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Sombor Index in Chemical SuperHyperGraph

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Abstract

A hypergraph extends an ordinary graph by allowing each edge to join an arbitrary nonempty subset of the vertex set. If one iterates the powerset construction further, one obtains nested (higher-order) vertex objects and, in turn, finite SuperHyperGraphs whose vertices and edges may be set-valued across multiple levels. Topological indices are numerical graph invariants—typically degree- or distance-based—that compactly encode structural information and often correlate with physical, chemical, or network properties. Among them, the Sombor index is a widely studied representative.

In this paper, we first review the Sombor index in the setting of SuperHyperGraphs. We then introduce two related notions, namely the *Sombor index in Chemical SuperHyperGraphs* and the *Multiplicative Sombor index in SuperHyperGraphs*, and we briefly examine their fundamental properties.

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1 Introduction

1.1 Graph, hypergraph, and superhypergraph

A wide range of networked systems can be modeled by graphs, where vertices represent entities and edges encode pairwise relationships [18]. This classical paradigm is effective when interactions are essentially binary, but it becomes less adequate in settings where three or more entities participate in a single interaction. Hypergraphs provide a natural remedy: a hyperedge may connect any nonempty subset of the vertex set, so multiway interactions can be represented directly [21].

In many applications, however, complexity arises not only from multiway interactions but also from *hierarchy*: groups may contain subgroups, and relations may occur across multiple abstraction levels. To address such nested organization, Smarandache proposed the notion of a *SuperHyperGraph*. SuperHyperGraphs rely on iterated powerset constructions to create set-valued (nested) vertex objects and the corresponding superedges, thereby enabling connectivity patterns to be expressed across several levels of granularity [28, 68].

Graphs and hypergraphs already play central roles in areas such as artificial intelligence, network science, data mining, informatics, chemistry, and physics [8, 13, 35]. By explicitly incorporating multi-tier structure, SuperHyperGraphs offer a flexible language for analyzing increasingly complex networked data (see, e.g., [5]). Table 1 summarizes the principal distinctions among graphs, hypergraphs, and superhypergraphs. Unless stated otherwise, n is assumed to be a natural number throughout. Readers seeking further background on SuperHyperGraphs may consult, for instance, [31].

1.2 Molecular graph and chemical graph

Graph-based formalisms have long been influential in chemical modeling. A *molecular graph* represents atoms as vertices and chemical bonds as edges, emphasizing connectivity and topological structure [37, 73]. A *chemical graph* is typically understood as a molecular graph that respects

Table 1. Key distinctions among graph, hypergraph, and superhypergraph

Concept	Notation	Edge Type	Extension Mechanism
Graph [18]	$G = (V, E)$	$E \subseteq \{\{u, v\} \mid u, v \in V,\ u \neq v\}$	Edges represent pairwise relations.
Hypergraph [7]	$H = (V, E)$	$E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$	Hyperedges represent multiway relations among vertex subsets.
Superhypergraph [68]	$\mathrm{SHG}^{(n)} = (V_0, V, E)$	$V \subseteq \mathcal{P}^n(V_0), \quad E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$	Iterated powersets produce nested vertices and multi-level connectivity.

Notation. $\mathcal{P}(X) = \{A \subseteq X\}$ and $\mathcal{P}^0(X) = X,\ \mathcal{P}^{k+1}(X) = \mathcal{P}(\mathcal{P}^k(X))$.

valence constraints, often expressed as a bounded maximum degree (commonly at most four) in accordance with standard bonding patterns [55,58]. These ideas extend naturally beyond graphs: hypergraph and superhypergraph formulations have been proposed to encode multi-atom relations and hierarchical substructures, leading to notions such as molecular hypergraphs [12, 45], molecular superhypergraphs [26], chemical hypergraphs [11, 22], and chemical superhypergraphs [23].

1.3 Topological indices in graph

Topological indices are numerical invariants derived from a graph—often from degree-based or distance-based information—that summarize structural properties and are frequently used to correlate graph structure with physical, chemical, or network characteristics. Prominent examples include the Zagreb index [42, 59], the Sombor index [32, 70, 71], the ABC index [15,33,62], the Randić index [46,72], the hyper-Zagreb index [36,41], as well as the Harary and Wiener indices. Such indices are important both within graph theory and in chemical applications, where they have been studied extensively (cf. [30]).

1.4 Our contributions

The considerations above highlight the significance of research on graph and hypergraph models, superhypergraph extensions, chemical graph formalisms, and degree-/distance-based topological indices. Although the literature on superhypergraph indices is expanding, the area remains technically demanding and far from fully systematized. Given the potential of superhypergraphs to encode highly intricate chemical structures in a principled, hierarchical manner, we view further development of topological indices in this setting as both timely and well motivated.

Accordingly, we first review the Sombor index for SuperHyperGraphs introduced in [31]. We then introduce two related notions—the *Sombor index in Chemical SuperHyperGraphs* and the *Multiplicative Sombor index in SuperHyperGraphs*—and provide a brief analysis of their basic properties. Table 2 summarizes the Sombor-index formulations for graphs, hypergraphs, and superhypergraphs.

Table 2. Comparison of Sombor index for graphs, hypergraphs, and superhypergraphs

Framework	**Underlying structure**	**Sombor index**
Graph	Simple graph $G = (V, E)$ with pairwise edges.	$SO(G) = \sum_{uv \in E} \sqrt{d_G(u)^2 + d_G(v)^2}.$
Hypergraph	Hypergraph $H = (V, E)$ with hyperedges $e \subseteq V$, $e \neq \emptyset$.	$SO(H) = \sum_{e \in E} \sqrt{\sum_{v \in e} d_H(v)^2}.$
SuperHypergraph	Level-n SuperHyperGraph $\mathrm{SHG}^{(n)} = (V, E, \partial)$ with n-supervertices and n-superedges.	$SO\big(\mathrm{SHG}^{(n)}\big) = \sum_{e \in E} \sqrt{\sum_{v \in \partial(e)} d_{\mathrm{SHG}^{(n)}}(v)^2}.$

2 Preliminaries

This section summarizes the notation and background concepts needed in the sequel.

2.1 SuperHyperGraphs

Graphs are a standard formalism for encoding relational data: vertices represent objects and edges represent pairwise relations, and the resulting structure supports a rich theory of connectivity, structure, and algorithms [18]. In many settings, however, interactions are not purely binary; one often needs to model relations among several entities at once. Hypergraphs provide an appropriate generalization by allowing each hyperedge to be an arbitrary nonempty subset of the vertex set, thereby capturing higher-order interactions directly [21, 34]. Such higher-order models have gained further prominence in contemporary applications, including recent work in neural and graph-based learning [10, 12, 19, 21, 44].

To represent *hierarchical* or *nested* entities (for instance, groups of groups), one may iterate the powerset construction beyond the hypergraph level. This yields finite *SuperHyperGraphs*, whose vertex objects may themselves be set-valued across multiple layers, and whose edges connect these higher-order vertices [6, 27]. Such layered representations arise naturally in molecular design, complex-network analysis, and related learning pipelines [2, 5, 52]. Further developments include directed extensions and meta-level variants [24, 25, 29].

Throughout the paper, the parameter n in
$\mathcal{P}^n(\cdot)$ and in an n-SuperHyperGraph is always a nonnegative integer.

Definition 1 (Base set)**.** A *base set* S is the underlying universe of discourse:

$$S \;=\; \{\, x \mid x \text{ is an admissible object in the given context} \,\}.$$

All sets appearing in $\mathcal{P}(S)$ and in the iterated powersets $\mathcal{P}^n(S)$ are ultimately built from elements of S.

Definition 2 (Powerset)**.** (see [43, 56, 63]) For a set S, the *powerset* of S is

$$\mathcal{P}(S) \;=\; \{\, A \mid A \subseteq S \,\}.$$

In particular, $\emptyset \in \mathcal{P}(S)$ and $S \in \mathcal{P}(S)$.

Definition 3 (Hypergraph)**.** [4,7] A *hypergraph* is a pair $H = (V, E)$ such that:

- V is a finite set (the *vertices*), and
- E is a finite family of nonempty subsets of V (the *hyperedges*).

Thus, a hyperedge may contain more than two vertices, representing genuinely multiway relations.

Definition 4 (Iterated powerset and flattening)**.** Let V_0 be a finite nonempty set. Define $\mathcal{P}^0(V_0) := V_0$ and $\mathcal{P}^{k+1}(V_0) := \mathcal{P}\big(\mathcal{P}^k(V_0)\big)$ for $k \geq 0$. For each $k \geq 0$, define the flattening map

$$\mathrm{Flat}_k : \mathcal{P}^k(V_0) \setminus \{\emptyset\} \longrightarrow \mathcal{P}(V_0) \setminus \{\emptyset\}$$

recursively by

$$\mathrm{Flat}_0(x) := \{x\} \quad (x \in V_0),$$

$$\mathrm{Flat}_{k+1}(X) := \bigcup_{Y \in X} \mathrm{Flat}_k(Y) \quad (X \in \mathcal{P}^{k+1}(V_0) \setminus \{\emptyset\}).$$

Definition 5 (n-SuperHyperGraph)**.** (see [68]) Let V_0 be a finite, nonempty base set. Define

$$\mathcal{P}^0(V_0) := V_0, \qquad \mathcal{P}^{\,k+1}(V_0) := \mathcal{P}\big(\mathcal{P}^{\,k}(V_0)\big) \quad (k \in \mathbb{N}).$$

For $n \geq 0$, an *n-SuperHyperGraph on V_0* is a pair

$$\mathrm{SHG}^{(n)} = (V, E)$$

satisfying

$$V \subseteq \mathcal{P}^{\,n}(V_0) \quad \text{and} \quad E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}.$$

Elements of V are called *n-supervertices*, and elements of E are called *n-superedges* (i.e., each n-superedge is a nonempty subset of V).

Example 1 (n-SuperHyperGraph for enterprise IT portfolio governance)**.** An enterprise IT portfolio is naturally hierarchical: tasks form projects,

projects form programs, and programs are governed at a portfolio level. Let

$$V_0 = \{T_{\text{cloud}}, T_{\text{data}}, T_{\text{sec}}, T_{\text{ui}}\}, \qquad n = 3.$$

Define three 3-supervertices (programs)

$$p_1 = \big\{\{\{T_{\text{cloud}}, T_{\text{sec}}\}\}, \{\{T_{\text{data}}\}\}\big\},$$

$$p_2 = \big\{\{\{T_{\text{ui}}\}\}, \{\{T_{\text{cloud}}, T_{\text{data}}\}\}\big\},$$

$$p_3 = \big\{\{\{T_{\text{sec}}\}\}, \{\{T_{\text{data}}, T_{\text{ui}}\}\}\big\},$$

and set $V = \{p_1, p_2, p_3\} \subseteq \mathcal{P}^3(V_0)$. Let

$$e_1 = \{p_1, p_2\}, \qquad e_2 = \{p_2, p_3\}, \qquad E = \{e_1, e_2\} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}.$$

Then $\text{SHG}^{(3)} = (V, E)$ is a valid 3-SuperHyperGraph, where each superedge represents a portfolio-level governance relation spanning multiple programs. For reference, an overview diagram of this example is shown in Figure 1.

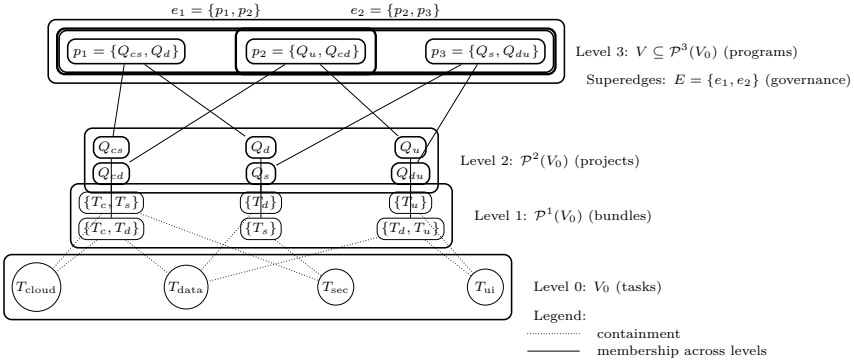

Figure 1. A compact layered schematic for the enterprise IT portfolio example ($n = 3$).

2.2 Chemical SuperHyperGraphs

Chemical systems often exhibit natural hierarchies: atoms form bonds and functional groups, functional groups assemble into molecular substructures, and molecules may further organize into aggregates or reaction networks. A *chemical superhypergraph* is intended to encode such multilevel organization by allowing successive layers of set-valued objects together with quantitative annotations (e.g., strengths, rates, or affinities).

Definition 6 (Chemical SuperHyperGraph)**.** Fix integers $m \geq 1$ and $n \geq 0$. A *chemical superhypergraph* is an m-level structure

$$\mathcal{CSH}^{(m,n)} = \big(V_0,\, E_1,\, E_2,\, \ldots,\, E_m,\, w_1,\, w_2,\, \ldots,\, w_m\big),$$

where:

- V_0 is a finite set of *atoms*.
- $E_1 \subseteq \mathcal{P}^{\,n}(V_0) \setminus \{\emptyset\}$ is a finite family of first-level chemical units (e.g., bonds, small motifs, or functional groups), represented as nonempty elements of $\mathcal{P}^{\,n}(V_0)$.
- For each $\ell = 2, \ldots, m$, the set $E_\ell \subseteq \mathcal{P}(E_{\ell-1}) \setminus \{\emptyset\}$ is a finite family of ℓ-th level aggregates built from nonempty collections of $(\ell-1)$-th level units (e.g., substructures, molecules, and higher-order assemblies).
- For each $\ell = 1, \ldots, m$, the map $w_\ell : E_\ell \to \mathbb{R}_{\geq 0}$ assigns a nonnegative weight encoding a quantitative property at level ℓ (e.g., bond strength, interaction energy, or reaction rate), with the precise interpretation depending on the modeling objective.

Example 2 (A concise chemical superhypergraph for a small molecule)**.** Consider the water molecule H_2O. Let the base set of atoms be

$$V_0 = \{\mathrm{O}, \mathrm{H}_1, \mathrm{H}_2\}.$$

Take $m = 2$ and $n = 0$, so $\mathcal{P}^0(V_0) = V_0$ and $E_1 \subseteq \mathcal{P}^0(V_0) \setminus \{\emptyset\} = V_0 \setminus \{\emptyset\}$.

Define the first-level chemical units (bonds) by

$$E_1 = \big\{\, b_1 = \{\mathrm{O}, \mathrm{H}_1\},\ b_2 = \{\mathrm{O}, \mathrm{H}_2\} \,\big\},$$

and define the second-level aggregate (the molecule) by

$$E_2 = \big\{\, M = \{b_1, b_2\} \,\big\} \ \subseteq\ \mathcal{P}(E_1) \setminus \{\emptyset\}.$$

Assign weights

$$w_1(b_1) = w_1(b_2) = 1, \qquad w_2(M) = 1,$$

interpreting w_1 as a normalized bond-strength score and w_2 as a normalized stability score of the molecule.

Then

$$\mathcal{CSH}^{(2,0)} = \big(V_0, E_1, E_2, w_1, w_2\big)$$

is a valid chemical superhypergraph: atoms form first-level units (bonds), and bonds are grouped into a second-level aggregate representing the molecule. For reference, an overview diagram of this example is provided in Figure 2.

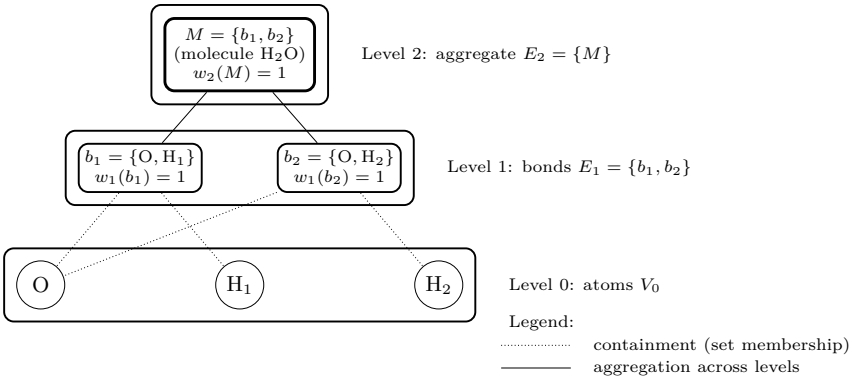

Figure 2. A schematic diagram of the chemical superhypergraph $\mathcal{CSH}^{(2,0)}$ for H_2O: atoms (V_0) form bonds (E_1), and bonds are aggregated into the molecule (E_2).

Example 3 (A chemical superhypergraph: ethanol C_2H_5OH)**.** Consider

ethanol C_2H_5OH. Let the base set of atoms be

$$V_0 = \{C_1, C_2, O, H_1, H_2, H_3, H_4, H_5, H_6\}.$$

Take $m = 3$ and $n = 0$.

Level 1 (bonds). Let E_1 be the set of covalent bonds:

$$E_1 = \{b_{12} = \{C_1, C_2\},\ b_{2O} = \{C_2, O\},\ b_{OH} = \{O, H_6\},$$
$$b_{1i} = \{C_1, H_i\}\ (i = 1, 2, 3),\ b_{2j} = \{C_2, H_j\}\ (j = 4, 5)\}.$$

Level 2 (functional group / substructure). Define the hydroxyl substructure (the "C−O−H" motif) by

$$g_{\mathrm{OH}} = \{b_{2O}, b_{OH}\} \in \mathcal{P}(E_1) \setminus \{\emptyset\},$$

and set

$$E_2 = \{g_{\mathrm{OH}}\} \subseteq \mathcal{P}(E_1) \setminus \{\emptyset\}.$$

Level 3 (molecule as an aggregate of substructures and bonds). Let the molecule aggregate be

$$M = \{\, g_{\mathrm{OH}},\, b_{12},\, b_{11},\, b_{12'},\, b_{13},\, b_{24},\, b_{25} \,\} \in \mathcal{P}(E_2 \cup E_1) \setminus \{\emptyset\},$$

where we abbreviate $b_{11} = \{C_1, H_1\}$, $b_{12'} = \{C_1, H_2\}$, etc. Set

$$E_3 = \{M\}.$$

Weights. Assign normalized weights by

$$w_1(b) = 1 \quad (\forall b \in E_1), \qquad w_2(g_{\mathrm{OH}}) = 1, \qquad w_3(M) = 1,$$

where w_1 may represent bond strength, w_2 the significance of the hydroxyl functional group, and w_3 the overall molecular stability (all normalized here for simplicity).

Then

$$\mathcal{CSH}^{(3,0)} = \big(V_0, E_1, E_2, E_3, w_1, w_2, w_3\big)$$

is a valid chemical superhypergraph: atoms form bonds, selected bonds form a functional group, and the molecule is modeled as a higher-level aggregate collecting the functional group together with the remaining bonds. For reference, an overview diagram of this example is provided in Figure 3.

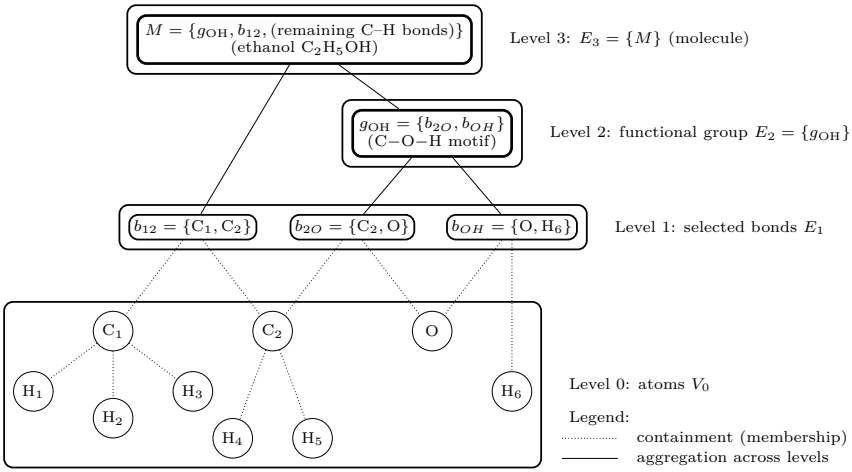

Figure 3. A layered schematic of the chemical superhypergraph $\mathcal{CSH}^{(3,0)}$ for ethanol C_2H_5OH: atoms (V_0) form bonds (E_1), selected bonds form the hydroxyl group (E_2), and these are aggregated into the molecule (E_3).

3 Reviews and results: Sombor index of SuperHyperGraphs

The Sombor index is a degree-based topological index originally defined for graphs by summing, over edges, the Euclidean norm of the endpoint degree pair; it is commonly used to quantify structural complexity in (chemical) networks [14, 57, 61]. Subsequent work has investigated numerous extensions and applications, including chemical graphs [20, 49], fuzzy graphs [70, 71], and neutrosophic graphs [1, 32]. Several related degree-based indices are also widely studied, such as modified Sombor indices [16, 39, 75], Zagreb-type indices [38, 41, 48, 50, 65], and the ABC and GA indices [15, 33, 60, 62].

For hypergraphs, one natural generalization aggregates squared vertex degrees inside each hyperedge and then sums the resulting Euclidean norms over all hyperedges [64]. For superhypergraphs, the same philosophy can be applied at the level of superedges, thereby capturing degree-driven information in hierarchical, set-valued connectivity patterns.

Definition 7 (Sombor index of a hypergraph)**.** [64] Let $H = (V, E)$ be a finite hypergraph, where V is a nonempty finite vertex set and $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ is a finite family of nonempty subsets of V. For each vertex $v \in V$, the *degree* of v in H is

$$d_H(v) \;:=\; \big|\{\, e \in E \mid v \in e \,\}\big|.$$

The *Sombor index* of H is defined by

$$SO(H) \;:=\; \sum_{e \in E} \sqrt{\sum_{v \in e} d_H(v)^2}\,.$$

When H is 2-uniform, this reduces to the classical Sombor index of a simple graph.

Definition 8 (Degree in an n-SuperHyperGraph)**.** Let $\mathrm{SHG}^{(n)} = (V, E)$ be an n-SuperHyperGraph. For each $x \in V$, define the *degree* of x by

$$d_{\mathrm{SHG}^{(n)}}(x) \;:=\; \big|\{\, e \in E \mid x \in e \,\}\big|.$$

Definition 9 (Sombor index of an n-SuperHyperGraph)**.** Let $\mathrm{SHG}^{(n)} = (V, E)$ be an n-SuperHyperGraph and let $d_{\mathrm{SHG}^{(n)}}(\cdot)$ be as in Definition 8. The *Sombor index* of $\mathrm{SHG}^{(n)}$ is defined by

$$SO\big(\mathrm{SHG}^{(n)}\big) \;:=\; \sum_{e \in E} \sqrt{\sum_{x \in e} d_{\mathrm{SHG}^{(n)}}(x)^2}\,.$$

Remark. If a hypergraph $H = (V, E)$ is viewed as an 0-SuperHyperGraph by taking the same vertex set V and the same hyperedge family $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$, then Definition 9 coincides with Definition 7.

4 Results: Sombor index of SuperHypergraphs

Sombor index of a graph sums, over edges, the square root of squared endpoint degrees, capturing degree-based structural complexity information [14,57,61]. These concepts have been further extended and studied in various settings, including chemical graphs [20, 49], fuzzy graphs [70, 71], and neutrosophic graphs [1, 32]. Moreover, related concepts such as the modified Sombor index [75], the Zagreb index [38, 50], the Hyper-Zagreb Index [48], the ABC index [62], and the GA index [33, 60] are also well known.

Sombor index of a hypergraph generalizes this by summing square-rooted degree squares over each hyperedge's incident vertices within complex interactions [64]. Sombor index of a superhypergraph extends further, aggregating degree-squared contributions over multi-tier superedges, reflecting hierarchical connectivity across nested structural levels.

Definition 10 (Sombor index of a hypergraph)**.** [64] Let $H = (V, E)$ be a finite hypergraph, where V is a nonempty finite vertex set and $E \subseteq \mathcal{P}^*(V)$ is a finite family of nonempty subsets of V (the hyperedges).

For each vertex $v \in V$, the *degree* of v in H is

$$d_H(v) \;:=\; \big|\{\, e \in E \mid v \in e \,\}\big|.$$

The *Sombor index* of the hypergraph H is defined by

$$SO(H) \;:=\; \sum_{e \in E} \sqrt{\sum_{v \in e} d_H(v)^2}\,.$$

When H is 2-uniform (i.e., every hyperedge has size 2), this reduces to the classical Sombor index of a simple graph.

Definition 11 (Degree in an n-SuperHyperGraph)**.** Let $\mathrm{SHG}^{(n)} = (V, E, \partial)$ be a level-n SuperHyperGraph. For each $v \in V$, the *degree* of v in $\mathrm{SHG}^{(n)}$ is

$$d_{\mathrm{SHG}^{(n)}}(v) \;:=\; \big|\{\, e \in E \mid v \in \partial(e) \,\}\big|.$$

Definition 12 (Sombor index of an n-SuperHyperGraph)**.** Let $\mathrm{SHG}^{(n)} = (V, E, \partial)$ be a level-n SuperHyperGraph. The *Sombor index* of $\mathrm{SHG}^{(n)}$ is defined by

$$SO\big(\mathrm{SHG}^{(n)}\big) := \sum_{e \in E} \sqrt{\sum_{v \in \partial(e)} d_{\mathrm{SHG}^{(n)}}(v)^2}\,.$$

Remark. If we view a hypergraph $H = (V, E)$ in incidence form by taking $\partial(e) = e$ for all $e \in E$, then the above formula coincides with the Sombor index of a hypergraph.

Example 4 (Sombor index of an n-SuperHyperGraph)**.** Let $n = 1$ and take the base set $V_0 = \{1, 2, 3\}$. Define three 1-supervertices

$$v_1 = \{1, 2\}, \qquad v_2 = \{2, 3\}, \qquad v_3 = \{1, 3\},$$

so $V = \{v_1, v_2, v_3\} \subseteq \mathcal{P}^1(V_0)$. Let the (undirected) superedge set be

$$E = \{e_1, e_2\}, \qquad e_1 = \{v_1, v_2\}, \quad e_2 = \{v_2, v_3\},$$

and take the natural incidence map $\partial(e) = e$ for all $e \in E$.

Then the degrees are

$$d_{\mathrm{SHG}^{(1)}}(v_1) = 1, \qquad d_{\mathrm{SHG}^{(1)}}(v_2) = 2, \qquad d_{\mathrm{SHG}^{(1)}}(v_3) = 1.$$

Hence, by the definition of the Sombor index,

$$SO\big(\mathrm{SHG}^{(1)}\big) = \sum_{e \in E} \sqrt{\sum_{v \in \partial(e)} d_{\mathrm{SHG}^{(1)}}(v)^2} = \sqrt{1^2 + 2^2} + \sqrt{2^2 + 1^2} = 2\sqrt{5}.$$

Therefore, the Sombor index of this 1-SuperHyperGraph equals $2\sqrt{5}$.

5 Results: Sombor index in chemical SuperHyperGraph

In a chemical graph, the Sombor index sums over bonds the square root of squared endpoint degrees, quantifying degree-based molecular branching

complexity in a molecule. In a chemical hypergraph, the Sombor index sums over hyperedges the square root of summed squared vertex degrees, capturing multi-atom interactions beyond pairwise bonds naturally. In a chemical superhypergraph, the Sombor index sums over superedges the square root of squared supervertex degrees, measuring hierarchical nested organization of molecular interactions quantitatively.

Definition 13 (Sombor index of a chemical graph)**.** Let $G = (V, E)$ be a chemical graph, and for each vertex $v \in V$ let

$$d_G(v) \ := \ |\{u \in V : \ uv \in E\}|$$

be its (crisp) degree. The *Sombor index* of G is

$$SO(G) \ := \ \sum_{uv \in E} \sqrt{d_G(u)^2 + d_G(v)^2}\,.$$

Definition 14 (Sombor index of a chemical hypergraph)**.** Let $H = (V, E)$ be a chemical hypergraph. The *Sombor index* of H is defined by

$$SO(H) \ := \ \sum_{e \in E} \sqrt{\sum_{v \in e} d_H(v)^2}\ .$$

Definition 15 (Sombor index of a chemical n-SuperHyperGraph)**.** Let $\mathrm{SHG}^{(n)} = (V, E)$ be a chemical n-SuperHyperGraph. The *Sombor index* of $\mathrm{SHG}^{(n)}$ is defined by

$$SO\big(\mathrm{SHG}^{(n)}\big) \ := \ \sum_{e \in E} \sqrt{\sum_{x \in e} d_{\mathrm{SHG}^{(n)}}(x)^2}\ .$$

Example 5 (Sombor index of a chemical n-SuperHyperGraph: water as a chemical 0-SuperHyperGraph)**.** Consider the water molecule $\mathrm{H_2O}$. Model it as a chemical 0-SuperHyperGraph $\mathrm{SHG}^{(0)} = (V, E)$ (so it is also a chemical hypergraph).

Let the vertex set (atoms) be

$$V = \{\mathrm{O}, \mathrm{H}_1, \mathrm{H}_2\},$$

and let the edge set (bonds) be

$$E = \big\{e_1 = \{\mathrm{O}, \mathrm{H}_1\},\ e_2 = \{\mathrm{O}, \mathrm{H}_2\}\big\}.$$

Then the (crisp) degrees are

$$d_{\mathrm{SHG}^{(0)}}(\mathrm{O}) = 2, \qquad d_{\mathrm{SHG}^{(0)}}(\mathrm{H}_1) = 1, \qquad d_{\mathrm{SHG}^{(0)}}(\mathrm{H}_2) = 1.$$

By Definition 15,

$$SO\big(\mathrm{SHG}^{(0)}\big) = \sum_{e\in E} \sqrt{\sum_{x\in e} d_{\mathrm{SHG}^{(0)}}(x)^2} = \sqrt{2^2+1^2} + \sqrt{2^2+1^2} = 2\sqrt{5}.$$

Thus the Sombor index of this chemical 0-SuperHyperGraph equals $2\sqrt{5}$.

Theorem 1 (Chemical SuperHyperGraph Sombor index generalizes the chemical hypergraph case)**.** *Let $H = (V, E)$ be a chemical hypergraph. Set $V_0 := V$ and $n := 0$, and regard H as the 0-SuperHyperGraph*

$$\mathrm{SHG}^{(0)} := (V, E),$$

where $V \subseteq \mathcal{P}^0(V_0) = V_0$ and $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$. Then

$$SO\big(\mathrm{SHG}^{(0)}\big) = SO(H).$$

Proof. When $n = 0$, we have $\mathcal{P}^0(V_0) = V_0 = V$, so the supervertex set of $\mathrm{SHG}^{(0)}$ is exactly V, and each superedge is exactly a hyperedge $e \in E$. For any $v \in V$,

$$d_{\mathrm{SHG}^{(0)}}(v) = |\{\, e \in E :\ v \in e \,\}| = d_H(v)$$

. Substituting $d_{\mathrm{SHG}^{(0)}}(v) = d_H(v)$ into Definition 15 yields

$$SO\big(\mathrm{SHG}^{(0)}\big) = \sum_{e\in E} \sqrt{\sum_{v\in e} d_{\mathrm{SHG}^{(0)}}(v)^2} = \sum_{e\in E} \sqrt{\sum_{v\in e} d_H(v)^2} = SO(H),$$

which proves the claim. ∎

Theorem 2 (Nonnegativity and trivial case)**.** *Let* $\mathrm{SHG}^{(n)} = (V, E)$ *be a chemical n-SuperHyperGraph. Then*

$$SO\big(\mathrm{SHG}^{(n)}\big) \;\geq\; 0,$$

and $SO\big(\mathrm{SHG}^{(n)}\big) = 0$ *if and only if* $E = \emptyset$*.*

Proof. Each term $\sqrt{\sum_{x\in e} d_{\mathrm{SHG}^{(n)}}(x)^2}$ is a square root of a sum of squares, hence is nonnegative. Therefore the sum over $e \in E$ is nonnegative. If $E = \emptyset$, the sum is empty and equals 0. Conversely, if $E \neq \emptyset$, pick $e \in E$. Then $e \neq \emptyset$, and for every $x \in e$ we have $d_{\mathrm{SHG}^{(n)}}(x) \geq 1$ (since x is incident to at least the edge e). Hence $\sum_{x\in e} d_{\mathrm{SHG}^{(n)}}(x)^2 \geq 1$, so the corresponding summand is > 0, and thus $SO(\mathrm{SHG}^{(n)}) > 0$. ■

Theorem 3 (Lower bound by edge sizes)**.** *Let* $\mathrm{SHG}^{(n)} = (V, E)$ *be a chemical n-SuperHyperGraph. Then*

$$SO\big(\mathrm{SHG}^{(n)}\big) \;\geq\; \sum_{e\in E} \sqrt{|e|}.$$

Proof. Fix $e \in E$. For any $x \in e$, $d_{\mathrm{SHG}^{(n)}}(x) \geq 1$. Therefore

$$\sum_{x\in e} d_{\mathrm{SHG}^{(n)}}(x)^2 \;\geq\; \sum_{x\in e} 1^2 \;=\; |e|.$$

Taking square roots gives $\sqrt{\sum_{x\in e} d(x)^2} \geq \sqrt{|e|}$. Summing over $e \in E$ yields the claim. ■

Theorem 4 (Upper bound using the maximum degree)**.** *Let* $\mathrm{SHG}^{(n)} = (V, E)$ *be a chemical n-SuperHyperGraph and let*

$$\Delta \;:=\; \max_{x\in V} d_{\mathrm{SHG}^{(n)}}(x).$$

Then

$$SO\big(\mathrm{SHG}^{(n)}\big) \;\leq\; \Delta \sum_{e\in E} \sqrt{|e|}.$$

Proof. Fix $e \in E$. Since $d_{\mathrm{SHG}^{(n)}}(x) \leq \Delta$ for all $x \in V$,

$$\sum_{x \in e} d_{\mathrm{SHG}^{(n)}}(x)^2 \;\leq\; \sum_{x \in e} \Delta^2 \;=\; |e|\Delta^2.$$

Taking square roots gives $\sqrt{\sum_{x \in e} d(x)^2} \leq \Delta\sqrt{|e|}$. Summing over $e \in E$ yields the result. ■

Theorem 5 (Exact value for Δ-regular chemical n-SuperHyperGraphs)**.** *Assume* $\mathrm{SHG}^{(n)} = (V, E)$ *is* Δ*-regular, i.e.,* $d_{\mathrm{SHG}^{(n)}}(x) = \Delta$ *for all* $x \in V$*. Then*

$$SO\big(\mathrm{SHG}^{(n)}\big) \;=\; \Delta \sum_{e \in E} \sqrt{|e|}.$$

Proof. If $d(x) = \Delta$ for all $x \in V$, then for each $e \in E$,

$$\sum_{x \in e} d(x)^2 \;=\; \sum_{x \in e} \Delta^2 \;=\; |e|\Delta^2,$$

hence $\sqrt{\sum_{x \in e} d(x)^2} \;=\; \Delta\sqrt{|e|}$. Summing over $e \in E$ gives the stated formula. ■

Theorem 6 (Additivity over disjoint unions)**.** *Let* $\mathrm{SHG}_1^{(n)} = (V_1, E_1)$ *and* $\mathrm{SHG}_2^{(n)} = (V_2, E_2)$ *be chemical* n*-SuperHyperGraphs with* $V_1 \cap V_2 = \emptyset$*. Define their disjoint union by*

$$\mathrm{SHG}_1^{(n)} \,\dot\cup\, \mathrm{SHG}_2^{(n)} \;:=\; (V_1 \cup V_2,\; E_1 \cup E_2).$$

Then

$$SO\big(\mathrm{SHG}_1^{(n)} \dot\cup \mathrm{SHG}_2^{(n)}\big) \;=\; SO\big(\mathrm{SHG}_1^{(n)}\big) \;+\; SO\big(\mathrm{SHG}_2^{(n)}\big).$$

Proof. If $V_1 \cap V_2 = \emptyset$, then degrees computed in the union agree with the degrees computed in each component: for $x \in V_i$, the incident superedges in the union are exactly those in E_i, so $d_{\mathrm{union}}(x) = d_i(x)$. Moreover, every superedge of the union belongs either to E_1 or to E_2, and the defining sum

splits as

$$SO(\text{union}) = \sum_{e\in E_1} \sqrt{\sum_{x\in e} d_1(x)^2} + \sum_{e\in E_2} \sqrt{\sum_{x\in e} d_2(x)^2}$$

$$= SO(\text{SHG}_1^{(n)}) + SO(\text{SHG}_2^{(n)}). \qquad \blacksquare$$

6 Additional results: multiplicative Sombor index in SuperHyperGraph

It multiplies over all superedges the square root of squared supervertex-degree sums, quantifying hierarchical connectivity intensity in superhypergraphs overall networks. The multiplicative Sombor index in graphs is a concept that has been studied in several papers [17, 40, 47, 53].

Definition 16 (Multiplicative Sombor index of a graph)**.** [47] Let $G = (V, E)$ be a finite simple graph. For $v \in V$, let $d_G(v)$ denote the (crisp) degree of v in G. The *multiplicative Sombor index* of G is defined by

$$\Pi_{SO}(G) \;:=\; \prod_{uv\in E} \sqrt{d_G(u)^2 + d_G(v)^2}\,.$$

Definition 17 (Multiplicative Sombor index of a hypergraph)**.** Let $H = (V, E)$ be a finite hypergraph. The *multiplicative Sombor index* of H is defined by

$$\Pi_{SO}(H) \;:=\; \prod_{e\in E} \sqrt{\sum_{v\in e} d_H(v)^2}\,.$$

Remark. If H is 2-uniform and simple (i.e., every hyperedge has size 2 and there are no repeated hyperedges), then H is naturally a graph and $\Pi_{SO}(H)$ coincides with $\Pi_{SO}(G)$ in Definition 16.

Definition 18 (Multiplicative Sombor index of an n-SuperHyperGraph)**.** Let $\text{SHG}^{(n)} = (V, E)$ be an n-SuperHyperGraph. The *multiplicative Som-*

bor index of $\mathrm{SHG}^{(n)}$ is defined by

$$\Pi_{SO}\big(\mathrm{SHG}^{(n)}\big) := \prod_{e\in E}\sqrt{\sum_{x\in e} d_{\mathrm{SHG}^{(n)}}(x)^2}\,.$$

Remark. When $n = 0$, one has $V \subseteq \mathcal{P}^0(V_0) = V_0$, so vertices are "base-level" objects and $\mathrm{SHG}^{(0)}$ reduces to an ordinary hypergraph on V. In this case, Definition 18 specializes to Definition 17.

Example 6 (Multiplicative Sombor index of a simple n-SuperHyperGraph)**.** Let $n = 1$ and take the base set $V_0 = \{1, 2, 3\}$. Define three 1-supervertices

$$v_1 = \{1, 2\}, \qquad v_2 = \{2, 3\}, \qquad v_3 = \{1, 3\},$$

so $V = \{v_1, v_2, v_3\} \subseteq \mathcal{P}^1(V_0)$. Let the superedge set be

$$E = \{e_1, e_2\}, \qquad e_1 = \{v_1, v_2\}, \quad e_2 = \{v_2, v_3\}.$$

Then the supervertex degrees are

$$d_{\mathrm{SHG}^{(1)}}(v_1) = 1, \qquad d_{\mathrm{SHG}^{(1)}}(v_2) = 2, \qquad d_{\mathrm{SHG}^{(1)}}(v_3) = 1.$$

By Definition 18,

$$\Pi_{SO}\big(\mathrm{SHG}^{(1)}\big) = \prod_{e\in E}\sqrt{\sum_{x\in e} d_{\mathrm{SHG}^{(1)}}(x)^2} = \sqrt{1^2 + 2^2}\cdot\sqrt{2^2 + 1^2} = \sqrt{5}\cdot\sqrt{5} = 5.$$

Hence, the multiplicative Sombor index of this 1-SuperHyperGraph equals 5.

Theorem 7 (SuperHyperGraph multiplicative Sombor index generalizes the graph case)**.** *Let $G = (V, E)$ be a finite simple graph. Define $V_0 := V$ and $n := 0$, and regard G as the 0-SuperHyperGraph*

$$\mathrm{SHG}^{(0)} := (V, E),$$

where each graph edge $uv \in E$ is identified with the 0-superedge $\{u, v\} \subseteq V$.

Then

$$\Pi_{SO}\big(\mathrm{SHG}^{(0)}\big) = \Pi_{SO}(G).$$

Proof. Since $n = 0$, we have $\mathcal{P}^0(V_0) = V_0 = V$, so the vertex set of $\mathrm{SHG}^{(0)}$ is V. Moreover, the superedge set $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ consists precisely of the 2-element sets $\{u, v\}$ corresponding to edges $uv \in E(G)$. For each $v \in V$, the degree in $\mathrm{SHG}^{(0)}$ is

$$d_{\mathrm{SHG}^{(0)}}(v) = \big|\{\, e \in E : \ v \in e \,\}\big| = \big|\{\, uv \in E(G) : \ v \in \{u, v\} \,\}\big| = d_G(v).$$

Therefore, by Definition 18,

$$\Pi_{SO}\big(\mathrm{SHG}^{(0)}\big) = \prod_{\{u,v\}\in E} \sqrt{d_{\mathrm{SHG}^{(0)}}(u)^2 + d_{\mathrm{SHG}^{(0)}}(v)^2}$$

$$= \prod_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} = \Pi_{SO}(G),$$

which proves the claim. ∎

7 Conclusion

In this paper, we defined a new class of graphs called Tree-Vertex Graphs. We expect that future work will explore extensions based on fuzzy sets [76], neutrosophic sets [9, 74], soft sets [51, 54], hypersoft sets [66, 69], and plithogenic sets [3, 67], as well as applications to methods such as neural networks. Since this paper is primarily theoretical, we also anticipate further progress on algorithm design, complexity analysis, and quantitative investigations supported by computational experiments.

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