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On Sum Lordeg index: theory and applications

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Abstract. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. The *sum lordeg index* is defined as

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

The aim of this paper is to obtain new results for the Sum Lordeg Index. We provide some relations between the Sum Lordeg Index and other classic topological indices. Moreover, we show upper and lower bounds for this topological index on unicyclic graphs and find the corresponding extremal graphs. Finally, we show that the Sum Lordeg Index is an important tool for predicting the boiling point of cycloalkanes isomers.

1. Introduction

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, they play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [34]. The *Wiener index* of G is defined as

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

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

Topological indices based on end-vertex degrees of edges have been used over 50 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) [25].

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5.85×10^{21} [31]. Hence, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species. The main reason for the use of topological indices is to obtain predictions of some property of certain molecules (see, e.g., [9], [11], [13], [26]). Therefore, given some fixed parameters, a natural problem is to find the graphs that minimize (or maximize) the value of a topological index (which correlates with a physico-chemical property) on the set of graphs satisfying the restrictions given by the parameters (see, e.g., [2], [3], [4], [5], [6], [7], [8], [12], [18], [27], [28]).

The *sum lordeg index* is one of the Adriatic indices introduced in [33]. It is defined as

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

This index is interesting from an applied viewpoint since it is a good predictor of octanol-water partition coefficient for octane isomers [33], and so, it appears in numerical packages for the computation of topological indices [30]. For these reasons, in [32] is stated the open problem of find (sharp) lower and upper bounds for this index.

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite connected simple (without multiple edges and loops) non-trivial ($E(G) \neq \emptyset$) graph. Note that the connectivity of G is not an important restriction, since every molecular graph is connected. A main topic in the study of topological indices is to find bounds of the indices involving several parameters.

A *unicyclic* graph is a graph containing exactly one cycle [14, p.41]. It is well known that if G is a unicyclic graph with n vertices, then G has n edges.

2. Inequalities involving other topological indices

The *first and second variable Zagreb indices* are defined in [16], [17], [21] as

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

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

Note that several well-known indices are particular cases of these two. For example, M_1^1 is the first Zagreb index M_1, $M_1^{-1/2}$ is the inverse index ID [10], $M_1^{3/2}$ is the forgotten index F, etc. Similarly, $M_2^{-1/2}$ is the Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified Zagreb index [23], etc.

In [33] are introduced the Adriatic indices. In particular, a family of indices is defined as

$$L_a(G) = \sum_{u \in V(G)} \left(\log d_u\right)^a.$$

Theorem 2.1. *Let G be a graph and $\alpha > 1$. Then*

$$SL(G) \leq M_1^{\alpha}(G)^{1/\alpha} L_{\alpha/(2\alpha-2)}(G)^{(\alpha-1)/\alpha},$$

and the equality is attained if G is regular. Besides, if $\alpha \geq 1 + 1/(2\log 2)$, then the equality is attained if and only if G is a regular graph.

Proof. Hölder inequality gives

$$SL(G) = \sum_{u\in V(G)} d_u\Big(\log d_u\Big)^{1/2} \le \Big(\sum_{u\in V(G)} d_u^\alpha\Big)^{1/\alpha}\Big(\sum_{u\in V(G)}\Big(\log d_u\Big)^{\alpha/(2\alpha-2)}\Big)^{(\alpha-1)/\alpha}$$
$$= M_1^\alpha(G)^{1/\alpha} L_{\alpha/(2\alpha-2)}(G)^{(\alpha-1)/\alpha}.$$

If G is a regular graph with n vertices and degree Δ, then $SL(G) = n\Delta\sqrt{\log\Delta}$, $M_1^\alpha(G) = n\Delta^\alpha$, $L_{\alpha/(2\alpha-2)}(G) = n\Big(\log\Delta\Big)^{\alpha/(2\alpha-2)}$, and the equality holds.

Assume now that the equality is attained for some $\alpha \ge 1 + 1/(2\log 2)$. Thus, $2^{2\alpha-2} \ge e$. By Hölder inequality, there exist $a, b \ge 0$, not both of them zero, such that $a\,d_u^\alpha = b\Big(\log d_u\Big)^{\alpha/(2\alpha-2)}$ for every $u \in V(G)$, i.e., $a^{(2\alpha-2)/\alpha} d_u^{2\alpha-2} = b^{(2\alpha-2)/\alpha}\log d_u$ for every $u \in V(G)$.

Note that, since the function e^{x-1} is strictly convex on $\mathbb{R}$ and $y = x$ is its tangent at $x = 1$, we have $e^{x-1} > x$ for every $x \in \mathbb{R}\setminus\{1\}$, and so,

$$t^{x-1} > x \tag{1}$$

for every $t \ge e$ and $x > 1$.

If $b = 0$, then $a \ne 0$ and $1 \le d_u = 0$ for every $u \in V(G)$, a contradiction.

Therefore, $b \ne 0$. If $a = 0$, then $\log d_u = 0$ for every $u \in V(G)$; thus, $d_u = 1$ for every $u \in V(G)$ and so, G is regular. Hence, we can assume that $a, b > 0$ and so,

$$\frac{\log d_u}{d_u^{2\alpha-2}} = \frac{\log d_v}{d_v^{2\alpha-2}} \tag{2}$$

for every $u, v \in V(G)$.

If $d_v = 1$ for some $v \in V(G)$, then (2) gives $d_u = 1$ for every $u \in V(G)$ and so, G is regular.

Assume $d_u \ge 2$ for every $u \in V(G)$. Seeking for a contradiction assume that G is not a regular graph. Thus, there exist $u, v \in V(G)$ such that $d_u \ne d_v$ and (2) holds. Without loss of generality we can assume that $2 \le d_u < d_v$. Therefore, $d_v = d_u^x$ for some $x > 1$ and we have

$$\frac{\log d_u}{d_u^{2\alpha-2}} = \frac{\log d_u^x}{d_u^{(2\alpha-2)x}} \qquad \Rightarrow \qquad (d_u^{2\alpha-2})^{x-1} = x,$$

which contradicts (1) since $d_u^{2\alpha-2} \ge 2^{2\alpha-2} \ge e$. Hence, G is regular. □

The *Narumi-Katayama index* defined in [22] as

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

Since $2 > 1 + 1/(2\log 2)$ and $L_1 = \log NK$, Theorem 2.1 provides the following inequality relating SL with the first Zagreb and the Narumi-Katayama indices.

Theorem 2.2. *Let G be a graph. Then*

$$SL(G) \le \sqrt{M_1(G)\log NK(G)}\,,$$

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

We need the following Chebyshev inequality (see, e.g., [1, Theorem 2.1, p.21]).

Lemma 2.3. *If $0 < a_1 \le a_2 \le \cdots \le a_n$ and $0 < b_1 \le b_2 \le \cdots \le b_n$, then*

$$\sum_{j=1}^{n} a_j b_j \ge \frac{1}{n} \sum_{j=1}^{n} a_j \sum_{j=1}^{n} b_j \,,$$

and the equality is attained if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

The following Kober's inequality appears in [15] (see also [35, Lemma 1]).

Lemma 2.4. *If $a_j \ge 0$ for $1 \le j \le n$, then*

$$\Big(\sum_{j=1}^{n} \sqrt{a_j} \Big)^2 \ge \sum_{j=1}^{n} a_j + n(n-1) \Big(\prod_{j=1}^{n} a_j \Big)^{1/n}.$$

Theorem 2.5. *If G is a graph with n vertices, m edges and minimum degree δ, then*

$$SL(G) \ \ge \ \frac{2m}{n} \Big(\log NK(G) + n(n-1) \log \delta \Big)^{1/2},$$

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

Proof. Since $\sqrt{\log t}$ is a strictly increasing function on $[1, \infty)$, Lemma 2.3 gives

$$\begin{aligned} SL(G) &= \sum_{u \in V(G)} d_u \sqrt{\log d_u} \ge \frac{1}{n} \sum_{u \in V(G)} d_u \sum_{u \in V(G)} \sqrt{\log d_u} \\ &= \frac{2m}{n} \sum_{u \in V(G)} \sqrt{\log d_u} \ . \end{aligned}$$

Lemma 2.4 gives

$$\begin{aligned} \Big(\sum_{u \in V(G)} \sqrt{\log d_u} \Big)^2 &\ge \sum_{u \in V(G)} \log d_u + n(n-1) \Big(\prod_{u \in V(G)} \log d_u \Big)^{1/n} \\ &\ge \ \log NK(G) + n(n-1) \log \delta \,, \end{aligned}$$

and so,

$$SL(G) \ge \frac{2m}{n} \sum_{u \in V(G)} \sqrt{\log d_u} \ \ge \ \frac{2m}{n} \Big(\log NK(G) + n(n-1) \log \delta \Big)^{1/2}.$$

Lemma 2.3 gives that if the equality holds then we have $d_u = d_v$ for every $u, v \in V(G)$ or $\sqrt{\log d_u} = \sqrt{\log d_v}$ for every $u, v \in V(G)$, and so, G is regular.

If G is regular, then $SL(G) = n\delta \sqrt{\log \delta}$, $2m = n\delta$ and $\log NK(G) = n \log \delta$, and thus, the equality holds. □

3. Extremal problems on unicyclic graphs

In [32] is stated the open problem of finding (sharp) lower and upper bounds for the sum lordeg index. When the number of vertices is fixed, we solve in [19] this open problem in the case of graphs, graphs with a fixed maximum degree Δ, trees and trees with a fixed number of pendant vertices. Also, we characterized therein the extremal graphs or trees. When the number of vertices is fixed, in [24] is solved this open problem in the case of graphs with a fixed minimum degree δ.

Given $n \ge 3$, let S_{2n} be the set of n-tuples $\mathbf{x} \in \mathbb{N}^n$ such that $x_{j+1} \le x_j$ for every $1 \le j < n$ and $\sum_{j=1}^{n} x_j = 2n$, and let $S_{2n,p}$ be the set of n-tuples $\mathbf{x} \in S_{2n}$ such that $x_j = 1$ if and only if $j > n - p$. Note that if G is a unicyclic graph with n vertices and p pendant vertices and $\mathbf{x}_G$ is its (non-increasing) degree sequence, then $\mathbf{x}_G \in S_{2n,p}$.

Let us recall the following result from [20].

If G is a unicyclic graph with $n \ge 4$ vertices and $1 \le p \le n-3$ pendant vertices, $m = \left\lfloor \frac{2n-p}{n-p} \right\rfloor$, $t = 2n - p - m(n-p)$, let $\mathbf{a} = (a_1, a_2, \dots, a_n)$ be such that

- $a_j = m + 1$ for every $1 \le j \le t$,
- $a_j = m$ for every $t < j \le n - p$,
- $a_j = 1$ for every $n - p < j \le n$,

and $\mathbf{b} = (b_1, b_2, \dots, b_n)$ be such that

- $b_1 = p + 2$,
- $b_j = 2$ for every $1 < j \le n - p$,
- $b_j = 1$ for every $n - p < j \le n$.

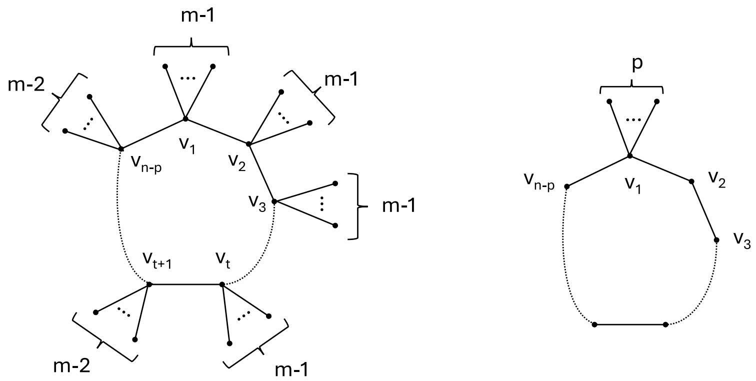

Figure 1: Unicyclic graphs with degree sequence **a**, on the left, and degree sequence **b**, on the right.

Given any function $f : [1, \infty) \to \mathbb{R}$, let us define the index

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

Theorem 3.1. *[20, Theorem 5.2] If G is a unicyclic graph with $n \ge 4$ vertices and $1 \le p \le n - 3$ pendant vertices, $m = \left\lfloor \frac{2n-p}{n-p} \right\rfloor$, $t = 2n - p - m(n - p)$ and $f : [2, \infty) \to \mathbb{R}$ is a convex function, then*

$$tf(m + 1) + (n - p - t)f(m) + pf(1) \le I_f(G) \le f(p + 2) + (n - p - 1)f(2) + pf(1),$$

and both inequalities are attained.

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

$$f'(t) = \frac{1}{2}\Big(\log t\Big)^{-1/2}\Big(2\log t + 1\Big),$$
$$f''(t) = \frac{1}{4t}\Big(\log t\Big)^{-3/2}\Big(2\log t - 1\Big),$$

and so, f is concave on $[1, e^{1/2}]$ and it is convex on $[e^{1/2}, \infty)$. Thus, f is not convex on $[1, \infty)$, but it is strictly convex on $[2, \infty)$, and Theorem 3.1 gives the following result.

Theorem 3.2. *If G is a unicyclic graph with $n \ge 4$ vertices and $0 \le p \le n - 3$ pendant vertices, $m = \left\lfloor \frac{2n-p}{n-p} \right\rfloor$, $t = 2n - p - m(n - p)$, then*

$$t(m + 1)\sqrt{\log(m + 1)} + m(n - p - t)\sqrt{\log m} \le SL(G) \le (p + 2)\sqrt{\log(p + 2)} + 2(n - p - 1)\sqrt{\log 2}\,,$$

and the lower bound is attained if and only if G has the degree sequence **a** *and the upper bound is attained if and only if G has the degree sequence* **b**.

Proof. Theorem 3.1 gives that if G is a unicyclic graph with $n \geq 4$ vertices and $1 \leq p \leq n-3$ pendant vertices, $m = \left\lfloor \frac{2n-p}{n-p} \right\rfloor$, $t = 2n - p - m(n-p)$, then

$$t(m+1)\sqrt{\log(m+1)} + m(n-p-t)\sqrt{\log m} \leq SL(G) \leq (p+2)\sqrt{\log(p+2)} + 2(n-p-1)\sqrt{\log 2}\,,$$

and the lower bound is attained if G has the degree sequence **a** and the upper bound is attained if G has the degree sequence **b**.

If $p = 0$, then G is a cycle, $SL(G) = 2n\sqrt{\log(2)}$ and the theorem is trivially satisfied.

Finally, since $f(t) = t\sqrt{\log t}$ is stricly convex on $[2, \infty)$, it follows immediately from the proof of Lemma 5.1 in [20] that the unique degree sequences that give the lower and upper bound, respectively, are **a** and **b**. □

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

$$I_f(G) \leq \max\Big\{nf(2),\ f(n-1) + 2f(2) + (n-3)f(1)\Big\}.$$

Proof. Since the number p of pendant vertices satisfies $0 \leq p \leq n-3$, Theorem 3.1 gives

$$I_f(G) \leq \max_{0\leq p\leq n-3}\Big(f(p+2) + (n-p-1)f(2) + pf(1)\Big).$$

Let us consider the function $F : [0, n-3] \to \mathbb{R}$ given by $F(s) = f(s+2) + (n-s-1)f(2) + sf(1)$. Since f is a convex function on $[2, \infty)$ and $(n-s-1)f(2) + sf(1)$ is a polynomial of degree 1, F is convex on $[0, n-3]$ and so,

$$\max\Big\{F(0),\ F(n-3)\Big\} \leq \max_{0\leq p\leq n-3} F(p) \leq \max_{s\in[0,n-3]} F(s) = \max\Big\{F(0),\ F(n-3)\Big\}.$$

Therefore,

$$\max_{0\leq p\leq n-3}\Big(f(p+2) + (n-p-1)f(2) + pf(1)\Big) = \max\Big\{nf(2),\ f(n-1) + 2f(2) + (n-3)f(1)\Big\},$$

and this finishes the proof. □

Given $n \geq 4$, let J_n be the graph obtained by identifying a vertex from a cycle C_3 and the vertex with degree $n-3$ of a star graph with $n-2$ vertices, S_{n-2}.

Theorem 3.4. *Let G be a unicyclic graph with $n \geq 3$ vertices.*

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

$$SL(G) \leq 2n\sqrt{\log 2}\,,$$

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

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

$$SL(G) \leq (n-1)\sqrt{\log(n-1)} + 4\sqrt{\log 2}\,,$$

and the equality is attained if and only if G has degree sequence $(n-1, 2, 2, 1, \dots, 1)$, i.e., $G = J_n$.

Proof. By Theorem 3.3 we have that

$$SL(G) \leq \max\Big\{nf(2),\ f(n-1) + 2f(2) + (n-3)f(1)\Big\},$$

with $f(t) = t\sqrt{\log t}$. Furthermore, if $nf(2) > f(n-1) + 2f(2) + (n-3)f(1)$, then the equality is attained if and only if G is the cycle graph, and if $nf(2) < f(n-1) + 2f(2) + (n-3)f(1)$, then the equality is attained if and only if G has degree sequence $(n-1, 2, 2, 1, \dots, 1)$.

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

Let us consider the functions

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

We have

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

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

One can check that $2(n-2)\sqrt{\log 2} > (n-1)\sqrt{\log(n-1)}$ for $3 < n < 10$, and therefore, $2n\sqrt{\log 2} > (n-1)\sqrt{\log(n-1)} + 4\sqrt{\log 2}$ for $3 < n < 10$, finishing the proof. □

Proposition 3.5. *Let G be a unicyclic graph with $3 \leq n \leq 6$ vertices.*

- *If $n = 3$, then G is the 3-cycle and $SL(G) = 6\sqrt{\log 2}$.*
- *If $n = 4$, then*

$$SL(G) \geq 3\sqrt{\log 3} + 4\sqrt{\log 2},$$

  and the equality is attained if and only if G is a 3-cycle with an extra edge attached to some vertex.
- *If $n = 5$, then*

$$SL(G) \geq 6\sqrt{\log 3} + 2\sqrt{\log 2},$$

  and the equality is attained if and only if G is a 3-cycle with two extra edges attached to different vertices.
- *If $n = 6$, then*

$$SL(G) \geq 9\sqrt{\log 3},$$

  and the equality is attained if and only if G is a 3-cycle with a pendant vertex attached to each vertex.

Proof. If $n = 3$, then G is the 3-cycle and the result is trivial.

If $n = 4$, then G has degree sequence either $(3,2,2,1)$ or $(2,2,2,2)$ and since

$$6.47 \approx 3\sqrt{\log 3} + 4\sqrt{\log 2} = SL(S_4) < SL(P_4) = 8\sqrt{\log 2} \approx 6.66,$$

the first one gives the minimum.

If $n = 5$, then G has one of the following degree sequences: $(4,2,2,1,1)$, $(3,3,2,1,1)$, $(3,2,2,2,1)$ or $(2,2,2,2,2)$, see Figure 2. Then, it is immediate to compute that the sequence $(3,3,2,1,1)$ gives the minimum.

If $n = 6$, then G has one of the following degree sequences: $(5,2,2,1,1,1)$, $(4,3,2,1,1,1)$, $(4,2,2,2,1,1)$, $(3,3,3,1,1,1)$, $(3,3,2,2,1,1)$, $(3,2,2,2,2,1)$ or $(2,2,2,2,2,2)$, see Figure 3. Then, it is immediate to compute that the sequence $(3,3,3,1,1,1)$ gives the minimum. □

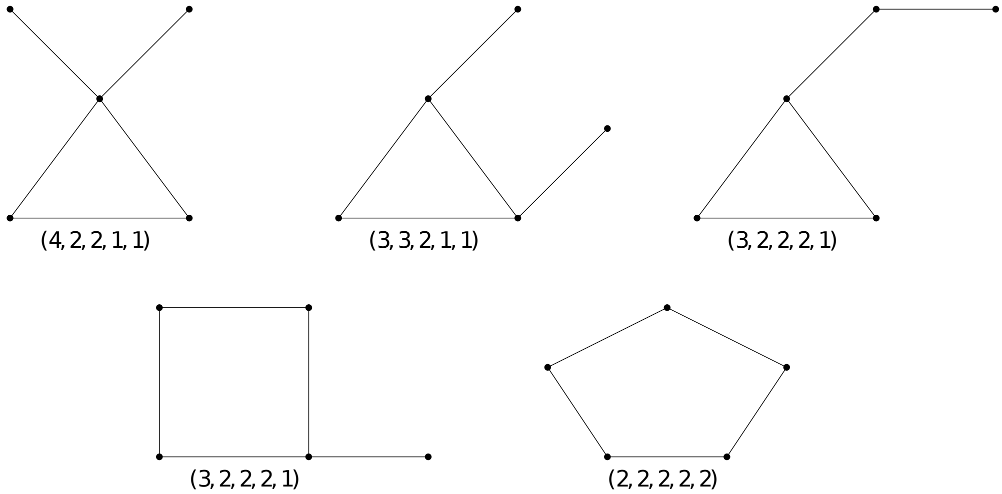

Figure 2: Unicyclic graphs with 5 vertices and their degree sequences.

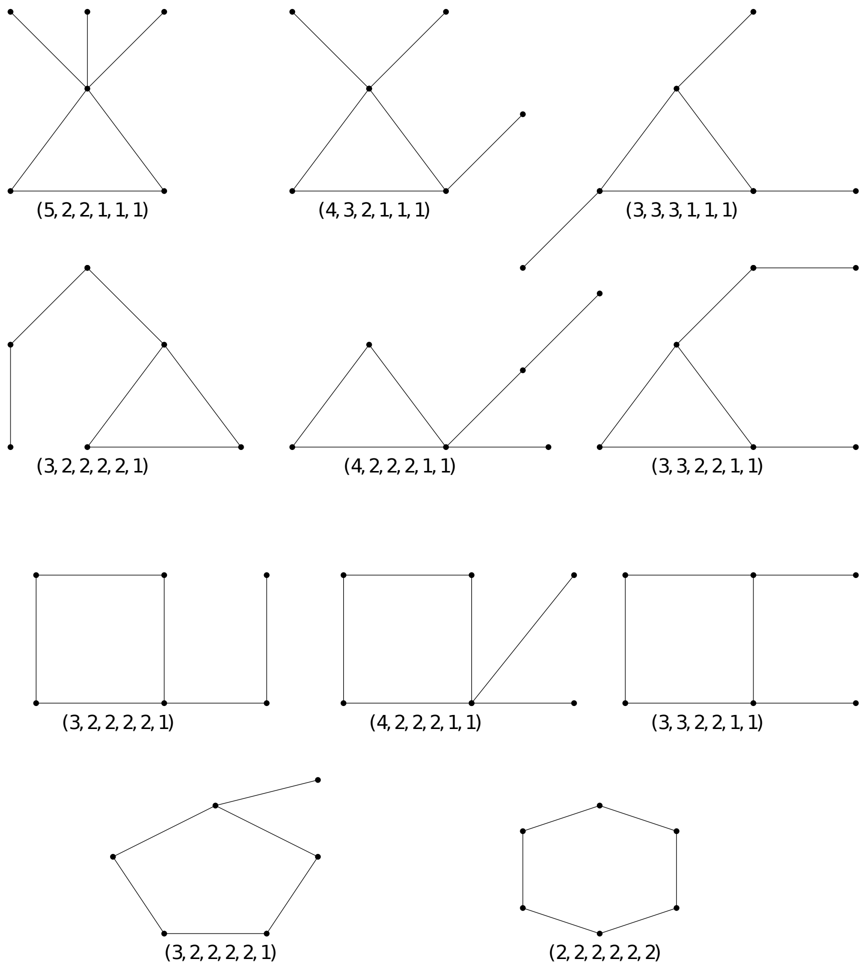

Figure 3: Unicyclic graphs with 6 vertices and their degree sequences.

Let us recall the two following results from [19]:

Lemma 3.6. *If $d \geq 6$, then*

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

and if $3 \leq d \leq 5$, then

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

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

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

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

Theorem 3.7. *Let G be a graph with $n \geq 6$ vertices. If $r = \left\lceil \frac{n-2}{3} \right\rceil$ and $s = 3r - n + 2$, then*

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

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

The proof of Theorem 3.7, partially based on Lemma 3.6, can be easily adapted to obtain Theorem 3.8 below.

Let $n \geq 6$. If $r' = \left\lceil \frac{n}{3} \right\rceil$ and $s' = 3r' - n$, let us define $\mathbf{z}' = (z'_1, z'_2, \dots, z'_n)$ as

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

Note that $0 \leq s' \leq 2 \leq r' \leq n - 4$, and $\mathbf{z}' \in S_{2n}$.

Theorem 3.8. *Let G be a unicyclic graph with $n \geq 7$ vertices. If $r' = \left\lceil \frac{n}{3} \right\rceil$ and $s' = 3r' - n$, then*

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

and the equality is attained if and only if the degree sequence of G is $\mathbf{z}'$.

Proof. Suppose G is a unicylic graph which is minimal for SL and has maximum degree Δ. Let C be the cycle in G.

Claim 1: $\Delta \leq 5$. Seeking for a contradiction suppose there is a vertex w with $deg_G(w) = d \geq 6$. Then consider any adjacent vertex v to w in a connected component of $G \setminus \{w\}$ not intersecting the cycle C and any pendant vertex u in the connected component of $G \setminus \{wv\}$ containing w. Then, let

$$G' = \big(G \setminus \{wv\}\big) \cup \{uv\}.$$

Thus, in G', $deg_{G'}(w) = d - 1$, $deg_{G'}(u) = 2$ and, by Lemma 3.6,

$$SL(G) - SL(G') = d\sqrt{\log d} - (d-1)\sqrt{\log(d-1)} - 2\sqrt{\log 2} > 0,$$

leading to contradiction.

Claim 2: $\Delta \leq 4$. Suppose there is a vertex w with $deg_G(w) = 5$. Let v_1, v_2 be two vertices adjacent to w which belong to two connected components of $G \setminus \{w\}$ not intersecting C. Let u be a pendant vertex in the connected component of $G \setminus \left(\{wv_1\} \cup \{wv_2\}\right)$ containing w, and let

$$G' = \left(G \setminus \left(\{wv_1\} \cup \{wv_2\}\right)\right) \cup \{uv_1\} \cup \{uv_2\}.$$

Thus, in G', $deg_{G'}(w) = 3$, $deg_{G'}(u) = 3$ and

$$SL(G) - SL(G') = 5\sqrt{\log 5} - 6\sqrt{\log 3} > 0,$$

and we obtain a contradiction.

Claim 3: No vertex has degree 2. Suppose there is a vertex w with degree 2. Since

$$\sum_{u \in V(G),\, d_u > 1} (d_u - 1) = \sum_{u \in V(G),\, d_u > 1} d_u - n = n \geq 6,$$

there exists a vertex v in G distinct from w with $deg_G(v) > 1$, and so, $2 \leq deg_G(v) \leq 4$. Let u_1, u_2 be the vertices adjacent to w (with possibly $v \in \{u_1, u_2\}$)

- If $deg_G(v) = 2$, let
$$G' = \left(G \setminus \left(\{wu_1\} \cup \{wu_2\}\right)\right) \cup \{u_1u_2\} \cup \{wv\}.$$
Thus, in G', $deg_{G'}(w) = 1$, $deg_{G'}(v) = 3$, $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v, w\}$ and
$$SL(G) - SL(G') = 4\sqrt{\log 2} - 3\sqrt{\log 3} > 0,$$
leading to contradiction.

- If $deg_G(v) = 3$, let
$$G' = \left(G \setminus \left(\{wu_1\} \cup \{wu_2\}\right)\right) \cup \{u_1u_2\} \cup \{wv\}.$$
Thus, in G', $deg_{G'}(w) = 1$, $deg_{G'}(v) = 4$, $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v, w\}$ and
$$SL(G) - SL(G') = 2\sqrt{\log 2} + 3\sqrt{\log 3} - 4\sqrt{\log 4} > 0,$$
leading to contradiction.

- If $deg_G(v) = 4$, let u_0 be a vertex adjacent to v such that w, v and C are in the same connected component of $G \setminus \{u_0\}$. Then, let
$$G' = \left(G \setminus \{vu_0\}\right) \cup \{u_0w\}.$$
Thus, in G', $deg_{G'}(w) = 3$, $deg_{G'}(v) = 3$, $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v, w\}$ and
$$SL(G) - SL(G') = 2\sqrt{\log 2} + 4\sqrt{\log 4} - 6\sqrt{\log 3} > 0,$$
leading to contradiction.

Claim 4: There are at most two vertices with degree 3. Suppose there exist three vertices v_1, v_2, v_3 with $deg(v_i) = 3$ for $1 \leq i \leq 3$.

- If $v_1, v_2, v_3 \in C$, let u_1, u_2 be the two vertices in the cycle adjacent to v_1 (with possibly $\{u_1, u_2\} \cap \{v_2, v_3\} \neq \emptyset$) and u_3 the other vertex adjacent to v_1.

  If the cycle has at least length four, let

$$G' = \Big(G \setminus \big(\{v_1u_1\} \cup \{v_1u_2\} \cup \{v_1, u_3\}\big)\Big) \cup \big(\{u_1u_2\} \cup \{v_1v_2\} \cup \{v_3u_3\}\big).$$

  Thus, in G', $deg_{G'}(v_1) = 1$, $deg_{G'}(v_2) = 4$, $deg_{G'}(v_3) = 4$, $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v_1, v_2, v_3\}$ and

$$SL(G) - SL(G') = 9\sqrt{\log 3} - 8\sqrt{\log 4} > 0,$$

  leading to a contradiction.

  Otherwise, suppose that the cycle has length three and, therefore, its vertices are precisely $\{v_1, v_2, v_3\}$. Since $n \geq 7$, there is some other vertex v_4 with $deg(v_4) > 1$. From the previous claims, either $deg(v_4) = 3$ or $deg(v_4) = 4$. Also notice that since there are no vertices with degree 2, we may assume that v_4 is adjacent to the cycle. In particular, let us suppose (with no loss of generality) that it is adjacent to v_3. Let us denote $deg(v_4) = r$ and let w_i for $1 \leq i \leq r-1$ the vertices adjacent to v_4 different from v_3 and let

$$G' = \Big(G \setminus \cup_{1\leq i\leq r-1}\{v_4w_i\}\Big) \cup \Big(\cup_{1\leq j\leq r-1} \{v_iw_i\}\Big).$$

  Thus, in G', $deg_{G'}(v_i) = 4$ for every $1 \leq i \leq r-1$, $deg_{G'}(v_4) = 1$, and $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v_1, v_2, v_{r-1}, v_4\}$. Therefore (recall that we have either $r = 3$ or $r = 4$)

$$SL(G) - SL(G') = (r-1)3\sqrt{\log 3} + r\sqrt{\log r} - (r-1)4\sqrt{\log 4} = 9\sqrt{\log 3} - 8\sqrt{\log 4} > 0,$$

  leading to a contradiction.

- If $v_1 \notin C$ (similarly for v_2 or v_3), let u_1, u_2 be the two adjacent vertices to v_1 which are not in the connected component of $G \setminus \{v_1\}$ intersecting C. Then, let

$$G' = \Big(G \setminus \big(\{v_1u_1\} \cup \{v_1u_2\}\big)\Big) \cup \big(\{v_2u_1\} \cup \{v_3u_2\}\big).$$

  Thus, in G', $deg_{G'}(v_1) = 1$, $deg_{G'}(v_2) = 4$, $deg_{G'}(v_3) = 4$ and $deg_G(u) = deg_{G'}(u)$ for every $u \in V(G) \setminus \{v_1, v_2, v_3\}$. Hence,

$$SL(G) - SL(G') = 9\sqrt{\log 3} - 8\sqrt{\log 4} > 0,$$

  and we obtain a contradiction.

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

4. QSPR study on boiling point of cycloalkanes

The sum lordeg index was selected in [33] as a significant predictor of octanol-water partition coefficient for octane isomers. In this section we perform a quantitative structure property relationship (QSPR) study to model the boiling point (BP) of 41 cycloalkanes isomers. The selected compounds belong to the set of cycloalkane isomers with chemical formula C_nH_{2n} ($n \leq 8$) and whose corresponding graph is unicyclic (see Figure 4). Experimental BP data were obtained from https://webbook.nist.gov.

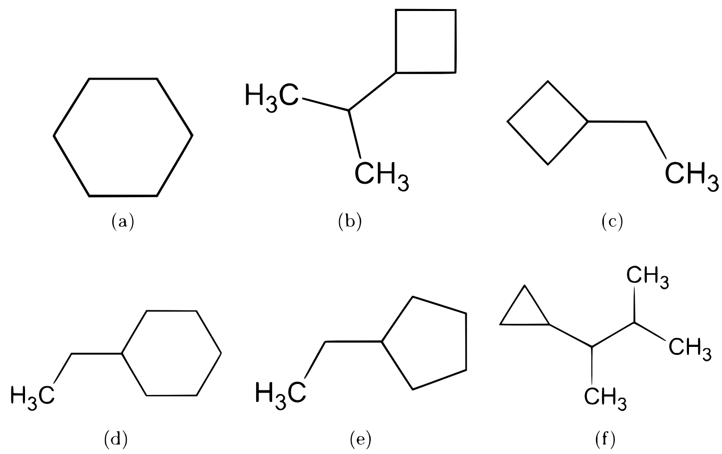

Figure 4: Some examples of selected cycloalkane isomers: (a) Cyclohexane; (b) Cyclobutane, isopropyl-; (c) Cyclobutane, ethyl-; (d) Cyclohexane, ethyl-; (e) Cyclopentane, ethyl-; (f) Cyclopropane,1, 2−dimethylpropyl-.

To construct the model in Equation (3), we use the multiple linear regression method. We take as dependent variable BP and as independent variables the SL index and the number of vertices of the graph n.

$$BP = 63.42\,SL - 72.37n + 152.65\,. \tag{3}$$

In Figure 4 we show the values of the boiling point predicted by the previous model (BP_{pre}) vs. the experimental values of the boiling point (BP_{exp}).

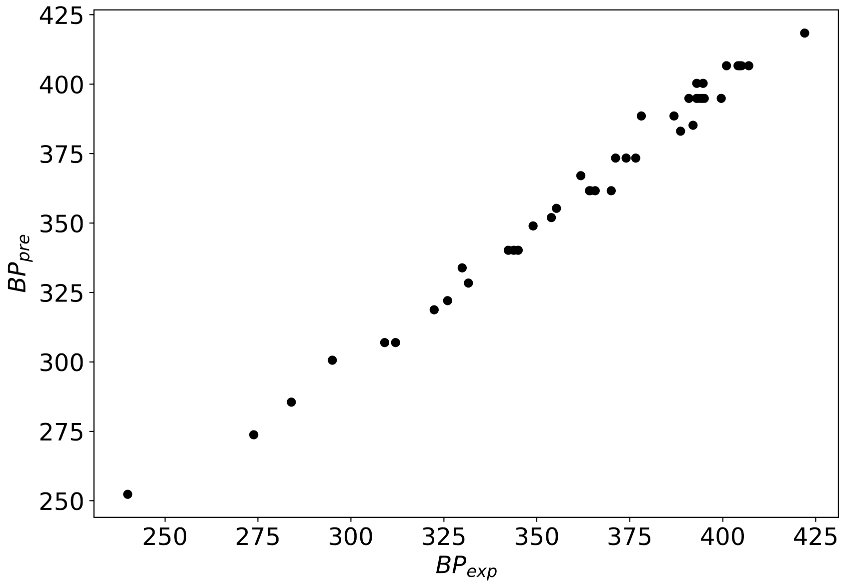

Figure 5: Experimental and predicted values of the boiling point (BP) of cycloalkanes compounds by the model in Eq. 3.

The statistical parameters of the model in Equation (3) are, number of observations $N = 41$, determination coefficient $R^2 = 0.988$, adjusted determination coefficient $R^2_{adj} = 0.987$, standard error $SE = 4.665$, significance test F ($F = 1515.102$, $p = 5.8 \times 10^{-37}$). Figure 4 shows the standard residuals obtained in the model.

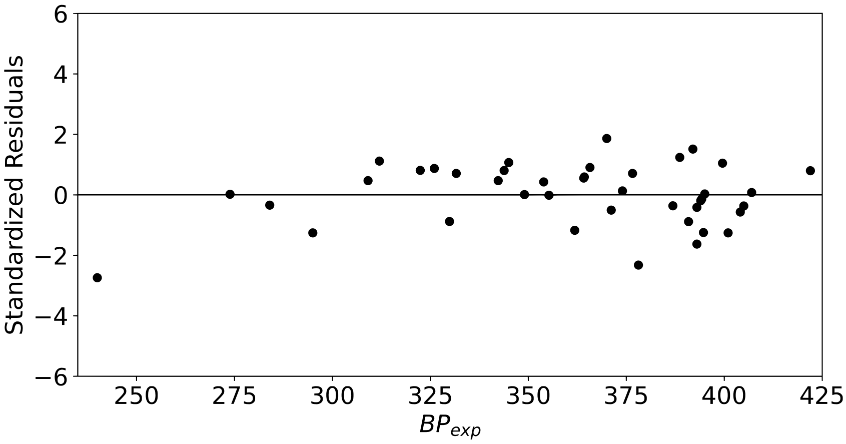

Figure 6: Standard residuals obtained in the model in Equation (3)

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