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A Family of Falling-Factorial Degree-Based Topological Indices: Comparison with the Sombor and Degree Ratio Sombor Indices

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Abstract

Degree-based topological indices are fundamental molecular descriptors for characterizing molecular structures. To develop more flexible and informative structural descriptors for molecular graphs, we introduce a family of falling-factorial degree-based indices (FFDBIs) and derive explicit expressions using the M-polynomial of Sierpiński fractal networks and Stirling numbers of the second kind. The proposed framework establishes algebraic connections between the FFDBIs and several classical degree-based indices, including the second Zagreb, redefined third Zagreb, reduced second Zagreb, Forgotten, and Sombor-related indices. To assess their structural discrimination and descriptive capability, we compare selected FFDBIs with the Sombor and degree-ratio Sombor indices across all 35 nonane isomers. The results show that several FFDBIs exhibit higher sensitivity to structural differences among the isomers, and scatter-plot analysis reveals complementary, parameter-dependent structural responses. Their physicochemical relevance is further evaluated using the enthalpy of fusion of the nonane isomers. The selected FFDBIs exhibit stronger correlations with the enthalpy of fusion than the Sombor and degree-ratio Sombor indices. These results demonstrate

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that FFDBIs provide a tunable family of structural descriptors with enhanced sensitivity and physicochemical relevance.

1 Introduction

Chemical graph theory provides a mathematical framework for representing molecules as graphs [3], where the vertices correspond to the atoms and the edges correspond to the chemical bonds [30]. By transforming discrete molecular structures into numerical descriptors, computational models enable prediction of the physicochemical properties and biological activities of compounds prior to experimental synthesis [4, 25]. In this context, graph-theoretical topological indices represent molecules as hydrogen-depleted networks and serve as quantitative descriptors capturing molecular connectivity, topological branching, graph symmetry [2], and geometric complexity, thereby supporting applications in drug discovery and structural similarity analysis [7].

Various degree-based topological indices have been developed to characterize molecular structures in terms of valency constraints and connectivity patterns. Classical examples include the first and second Zagreb indices [20], the Randić branching index [28], and the harmonic index [12]. In recent years, Sombor-type indices [18] and their various generalizations [19, 22, 26, 27] have attracted considerable attention due to their sensitivity to structural variations. In parallel, studies of distance-based topological indices and related graph invariants [9,21] have further strengthened the link between discrete combinatorics and cheminformatics.

To derive degree-based topological indices, the M-polynomial is introduced as an effective algebraic tool to encode edge-degree distributions. However, high-order power-based degree descriptors may overemphasize high-degree vertices and produce highly correlated descriptor sequences, which can reduce their stability and discriminative reliability in computational modeling. This limitation calls for a bounded and well-conditioned family of descriptors capable of capturing structural information more effectively.

In this paper, we propose a family of falling-factorial degree-based topo-

logical indices (FFDBIs), which is given by

$$\mathcal{F}_{m,n}(G) = \sum_{uv \in E} \frac{(d_u)_m (d_v)_n + (d_u)_n (d_v)_m}{1 + \delta_{m,n}}, \tag{1}$$

where d_u and d_v denote the degrees of two adjacent vertices u and v that form an edge $uv \in E$, $(x)_m = x(x-1)\cdots(x-m+1)$ denotes the falling factorial of order m. For example, $(d_u)_m$ counts ordered selections of m distinct incident edges, avoids repeated selection, and vanishes when $m > d_u$. The symbol $\delta_{m,n}$ is the Kronecker delta function [24]. The denominator $1 + \delta_{m,n}$ prevents double counting by dividing the identical numerator terms by 2 when $m = n$, while remaining 1 when $m \neq n$.

For finite organic molecules, particularly sp^3-hybridized carbon networks [3], the degree of the vertex is structurally constrained by the maximum valency $\Delta \leq 4$. Hence, the parameters are restricted to $m, n \in \{1, 2, 3, 4\}$. Since molecular graphs are undirected, the proposed indices are symmetric with respect to the two endpoints of each edge. Consequently, FFDBIs consist of ten distinct descriptors. To illustrate their structural connections with classical degree-based indices, we present their explicit expansions below.

1. $\mathcal{F}_{1,1}(G)$ $(m = 1, n = 1)$**:**

$$\begin{aligned}\mathcal{F}_{1,1}(G) &= \sum_{uv \in E} \frac{(d_u)_1 (d_v)_1 + (d_u)_1 (d_v)_1}{1+1} \\ &= \sum_{uv \in E} \frac{d_u d_v + d_u d_v}{2} = \sum_{uv \in E} d_u d_v. \end{aligned} \tag{2}$$

This index coincides with the second Zagreb index [20].

2. $\mathcal{F}_{1,2}(G)$ $(m = 1, n = 2)$**:**

$$\begin{aligned}\mathcal{F}_{1,2}(G) &= \sum_{uv \in E} \frac{(d_u)_1 (d_v)_2 + (d_u)_2 (d_v)_1}{1+0} \\ &= \sum_{uv \in E} \left[d_u \cdot d_v (d_v - 1) + d_u (d_u - 1) \cdot d_v \right] \end{aligned}$$

$$= \sum_{uv \in E} d_u d_v \left(d_u + d_v - 2\right). \tag{3}$$

For an edge $e = uv$, its edge degree is $d(e) = d_u + d_v - 2$. Hence, the contribution of e to $\mathcal{F}_{1,2}(G)$ is $d_u d_v d(e)$. Then Eq. (3) becomes

$$\mathcal{F}_{1,2}(G) = \sum_{uv \in E} d_u d_v \left(d_u + d_v\right) - 2 \sum_{uv \in E} d_u d_v.$$

This identity shows that $\mathcal{F}_{1,2}(G)$ is a linear combination of the redefined third Zagreb and second Zagreb indices [20, 29]. The factor $d_u + d_v - 2$ also occurs in the definition of the atom-bond connectivity index [10].

3. $\mathcal{F}_{2,2}(G)$ $(m = 2, n = 2)$**:**

$$\begin{aligned}
\mathcal{F}_{2,2}(G) &= \sum_{uv \in E} \frac{(d_u)_2 (d_v)_2 + (d_u)_2 (d_v)_2}{1+1} \\
&= \sum_{uv \in E} \frac{2 \cdot d_u (d_u - 1) d_v (d_v - 1)}{2} \\
&= \sum_{uv \in E} d_u d_v (d_u - 1)(d_v - 1). \qquad (4)
\end{aligned}$$

For each edge uv, $d_u d_v$ is its contribution to the second Zagreb index [20]. Similarly, $(d_u - 1)(d_v - 1)$ is its contribution to the reduced second Zagreb index [15].

4. $\mathcal{F}_{1,3}(G)$ $(m = 1, n = 3)$**:**

$$\begin{aligned}
\mathcal{F}_{1,3}(G) &= \sum_{uv \in E} \left[(d_u)_1 (d_v)_3 + (d_u)_3 (d_v)_1\right] \\
&= \sum_{uv \in E} \left[d_u \cdot d_v (d_v - 1)(d_v - 2) + d_u (d_u - 1)(d_u - 2) \cdot d_v\right] \\
&= \sum_{uv \in E} d_u d_v \left(d_u^2 + d_v^2 - 3\left(d_u + d_v\right) + 4\right). \qquad (5)
\end{aligned}$$

The bracketed polynomial in Eq. (5) contains $d_u^2 + d_v^2$. Its sum over all edges, $\sum_{uv \in E} \left(d_u^2 + d_v^2\right)$, defines the Forgotten topological index [14].

5. $\mathcal{F}_{2,3}(G)$ $(m=2,n=3)$**:**

$$\begin{aligned}\mathcal{F}_{2,3}(G) &= \sum_{uv\in E}\left[(d_u)_2\,(d_v)_3+(d_u)_3\,(d_v)_2\right]\\ &= \sum_{uv\in E}\left[d_u\,(d_u-1)\cdot d_v\,(d_v-1)\,(d_v-2)\right.\\ &\qquad \left.+\,d_u\,(d_u-1)\,(d_u-2)\cdot d_v\,(d_v-1)\right]\\ &= \sum_{uv\in E} d_u d_v\,(d_u-1)\,(d_v-1)\,(d_u+d_v-4)\,. \end{aligned} \tag{6}$$

6. $\mathcal{F}_{3,3}(G)$ $(m=3,n=3)$**:**

$$\begin{aligned}\mathcal{F}_{3,3}(G) &= \sum_{uv\in E}\frac{(d_u)_3\,(d_v)_3+(d_u)_3\,(d_v)_3}{2}\\ &= \sum_{uv\in E} d_u\,(d_u-1)\,(d_u-2)\cdot d_v\,(d_v-1)\,(d_v-2)\,. \end{aligned} \tag{7}$$

7. $\mathcal{F}_{1,4}(G)$ $(m=1,n=4)$**:**

$$\begin{aligned}\mathcal{F}_{1,4}(G) &= \sum_{uv\in E}\left[(d_u)_1\,(d_v)_4+(d_u)_4\,(d_v)_1\right]\\ &= \sum_{uv\in E} d_u d_v\left(d_u^3+d_v^3-6\left(d_u^2+d_v^2\right)+11\,(d_u+d_v)-12\right). \end{aligned} \tag{8}$$

8. $\mathcal{F}_{2,4}(G)$ $(m=2,n=4)$**:**

$$\begin{aligned}\mathcal{F}_{2,4}(G) &= \sum_{uv\in E}\left[(d_u)_2\,(d_v)_4+(d_u)_4\,(d_v)_2\right]\\ &= \sum_{uv\in E} d_u d_v\,(d_u-1)\,(d_v-1)\left(d_u^2+d_v^2-5\,(d_u+d_v)+12\right). \end{aligned} \tag{9}$$

9. $\mathcal{F}_{3,4}(G)$ $(m=3,n=4)$**:**

$$\mathcal{F}_{3,4}(G) = \sum_{uv\in E}\left[(d_u)_3\,(d_v)_4+(d_u)_4\,(d_v)_3\right]$$

$$= \sum_{uv \in E} d_u d_v \left(d_u - 1\right) \left(d_v - 1\right) \left(d_u - 2\right) \left(d_v - 2\right) \left(d_u + d_v - 6\right). \tag{10}$$

10. $\mathcal{F}_{4,4}\left(G\right)$ **(**$m = 4, n = 4$**):**

$$\begin{aligned} \mathcal{F}_{4,4}\left(G\right) &= \sum_{uv \in E} \frac{\left(d_u\right)_4 \left(d_v\right)_4 + \left(d_u\right)_4 \left(d_v\right)_4}{2} \\ &= \sum_{uv \in E} d_u \left(d_u - 1\right) \left(d_u - 2\right) \left(d_u - 3\right) \\ &\quad \cdot d_v \left(d_v - 1\right) \left(d_v - 2\right) \left(d_v - 3\right). \end{aligned} \tag{11}$$

2 Mathematical derivations

In this section, we present analytical derivations based on generating functions and Eulerian differential operators [11].

2.1 Sierpiński fractal networks

Let $S_n = (V_n, E_n)$ for $n \in \mathbb{N}^+$ denote the n-th order Sierpiński fractal networks [13]. The rules of topological evolution are defined as follows:

(i) For $n = 1$, the base graph S_1 is a cycle graph, which includes three $(2, 2)$-edges.

(ii) For $n \geq 2$, the graph S_n is obtained recursively. When three copies of S_{n-1} are connected and their peripheral vertices are identified, the degrees of bridging vertices increase to $2 + 2 = 4$.

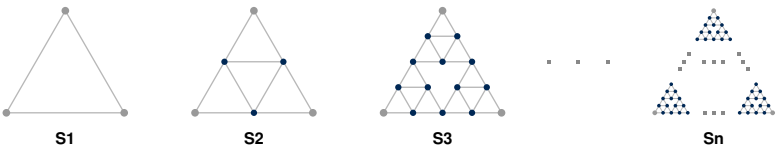


Figure 1. Constructions of Sierpiński fractal networks.

In this topological evolution, the maximum degree of the network remains bounded by $\Delta = 4$. Consequently, the edge partition induced by the degrees of adjacent vertices consists of three classes: $E_{(2,2)}$, $E_{(2,4)}$, and $E_{(4,4)}$, where $E_{(i,j)}$ denotes the set of edges connecting vertices of degrees i and j. Define the state vector of the edge partition for the Sierpiński fractal network as

$$X_n = \left[m_{2,2}(n), m_{2,4}(n), m_{4,4}(n) \right]^{\mathrm{T}},$$

where $m_{i,j}(n) = |E_{(i,j)}|$ denotes the number of edges in the class $E_{(i,j)}$.

2.2 M-polynomial and graph Invariants

For variables x and y, the M-polynomial [8] is defined as $M(S_n; x, y) = m_{2,2}(n) x^2 y^2 + m_{2,4}(n) x^2 y^4 + m_{4,4}(n) x^4 y^4$. The generating function of the state X_n with respect to a variable $z \in \mathbb{R}$ is formalized as

$$F(z) = \sum_{n=1}^{\infty} X_n z^n. \tag{12}$$

To establish the connection between the Eulerian differential operators and the proposed FFDBIs, we then introduce the sequence

$$\{Z_k(S_n)\}_{k \geq 1},$$

defined by

$$\mathcal{Z}_k(S_n) = (D_x D_y)^k M(S_n; x, y)\Big|_{x=y=1},$$

and $D_x = x\frac{\partial}{\partial x}$ and $D_y = y\frac{\partial}{\partial y}$.

Lemma 1. *The recursive expression of the state X_{n+1} is governed by a transition matrix $\mathbf{T}$, which is given by*

$$X_{n+1} = \mathbf{T} X_n, \quad n \geq 1, \tag{13}$$

where the matrix $\mathbf{T}$ *and the initial condition* X_1 *read as*

$$\mathbf{T} = \begin{bmatrix} 0 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 2 & 3 \end{bmatrix}, \quad X_1 = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}. \tag{14}$$

2.3 Explicit expressions of FFDBIs

Based on this generating function, we derive explicit expressions for this family of falling-factorial degree-based indices.

Theorem 1. *The M-polynomial of the Sierpiński fractal networks* S_n *is*

$$M(S_n; x, y) = 6x^2y^4 + (3^n - 6)\, x^4y^4, \quad n \geq 2, \tag{15}$$

and $M(S_1; x, y) = 3x^2y^2$.

Proof. Multiplying Eq. (13) by z^{n+1} yields

$$\sum_{n=1}^{\infty} X_{n+1} z^{n+1} = z\mathbf{T} \sum_{n=1}^{\infty} X_n z^n. \tag{16}$$

It follows from the definition of $F(z)$ in Eq. (12) and the identity $F(z) - zX_1 = z\mathbf{T}F(z)$ that

$$(\mathbf{I} - z\mathbf{T})\, F(z) = zX_1 \implies F(z) = z\,(\mathbf{I} - z\mathbf{T})^{-1} X_1, \tag{17}$$

where $\mathbf{I}$ represents the 3×3 identity matrix. The characteristic equation of the matrix $\mathbf{T}$ is $\det(\lambda\mathbf{I} - \mathbf{T}) = \lambda(1 - \lambda)(3 - \lambda) = 0$. By the Cauchy–Hadamard theorem, the radius of convergence for $F(z)$ resolves to $R = 1/3$.

The inverse of the matrix $(\mathbf{I} - z\mathbf{T})$ reads as

$$\begin{aligned}(\mathbf{I} - z\mathbf{T})^{-1} &= \begin{bmatrix} 1 & 0 & 0 \\ -2z & 1-z & 0 \\ -z & -2z & 1-3z \end{bmatrix}^{-1} \\ &= \begin{bmatrix} 1 & 0 & 0 \\ \frac{2z}{1-z} & \frac{1}{1-z} & 0 \\ \frac{z+3z^2}{(1-z)(1-3z)} & \frac{2z}{(1-z)(1-3z)} & \frac{1}{1-3z} \end{bmatrix}.\end{aligned} \tag{18}$$

Substituting the initial condition $X_1 = [3, 0, 0]^{\mathrm{T}}$ into Eq. (17), $F(z)$ becomes

$$F(z) = \begin{bmatrix} 3z \\ \frac{6z^2}{1-z} \\ \frac{3z^2+9z^3}{(1-z)(1-3z)} \end{bmatrix}, \ z \in (-1/3, 1/3). \tag{19}$$

Applying partial fraction decomposition to $F_3(z)/z^2$ yields

$$\frac{3+9z}{(1-z)(1-3z)} = \frac{A}{1-z} + \frac{B}{1-3z}.$$

Evaluating at $z = 1$ yields $A = -6$, and at $z = 1/3$ yields $B = 9$. The third component is then rewritten as

$$\begin{aligned}F_3(z) &= z^2 \left(\frac{9}{1-3z} - \frac{6}{1-z} \right) \\ &= z^2 \left(9 \sum_{k=0}^{\infty} (3z)^k - 6 \sum_{k=0}^{\infty} z^k \right) \\ &= \sum_{k=0}^{\infty} \left(9 \cdot 3^k - 6 \right) z^{k+2}.\end{aligned} \tag{20}$$

Substituting $n = k + 2$, the coefficient $m_{4,4}(n)$ of z^n is

$$m_{4,4}(n) = [z^n] F_3(z) = 9 \cdot 3^{n-2} - 6 = 3^n - 6, \quad n \geq 2. \tag{21}$$

In the same way, $m_{2,4}(n)$ is

$$m_{2,4}(n) = [z^n]\frac{6z^2}{1-z} = [z^n]\sum_{k=0}^{\infty} 6z^{k+2} = 6, \quad n \geq 2. \tag{22}$$

Substituting these derived scalar coefficients into the M-polynomial formula verifies Eq. (15). ■

Theorem 2. *For $k \geq 1$, the expression of $\mathcal{Z}_k(S_n)$ is given by*

$$\begin{aligned}\mathcal{Z}_k(S_n) = 6&\left[\sum_{m=1}^{\min(k,2)} \left\{ {k \atop m} \right\} (2)_m\right] \mathcal{S}_4(k) \\ &+ (3^n - 6)\left[\sum_{m=1}^{\min(k,4)} \left\{ {k \atop m} \right\} (4)_m\right] \mathcal{S}_4(k),\end{aligned} \tag{23}$$

where $(i)_m = i(i-1)\cdots(i-m+1)$ denotes the falling factorial of order m, $\left\{ {k \atop m} \right\}$ denotes the Stirling numbers of the second kind [11, 17], and $\mathcal{S}_4(k) = \sum_{l=1}^{\min(k,4)} \left\{ {k \atop l} \right\} (4)_l$.

Proof. Applying the differential operator $D_x = x\frac{\partial}{\partial x}$ consecutively k times to a monomial x^i yields a linear combination of derivatives, where the coefficients are the Stirling numbers of the second kind. Evaluating this expansion at $x = 1$ yields

$$\begin{aligned}(D_x)^k x^i\Big|_{x=1} &= \left[\sum_{m=1}^{k} \left\{ {k \atop m} \right\} x^m \frac{\partial^m}{\partial x^m}\right] x^i\Bigg|_{x=1} \\ &= \sum_{m=1}^{k} \left\{ {k \atop m} \right\} (i)_m.\end{aligned} \tag{24}$$

The algebraic truncation is a property of the falling factorial $(i)_m$. Since the maximum vertex degree of the Sierpiński fractal networks is bounded by $\Delta = 4$, whenever $m > i$, the factor $(i - i) = 0$ appears in the product defining $(i)_m$, implying that $(i)_m = 0$. Consequently, since $i \leq 4$, we have $(i)_m = 0$ for all $m > 4$.

Moreover, this truncation is independent of the iteration k. Therefore,

the summation terminates at $m = \min(k, i) \leq 4$. Applying the operator $(D_x D_y)^k$ to the M-polynomial in Eq. (15) establishes the finite expansion given in Eq. (23). ■

Remark. The algebraic truncation established in Theorem 2 depends on the property of the falling factorial and the finite-degree constraint $\Delta \leq 4$, independent of the specific network topology. Thus, this property extends to any finite network G with a bounded maximum degree. The graph invariant for G is also calculated via its M-polynomial as $\mathcal{Z}_k(G) = (D_x D_y)^k M(G; x, y)\big|_{x=y=1}$.

Theorem 3. *Let $G = (V, E)$ be a finite molecular network with a maximum vertex degree $\Delta \leq 4$. $\mathcal{Z}_k(G)$ reduces to a finite combination of ten descriptors in the set $\mathcal{B} = \{\mathcal{F}_{m,n}(G)\}_{1 \leq m \leq n \leq 4}$.*

Proof. Let $M(G; x, y) = \sum_{1 \leq i \leq j \leq \Delta} m_{i,j} x^i y^j$ be the M-polynomial of the network G, where the coefficient $m_{i,j}$ denotes the number of edges connecting vertices of degree i and j. By the linearity of the differential operator, applying $(D_x D_y)^k$ to $M(G; x, y)$ yields

$$\mathcal{Z}_k(G) = \sum_{1 \leq i \leq j \leq \Delta} m_{i,j} \Big[(D_x)^k x^i \big|_{x=1} \Big] \Big[(D_y)^k y^j \big|_{y=1} \Big]. \tag{25}$$

It follows from Eq. (24) that $(D_x)^k x^i\big|_{x=1} = \sum_{m=1}^{\min(k,i)} \left\{ {k \atop m} \right\} (i)_m$. Since the maximum degree is bounded by $\Delta \leq 4$, we have $i, j \leq 4$. The falling factorials $(i)_m$ and $(j)_n$ evaluate to zero for $m > i$ and $n > j$, respectively. Consequently, the summations are truncated at $m, n \leq \Delta \leq 4$, independent of k.

Because the graph G is undirected, the descriptor is symmetric for m and n, i.e.,

$$\mathcal{F}_{m,n}(G) = \mathcal{F}_{n,m}(G).$$

Therefore, condition $1 \leq m \leq n \leq 4$ produces ten distinct parameter pairs, then the set $\mathcal{B}$ contains ten topological descriptors.

In contrast, if the maximum degree of the vertex is unbounded ($\Delta \to \infty$), the indices i and j can increase with k. For $m \leq k$, the falling factorial

$(i)_m$ would not vanish, preventing the summation from truncating. Thus, condition $\Delta < \infty$ is necessary. ■

Theorem 4. *Let $G = (V, E)$ represent a finite molecule network with maximum vertex degree $\Delta \leq 4$. The expression of $\mathcal{Z}_k(G)$ reads as*

$$\mathcal{Z}_k(G) = \sum_{1 \leq m \leq n \leq \Delta} \lambda_{m,n}^{(k)} \mathcal{F}_{m,n}(G), \tag{26}$$

where

$$\mathcal{F}_{m,n}(G) = \sum_{uv \in E} \frac{(d_u)_m (d_v)_n + (d_u)_n (d_v)_m}{1 + \delta_{m,n}},$$

and $\lambda_{m,n}^{(k)} = \left\{ {k \atop m} \right\} \left\{ {k \atop n} \right\}$ is the product of two Stirling numbers of the second kind.

Proof. Substituting the Stirling expansion $i^k = \sum_{m=1}^{\Delta} \left\{ {k \atop m} \right\} (i)_m$ yields

$$\begin{aligned} \mathcal{Z}_k(G) &= \sum_{uv \in E} \left[\sum_{m=1}^{\Delta} \left\{ {k \atop m} \right\} (d_u)_m \right] \left[\sum_{n=1}^{\Delta} \left\{ {k \atop n} \right\} (d_v)_n \right] \\ &= \sum_{m=1}^{\Delta} \sum_{n=1}^{\Delta} \left\{ {k \atop m} \right\} \left\{ {k \atop n} \right\} \left[\sum_{uv \in E} (d_u)_m (d_v)_n \right]. \end{aligned} \tag{27}$$

To avoid double counting when $m = n$, we introduce the Kronecker delta function $\delta_{m,n}$ [24], which produces the following family of falling-factorial degree-based indices. Then, $\mathcal{Z}_k(G)$ becomes

$$\mathcal{Z}_k(G) = \sum_{1 \leq m \leq n \leq \Delta} \lambda_{m,n}^{(k)} \mathcal{F}_{m,n}(G),$$

where $\lambda_{m,n}^{(k)} = \left\{ {k \atop m} \right\} \left\{ {k \atop n} \right\}$, and

$$\mathcal{F}_{m,n}(G) = \sum_{uv \in E} \frac{(d_u)_m (d_v)_n + (d_u)_n (d_v)_m}{1 + \delta_{m,n}}.$$

Because $(d)_m = 0$ whenever $m > d$, only the orders $1 \leq m, n \leq \Delta$ contribute for a graph with maximum degree Δ. Hence, the FFDBI family is finite; for $\Delta = 4$, it consists of ten distinct descriptors. ■

3 Comparison with the Sombor and degree ratio Sombor indices

3.1 Sombor and degree ratio Sombor indices

The Sombor index (SO) [18] and the degree ratio Sombor index (DRSO) [27] are given by

$$\mathrm{SO}\,(G) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}, \tag{28}$$

$$\mathrm{DRSO}\,(\mathrm{G}) = \sum_{uv \in E} \sqrt{\left(\frac{d_u}{d_v}\right)^2 + \left(\frac{d_v}{d_u}\right)^2}. \tag{29}$$

3.2 Experimental design

To evaluate the structural discriminative power and geometric sensitivity of the proposed indices, we perform a comparative analysis based on isomer distinguishability. In chemical graph theory, a meaningful assessment of a topological index requires controlling atomic properties so that the influence of skeletal branching can be examined independently. Accordingly, our dataset consists of the complete set of 35 nonane isomers (C_9H_{20}), corresponding to the family of 9-vertex chemical trees [3].

All isomers share the same molecular formula, containing nine carbon atoms and identical atom types, thereby fixing the number of vertices and chemical composition. Consequently, the skeletal branching topology is the only varying structural feature. This controlled setting enables an objective comparison of the ability of the proposed FFDBIs and classical degree-based descriptors to distinguish structural variations. An overview of the complete set of 35 nonane isomers is presented in Figure 2.

3.3 Degeneracy and structural sensitivity

Let Ω denote the set of 35 nonane isomer trees, and let $N_{\mathrm{dist}}\,(I)$ be the number of distinct values assigned by an index I to the members of Ω.

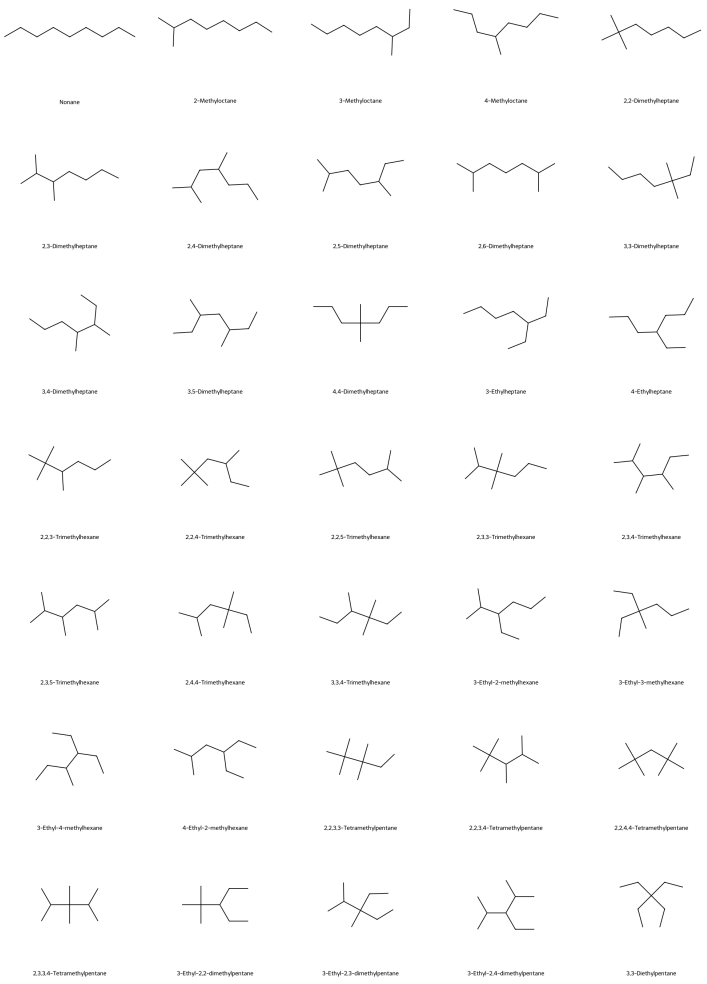


Figure 2. 35 nonane isomers represented by trees with 9 vertices.

The degeneracy count [5, 6, 23] is defined as

$$D(I) = |\Omega| - N_{\text{dist}}(I). \tag{30}$$

For each $G \in \Omega$, let $\mathcal{S}(G)$ contain one representative of each isomorphism class of connected chemical trees obtained from G by deleting one

edge and inserting another edge, including G itself. The structure sensitivity and abruptness [16] are given by

$$\mathrm{SS}(I) = \frac{1}{|\Omega|} \sum_{G \in \Omega} \frac{1}{|\mathcal{S}(G)|} \sum_{H \in \mathcal{S}(G)} \left| \frac{I(H) - I(G)}{I(G)} \right|, \tag{31}$$

$$\mathrm{Abr}(I) = \frac{1}{|\Omega|} \sum_{G \in \Omega} \max_{H \in \mathcal{S}(G)} \left| \frac{I(H) - I(G)}{I(G)} \right|. \tag{32}$$

We then calculate the structure sensitivity and abruptness of three FFDBIs compared to those of SO and DRSO. The corresponding values are listed in Table 1. The results show that $\mathcal{F}_{1,2}$ and $\mathcal{F}_{2,2}$ exhibit stronger responses to local structural changes than SO and DRSO.

Table 1. Values of degeneracy, structure sensitivity, and abruptness for the 35 nonane isomers.

Index	D	SS	Abr
$\mathcal{F}_{1,1}$	19	0.0955	0.2489
$\mathcal{F}_{1,2}$	11	0.2532	0.6829
$\mathcal{F}_{2,2}$	15	0.4497	1.4289
SO	7	0.0808	0.1866
DRSO	7	0.1382	0.3152

3.4 Geometric comparison

In this subsection, we select $\mathcal{F}_{1,1}$, $\mathcal{F}_{1,2}$, $\mathcal{F}_{1,3}$, $\mathcal{F}_{2,2}$, and $\mathcal{F}_{2,3}$ for geometric comparison. Each descriptor is plotted against DRSO in the left column and against SO in the right column of Figure 3.

Figure 3 contains overlapping markers because each plotted pair yields only 28 distinct coordinate pairs. The seven collisions of SO and DRSO correspond to identical endpoint-degree distributions. Since every FFDBI descriptor considered here is also determined by these distributions, adding it as a second coordinate cannot separate the degenerate classes. However, the scatter plots show different numerical spreads among the descriptors. This geometric variation is consistent with the structure-sensitivity results

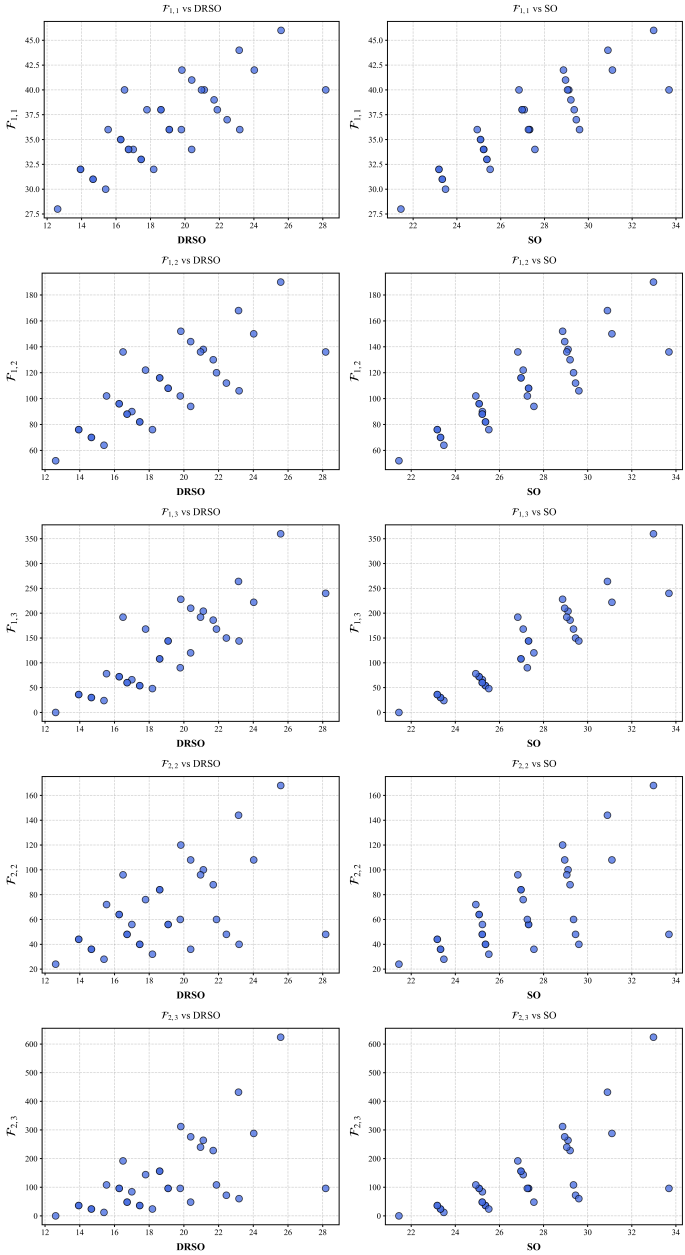


Figure 3. Pairwise scatter plots of five selected FFDBIs against DRSO (left column) and SO (right column) for the 35 nonane isomers.

in Table 1. It reflects differences in response magnitude, rather than an increase in the number of distinguishable nonane isomers.

3.5 Correlation with physicochemical properties

To assess the chemical relevance of the considered descriptors, we examine their correlations with the octanol–water partition coefficient ($\log P$) and the enthalpy of fusion (ΔH_{fus}). The reported property values for the same 35 nonane isomers are taken from [1]. All 35 observations are used without imputation.

For a topological index $\mathcal{J}$ and a physicochemical property P, the Pearson correlation coefficient is defined as

$$C(\mathcal{J}, P) = \frac{\sum_{i=1}^{35} \left(\mathcal{J}_i - \overline{\mathcal{J}}\right)\left(P_i - \overline{P}\right)}{\sqrt{\sum_{i=1}^{35} \left(\mathcal{J}_i - \overline{\mathcal{J}}\right)^2} \sqrt{\sum_{i=1}^{35} \left(P_i - \overline{P}\right)^2}}, \tag{33}$$

where $\mathcal{J}_i$ and P_i are the index and property values of the i-th isomer, respectively, and $\overline{\mathcal{J}}$ and $\overline{P}$ are their sample means.

Table 2. Correlation coefficients between the selected topological indices and physicochemical properties of the 35 nonane isomers.

Index	$C(\mathcal{J}, \log P)$	$C(\mathcal{J}, \Delta H_{\mathrm{fus}})$
$\mathcal{F}_{1,1}$	−0.8737	0.4830
$\mathcal{F}_{1,2}$	−0.8606	0.5018
$\mathcal{F}_{1,3}$	−0.8416	0.4966
$\mathcal{F}_{2,2}$	−0.7041	0.5219
$\mathcal{F}_{2,3}$	−0.7257	0.5295
SO	−0.9301	0.3554
DRSO	−0.9106	0.2729

Table 2 presents the correlation coefficients between the selected topological indices and the physicochemical properties. The selected FFDBIs show negative correlations with the octanol–water partition coefficient and

positive correlations with the enthalpy of fusion. Notably, the selected FFDBIs exhibit stronger correlations with the enthalpy of fusion than the Sombor and degree-ratio Sombor indices.

4 Conclusion

In this paper, we have introduced the falling-factorial degree-based indices (FFDBIs) and established their explicit formulations through the M-polynomial of Sierpiński fractal networks and Stirling numbers of the second kind. The proposed framework unifies several degree-based topological descriptors within a common algebraic formulation. The results obtained show that some of the proposed FFDBIs can characterize structural variations more effectively than the Sombor and degree ratio Sombor indices. The proposed topological indices offer a flexible foundation for the construction and analysis of novel degree-based descriptors. Future work will investigate extremal values and sharp bounds and extend the physicochemical evaluation to independently curated molecular-property datasets and broader classes of molecular and complex networks.

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