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On the Degree-Ratio Sombor Index: Corrections and New Bounds

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Abstract

The degree-ratio Sombor index (DRSO) is a recently introduced geometric degree-based topological invariant. First, we correct an erroneous lower bound involving the Sombor index and rectify the characterization of extremal graphs from the original work on this index [11]. Subsequently, we investigate the relationship between the DRSO index and the spectral radius of a graph. Sharp upper and lower bounds involving the graph's order, size, minimum and maximum degree are obtained. Finally, we establish several relations between DRSO and other classical indices, including the Diminished Sombor index, the Sombor index, the Randić index, the harmonic index, and the first Zagreb index.

1 Introduction

Let $G = (V, E)$ be a simple, connected graph without isolated vertices. The number of vertices and edges are denoted by $n = |V|$ and $m = |E|$, respectively. The degree of a vertex u is written $d(u)$, and the minimum

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and maximum degrees are δ and Δ. The *spectral radius* $\lambda_1(G)$ is the largest eigenvalue of the adjacency matrix of G. We refer to the path, cycle and star on n vertices as P_n, C_n and S_n, respectively.

Degree-based topological indices play a central role in chemical graph theory [5,6]. The recently introduced *Degree-Ratio Sombor index* (DRSO) [11] is defined by

$$\mathrm{DRSO}(G) \;=\; \sum_{uv\in E(G)} \sqrt{\left(\frac{d(u)}{d(v)}\right)^2 + \left(\frac{d(v)}{d(u)}\right)^2} \;=\; \sum_{uv\in E(G)} \frac{\sqrt{d(u)^4 + d(v)^4}}{d(u)\,d(v)}. \tag{1}$$

This index admits a geometric interpretation as the sum of Euclidean lengths of the vectors $(d_u/d_v,\, d_v/d_u)$ associated to edges. For more details see [8].

The original paper [11] investigated basic mathematical properties and extremal values of DRSO. However, it contains two errors that we correct in Section 3. Beyond these corrections, the connections between DRSO and other graph invariants have not been explored. In the present paper we fill this gap. Section 2 fixes notation and lists auxiliary results. In Section 4 we prove sharp bounds that relate DRSO with the spectral radius. Section 5 establishes tight relations with the Diminished Sombor index, the Sombor index, and the Randić index.

2 Preliminaries

For an edge uv, define the *edge-weight function*

$$\varphi(x,y) = \frac{\sqrt{x^4+y^4}}{xy}, \qquad x,y>0.$$

The following elementary properties are immediate.

Lemma 1. *For any $x, y \in [\delta, \Delta]$,*

$$\sqrt{2} \;\le\; \varphi(x,y) \;\le\; \frac{\sqrt{\Delta^4+\delta^4}}{\Delta\delta} =: K.$$

Equality on the left holds iff $x = y$; equality on the right holds iff $\{x, y\} =$

$\{\delta, \Delta\}$.

Proof. Let $r = \max\{x/y,\, y/x\} \geq 1$. Then $\varphi(x, y) = \sqrt{r^2 + r^{-2}}$. The function $r \mapsto \sqrt{r^2 + r^{-2}}$ is strictly increasing for $r \geq 1$. Thus the minimum is attained at $r = 1$ (i.e., $x = y$) and equals $\sqrt{2}$. The maximum is attained at the largest possible ratio $r = \Delta/\delta$, giving $\varphi = \sqrt{(\Delta/\delta)^2 + (\delta/\Delta)^2} = \frac{\sqrt{\Delta^4+\delta^4}}{\Delta\delta}$. ∎

The bounds in Lemma 1 are closely related to Theorem 1 of [11] and Proposition 1 of [1]; we present them here with a new, self-contained proof based on a monotonicity argument, as they are needed for the original results in Sections 4 and 5.

From Lemma 1 we obtain the global bounds

Corollary. *Let G be a graph of size m, then*

$$m\sqrt{2} \;\leq\; \mathrm{DRSO}(G) \;\leq\; mK. \tag{2}$$

We will also need the following well-known spectral inequalities for a connected graph G:

$$\delta \leq \lambda_1 \leq \Delta, \tag{3}$$

$$\lambda_1 \geq \frac{2m}{n}, \tag{4}$$

$$\lambda_1 \leq \sqrt{2m - n + 1}, \tag{5}$$

with equalities in (3) and (4) iff G is regular [2, 13], and equality in (5) iff $G \cong S_n$ or $G \cong K_n$ [9].

Recall the definitions of the indices that will appear later:

- **Sombor index** [7]: $\mathrm{SO}(G) = \displaystyle\sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$.
- **Diminished Sombor index** [10]:

$$\mathrm{DSO}(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2}}{d(u) + d(v)}.$$

- **Randić index** [12]: $\mathrm{R}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)\,d(v)}}$.
- **Harmonic index** [3]: $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$.
- **First Zagreb index**: $M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v))$.

3 Corrections of previous results

3.1 Theorem 3 of [11]: an invalid lower bound

In [11], Theorem 3 asserts that

$$\frac{\sqrt{\delta^2 + \Delta^2}}{\sqrt{2}\,\delta\Delta}\ \mathrm{SO}(G) \ \le\ \mathrm{DRSO}(G) \ \le\ \frac{1}{\delta}\ \mathrm{SO}(G).$$

While the upper bound is correct, the lower bound is false in general. The proof attempted to use the pointwise inequality

$$\frac{\sqrt{x^2 + y^2}}{xy} \le \frac{\sqrt{\delta^2 + \Delta^2}}{\delta\Delta}, \qquad (\delta \le x, y \le \Delta),$$

but this inequality fails, e.g., for $\delta = 1$, $\Delta = 10$ and $(x, y) = (1, 2)$:

$$\frac{\sqrt{5}}{2} \approx 1.118 > \frac{\sqrt{101}}{10} \approx 1.005.$$

Hence the claimed lower bound does not hold. The correct statement is as follows.

Theorem 1 (Refinement of Theorem 3 in [11])**.** *For every connected graph G,*

$$\mathrm{DRSO}(G) \ \le\ \frac{1}{\delta}\ \mathrm{SO}(G).$$

The best possible uniform lower bound that can be obtained directly from the edge weights remains $\mathrm{DRSO}(G) \ge m\sqrt{2}$.

Proof. For any edge uv,

$$\frac{\sqrt{d(u)^4 + d(v)^4}}{d(u)\,d(v)} \;\le\; \frac{\max\{d(u),d(v)\}\sqrt{d(u)^2 + d(v)^2}}{d(u)\,d(v)} \;\le\; \frac{1}{\delta}\,\sqrt{d(u)^2 + d(v)^2},$$

since $\max\{d(u),d(v)\}/(d(u)\,d(v)) \le 1/\delta$. Summing over all edges gives $\mathrm{DRSO}(G) \le \delta^{-1}\,\mathrm{SO}(G)$. The lower bound $m\sqrt{2}$ follows directly from Lemma 1. ∎

3.2 Theorem 6 of [11]

Theorem 6 in [11] claims that for any connected graph on $n \ge 3$ vertices,

$$\mathrm{DRSO}(C_n) \le \mathrm{DRSO}(G) \le \mathrm{DRSO}(S_n),$$

with equality on the left only for C_n. This statement is false. A counterexample is $n = 4$:

$$\mathrm{DRSO}(P_4) = \sqrt{17} + \sqrt{2} \approx 5.537, \qquad \mathrm{DRSO}(C_4) = 4\sqrt{2} \approx 5.657,$$

so $\mathrm{DRSO}(P_4) < \mathrm{DRSO}(C_4)$. Hence the cycle does *not* give the minimum.

To provide further numerical evidence and motivation, we compute the DRSO values for the four basic families of graphs (star S_n, path P_n, cycle C_n, and complete graph K_n) for $n = 3$ to 7. The results are summarised in Table 1.

From the table we observe that for every $n \ge 3$ (except $n = 3$ where $P_3 = S_3$), the following strict inequalities hold:

$$\mathrm{DRSO}(P_n) \;<\; \mathrm{DRSO}(C_n) \;<\; \mathrm{DRSO}(K_n) \;<\; \mathrm{DRSO}(S_n).$$

In particular, the path consistently gives a smaller value than the cycle, and the star gives the largest value among all these standard graphs. This numerical evidence strongly suggests that, among all connected graphs on n vertices, the path P_n minimises DRSO and the star S_n maximises it.

Consequently, Theorem 6 of [11] is incorrect in asserting that the cycle is the minimiser. The correct extremal candidates remain to be rigorously determined. Therefore we state the following open problem:

Table 1. Values of DRSO for S_n, P_n, C_n, K_n ($n = 3, \ldots, 7$). Approximate numerical values are given in parentheses.

n	Graph	DRSO
3	$S_3 = P_3$	$\sqrt{17} \approx 4.1231$
3	$C_3 = K_3$	$3\sqrt{2} \approx 4.2426$
4	P_4	$\sqrt{17} + \sqrt{2} \approx 5.5373$
4	C_4	$4\sqrt{2} \approx 5.6569$
4	K_4	$6\sqrt{2} \approx 8.4853$
4	S_4	$\sqrt{82} \approx 9.0554$
5	P_5	$\sqrt{17} + 2\sqrt{2} \approx 6.9515$
5	C_5	$5\sqrt{2} \approx 7.0711$
5	K_5	$10\sqrt{2} \approx 14.1421$
5	S_5	$\sqrt{257} \approx 16.0312$
6	P_6	$\sqrt{17} + 3\sqrt{2} \approx 8.3657$
6	C_6	$6\sqrt{2} \approx 8.4853$
6	K_6	$15\sqrt{2} \approx 21.2132$
6	S_6	$\sqrt{626} \approx 25.0200$
7	P_7	$\sqrt{17} + 4\sqrt{2} \approx 9.7800$
7	C_7	$7\sqrt{2} \approx 9.8995$
7	K_7	$21\sqrt{2} \approx 29.6985$
7	S_7	$\sqrt{1297} \approx 36.0139$

Problem 1. For every connected graph G on $n \geq 3$ vertices, is it true that

$$\mathrm{DRSO}(P_n) \;\leq\; \mathrm{DRSO}(G) \;\leq\; \mathrm{DRSO}(S_n),$$

with equality on the left if and only if $G \cong P_n$, and equality on the right if and only if $G \cong S_n$?

The errors in Theorems 3 and 6 of [11] are also noted in [1]. We include a concise discussion here because a clear statement of these corrections is essential for formulating the open problem that follows; that problem is not addressed in either of the above references and constitutes one of the contributions of the present work.

4 Relations with the spectral radius

We now present several inequalities that connect $\mathrm{DRSO}(G)$ with the spectral radius $\lambda_1(G)$. The first result follows directly from the global bounds (2) and the spectral sandwich $\delta \le \lambda_1 \le \Delta$.

Theorem 2. *For any connected graph G on $n \ge 3$ vertices,*

$$\frac{m\sqrt{2}}{\Delta}\,\lambda_1 \;\le\; \mathrm{DRSO}(G) \;\le\; \frac{mK}{\delta}\,\lambda_1,$$

where $K = \frac{\sqrt{\Delta^4+\delta^4}}{\Delta\delta}$. Both equalities hold simultaneously if and only if G is regular.

Proof. From (2) and $\delta \le \lambda_1 \le \Delta$ we obtain

$$\frac{\mathrm{DRSO}(G)}{\lambda_1} \ge \frac{m\sqrt{2}}{\lambda_1} \ge \frac{m\sqrt{2}}{\Delta}, \qquad \frac{\mathrm{DRSO}(G)}{\lambda_1} \le \frac{mK}{\lambda_1} \le \frac{mK}{\delta}.$$

Multiplying by λ_1 yields the bounds. If G is regular, then $\delta = \Delta$, $K = \sqrt{2}$, and both bounds collapse to $m\sqrt{2}$, so equality holds in both. Conversely, equality in the lower bound forces $\varphi(d_u, d_v) = \sqrt{2}$ on every edge (hence G regular) and $\lambda_1 = \Delta$, which again forces regularity. The same conclusion follows from the upper bound. ∎

Using $\lambda_1 \ge 2m/n$ we can eliminate m from the upper bound.

Corollary. $\mathrm{DRSO}(G) \;\le\; \dfrac{n}{2}\,K\,\lambda_1$, *with equality iff G is regular.*

Proof. From (4), $m \le n\lambda_1/2$. Insert into $\mathrm{DRSO}(G) \le mK$. Equality conditions are the same as in Theorem 2. ∎

A lower bound that depends only on n, δ and λ_1 is obtained via Hong's inequality (5).

Theorem 3. *Let G be a connected graph on $n \ge 3$ vertices with minimum degree δ.*

1. *If $\delta = 1$, then* $\mathrm{DRSO}(G) > \lambda_1\sqrt{2(n-1)}$.

2. *If* $\delta \geq 2$, *then* $\mathrm{DRSO}(G) \geq \lambda_1 \, n\sqrt{\dfrac{2}{n+1}}$. *Equality holds if and only if* $n = 3$ *and* $G \cong C_3$.

Proof. From Corollary 2 we have $\mathrm{DRSO}(G) \geq m\sqrt{2}$, and Hong's bound [9] states $\lambda_1 \leq \sqrt{2m - n + 1}$. Combining these gives

$$\frac{\mathrm{DRSO}(G)}{\lambda_1} \geq \frac{m\sqrt{2}}{\sqrt{2m-n+1}} = \sqrt{2}\, f(m), \qquad f(m) = \frac{m}{\sqrt{2m-n+1}}.$$

The derivative is

$$f'(m) = \frac{\sqrt{2m-n+1} - \frac{m}{\sqrt{2m-n+1}}}{2m-n+1} = \frac{m-n+1}{(2m-n+1)^{3/2}}.$$

For $m \geq n-1$ we have $m - n + 1 \geq 0$, hence $f'(m) \geq 0$ and f is non-decreasing on $[n-1, \infty)$.

Case 1: $\delta = 1$**.** Connectivity forces $m \geq n-1$. Thus $f(m) \geq f(n-1)$, with strict inequality when $m > n-1$. Evaluating, $f(n-1) = \frac{n-1}{\sqrt{2(n-1)-n+1}} = \sqrt{n-1}$. Hence

$$\frac{\mathrm{DRSO}(G)}{\lambda_1} \geq \sqrt{2}\sqrt{n-1} = \sqrt{2(n-1)}.$$

Equality would require $m = n-1$ (so G is a tree) and equality in both constituent bounds, i.e. $\mathrm{DRSO}(G) = m\sqrt{2}$ and $\lambda_1 = \sqrt{2m-n+1}$. $\mathrm{DRSO}(G) = m\sqrt{2}$ forces every edge to join vertices of equal degree (Lemma 1). In a tree with $n \geq 3$, there is at least one leaf (degree 1) connected to a vertex of degree at least two, so that edge fails the condition $d(u) = d(v)$. Hence equality cannot hold, and the inequality is strict.

Case 2: $\delta \geq 2$**.** Then every vertex has degree at least two, implying $m \geq n$ (since $2m = \sum \deg v \geq 2n$). Monotonicity of f gives $f(m) \geq f(n)$, with equality only for $m = n$. We have $f(n) = \frac{n}{\sqrt{2n-n+1}} = \frac{n}{\sqrt{n+1}}$, so

$$\frac{\mathrm{DRSO}(G)}{\lambda_1} \geq n\sqrt{\frac{2}{n+1}}.$$

If equality holds, then $m = n$ and both $\mathrm{DRSO}(G) = n\sqrt{2}$ and $\lambda_1 =$

$\sqrt{n+1}$. $\mathrm{DRSO}(G) = n\sqrt{2}$ forces G to be regular; with $m = n$ the only regular connected graph is the cycle C_n, which gives $\lambda_1(C_n) = 2$. Hence $\sqrt{n+1} = 2$, so $n = 3$. The triangle C_3 indeed attains equality (both sides equal $3\sqrt{2}$). Note that equality in Hong's bound requires G to be a star or a complete graph; with $m = n$ the only such graph is $K_3 \cong C_3$, which is consistent with our conclusion. ■

Finally, we combine the upper bound with a spectral lower bound for the Randić index.

Corollary. $\mathrm{DRSO}(G) \le K\,\lambda_1\,\mathrm{R}(G)$.

Proof. Favaron et al. [4] proved $\lambda_1 \ge m/\,\mathrm{R}(G)$, thus $1/\lambda_1 \le \mathrm{R}(G)/m$. From $\mathrm{DRSO}(G) \le mK$ we obtain $\mathrm{DRSO}(G)/\lambda_1 \le K\ \mathrm{R}(G)$. ■

5 Relations with other topological indices

In this section we often use the constant $K = \frac{\sqrt{\Delta^4+\delta^4}}{\Delta\delta}$ from Lemma 1. All bounds are expressed in terms of K to make the relations clearer and to highlight the common role of the extreme degree ratio.

5.1 Diminished Sombor index

Theorem 4. *For any connected graph G without isolated vertices,*

$$2\ \mathrm{DSO}(G) \ \le\ \mathrm{DRSO}(G) \ <\ \frac{(\delta+\Delta)\sqrt{\delta^2+\Delta^2}}{\delta\Delta}\ \mathrm{DSO}(G).$$

Equality in the lower bound holds if and only if G is regular. The upper bound is strict for every such graph G.

Proof. For an edge uv with $x = d(u)$, $y = d(v)$, set

$$f(x,y) = \frac{\sqrt{x^4+y^4}}{xy}, \qquad g(x,y) = \frac{\sqrt{x^2+y^2}}{x+y}.$$

We examine the ratio

$$\frac{f(x,y)}{g(x,y)} = \frac{\sqrt{x^4+y^4}\,(x+y)}{xy\,\sqrt{x^2+y^2}}.$$

Lower bound. By the AM–QM inequality, $\sqrt{x^4+y^4} \geq \frac{x^2+y^2}{\sqrt{2}}$. Hence

$$\frac{f}{g} \geq \frac{(x^2+y^2)(x+y)}{\sqrt{2}\,xy\,\sqrt{x^2+y^2}} = \frac{(x+y)\sqrt{x^2+y^2}}{\sqrt{2}\,xy}.$$

Now, $(x+y)^2(x^2+y^2) \geq 8x^2y^2$ (squaring the AM–GM inequalities $x^2+y^2 \geq 2xy$ and $(x+y)^2 \geq 4xy$ gives the product $\geq 8x^2y^2$). Taking square roots yields $(x+y)\sqrt{x^2+y^2} \geq 2\sqrt{2}\,xy$. Therefore

$$\frac{f}{g} \geq \frac{2\sqrt{2}\,xy}{\sqrt{2}\,xy} = 2.$$

Equality requires $x = y$ (both AM–GM equalities become equalities). Summing over all edges gives $\mathrm{DRSO}(G) \geq 2\,\mathrm{DSO}(G)$, with equality iff $d(u) = d(v)$ on every edge, i.e., G is regular.

Upper bound. Because $(x^2+y^2)^2 = x^4+y^4+2x^2y^2 > x^4+y^4$ for all $x, y > 0$, we have the strict inequality $\sqrt{x^4+y^4} < x^2+y^2$. Consequently,

$$\frac{f}{g} < \frac{(x^2+y^2)(x+y)}{xy\,\sqrt{x^2+y^2}} = \frac{(x+y)\sqrt{x^2+y^2}}{xy} = \Big(\frac{1}{x}+\frac{1}{y}\Big)\sqrt{x^2+y^2}.$$

The function $h(x,y) = (1/x+1/y)\sqrt{x^2+y^2}$ attains its maximum on $[\delta,\Delta]^2$ at the pair (δ,Δ) (or (Δ,δ)). Indeed, setting $r = \max\{x/y,\, y/x\} \geq 1$ and $t = \min\{x,y\}$, we have $x = t$, $y = tr$ (or vice-versa), giving $h = (1/t)(1+1/r)\cdot t\sqrt{1+r^2} = (1+1/r)\sqrt{1+r^2}$, which is independent of t and strictly increasing in r. Hence its maximum on the feasible set $1 \leq r \leq \Delta/\delta$ is attained at $r = \Delta/\delta$, corresponding to the extreme pair (δ,Δ). Thus

$$\frac{f}{g} < \frac{(\delta+\Delta)\sqrt{\delta^2+\Delta^2}}{\delta\Delta}.$$

Summing over all edges gives the strict upper bound

$$\mathrm{DRSO}(G) < \frac{(\delta+\Delta)\sqrt{\delta^2+\Delta^2}}{\delta\Delta}\ \mathrm{DSO}(G),$$

which holds for every connected graph without isolated vertices. ■

5.2 The Sombor index

Theorem 5. *For a connected graph G with minimum degree δ and maximum degree Δ,*

$$\frac{\delta}{\Delta^2}\ \mathrm{SO}(G)\ \le\ \mathrm{DRSO}(G)\ \le\ \frac{K}{\sqrt{2}\,\delta}\ \mathrm{SO}(G).$$

Equality in both bounds holds if and only if G is regular.

Proof. Recall $K = \frac{\sqrt{\Delta^4+\delta^4}}{\Delta\delta}$. For each edge uv,

$$\frac{\varphi(d(u),d(v))}{\sqrt{d(u)^2+d(v)^2}} = \frac{\sqrt{d(u)^4+d(v)^4}}{d(u)d(v)\sqrt{d(u)^2+d(v)^2}}.$$

Using $\sqrt{d(u)^4+d(v)^4} \ge \frac{d(u)^2+d(v)^2}{\sqrt{2}}$,

$$\begin{aligned}\frac{\varphi(d(u),d(v))}{\sqrt{d(u)^2+d(v)^2}} &\ge \frac{d(u)^2+d(v)^2}{\sqrt{2}\,d(u)d(v)\sqrt{d(u)^2+d(v)^2}}\\ &= \frac{\sqrt{d(u)^2+d(v)^2}}{\sqrt{2}\,d(u)d(v)} \ge \frac{\sqrt{2\delta^2}}{\sqrt{2}\,\Delta^2} = \frac{\delta}{\Delta^2}.\end{aligned}$$

Summing yields the lower bound. Equality in the chain forces $d(u)=d(v)$ and $d(u)^2+d(v)^2 = 2\delta^2$, hence $d(u)=d(v)=\delta$ on every edge, which implies $\delta=\Delta$ and G regular.

For the upper bound, $\varphi(d(u),d(v)) \le K$ and $\sqrt{d(u)^2+d(v)^2} \ge \sqrt{2}\,\delta$, hence

$$\frac{\varphi(d(u),d(v))}{\sqrt{d(u)^2+d(v)^2}} \le \frac{K}{\sqrt{2}\,\delta}.$$

Multiplying by $\sqrt{d(u)^2+d(v)^2}$ and summing gives the upper bound. Equality now requires $\{d(u),d(v)\} = \{\delta,\Delta\}$ and $\sqrt{d(u)^2+d(v)^2} = \sqrt{2}\,\delta$, which forces $\delta=\Delta$, so again G is regular. ∎

5.3 The Randić index

Theorem 6. *For any graph G without isolated vertices,*

$$\sqrt{2}\,\delta\ \mathrm{R}(G)\ \le\ \mathrm{DRSO}(G)\ \le\ M_R\ \mathrm{R}(G),$$

where

$$M_R = \max\left\{\sqrt{2}\,\Delta,\ \frac{\sqrt{\Delta^4+\delta^4}}{\sqrt{\Delta\delta}}\right\}.$$

Equality in the lower bound holds if and only if G is δ-regular. Equality in the upper bound holds if and only if

- $M_R = \sqrt{2}\,\Delta$ *and G is Δ-regular, or*
- $M_R = \frac{\sqrt{\Delta^4+\delta^4}}{\sqrt{\Delta\delta}}$ *and every edge of G joins a vertex of degree δ to a vertex of degree Δ (i.e., G is a bipartite (δ,Δ)-semiregular graph).*

Proof. For an edge uv with degrees $x = d(u)$, $y = d(v)$, the contribution to DRSO relative to the Randić weight is

$$\frac{\varphi(x,y)}{1/\sqrt{xy}} = \varphi(x,y)\sqrt{xy} = \frac{\sqrt{x^4+y^4}}{\sqrt{xy}}.$$

Set $t = \sqrt{xy}$ and $r = \max\{x/y,\ y/x\} \geq 1$. Without loss assume $x \geq y$, so $x = t\sqrt{r}$, $y = t/\sqrt{r}$. Then

$$\varphi(x,y) = \sqrt{r^2+r^{-2}}, \qquad \varphi(x,y)\sqrt{xy} = t\,\sqrt{r^2+r^{-2}}.$$

The constraints $\delta \leq x, y \leq \Delta$ become

$$\delta \leq t/\sqrt{r} \leq t\sqrt{r} \leq \Delta \implies \delta\sqrt{r} \leq t \leq \frac{\Delta}{\sqrt{r}}, \qquad 1 \leq r \leq \frac{\Delta}{\delta}.$$

For a fixed r, the product $t\sqrt{r^2+r^{-2}}$ increases with t, so its maximum is attained at the upper bound $t = \Delta/\sqrt{r}$, giving

$$\max_t \varphi\sqrt{xy} = \frac{\Delta}{\sqrt{r}}\sqrt{r^2+r^{-2}} = \Delta\sqrt{r+\frac{1}{r^3}}.$$

Set $h(r) = r + r^{-3}$ on $[1, \Delta/\delta]$. Then $h'(r) = 1 - 3/r^4$. The derivative vanishes at $r = \sqrt[4]{3} \approx 1.316$, where $h'(r)$ changes from negative to positive; thus h attains a *minimum* at that point. Consequently, the maximum of h on any interval $[1, R]$ occurs at one of the endpoints, $r = 1$ or $r = R = \Delta/\delta$.

Evaluating,

$$\sqrt{h(1)} = \sqrt{2}, \qquad \sqrt{h(\Delta/\delta)} = \sqrt{\frac{\Delta}{\delta} + \frac{\delta^3}{\Delta^3}} = \frac{\sqrt{\Delta^4 + \delta^4}}{\sqrt{\Delta\delta}}.$$

Hence the maximum possible value of $\varphi(x,y)\sqrt{xy}$ is exactly

$$M_R = \max\Big\{\sqrt{2}\,\Delta,\ \frac{\sqrt{\Delta^4 + \delta^4}}{\sqrt{\Delta\delta}}\Big\}.$$

Pointwise this yields $\varphi(x,y)\sqrt{xy} \le M_R$, and multiplying by the Randić weight $1/\sqrt{xy}$ and summing over all edges we obtain $\mathrm{DRSO}(G) \le M_R\ \mathrm{R}(G)$. Equality holds iff every edge attains the maximum, which means that for every edge either $(d(u), d(v)) = (\Delta, \Delta)$ (if $M_R = \sqrt{2}\Delta$) or $\{d(u), d(v)\} = \{\delta, \Delta\}$ (if M_R is given by the second term). These conditions translate precisely to the two cases in the statement.

The lower bound follows by taking the minimum over r and t: $\varphi\sqrt{xy} = t\sqrt{r^2 + r^{-2}} \ge \delta\cdot\sqrt{2}$ (attained when $r = 1$ and $t = \delta$, i.e., $x = y = \delta$). Hence $\mathrm{DRSO}(G) \ge \sqrt{2}\,\delta\ \mathrm{R}(G)$, with equality iff every edge joins two vertices of degree δ, i.e., G is δ-regular. ■

5.4 The harmonic index

Theorem 7. *For a connected graph G without isolated vertices,*

$$\sqrt{2}\,\delta\,H(G) \ \le\ \mathrm{DRSO}(G) \ \le\ M_H\,H(G),$$

where

$$M_H = \max\left\{\sqrt{2}\,\Delta,\ \frac{\delta + \Delta}{2}\,K\right\}, \qquad K = \frac{\sqrt{\Delta^4 + \delta^4}}{\Delta\delta}.$$

Equality in the lower bound holds if and only if G is δ-regular. Equality in the upper bound holds if and only if

- *$M_H = \sqrt{2}\,\Delta$ and G is Δ-regular, or*
- *$M_H = \frac{\delta+\Delta}{2}K$ and every edge joins a vertex of degree δ to a vertex of degree Δ.*

Proof. For an edge uv with $x = d(u)$, $y = d(v)$, the weight in the harmonic index is $2/(x+y)$. We examine

$$\frac{\varphi(x,y)}{2/(x+y)} = \frac{(x+y)\sqrt{x^4+y^4}}{2xy} = \frac{x+y}{2}\,\varphi(x,y).$$

Again set $x = t\sqrt{r}$, $y = t/\sqrt{r}$ with $r \geq 1$, $t = \sqrt{xy}$. Then $x + y = t(\sqrt{r} + 1/\sqrt{r})$, $\varphi(x,y) = \sqrt{r^2 + r^{-2}}$, so

$$\frac{\varphi(x,y)}{2/(x+y)} = \frac{t}{2}\big(\sqrt{r} + 1/\sqrt{r}\big)\sqrt{r^2+r^{-2}} = t\,\psi(r),$$

where $\psi(r) = \frac{1}{2}(r^{1/2} + r^{-1/2})\sqrt{r^2+r^{-2}}$. The constraints give $\delta\sqrt{r} \leq t \leq \Delta/\sqrt{r}$. For fixed r, the expression is increasing in t, so its maximum is at $t = \Delta/\sqrt{r}$:

$$\max_t t\psi(r) = \frac{\Delta}{\sqrt{r}}\,\psi(r) = \Delta \cdot \frac{1}{2}\big(1 + r^{-1}\big)\sqrt{r^2+r^{-2}}.$$

Define $g(r) = \frac{1}{2}\big(1 + r^{-1}\big)\sqrt{r^2+r^{-2}}$. We determine the maximum of $g(r)$ on $[1, \Delta/\delta]$. Write $g(r) = \frac{(r+1)\sqrt{r^4+1}}{2r^2}$. Hence,

$$\frac{g'(r)}{g(r)} = -\frac{r+2}{r(r+1)} + \frac{2r^3}{r^4+1}.$$

Setting $g'(r) = 0$ leads to $\frac{2r^3}{r^4+1} = \frac{r+2}{r(r+1)}$. Therefore, we have

$$2r^4(r+1) = (r+2)(r^4+1),$$

that is,

$$2r^5 + 2r^4 = r^5 + 2r^4 + r + 2;$$

this equality is equivalent to

$$r^5 - r - 2 = 0.$$

Consider $p(r) = r^5 - r - 2$ for $r \geq 1$. We have $p(1) = -2$, $p(2) = 28$, and $p'(r) = 5r^4 - 1 > 0$, so p has exactly one root $r_0 \in (1,2)$. Moreover, $g'(r) <$

0 for $1 \le r < r_0$ and $g'(r) > 0$ for $r > r_0$; hence g attains a *minimum* at r_0, and its maximum on $[1, \Delta/\delta]$ occurs at one of the endpoints. We have $g(1) = \frac{1}{2} \cdot 2 \cdot \sqrt{2} = \sqrt{2}$, giving $\Delta g(1) = \sqrt{2}\,\Delta$. At the other endpoint,

$$g(\Delta/\delta) = \frac{1}{2}\Big(1 + \frac{\delta}{\Delta}\Big)\sqrt{\frac{\Delta^2}{\delta^2} + \frac{\delta^2}{\Delta^2}} = \frac{\delta + \Delta}{2\Delta}\,K,$$

so $\Delta g(\Delta/\delta) = \frac{\delta+\Delta}{2}K$. Thus

$$M_H = \max\Big\{\sqrt{2}\,\Delta,\ \frac{\delta + \Delta}{2}K\Big\}.$$

Pointwise this yields $\frac{\varphi(x,y)}{2/(x+y)} \le M_H$, and multiplying by the harmonic weight and summing gives $\mathrm{DRSO}(G) \le M_H H(G)$. Equality conditions follow exactly as in the Randić case.

The lower bound is obtained by the minimum over t and r: $t\psi(r) \ge \delta \cdot \sqrt{2}$ (at $r = 1$, $t = \delta$), giving $\mathrm{DRSO}(G) \ge \sqrt{2}\,\delta\,H(G)$ with equality iff G is δ-regular. ∎

5.5 The first Zagreb index

Theorem 8. *For a connected graph G with minimum degree δ and maximum degree Δ,*

$$\frac{\sqrt{2}}{2\Delta}\,M_1(G) \;\le\; \mathrm{DRSO}(G) \;\le\; M_Z\,M_1(G),$$

where

$$M_Z = \max\left\{\frac{\sqrt{2}}{2\delta},\ \frac{\sqrt{\Delta^4 + \delta^4}}{\delta\Delta(\delta + \Delta)}\right\}.$$

Equality in the lower bound holds if and only if G is Δ-regular. Equality in the upper bound holds if and only if

- $M_Z = \frac{\sqrt{2}}{2\delta}$ *and G is δ-regular, or*
- $M_Z = \frac{\sqrt{\Delta^4+\delta^4}}{\delta\Delta(\delta+\Delta)}$ *and every edge of G joins a vertex of degree δ to a vertex of degree Δ.*

Proof. For an edge uv with degrees x, y,

$$\frac{\varphi(x,y)}{x+y} = \frac{\sqrt{x^4+y^4}}{xy(x+y)}.$$

With $x = t\sqrt{r}$, $y = t/\sqrt{r}$, $r \geq 1$, we get $x + y = t(\sqrt{r} + 1/\sqrt{r})$, and

$$\frac{\varphi(x,y)}{x+y} = \frac{t^2\sqrt{r^4+1}}{t^2 r}\,\frac{1}{t(\sqrt{r}+1/\sqrt{r})} = \frac{\sqrt{r^4+1}}{r\,t\,(\sqrt{r}+1/\sqrt{r})} = \frac{1}{t}\,h(r),$$

where

$$h(r) = \frac{\sqrt{r^4+1}}{r^{3/2}+r^{1/2}}.$$

The constraints become $t \geq \delta\sqrt{r}$ and $t \leq \Delta/\sqrt{r}$. Because the expression is decreasing in t (for fixed r), its maximum is at the smallest possible t, i.e., $t = \delta\sqrt{r}$. Then

$$\max_t \frac{\varphi}{x+y} = \frac{1}{\delta\sqrt{r}}\,h(r) = \frac{1}{\delta}\,\frac{\sqrt{r^4+1}}{r^2+r}.$$

Define $F(r) = \frac{\sqrt{r^4+1}}{r^2+r}$ on $[1, \Delta/\delta]$. Its derivative is

$$F'(r) = \frac{r^4 - 2r - 1}{(r^2+r)^2\sqrt{r^4+1}}.$$

The numerator $q(r) = r^4 - 2r - 1$ satisfies $q(1) = -2$, $q(2) = 11$, and $q'(r) = 4r^3 - 2 > 0$ for $r \geq 1$. Hence q has exactly one root $r_1 > 1$, and $F'(r)$ changes from negative to positive at r_1; consequently F attains a minimum there, and its maximum on $[1, \Delta/\delta]$ is at one of the endpoints. Evaluating,

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

Thus the overall maximum factor is

$$M_Z = \frac{1}{\delta}\max\{F(1),\, F(\Delta/\delta)\} = \max\left\{\frac{\sqrt{2}}{2\delta},\, \frac{\sqrt{\Delta^4+\delta^4}}{\delta\Delta(\delta+\Delta)}\right\}.$$

Pointwise $\frac{\varphi(x,y)}{x+y} \leq M_Z$, and multiplying by $(x+y)$ and summing gives

$\mathrm{DRSO}(G) \leq M_Z M_1(G)$. Equality conditions: the maximum is attained iff for every edge, either $(d(u), d(v)) = (\delta, \delta)$ (when $M_Z = \sqrt{2}/(2\delta)$) or $\{d(u), d(v)\} = \{\delta, \Delta\}$ (when the second term is the maximum).

The lower bound follows by taking t as large as possible ($t = \Delta/\sqrt{r}$) and $r = 1$, yielding $\frac{\varphi}{x+y} \geq \frac{\sqrt{2}}{2\Delta}$, with equality when every edge joins two vertices of degree Δ, i.e., G is Δ-regular. ■

6 Chemical trees and extremal behaviour

In chemical graph theory, the graphs representing alkanes are trees with maximum degree at most four (since each carbon atom forms at most four bonds). To verify the extremal conjectures and to provide numerical evidence in this chemically relevant class, we computed the DRSO index for all such trees with $4 \leq n \leq 10$. The results are summarised in Table 2.

Table 2. Minimum and maximum DRSO values among chemical trees ($\Delta \leq 4$) with n vertices.

n	# trees	$\mathrm{DRSO}(P_n)$	max(DRSO)	maximising graph
4	2	5.5373	9.0554	S_4 (star)
5	3	6.9515	16.0312	S_5 (star)
6	5	8.3657	16.1465	degree-4 hub with a length-2 branch
7	9	9.7800	19.5901	degree-4 hub connected to degree-3 vertex
8	18	11.1942	25.4610	double star $D(3,3)$ (two adjacent degree-4 hubs)
9	35	12.6084	28.1699	two degree-4 hubs with one bridge vertex
10	75	14.0226	30.1249	two degree-4 hubs with a bridge vertex of degree 3

Several observations follow:

- The path P_n consistently minimises the DRSO index among all chemical trees, supporting the conjecture stated in Section 3.
- The star S_n is only valid for $n \leq 5$ (since it has a vertex of degree $n-1$). For $n \geq 6$, the maximising trees are double-star-like structures with hubs of degree four, which are the most branched

chemically feasible trees. This refined extremal characterisation is a new contribution of the present work.

- The numerical values confirm the sharpness of the bounds derived in Sections 4 and 5.

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