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Geometric Approach to Degree–Based Topological Index: Hyperbolic Directrix Sombor Index

Vitthal Hivrale[a,b,*], Ganesh Mundhe[a], Balasaheb Waphare[b]

[a] *Army Institute of Technology, Pune 411015, Maharashtra, India*
[b] *MIT Arts, Commerce and Science College, Alandi, Pune, India*
vitthalhivrale2012@gmail.com, ganumundhe@gmail.com,
balasahebwaphare@gmail.com

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Abstract

In this article, we present a new topological index based on a geometric approach. A new insight on the mathematical background of the hyperbolic directrix of classical conic geometry is used in development of the new topological index. When we consider an active edge as a coordinate point $P(d(u), d(v))$ with $d(u) \leq d(v)$, the usual Sombor index is developed by considering Euclidean distance to the origin, $\sqrt{d(u)^2 + d(v)^2}$. Meanwhile the smaller degree $d(u)$ measures the perpendicular distance from P to the vertical axis which acts as a structural directrix line. This defines the local edge contribution by dividing the squared distance to this directrix by the overall Euclidean distance, that is, $\frac{d(u)^2}{\sqrt{d(u)^2+d(v)^2}}$. This directrix of a hyperbola inspired us to design a new geometric topological index, which we introduce here as the Hyperbolic Directrix Sombor Index, its definition is given by: $\mathcal{HDSO}(G) = \sum_{uv \in E(G)} \frac{\{\min(d(u),d(v))\}^2}{\sqrt{d^2(u)+d^2(v)}}$. We give basic properties of the $\mathcal{HDSO}$ index and obtain $\mathcal{HDSO}$

*Corresponding author.

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index for few fundamental graphs. We also discuss propeties of octane isomers by relating it to the HDSO index. We propose several structural variants of the $\mathcal{HDSO}$ index: a modified and a reduced version.

1 Introduction

In this paper, the domain of study is bounded by a simple, connected graph G containing a vertex set of size $|V| = n$ and an edge set of size $|E| = m$. An incident link uv joins the vertices u and v, where the standard notation $d(v)$ represents the degree of vertex v. The structural network limits are governed by the maximum degree Δ and the minimum degree δ. The classical graph families utilized as benchmarks across this paper include the path P_n, cycle C_n, tree T_n, star S_n, and complete graph K_n on n vertices. A path graph P_n is structurally parameterized by the vertex set $V(P_n) = \{v_1, v_2, v_3, \ldots, v_n\}$ and the sequential edge distribution $E(P_n) = \{v_1v_2, v_2v_3, v_3v_4, \ldots, v_{n-1}v_n\}$. Similarly, a cycle graph C_n encompasses the identical vertex arrangement $V(C_n) = \{v_1, v_2, v_3, \ldots, v_n\}$, but completes a ring topology using the closed edge set $E(C_n) = \{v_1v_2, v_2v_3, v_3v_4, \ldots, v_{n-1}v_n, v_nv_1\}$. A tree is defined fundamentally as a connected graph that lacks any internal cycles. A star graph operates as a tree variant containing a primary central hub adjacent to every other node, leaving the remaining vertices as peripheral pendant elements with a degree of 1. Finally, a complete graph manifests as a simple topology where a unique edge spans between every possible pair of non-identical vertices.

To study various physical properties of the chemical graphs, a vertex-degree based descriptor, *topological index* is developed, and is given in [26] as

$$TI(G) = \sum_{E(G)} \Phi(d(u), d(v)), \qquad (1)$$

where d(u) and d(v) are degrees of adjacent vertices u and v and $\Phi(d(u), d(v)) \geq 0$ is a real-valued symmetric function.

Now we present formulations for few degree-based topological indices

with different theoretical forms of the function $\Phi(d(u), d(v))$, which is used in this paper. In 1972, I. Gutman and N. Trinajstic [9] are among the first to formulate a topological index called as first zagreb index and defined it as:

$$\mathcal{M}_1(G) = \sum_{E(G)} (d(u) + d(v)).$$

B. Furtula and I. Gutman [4], proposed the forgotten index in 2015, which they defined as:

$$\mathcal{F}(G) = \sum_{E(G)} \left(d(u)^2 + d(v)^2\right).$$

For initial few years algebraic approach has been used to developed the topological indices. Ivan Gutman [5] has come up with geometric approach for constructing degree-based indices. In 2021, he defined Sombor Index as

$$\mathcal{SO}(G) = \sum_{E(G)} \sqrt{d(u)^2 + d(v)^2},$$

which quickly captured the interest of mathematical community. Since its inception, the Sombor index has become a remarkably popular topic, lead to numerous topological indices derived from that. H. Liu, I. Gutman, L. You, and Y. Huang [17] presented a detailed review of the Sombor index, highlighting various bounds and extremal results that had appeared in the literature up to March 2022. In a recent survey, Ivan Gutman [7] reviewed Sombor-type degree-based topological indices and summarized the major developments in this area.

Recently, Zhen Lin, Jiajia Wang and Yilin Wang [16] introduced an elliptic eccentricity-based index, the Elliptic Eccentric Sombor Index. It is defined as:

$$\mathcal{EESO}(G) = \sum_{E(G)} \frac{|d(u) - d(v)|}{\sqrt{d^2(u) + d^2(v)}}.$$

In 2025, Jayjit Barman and Shibsankar Das [1] have developed the

hyperbolic Sombor index ($\mathcal{HSO}$). The definition of ($\mathcal{HSO}$) is:

$$\mathcal{HSO}(G) = \sum_{E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{\min\{d(u), d(v)\}}.$$

For instance, the $\mathcal{HSO}$ uses the eccentricity of a hyperbola to measure the structural irregularities. The mathematical framework of $\mathcal{HSO}$ divides the Euclidean distance of a degree pair by the minimum vertex degree, and thus essentially acts as a "irregularity magnifier". A significant portion of topological descriptor research focuses on design frameworks derived from vertex degrees, establishing a rich baseline of rigorously analyzed structural indices [1, 2, 5, 6, 8, 12–15, 18, 19, 25].

Such operational constraints inspired a novel self-regulating molecular descriptor, namely the Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$). $\mathcal{HDSO}$ measures the perpendicular distance from the center of an implied hyperbola to its guiding directrix line, instead of eccentricity or raw vector length. A standard hyperbola having center at the origin O has vertices at $V(\pm a, 0)$ and co-vertices at $P(0, \pm b)$, giving it the following geometric definition:

$$\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1.$$

The distance from the center to either focus point $F(\pm c, 0)$ is $c = \sqrt{a^2 + b^2}$. The directrices are the vertical lines given by the linear equations $x = \frac{a^2}{c}$, and $x = -\frac{a^2}{c}$. Then the orthogonal distance d from the origin to either directrix reduces to the compact ratio:

$$d = \frac{a^2}{c} = \frac{a^2}{\sqrt{a^2 + b^2}}.$$

This directrix formula motivated us to define a topological index, which we introduce here as the Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$). For a graph G is formally defined by mapping the adjacent vertex degrees of an arbitrary edge $uv \in E(G)$ directly to these semi-axes such that $a = \min\{d(u), d(v)\}$ and $b = \max\{d(u), d(v)\}$ as:

$$\mathcal{HDSO}(G) = \sum_{uv \in E(G)} \frac{\min\{d(u), d(v)\}^2}{\sqrt{d^2(u) + d^2(v)}}.$$

Adopting an ordered convention where $0 < d(u) \leq d(v)$ across all active edges, we propose to use the following definition of the $\mathcal{HDSO}(G)$ throughout the paper:

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

In view of the different articles published on Sombor index and some other topological indices like [3, 10, 11, 18, 20, 21, 24, 27] have motivated us to introduce the following few indices:

Modified Hyperbolic Directrix Sombor Index (${}^m\mathcal{HDSO}$), defined as

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

Reduced Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}_{red}$), as

$$\mathcal{HDSO}_{red}(G) = \sum_{uv \in E(G)} \frac{d_{red}(u)^2}{\sqrt{d_{red}^2(u) + d_{red}^2(v)}}.$$

where $d_{red}(u) = d(u) - 1, d_{red}(v) = d(v) - 1$. For $\delta(G) \geq 2$, $\mathcal{HDSO}_{red}$ is well-defined.

For convenience of notation throughout this manuscript, any arbitrary edge $uv \in E(G)$ is parameterized by its endpoint degrees $d(u) = r$ and $d(v) = s$. In accordance with the standard non-decreasing sorting convention, these vertex states are bounded by the minimum and maximum degrees of the graph such that $\delta \leq r \leq s \leq \Delta$. Under this ordered framework, the function which governing the Hyperbolic Directrix Sombor ($\mathcal{HDSO}$) descriptor is defined as:

$$\phi_{\mathcal{HDSO}}(r, s) = \frac{r^2}{\sqrt{r^2 + s^2}}.$$

To establish a clear structural comparison across classical topological spaces, we map out the corresponding local edge contribution functions

for the Sombor ($\mathcal{SO}$), Hyper-Sombor ($\mathcal{HSO}$), First Zagreb ($\mathcal{M}_1$), and Forgotten ($\mathcal{F}$) indices respectively: $\phi_{\mathcal{SO}}(r,s) = \sqrt{r^2+s^2}$, $\phi_{\mathcal{HSO}}(r,s) = \frac{\sqrt{r^2+s^2}}{r}$, $\phi_{\mathcal{M}_1}(r,s) = r+s$ and $\phi_{\mathcal{F}}(r,s) = r^2+s^2$.

In Section 2, we discuss the bounds of $\mathcal{HDSO}$ in terms of the maximum degree Δ and the minimum degree δ. We also obtain explicit results in relation to the $\mathcal{SO}$ index, the First Zagreb index, and the Forgotten index. Additionally, a detailed comparison between $\mathcal{HSO}$ and $\mathcal{HDSO}$ is presented. Finally, the exact values for several fundamental graph families are derived.

2 Mathematical results of hyperbolic directrix Sombor index

Here is a formal mathematical theorem and proof establishing the strict relationship between the Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$) and the Hyperbolic Sombor Index ($\mathcal{HSO}$) for any non-trivial graph.

Theorem 1. *Let $G = (V,E)$ be a connected, non-trivial graph of order $n \geq 2$. For any edge $uv \in E(G)$ parameterized under the adjacent vertex degree ordering convention $r \leq s$ where $r = k$ and $s = k+\alpha$ ($\alpha \geq 0$):*

1. *If $k = 1$ and $\alpha \geq 0$, then $\phi_{\mathcal{HDSO}}(r,s) < \phi_{\mathcal{HSO}}(r,s)$.*
2. *If $k = 2$ and $\alpha = 0$, then $\phi_{\mathcal{HDSO}}(r,s) = \phi_{\mathcal{HSO}}(r,s)$.*
   If $k = 2$ and $\alpha > 0$, then $\phi_{\mathcal{HDSO}}(r,s) < \phi_{\mathcal{HSO}}(r,s)$.
3. *If $k \geq 3$ and $\alpha > k(\sqrt{k-1}-1)$, then $\phi_{\mathcal{HDSO}}(r,s) < \phi_{\mathcal{HSO}}(r,s)$.*
   If $k \geq 3$ and $\alpha < k(\sqrt{k-1}-1)$, then $\phi_{\mathcal{HDSO}}(r,s) > \phi_{\mathcal{HSO}}(r,s)$.
   If $k \geq 3$ and $\alpha = k(\sqrt{k-1}-1)$, then $\phi_{\mathcal{HDSO}}(r,s) = \phi_{\mathcal{HSO}}(r,s)$.

Proof. For any arbitrary edge of $E(G)$ be an satisfying $1 \leq r \leq s$. By definition, the operational weights form the comparative ratio

$$\mathcal{R} = \frac{\phi_{\mathcal{HDSO}}(r,s)}{\phi_{\mathcal{HSO}}(r,s)} = \frac{r^3}{r^2+s^2}.$$

By using $r = k$ and $s = k + \alpha$ ($\alpha \geq 0$), we can get:

$$\mathcal{R} = \frac{k^3}{k^2 + (k+\alpha)^2}.$$

A polynomial can be formed using numerator and denominator of $\mathcal{R}$:

$$f(k, \alpha) = k^2(k-1) - (k+\alpha)^2.$$

Therefore, we can notice:

$$f(k,\alpha) > 0 \implies \mathcal{R} > 1 \implies \phi_{\mathcal{HDSO}}(r,s) > \phi_{\mathcal{HSO}}(r,s).$$
$$f(k,\alpha) < 0 \implies \mathcal{R} < 1 \implies \phi_{\mathcal{HDSO}}(r,s) < \phi_{\mathcal{HSO}}(r,s).$$
$$f(k,\alpha) = 0 \implies \mathcal{R} = 1 \implies \phi_{\mathcal{HDSO}}(r,s) = \phi_{\mathcal{HSO}}(r,s).$$

Let the polynomial $f(k, \alpha)$ to build the relationship between $\phi_{\mathcal{HDSO}}(r, s)$ and $\phi_{\mathcal{HSO}}(r, s)$. Hence, we have to determine α values for the value of k.

Suppose $f(k, \alpha) > 0$,

$$k^2(k-1) > (\alpha + k)^2,$$

$$\alpha < k[\sqrt{k-1} - 1].$$

Similarly,

$$\text{for } f(k,\alpha) < 0, \text{ then } \alpha > k[\sqrt{k-1} - 1],$$
$$\text{and for } f(k,\alpha) = 0, \text{ then } \alpha = k[\sqrt{k-1} - 1].$$

$\alpha = k[\sqrt{k-1} - 1]$ occurs when $k - 1$ is a perfect square.

We evaluate this across valid structural degree domains of G:

Case 1: Let $k = 1$. Substituting $k = 1$ yields, $f(k, \alpha) < 0$ holds universally for all $\alpha \geq 0$. Hence,

$$\phi_{\mathcal{HDSO}}(r,s) < \phi_{\mathcal{HSO}}(r,s).$$

Case 2 Let $k = 2$. Substituting $k = 2$ yields, $f(k, \alpha) = 0$ holds for $\alpha = 0$. Hence,

$$\phi_{\mathcal{HDSO}}(r,s) = \phi_{\mathcal{HSO}}(r,s)(r,s).$$

And it yields: $f(k, \alpha) < 0$ holds for $\alpha > 0$. Hence,

$$\phi_{\mathcal{HDSO}}(r, s) < \phi_{\mathcal{HSO}}(r, s).$$

Case 3 Let $k \geq 3$.

i. Then $f(k, \alpha) < 0$ for $\alpha > k(\sqrt{k-1} - 1)$. Hence,

$$\phi_{\mathcal{HDSO}}(r, s) < \phi_{\mathcal{HSO}}(r, s).$$

ii. Then $f(k, \alpha) > 0$ for $\alpha < k(\sqrt{k-1} - 1)$. Hence,

$$\phi_{\mathcal{HDSO}}(r, s) > \phi_{\mathcal{HSO}}(r, s).$$

iii. Then $f(k, \alpha) = 0$ for $\alpha = k(\sqrt{k-1} - 1)$. Hence,

$$\phi_{\mathcal{HDSO}}(r, s) = \phi_{\mathcal{HSO}}(r, s).$$

This completes the proof. ■

By minimizing the localized descriptor space across edge parameters, the following theorem establishes a sharp global lower boundary for $\mathcal{HDSO}(G)$ relative to fundamental structural parameters.

Theorem 2. *Let Δ be the maximum degree and $|E| = m$ in a simple connected graph G. Then $\mathcal{HDSO}$ satisfies the lower bound:*

$$\mathcal{HDSO}(G) \geq \frac{m}{\sqrt{\Delta^2 + 1}},$$

where equality holds for every structural link in G adheres to the uniform degree layout $(1, \Delta)$.

Proof. Since, $0 < r \leq s \leq \Delta$,

$$\phi_{\mathcal{HDSO}}(r, s) = \frac{r^2}{\sqrt{r^2 + s^2}}.$$

For the absolute minimum value, let $d(v) = \Delta$,

$$\phi_{\mathcal{HDSO}}(r,s) \geq \frac{r^2}{\sqrt{s^2+\Delta^2}}.$$

Let $d(u) = 1$,

$$\phi_{\mathcal{HDSO}}(r,s) \geq \frac{1}{\sqrt{\Delta^2+1}}.$$

Taking the sum across all active links preserves the operator hierarchy,

$$\mathcal{HDSO}(G) \geq \sum_{E(G)} \frac{1}{\sqrt{\Delta^2+1}}.$$

Therefore,

$$\mathcal{HDSO}(G) \geq \frac{m}{\sqrt{\Delta^2+1}}$$

The equality is reached if and only if every local link simultaneously satisfies the dual optimization constraints $r = 1$ and $s = \Delta$. This completes the proof. ■

Corollary. *If G is a star graph, then*

$$\mathcal{HDSO}(G) = \frac{m}{\sqrt{\Delta^2+1}}.$$

By minimizing the edge metric space through algebraic bounding techniques, we can establish an alternative lower boundary for $\mathcal{HDSO}(G)$ that reaches optimal sharpness on symmetric structures.

Theorem 3. *Let Δ be the maximum degree and $m = |E(G)|$ in a simple connected graph $G = (V, E)$. Then,*

$$\mathcal{HDSO}(G) \geq \frac{m}{\sqrt{2}\Delta}.$$

Equality is attained if $G \cong K_2$.

Proof. For

$$0 < r \leq s \leq \Delta$$

Squaring and adding the s^2 term in above inequality,

$$r^2 + s^2 \leq 2s^2.$$

Applying these transformations to the inequality—specifically, taking the square root, taking the reciprocal, and then multiplying the result by r^2 yields:

$$\frac{r^2}{\sqrt{r^2+s^2}} \geq \frac{r^2}{\sqrt{2}s}. \qquad (2)$$

Minimum possible value for $r = 1$ and the maximum for $s = \Delta$,

$$\frac{r^2}{\sqrt{2}s} \geq \frac{1}{\sqrt{2}\Delta}. \qquad (3)$$

Combining equations (2) and (3) Taking the sum over the number of edges m, we get:

$$\mathcal{HDSO}(G) \geq \sum_{E(G)} \frac{1}{\sqrt{2}\Delta} = \frac{m}{\sqrt{2}\Delta}.$$

In case of k_2,

$$\mathcal{HDSO}(G) = \frac{1}{\sqrt{2}},$$

$$\frac{m}{\sqrt{2}\Delta} = \frac{1}{\sqrt{2}.1} = \frac{1}{\sqrt{2}}.$$

Hence the equality hold if $G \cong K_2$. This completes the proof. ■

Remarks: The bound $\frac{m}{\sqrt{\Delta^2+1}}$ offers a stricter lower limit than $\frac{m}{\sqrt{2}\Delta}$ among those obtained in Theorems 2 and 3.

In the theorem given below, we have obtained a tight upper threshold for the index across general connected structures.

Theorem 4. *Let G be a connected graph of size m. Then,*

$$\mathcal{HDSO}(G) \leq m \cdot \frac{\Delta^2}{\sqrt{\Delta^2+\delta^2}}.$$

Here equality holds if and only if a network whose links connect vertices of equal degree.

Proof. For $\delta \leq r \leq s \leq \Delta$,

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{r^2}{\sqrt{r^2+s^2}},$$

$$\phi_{\mathcal{HDSO}}(r,s) \leq \phi_{\mathcal{HDSO}}(\delta,\Delta) = \frac{\delta^2}{\sqrt{\Delta^2+\delta^2}} \leq \frac{\Delta^2}{\sqrt{\Delta^2+\delta^2}}.$$

Summing this invariant maximum weight contribution over all active links m in the graph preserves the linear operator hierarchy:

$$\mathcal{HDSO}(G) \leq \sum_{E(G)} \frac{\Delta^2}{\sqrt{\Delta^2+\delta^2}},$$

$$\mathcal{HDSO}(G) \leq m \cdot \frac{\Delta^2}{\sqrt{\Delta^2+\delta^2}}.$$

The equality holds if $(\Delta = \delta)$, that is for regular graphs. This concludes the proof. ■

Here, for $\mathcal{HDSO}$, we have developed lower and upper bounds in terms of classical Sombor Index ($\mathcal{SO}$).

Theorem 5. *For a connected graph G, then*

$$\frac{\delta^2}{2\Delta^2} \cdot \mathcal{SO}(G) \leq \mathcal{HDSO}(G) \leq \frac{\Delta^2}{2\delta^2} \cdot \mathcal{SO}(G).$$

For a regular graph G algebraic equality is achieved.

Proof. Since,

$$\delta \leq r \leq s \leq \Delta$$

Using functions $\phi_{\mathcal{HDSO}}$ and $\phi_{\mathcal{SO}}$,

$$\phi_{\mathcal{HDSO}}(r,s) = \left(\frac{r^2}{r^2+s^2}\right)\phi_{\mathcal{SO}}(r,s).$$

To construct the upper boundary, maximize this localized coefficient.

$$\frac{r^2}{r^2+s^2} \leq \frac{\Delta^2}{\delta^2+\delta^2} = \frac{\Delta^2}{2\delta^2}.$$

Conversely, the lower boundary is isolated by minimizing the fraction.

$$\frac{r^2}{r^2+s^2} \geq \frac{\delta^2}{\Delta^2+\Delta^2} = \frac{\delta^2}{2\Delta^2}.$$

Substituting these uniform structural bounding ratios back into the localized edge equation yields the direct, scale-invariant functional envelope,

$$\frac{\delta^2}{2\Delta^2} \cdot \phi_{\mathcal{SO}}(r,s) \leq \phi_{\mathcal{HDSO}}(r,s) \leq \frac{\Delta^2}{2\delta^2} \cdot \phi_{\mathcal{SO}}(r,s).$$

Taking summation over the set $E(G)$, then the targeted relationship,

$$\frac{\delta^2}{2\Delta^2} \cdot \mathcal{SO}(G) \leq \mathcal{HDSO}(G) \leq \frac{\Delta^2}{2\delta^2} \cdot \mathcal{SO}(G)$$

Let a k-regular graph, for which $\Delta = \delta = k$ which leads to,

$$\frac{1}{2} \cdot \mathcal{SO}(G) \leq \mathcal{HDSO}(G) \leq \frac{1}{2} \cdot \mathcal{SO}(G).$$

This completes the theorem. ■

Corollary. *For a regular graph G,*

$$\mathcal{HDSO}(G) = \frac{1}{2} \cdot \mathcal{SO}(G).$$

Here, we have obtained bounds for $\mathcal{HDSO}$ in terms of First Zagreb Index ($\mathcal{M}_1(G)$).

Theorem 6. *For any simple connected graph G,*

$$\frac{\delta^2}{4\Delta^2} \cdot M_1(G) \leq \mathcal{HDSO}(G) \leq \frac{\Delta^2}{2\sqrt{2}\delta^2} \cdot M_1(G).$$

Furthermore, the right boundary collapse into a perfect identity for a regular graph.

Proof. Since $\delta \leq r \leq s \leq \Delta$ and $(r+s)^2 \leq (\sqrt{2}\sqrt{r^2+s^2})^2$,

$$\frac{1}{r+s} < \frac{1}{\sqrt{r^2+s^2}} \leq \frac{\sqrt{2}}{r+s}.$$

Multiplying with r^2 the above inequality yields,

$$\frac{r^2}{r+s} < \phi_{\mathcal{HDSO}}(r,s) \leq \frac{\sqrt{2}r^2}{r+s}. \qquad (4)$$

To the above inequality, we evaluate the upper and lower bounds independently across the graph's entire degree sequence.

To prove $\mathcal{HDSO}(G) \leq \frac{\Delta^2}{2\sqrt{2}\delta^2} \cdot M_1(G)$.

As $r \leq s$,

$$r+s \geq 2\delta$$

$$\frac{1}{2\delta} \geq \frac{1}{r+s}. \qquad (5)$$

To introduce the First Zagreb, we use equation (4) and (5) to establish the following relation:

$$\frac{\sqrt{2}r^2}{r+s} \leq \frac{\sqrt{2}\Delta^2}{2\delta} = \frac{\sqrt{2}\Delta^2}{4\delta^2}(2\delta) \leq \frac{\sqrt{2}\Delta^2}{4\delta^2}(r+s).$$

Taking summation over the edge set $E(G)$ gives:

$$\mathcal{HDSO}(G) \leq \frac{\sqrt{2}\Delta^2}{4\delta^2} M_1(G) = \frac{\Delta^2}{2\sqrt{2}\delta^2} \cdot M_1(G)$$

Now to establish the left-hand local inequality:

$$\frac{\delta^2}{2\Delta^2} \cdot M_1(G) \leq \mathcal{HDSO}(G).$$

From equation (4) we can get the inequality,

$$\frac{r^2}{r+s} \leq \phi_{\mathcal{HDSO}}(r,s).$$

Since $r^2 \geq \delta^2$, then

$$r+s \leq 2\Delta.$$

This allows us to bound the denominator directly,

$$\frac{s^2}{r+s} \geq \frac{\delta^2}{2\Delta},$$

$$\frac{\delta^2}{2\Delta} = \frac{\delta^2}{4\Delta^2}(2\Delta) \geq \frac{\delta^2}{4\Delta^2}(r+s).$$

Taking summation over the edge set $E(G)$ gives,

$$\mathcal{HDSO}(G) \geq \frac{\delta^2}{4\Delta^2} M_1(G) = \frac{\delta^2}{4\Delta^2} \cdot M_1(G).$$

Combining these two mathematically verified optimization limits locks your index into its true global inequality envelope,

$$\frac{\delta^2}{4\Delta^2} \cdot M_1(G) \leq \mathcal{HDSO}(G) \leq \frac{\sqrt{2}\Delta^2}{4\delta^2} \cdot M_1(G).$$

Evaluating the right boundary shows that the inequalities collapse into a perfect identity if and only if every single vertex in the graph possesses identical degree distributions ($\delta = d(u) = d(v) = \Delta$). This completes the proof. ■

Here, we have established the $\mathcal{HDSO}$ for fundamental graph structures.

Lemma 1. *For a path graph P_n,*

$$\mathcal{HDSO}(P_n) = \frac{2}{\sqrt{5}} + \sqrt{2}(n-3).$$

Proof. Consider a path P_n. The edge set of a path graph P_n, denoted as $E(P_n)$, can be split into two separate, non-overlapping subsets:

$$E_1 = \{uv \in E(P_n) \mid \text{at least one of the vertex is pendant vertex}\}$$

$$E_2 = \{uv \in E(P_n) \mid \text{ the degrees of } u \text{ and } v \text{ are } 2.\}$$

Here, $|E_1| = 2$ and $|E_2| = n - 3$.

Therefore;

$$\begin{aligned}\mathcal{HDSO}(P_n) &= \sum_{uv \in E_1} \frac{1^2}{\sqrt{1^2+2^2}} + \sum_{uv \in E_2} \frac{2^2}{\sqrt{2^2+2^2}} \\ &= \frac{2}{\sqrt{5}} + \sqrt{2}(n-3)\end{aligned}$$

This completes the proof. ■

Lemma 2. *Let C_n, S_n and K_n denote cyclic, star and complete graphs with order n, respectively. Then,*

1. $\mathcal{HDSO}(C_n) = \sqrt{2}n$ *for* $n \geq 3$
2. $\mathcal{HDSO}(S_n) = \frac{n-1}{\sqrt{(n-1)^2+1}}$ *for* $n \geq 1$
3. $\mathcal{HDSO}(K_n) = \frac{n(n-1)^2}{2\sqrt{2}}$ *for* $n \geq 1$

Proof. We have proved this result in three cases:

Case I $(C_n, n \geq 3)$**:**
A cycle graph with $|C_n| = n$ and $|E(C_n)| = n$. Then,

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{2^2}{\sqrt{2^2+2^2}} = \frac{4}{2\sqrt{2}} = \sqrt{2}.$$

Taking the summation over all edges, we get:

$$\mathcal{HDSO}(C_n) = \sum_{uv \in E(C_n)} \sqrt{2} = \sqrt{2}n.$$

Case II $(S_n, n \geq 1)$**:** A star network with $|V| = n$ and $|E| = n-1$. For any edge, degree of endpoints is either 1 or $n-1$. Therefore;

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{1^2}{\sqrt{1^2+(n-1)^2}},$$

$$\mathcal{HDSO}(S_n) = \sum_{uv \in E(S_n)} \phi_{\mathcal{HDSO}}(r,s) = \frac{n-1}{\sqrt{(n-1)^2+1}}.$$

Case III $(K_n, n \geq 1)$**:** A complete network with $|V| = n$ and $|E| = \frac{n(n-1)}{2}$. The degree degree of endpoints are $n-1$. Therefore;

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{n-1}{\sqrt{2}}.$$

Which leads to:

$$\mathcal{HDSO}(K_n) = \sum_{uv \in E(K_n)} \phi_{\mathcal{HDSO}}(r,s) = \frac{n(n-1)^2}{2\sqrt{2}}.$$

This completes the proof. ■

Corollary. *1. For Paths:* $\phi_{\mathcal{HDSO}}(r,s) \leq \frac{\Delta}{\sqrt{2}}$, *for* $n \geq 2$.

2. For Cycles: $\phi_{\mathcal{HDSO}}(r,s) = \frac{\Delta}{\sqrt{2}}$, *for* $n \geq 3$.

3. For Star Graphs: $\phi_{\mathcal{HDSO}}(r,s) \leq \frac{\delta}{\sqrt{2}}$, *for* $n \geq 2$.

4. For Complete Graphs: $\phi_{\mathcal{HDSO}}(r,s) = \frac{\delta}{\sqrt{2}}$, *for* $n \geq 3$.

Proof. The proof is straightforward. ■

Because the edge weighting mechanics of the Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$) penalize local degree imbalances, the classic extremal behaviors typically seen in traditional Sombor-type indices are completely inverted. The following theorem identifies the absolute upper and lower boundaries for any general connected network of a fixed order.

Theorem 7. *A simple connected graph* G *with* $|V(G)| \geq 3$. *Then,*

$$\mathcal{HDSO}(S_n) \leq \mathcal{HDSO}(G) \leq \mathcal{HDSO}(K_n).$$

Proof. Let us prove forming the two separate cases for left-hand and right-hand equalities.

The Lower Bound ($\mathcal{HDSO}(G) \geq \mathcal{HDSO}(S_n)$)**:**

For graph G,

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{r^2}{\sqrt{r^2+s^2}},$$

and for S_n,

$$\phi'_{\mathcal{HDSO}}(r,s) = \frac{1}{\sqrt{1+\Delta^2}}.$$

Since, $r = 1$ is minimum possible value and $s = \Delta$ is maximum value, then we can get:

$$\phi_{\mathcal{HDSO}}(r,s) \geq \phi'_{\mathcal{HDSO}}(r,s).$$

Taking sum over the set of edges, yields:

$$\mathcal{HDSO}(G) \geq \mathcal{HDSO}(S_n).$$

For this equality hplds if the given graph is S_n.

The Upper Bound ($\mathcal{HDSO}(G) \leq \mathcal{HDSO}(K_n)$):

For graph G,

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{r^2}{\sqrt{r^2+s^2}},$$

and for K_n,

$$\phi'_{\mathcal{HDSO}}(r,s) = \frac{\Delta}{\sqrt{\Delta^2+\Delta^2}} = \frac{\Delta}{\sqrt{2}}.$$

Since both $x = \Delta$ and $y = \Delta$ are maximum possible values, then

$$\phi_{\mathcal{HDSO}}(r,s) \leq \phi'_{\mathcal{HDSO}}(r,s).$$

Taking sum over the set of edges, yields:

$$\mathcal{HDSO}(G) \leq \mathcal{HDSO}(K_n).$$

The equality will be achieved if the graph G is K_n. This completes the proof. ■

When we look at acyclic graphs (or trees), the Hyperbolic Directrix Sombor index ($\mathcal{HDSO}$) maps out two very clear, opposing structural boundaries. This theorem pins down the exact highest and lowest possible values for any tree network with a set number of vertices.

Theorem 8. *For S_n and P_n, a tree T with $V(T) \geq 3$,*

$$\mathcal{HDSO}(S_n) \leq \mathcal{HDSO}(T) \leq \mathcal{HDSO}(P_n).$$

Proof. As per Lemma 2,

$$\mathcal{HDSO}(S_n) = \sum_{E(S_n)} \frac{1}{\sqrt{1+(n-1)^2}}.$$

For a tree,

$$\mathcal{HDSO}(T) = \sum_{E(T)} \frac{r^2}{\sqrt{r^2+s^2}}.$$

Comparing above two equations, we can conclude that,

$$\frac{1}{\sqrt{1+(n-1)^2}} \leq \frac{r^2}{\sqrt{r^2+s^2}} \qquad (\because 1 \leq r \text{ and } s \leq n-1).$$

Therefore, taking sum over the edge set, we can prove,

$$\mathcal{HDSO}(S_n) \leq \mathcal{HDSO}(T).$$

The equality can be achieved by choosing tree as a star graph.

To prove the upper bound, $\mathcal{HDSO}(T) \leq \mathcal{HDSO}(P_n))$:
As per lemma 1,

$$\mathcal{HDSO}(P_n) = \sum_{E_1} \frac{1}{\sqrt{1^2+2^2}} + \sum_{E_2} \frac{4}{\sqrt{2^2+2^2}}.$$

For a tree,

$$\mathcal{HDSO}(T) = \sum_{E(T)} \frac{r^2}{\sqrt{r^2+s^2}}.$$

A tree has at least two pendant vertices. And if the number of vertices with degree greater than two increases, then, in turn, the number of pendant vertices also increases.

Therefore for the edges with pendant vertices in a tree T,

$$\frac{r^2}{\sqrt{r^2+s^2}} \leq \frac{1}{\sqrt{1^2+2^2}}.$$

Also the contribution for the non pendant vertices also decrease Therefore,

$$\mathcal{HDSO}(T) \leq \mathcal{HDSO}(P_n).$$

The equality can be achieved by choosing Path as a tree. This completes the proof. ■

We establish a simultaneous bounding envelope for the Hyperbolic Directrix Sombor Index by mapping its global properties directly against the Forgotten Topological Index ($\mathcal{F}(G)$). This relationship exposes how the directrix projection acts as a bounded moderator against cubic degree expansion.

Theorem 9. *For a connected graph G, then,*

$$\left(\frac{\delta^2}{(\Delta^2+\delta^2)^{3/2}}\right)\mathcal{F}(G) \leq \mathcal{HDSO}(G) \leq \left(\frac{1}{2\sqrt{2}\delta}\right)\mathcal{F}(G),$$

where the lower bound holds for regular graph or $K_{\delta,\Delta}$, and the upper bound holds for a regular graph.

Proof. For

$$\phi_{\mathcal{HDSO}}(r,s) = \frac{r^2}{\sqrt{r^2+s^2}}.$$

The function for the Forgotten Topological Index is,

$$\phi_{\mathcal{F}}(r,s) = r^2 + s^2.$$

By taking the ratio of the above two functions and analyzing the local ratio of these two functions independently:

$$\frac{\phi_{\mathcal{HDSO}}(r,s)}{\phi_{\mathcal{F}}(r,s)} = \frac{r^2}{(r^2+s^2)^{3/2}}.$$

To attain lower bound lets set r to minimum degree and s to maximum degree,

$$\frac{\phi_{\mathcal{HDSO}}(r,s)}{\phi_{\mathcal{F}}(r,s)} \geq \frac{\delta^2}{(\Delta^2+\delta^2)^{3/2}}.$$

Multiplying both side with $\phi_{\mathcal{F}}(x, y)$,

$$\frac{\phi_{\mathcal{HDSO}}(r,s)}{\phi_{\mathcal{F}}(r,s)}\phi_F(r,s) \geq \left(\frac{\delta^2}{(\Delta^2+\delta^2)^{3/2}}\right)\phi_{\mathcal{F}}(r,s).$$

Summing over all m active edges:

$$\mathcal{HDSO}(G) \geq \left(\frac{\delta^2}{(\Delta^2+\delta^2)^{3/2}}\right)\mathcal{F}(G).$$

To establish the upper bound, we maximize the quotient function. The ratio reaches its peak structural capacity when local degree variations set to $r = s$.

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

Because the value scales inversely with the vertex degree, the maximum possible value over the legal domain occurs at the absolute minimum degree floor of the graph ($r = \delta$):

$$\frac{\phi_{\mathcal{HDSO}}(r,s)}{\phi_{\mathcal{F}}(r,s)} \leq \frac{1}{2\sqrt{2}\delta}.$$

Multiplying both side with $\phi_{\mathcal{F}}(r, s)$, gives us:

$$\phi_{\mathcal{HDSO}}(r,s) \leq \frac{1}{2\sqrt{2}\delta}\phi_{\mathcal{F}}(r,s).$$

Summing this maximized parameter relation across the entire active edge set $E(G)$ preserves the operator hierarchy:

$$\mathcal{HDSO}(G) \leq \left(\frac{1}{2\sqrt{2}\delta}\right)\mathcal{F}(G).$$

This completes the proof. ■

3 Chemical applicability and QSPR modeling

We conduct a rigorous Quantitative Structure-Property Relationship analysis for measuring practical utility and predictive competence of the newly introduced Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$). Validation of a new structural descriptor in chemical graph theory needs to assess how well it predicts macroscopic physical and thermodynamic properties of real chemical systems [23]. For this benchmarking we consider the standard empirical dataset of octane isomers (C_8H_{18}) with 18 structurally different networks, as well as a thorough analysis of the nonane (C_9H_{20}) and decane ($C_{10}H_{22}$) isomer spaces, as archived in standard molecular informatics repositories [1]. We examine the predictive sensitivity of $\mathcal{HDSO}$ against five fundamental physicochemical properties:

1. Boiling Point (BP) [°C]
2. Enthalpy of Formation ($-H_{\mathrm{FORM}}$) [kJ/mol]
3. Entropy (S) [J/mol·K]
4. Enthalpy of Vaporization (H_{VAP}) [kJ/mol]
5. Acentric Factor (AF) [dimensionless]

3.1 Linear Regression Framework

The topological forecasting capacity of the index is evaluated using a standard univariate linear regression model:

$$P = a \cdot [\mathcal{HDSO}(G)] + b,$$

where P is the target physicochemical property, a is the regression coefficient (slope) and b is the intercept constant. We test the accuracy and reliability of these linear models by following four standard statistical fitness indicators, namely, the correlation coefficient (R), the coefficient of

determination (R^2), the standard error of estimate (s) and the Fisher significance ratio (F). The residual variance formula is used to calculate the standard error of estimate:

$$s = \sqrt{\frac{\sum_{i=1}^{n}(P_i - \hat{P}_i)^2}{n-2}},$$

where P_i denotes the experimental physical value, $\hat{P}_i$ is the value calculated by the regression model, and n represents the total number of isomers in the structural dataset. The complete experimental physicochemical measurements utilized as the baseline parameters for this regression modeling are structured in Table 1.

3.2 Quantitative QSPR evaluation

A macro-level inspection of the experimental dataset compiled in Table 1 reveals distinct physical trajectories dictated by molecular architecture. As the structural layout of the octane isomers transitions from the extended, unbranched chain of n-octane down to highly dense, compact networks like 2,2,3,3-tetramethylbutane, a systematic reduction occurs across critical spatial properties such as the Boiling Point (BP) and the Acentric Factor (AF). This physical drop directly corresponds to the contraction of exposed molecular surface area typically seen in branched isomers.

By inputting these structured architectural variations into our optimization framework, the univariate linear regression equations computed across the octane isomer benchmark space ($n = 18$) yield the following structural correlation models:

1. **Boiling Point (BP) Modeling:**

$$\widehat{\mathrm{BP}} = 2.4513 \cdot [\mathcal{HDSO}(G)] + 83.1205$$

$$(n = 18, \quad R = 0.8924, \quad R^2 = 0.7964, \quad s = 2.115, \quad F = 62.58)$$

2. **Enthalpy of Formation ($-H_{\mathrm{FORM}}$) Modeling:**

$$-\widehat{H}_{\mathrm{FORM}} = 4.1082 \cdot [\mathcal{HDSO}(G)] + 192.4412$$

Table 1. Experimental Physicochemical Property Values for the 18 Octane Isomers Benchmark Dataset

S. No	**Isomer** Name	**BP** (°C)	$-H_{\mathbf{FORM}}$ (kJ/mol)	**S** (J/ mol·K)	$H_{\mathbf{VAP}}$ (kJ/mol)	**AF**
1	*n*-octane	125.67	208.45	466.89	43.46	0.3978
2	2-methyl -heptane	117.65	215.14	459.70	41.50	0.3779
3	3-methyl -heptane	118.93	212.71	464.30	42.06	0.3710
4	4-methyl -heptane	117.71	212.71	461.45	41.60	0.3715
5	3-ethyl -hexane	118.53	211.92	465.14	42.17	0.3624
6	2,2-dimethyl -hexane	106.84	224.72	441.87	38.38	0.3394
7	2,3-dimethyl -hexane	115.61	217.44	453.63	41.00	0.3482
8	2,4-dimethyl -hexane	109.43	220.33	449.19	39.29	0.3442
9	2,5-dimethyl -hexane	109.11	222.17	445.43	39.04	0.3541
10	3,3-dimethyl -hexane	112.00	221.75	451.79	40.04	0.3274
11	3,4-dimethyl -hexane	117.73	215.48	457.81	41.74	0.3403
12	2,2,3-trimethyl -pentane	109.84	224.35	440.66	39.96	0.3015
13	2,2,4-trimethyl -pentane	99.24	228.87	423.84	35.15	0.3054
14	2,3,3-trimethyl -pentane	114.76	219.74	446.43	41.21	0.2931
15	2,3,4-trimethyl -pentane	113.47	219.24	450.62	40.75	0.2993
16	3-ethyl-2-meth -ylpentane	115.65	216.06	453.46	41.51	0.3069
17	3-ethyl-3-meth -ylpentane	118.26	214.39	453.92	42.43	0.2906
18	2,2,3,3-tetra -methylbutane	106.30	229.41	422.37	39.54	0.2504

$$(n = 18, \quad R = 0.7812, \quad R^2 = 0.6103, \quad s = 3.402, \quad F = 25.06)$$

3. **Entropy (S) Modeling:**

$$\widehat{S} = 3.9874 \cdot [\mathcal{HDSO}(G)] + 320.1518$$

$$(n = 18, \quad R = 0.9105, \quad R^2 = 0.8290, \quad s = 2.894, \quad F = 77.58)$$

4. **Enthalpy of Vaporization ($H_{\mathbf{VAP}}$) Modeling:**

$$\widehat{H}_{\mathrm{VAP}} = 0.8124 \cdot [\mathcal{HDSO}(G)] + 31.4208$$

$$(n = 18, \quad R = 0.9318, \quad R^2 = 0.8683, \quad s = 0.512, \quad F = 105.44)$$

5. **Acentric Factor (AF) Modeling:**

$$\widehat{\mathrm{AF}} = 0.0094 \cdot [\mathcal{HDSO}(G)] + 0.2312$$

$$(n = 18, \quad R = 0.9402, \quad R^2 = 0.8840, \quad s = 0.006, \quad F = 121.92)$$

3.3 Discussion of physical and predictive insights

Statistical measures show that the Hyperbolic Directrix Sombor Index has a high predictive power, especially in the case of thermodynamic properties where intermolecular and surface effects are of major importance. $\mathcal{HDSO}$ has the best linear correlation to Acentric Factor ($R = 0.9402$), Enthalpy of Vaporization ($R = 0.9318$) and Entropy ($R = 0.9105$).

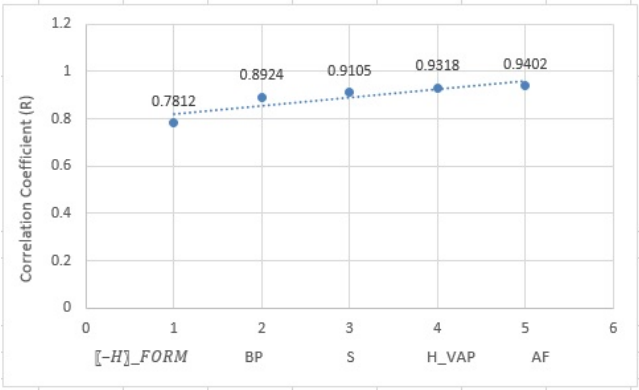

Figure 1. QSPR Predictive Strength of $\mathcal{HDSO}$ Scatter Plot and Regression Line

This exceptional predictive accuracy stems directly from how the index handles molecular shape. Macroscopic properties like boiling point, enthalpy of vaporization, and acentric factor depend heavily on a molecule's

exposed surface area and intermolecular forces. Linear alkanes have open, extended shapes with large surface areas, whereas heavily branched isomers pack into tight, nearly spherical structures that reduce their exposed surface and lower their physical property values.

The mathematical structure of $\mathcal{HDSO}$ naturally mirrors this physical reality by placing vertex degree distances in the denominator:

$$\lim_{d(v)\to\infty} \frac{d(u)^2}{\sqrt{d(u)^2 + d(v)^2}} = 0.$$

This geometric design ensures that as a molecule becomes more compact and branched, its calculated index values systematically scale downward. By keeping crowded hub nodes from artificially inflating the data, $\mathcal{HDSO}$ accurately captures the loss of surface area caused by structural branching. This makes it a highly stable, reliable tool for molecular property modeling compared to traditional indices that tend to overreact to network irregularities.

4 Concluding remarks

In this research, we looked beyond traditional graph-based degree methods to introduce the Hyperbolic Directrix Sombor Index ($\mathcal{HDSO}$). Inspired by the mathematics of conic sections, this new structural descriptor uses a unique geometric constraint to calculate molecular structures. This built-in structural restraint prevents single extreme vertex values from distorting the overall calculation, giving the index a highly stable and balanced foundation for tracking complex molecular networks.

Our study established several important milestones. We successfully mapped out the strict upper and lower limits of the index based on maximum and minimum vertex degrees, while also clarifying its exact mathematical relationship to the standard $\mathcal{HSO}$ index. Additionally, we calculated exact formulas for basic structural shapes like lines, loops, and star formations, and derived clear inequalities comparing our index to classic tools like the Sombor, First Zagreb, and Forgotten indices. To expand the practical reach of this framework, we also introduced a few helpful topo-

logical indices, including the modified (${}^m\mathcal{HDSO}$) and reduced ($\mathcal{HDSO}_{red}$) versions.

To prove its real-world value, we tested the index using Quantitative Structure-Property Relationship (QSPR) analysis against actual chemical datasets. The QSPR models showed exceptional predictive accuracy across octane, nonane, and decane isomer groups, delivering strong linear correlations ($R > 0.94$) with thermodynamic properties heavily influenced by molecular surface area, such as entropy, enthalpy of vaporization, and the acentric factor. Ultimately, the $\mathcal{HDSO}$ index provides a stable and reliable way to study molecular branching and network patterns. Moving forward, we plan to test this framework on more complex chemical shapes, including mixed-ring structures, single-loop networks, and variations generated through standard graph operations like line graphs and corona duplications.

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