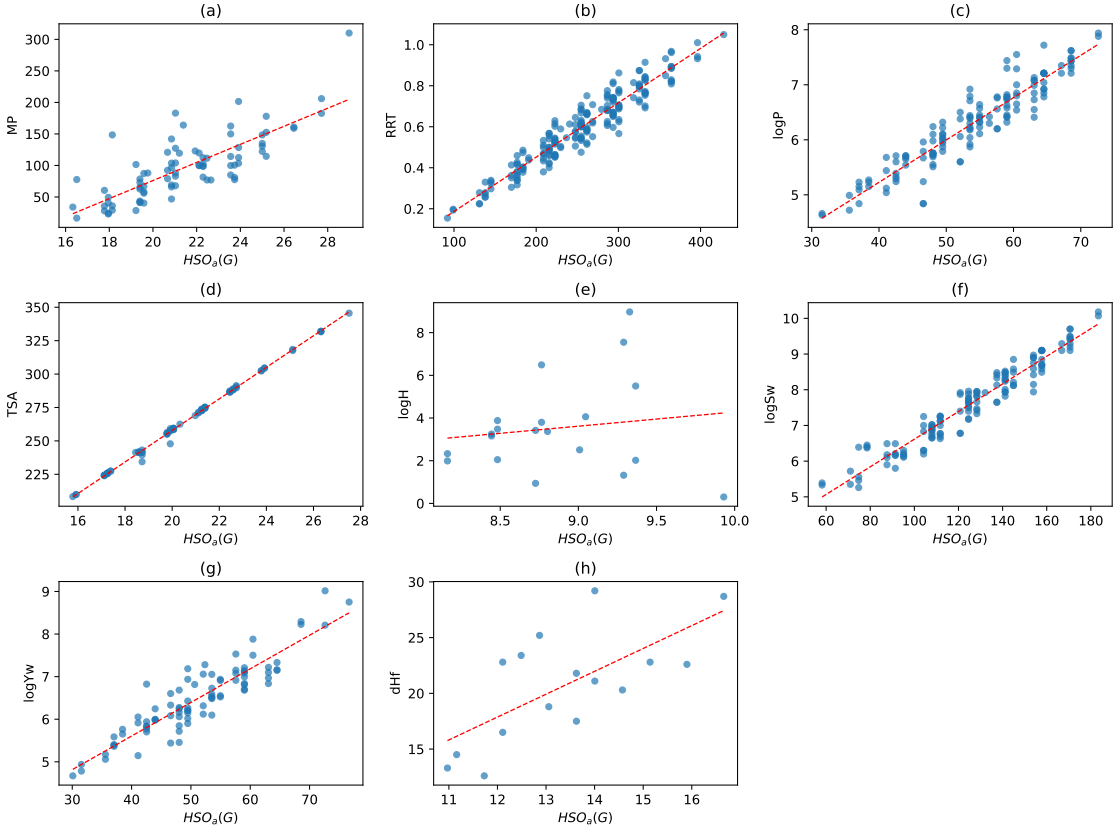

Figure 2: Scatter plots of experimental property values (P) versus $HSO_{a^*}(G)$. Panels correspond to: (a) MP, (b) RRT, (c) $\log P$, (d) TSA, (e) $\log H$, (f) $\log S_w$, (g) $\log Y_w$, and (h) dHf.

For properties exhibiting strong linear correlations ($R^2 > 0.800$), residual behaviour is examined using standard diagnostic tools. Figure 3 presents residuals versus fitted values and normal probability (Q–Q) plots, which are used to assess potential deviations from linearity, heteroscedasticity, and normality. Complementary residual metrics are reported in Table 2.

The results indicate that the parametrized index $HSO_a(G)$ captures systematic structural variability relevant to several physicochemical properties of PCBs. In particular, TSA exhibits an exceptionally strong linear association, with an optimized coefficient of determination approaching unity. High correlations are also observed for RRT, $\log P$, $\log S_w$, and $\log Y_w$, indicating that the corresponding properties are strongly influenced by the structural features encoded in the index.

Table 1: Regression parameters and statistical indicators for models based on $HSO_{a^*}(G)$. Here, c_1 and c_2 denote the slope and intercept, respectively; r is the Pearson correlation coefficient; R^2 is the coefficient of determination; SE is the standard error of the estimate; and F is the Fisher statistic with significance p_F.

Property	a^*	c_1	c_2	R^2	SE	F	p
MP	0.32	14.338	-210.663	0.611	31.821	123.874	< 0.001
RRT	3.18	0.003	-0.079	0.911	0.053	2122.199	< 0.001
logP	1.48	0.077	2.151	0.876	0.270	971.923	< 0.001
TSA	0.25	11.806	21.704	0.997	1.668	24456.173	< 0.001
logH	-1.10	0.667	-2.385	0.020	2.219	0.371	0.550
logSw	2.44	0.039	2.745	0.934	0.294	1889.883	< 0.001
logYw	1.48	0.079	2.448	0.827	0.354	410.424	< 0.001
dHf	-0.49	2.051	-6.736	0.461	3.763	11.992	0.004

Table 2: Residual statistics for strongly correlated models ($|r| > 0.900$). Here, $\overline{e}$ denotes the mean residual, $CV(e)$ the coefficient of variation of the residuals, R_{std} the standardized residual range, and $\max|e_{\mathrm{std}}|$ the maximum absolute standardized residual.

Property	a^*	$\overline{e}$	$CV(e)$	R_{std}	$\max\lvert e_{\mathrm{std}}\rvert$
RRT	3.18	0.000	0.089	5.533	2.842
logP	1.48	0.000	0.043	6.082	3.309
TSA	0.25	0.000	0.006	6.786	5.424
logSw	2.44	0.000	0.039	5.163	2.604
logYw	1.48	0.000	0.055	5.096	2.884

Conversely, properties such as $\log H$ and dHf display low R^2 values even after optimization of the parameter a. In these cases, the weak linear association suggests that their variability is dominated by factors not adequately represented by the topological information captured in $HSO_a(G)$.

The residual diagnostics provide additional insight into the validity of the linear models for the strongly correlated properties. For RRT, $\log P$, $\log S_w$, and $\log Y_w$, the residuals are approximately symmetrically distributed around zero and show no systematic trends with respect to the fitted values, indicating that the assumption of linearity is reasonable within the explored domain. The corresponding Q–Q plots exhibit only minor departures from normality, which are expected for data sets of this size and do not suggest severe model misspecification.

In the case of TSA, despite the exceptionally high coefficient of determination, the standardized residual analysis reveals the presence of an extreme observation, as evidenced by a large maximum absolute standardized residual. This behaviour is also reflected in the tails of the corresponding QQ-plot. While this point does not compromise the overall strength of the linear relationship, it indicates that individual observations may exert a non-negligible influence on the fitted model. Consequently, the TSA model should be interpreted as a highly predictive global trend rather than as a uniformly accurate description at the level of individual congeners.

Overall, this analysis demonstrates that allowing the parameter a to vary provides a systematic way to adapt the index to different physicochemical targets, enhancing its de-

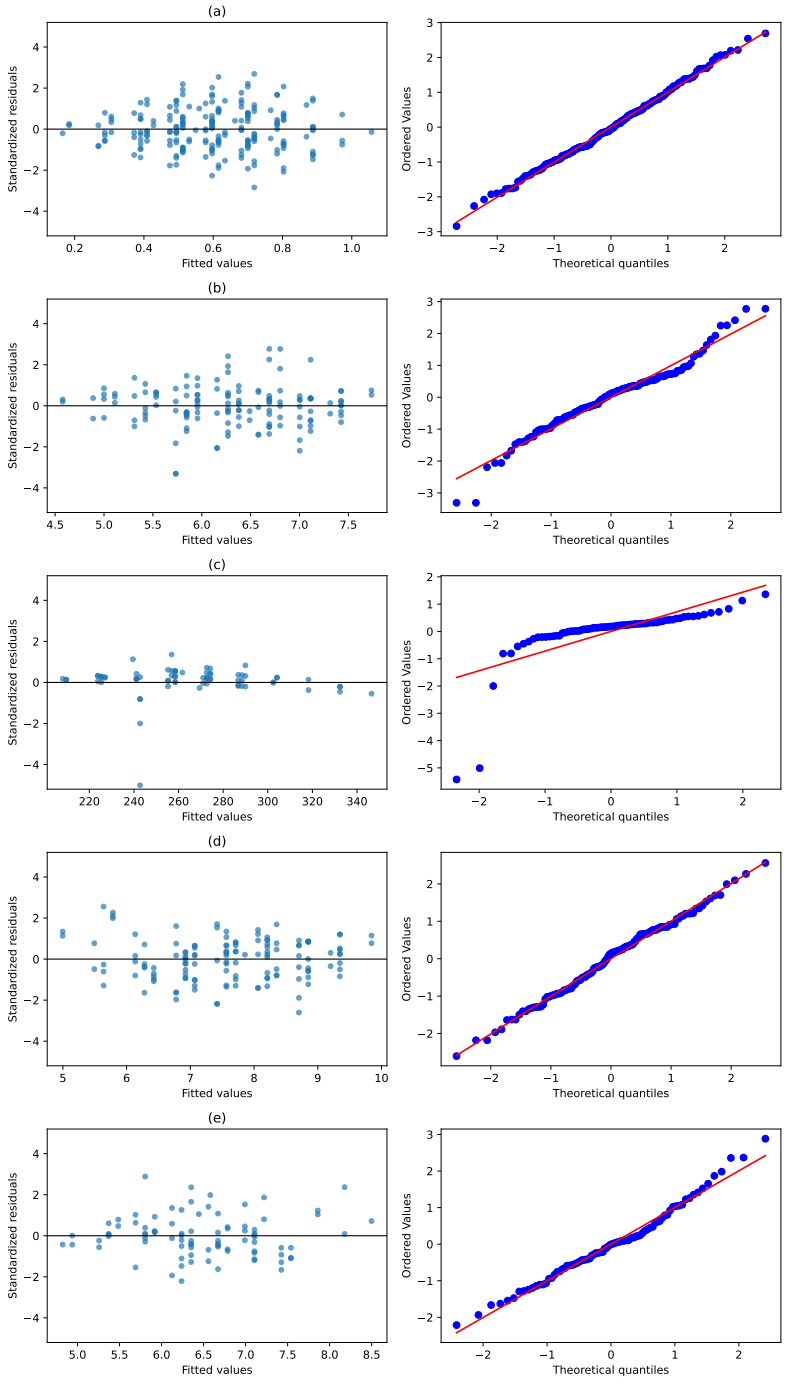

Figure 3: Residual diagnostics for strongly correlated properties. Rows correspond to: (a) RRT, (b) $\log P$, (c) TSA, (d) $\log S_w$, and (e) $\log Y_w$.

scriptive power where a genuine linear structure–property relationship exists, while leaving

weakly correlated properties unaffected.

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