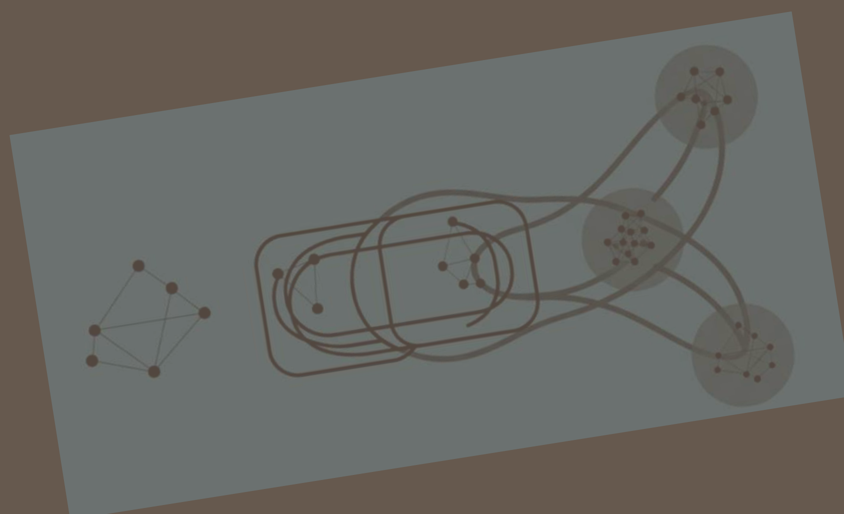
TAKAAKI FUJITA
FLORENTIN SMARANDACHE

HYPERGRAPH AND SUPERHYPERGRAPH THEORY WITH APPLICATIONS

V

REVISITING TOPOLOGICAL INDICES



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Chapter 1

Introduction

1.1 Graph, HyperGraph, and SuperHyperGraph

Network models are classically expressed by *graphs*, in which objects are represented by vertices and binary relationships by edges [5]. While this abstraction is effective for pairwise interactions, it becomes restrictive when the underlying system exhibits *simultaneous* interactions among three or more entities. *Hypergraphs* resolve this limitation by permitting each hyperedge to join an arbitrary nonempty subset of vertices, thereby representing higher-order relations directly [6].

Even so, many real-world datasets and engineered systems display relationships that are not only higher-order but also *layered*, *nested*, and intrinsically *hierarchical*. To capture such multi-level incidence patterns, F. Smarandache introduced the notion of a *SuperHyperGraph*. Informally, a SuperHyperGraph is built via iterative powerset-based constructions, which allow vertices ("supervertices") themselves to be set-valued objects and enable edges to encode nested connectivity across multiple levels [7, 8]. Consequently, SuperHyperGraphs have recently attracted growing attention in both theory and applications [9–14].

Graphs and hypergraphs also provide transparent visual metaphors for complex systems and support a broad spectrum of applications in artificial intelligence, network science, data mining, informatics, chemistry, physics, and related fields [15–17]. By explicitly incorporating hierarchical and multi-level relationships, SuperHyperGraphs offer a flexible framework for modeling and analyzing intricate structures in modern networked data (e.g., [18–27]). Table 1.1 summarizes the main set-theoretic distinctions among graphs, hypergraphs, and n-SuperHyperGraphs (in the supervertex model). Unless stated otherwise, $n \in \mathbb{N}_{\geq 1}$.

1.2 Molecular Graphs and Chemical Graphs

Graph-based representations have played a central role in chemical modeling for decades. A *molecular graph* encodes a compound by representing atoms as vertices and chemical bonds as edges, thereby highlighting connectivity and purely topological features of the structure [29, 30]. In many contexts, one further restricts attention to *chemical graphs*, namely molecular graphs that conform to basic valence considerations; a common abstraction is to require a bounded

Table 1.1: Key distinctions among graph, hypergraph, and n-superhypergraph (supervertex model).

Concept	*Notation*	*Edge family*	*Core extension principle*
Graph [5]	$G = (V, E)$	$E \subseteq \binom{V}{2}$	Edges are 2-element subsets of V, encoding *binary* (pairwise) incidence.
Hypergraph [28]	$H = (V, \mathcal{E})$	$\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$	Hyperedges may join *any* nonempty subset of V, enabling higher-order (multiway) interactions.
n-SuperHyperGraph [7]	$\mathrm{SHG}^{(n)} = (V_0, V, E)$	$V \subseteq \mathcal{P}^n(V_0), \quad E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$	Vertices themselves are *set-valued objects* drawn from an n-fold powerset hierarchy, so incidence can be represented across *nested* and *multi-level* layers.

Notation. $\mathcal{P}(X) = \{A \mid A \subseteq X\}$, $\mathcal{P}^0(X) = X$, and $\mathcal{P}^{k+1}(X) = \mathcal{P}(\mathcal{P}^k(X))$. Here $\binom{V}{2} = \{\{u, v\} \mid u, v \in V,\ u \neq v\}$. *Remark:* the superhypergraph row corresponds to the supervertex model (Model A); a dual nested-edge model (Model B) is recorded separately and related via support/flattening operators.

maximum vertex degree (often $\Delta \leq 4$), reflecting typical bonding patterns in organic chemistry [31, 32].

These ideas also admit higher-order extensions. Hypergraph and superhypergraph models have been proposed to represent multi-atom interactions and nested, hierarchical substructures that are difficult to capture with pairwise edges alone. This viewpoint leads to molecular hypergraphs [33, 34], molecular superhypergraphs [20], chemical hypergraphs [35, 36], and chemical superhypergraphs [37], among other related formalisms. As a reference, we present a concise comparison of chemical graphs, chemical hypergraphs, and chemical superhypergraphs in Table 1.2.

1.3 Topological Indices on Graphs

A *topological index* is a numerical invariant extracted from a graph—typically from degree information, distance data, or combinations thereof—designed to summarize structural aspects of the underlying network. In mathematical chemistry, such indices are widely used as descriptors to relate graph structure to physicochemical properties and to support QSPR/QSAR-type analyses. Well-studied examples include the Zagreb indices [38, 39], the Sombor index [40, 41], the atom–bond connectivity (ABC) index [42, 43], the Randić index [44, 45], the hyper-Zagreb indices [46, 47], and classical distance-based measures such as the Harary and Wiener indices. A broad literature investigates their extremal behavior, correlations, and applications; see, for example, [4].

Table 1.2: Chemical graph vs. chemical hypergraph vs. chemical superhypergraph (concise).

	Chemical graph	*Chemical hypergraph*	*Chemical superhypergraph*
Vertices / nodes	Atoms	Atoms (plus molecule-level units via nesting)	Nested entities (atoms, groups, molecules) as supervertices
Edges	Bonds (pairwise)	Hyperedges (multi-atom); optional directed reactions	Superedges among mixed-level supervertices
Key strength	Simple; classical indices apply	Models multiway interactions and reactions	Models multiway + hierarchical nesting in one object
Typical constraint	$\Delta \leq 4$ (valence)	Degree/incidence constraints on atoms	Degree constraints across levels (supervertices and/or base support)

Table 1.3: Topological indices on graphs, hypergraphs, and superhypergraphs (concise overview).

	Graphs	*Hypergraphs*	*SuperHyperGraphs*
Underlying structure	Vertices + pairwise edges	Vertices + multiway hyperedges	Supervertices (possibly nested) + superedges
Core ingredients	Degrees, distances, spectra, matchings	Generalized degrees, hyper-distances, incidence/spectral constructions	Superdegrees, superdistances, pair-incidence multiplicities, hierarchical support
How indices are formed	Sum/product over edges, vertices, or pairs	Replace edges by hyperedges; aggregate over pairs inside each hyperedge or via incidence graphs	Replace vertices by supervertices; aggregate over pairs inside each superedge or via flattening/levels
Typical outputs	$\mathbb{R}$-valued invariants	$\mathbb{R}$-valued invariants (choice of distance/incidence matters)	$\mathbb{R}$-valued invariants; can be level-aware or base-support-aware
Examples (families)	Wiener, Harary, Zagreb, Sombor, ABC, Randić	Hyper-Wiener, hyper-Zagreb, hyper-Sombor, hyper-ABC (via pair aggregation)	SuperHyper-Wiener, superhyper-Zagreb, superhyper-Sombor, superhyper-ABC (via superedge aggregation)

1.4 Our Contributions

In view of the above, research on topological indices for graphs and for SuperHyperGraphs is of considerable importance. As outlined in the table of contents, this book introduces and formalizes a variety of Chemical SuperHyperGraphs and numerous topological indices on SuperHyperGraphs. In addition, we briefly investigate a SuperHyperGraph counterpart of spectral graph theory. We expect that these concepts will provide useful tools for the analysis of complex real-world networks and hierarchical chemical structures.

Hypergraph and SuperHypergraph Theory with Applications (V): Revisiting Topological Indices

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Abstract

Hypergraphs generalize ordinary graphs by allowing a hyperedge to connect an arbitrary nonempty subset of the vertex set. By iterating the powerset construction, one obtains nested higher-order set-valued objects and, consequently, finite *SuperHyperGraphs*, in which both vertices and edges may carry multi-layer, set-valued structure. Topological indices are numerical invariants extracted from structural features—such as degrees, distances, and connectivity—and are widely used to compare networks and relate structure to intrinsic or application-driven properties. Despite this expressive framework, the systematic study of *SuperHyperGraph* properties and parameters remains relatively limited. In this book, we develop extensions of a variety of topological indices from graphs and hypergraphs to SuperHyperGraphs. The present volume continues and broadens the line of research initiated in [1–4]. Some notions may overlap with those discussed in earlier volumes of the series; we kindly ask the reader's indulgence.

Keywords: SuperHyperGraph, HyperGraph, Topological Indices

Chapter 2

Preliminaries

This chapter establishes notation and reviews the fundamental structures used throughout the book.

2.1 SuperHyperGraphs

Classical graph theory models a system of *vertices* linked by *edges*, and studies connectivity, structural invariants, and algorithmic problems motivated by mathematics, computer science, and many applied domains [5]. A *hypergraph* broadens this framework by allowing a single edge to connect an arbitrary nonempty subset of the vertex set; hence it is well suited to represent intrinsically multiway interactions (e.g., relations of arity greater than two) [6, 48]. Such higher-order relations have become especially prominent in contemporary learning and modeling pipelines, including neural architectures that directly leverage hypergraph incidence patterns [6, 34, 49–51].

By iterating the powerset operation, one can also permit *nested* set-valued entities at the vertex level. This leads to finite *SuperHyperGraphs*, in which both vertices and edges may occur at multiple levels of set nesting [52, 53]. Such hierarchical representations arise naturally in layered or multiscale relational settings, for instance in molecular design, complex-network analysis, and neural-network modeling, among other applications [19, 54–56]. Several related generalizations have also been investigated, including Directed SuperHyperGraphs [57, 58] and MetaSuperHyperGraphs [59]. Unless stated otherwise, the index n in $\mathcal{P}^n(\cdot)$ and in the term n-SuperHyperGraph always denotes a nonnegative integer.

Definition 2.1.1 (Base set)**.** A *base set* S is the ambient universe of discourse:

$$S = \{ x \mid x \text{ is an admissible object in the context under consideration} \}.$$

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

Definition 2.1.2 (Powerset)**.** (see [60]) 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 2.1.3 (Hypergraph)**.** [28,61] A *hypergraph* is a pair $H = (V, E)$ such that:

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

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

Example 2.1.4 (Real-life example of a hypergraph)**.** Consider the problem of organizing university courses and student enrollments. Let V be the set of all students in a department. For each course c, define a hyperedge

$$e_c := \{ s \in V \mid s \text{ is enrolled in course } c \}.$$

Then $H = (V, E)$, where $E = \{e_c : c \text{ is a course}\}$, is a hypergraph. Each hyperedge represents a multiway relation: all students jointly participating in the same course.

Definition 2.1.5 (Iterated powerset and flattening)**.** [62] Let V_0 be a finite nonempty set. Define $\mathcal{P}^0(V_0) := V_0$ and

$$\mathcal{P}^{k+1}(V_0) := \mathcal{P}\big(\mathcal{P}^k(V_0)\big) \qquad (k \geq 0).$$

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

$$\mathrm{Flat}_0(x) := \{x\} \quad (x \in V_0), \qquad \mathrm{Flat}_{k+1}(X) := \bigcup_{Y \in X} \mathrm{Flat}_k(Y) \quad (X \in \mathcal{P}^{k+1}(V_0) \setminus \{\emptyset\}).$$

Definition 2.1.6 (n-SuperHyperGraph)**.** (see [7]) 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

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

such that

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

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

Example 2.1.7 (A 1-SuperHyperGraph)**.** Let $V_0 = \{1, 2, 3\}$. Then $\mathcal{P}^1(V_0) = \mathcal{P}(V_0)$. Define the 1-supervertex set

$$V = \{\{1\}, \{2\}, \{3\}, \{1, 2\}\} \subseteq \mathcal{P}(V_0),$$

and define the 1-superedge family

$$E = \{ e_1, e_2 \} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}, \qquad e_1 = \{\{1\}, \{2\}, \{1, 2\}\}, \quad e_2 = \{\{2\}, \{3\}\}.$$

Then $\mathrm{SHG}^{(1)} = (V, E)$ is a 1-SuperHyperGraph on V_0. Here the supervertices are (nonempty) subsets of V_0, and superedges are nonempty families of such supervertices.

Example 2.1.8 (A 2-SuperHyperGraph)**.** Let $V_0 = \{a, b\}$. Then

$$\mathcal{P}^1(V_0) = \{\emptyset, \{a\}, \{b\}, \{a, b\}\}, \qquad \mathcal{P}^2(V_0) = \mathcal{P}\big(\mathcal{P}(V_0)\big).$$

Define the 2-supervertex set

$$V = \Big\{ \ \{\{a\}\}, \ \{\{b\}\}, \ \{\{a\}, \{b\}\} \ \Big\} \ \subseteq \ \mathcal{P}^2(V_0),$$

and define the 2-superedge family

$$E = \{ \, f \, \} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}, \qquad f = \Big\{ \ \{\{a\}\}, \ \{\{b\}\}, \ \{\{a\}, \{b\}\} \ \Big\}.$$

Then $\mathrm{SHG}^{(2)} = (V, E)$ is a 2-SuperHyperGraph on V_0. In this example, each supervertex is itself a set of subsets of V_0 (i.e., a nonempty element of $\mathcal{P}^2(V_0)$), illustrating the second-level nesting.

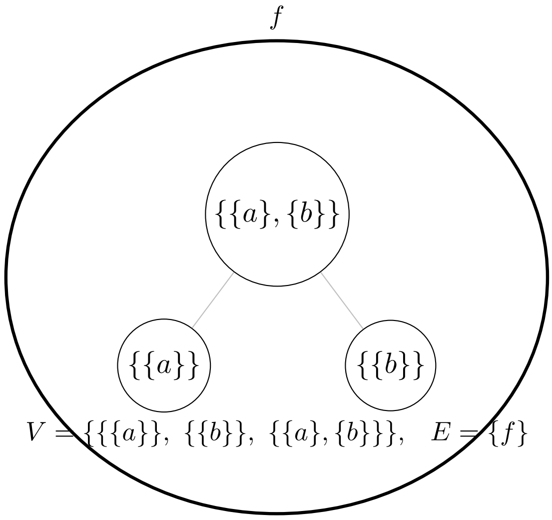

Figure 2.1: A 2-SuperHyperGraph $\mathrm{SHG}^{(2)} = (V, E)$ on $V_0 = \{a, b\}$ with one 2-superedge f containing all 2-supervertices.

Remark 2.1.9 (Two complementary models of SuperHyperGraphs and their correspondence)**.** Throughout this book, we intentionally work with two closely related formalizations of SuperHyperGraphs. They are equivalent after a canonical "support/flattening" translation, and different chapters adopt whichever model is more convenient for the intended construction (e.g., degree-based indices versus nested-edge combinatorics).

Model A (supervertex model; Chapter 2 as the default). Fix a nonempty base set V_0 and an integer $n \geq 1$. Let $\mathcal{P}^0(V_0) := V_0$ and $\mathcal{P}^{k+1}(V_0) := \mathcal{P}(\mathcal{P}^k(V_0))$. An *n-SuperHyperGraph in Model A* is a pair

$$\mathsf{H}_A = (V, E), \qquad V \subseteq \mathcal{P}^n(V_0), \qquad E \subseteq \mathcal{P}(V) \setminus \{\varnothing\},$$

where the elements of V are *n-supervertices* (set-valued vertices), and each $e \in E$ is a nonempty collection of supervertices.

Model B (nested superedge model; used in parts of Chapter 4, e.g. Hosoya-type constructions). Let V be a nonempty (base) vertex set. Let $\mathcal{P}_*(V) := \mathcal{P}(V) \setminus \{\varnothing\}$. Define iteratively $\mathcal{P}_*^{(1)}(V) := \mathcal{P}_*(V)$ and $\mathcal{P}_*^{(k+1)}(V) := \mathcal{P}_*(\mathcal{P}_*^{(k)}(V))$. An *n-SuperHyperGraph in Model B* is a pair

$$\mathsf{H}_B = (V, \mathbb{E}), \qquad \mathbb{E} \subseteq \mathcal{P}_*^{(n)}(V),$$

whose elements $\varepsilon \in \mathbb{E}$ are *nested superhyperedges* built from V. In this model, "higher-order" structure resides in the *edges* rather than in the vertex set.

Support/flattening and the translation between models. For $n \geq 1$, define the *support* map $\mathrm{supp}_n : \mathcal{P}_*^{(n)}(V) \to \mathcal{P}_*(V)$ recursively by

$$\mathrm{supp}_1(S) := S \quad (S \in \mathcal{P}_*(V)), \qquad \mathrm{supp}_n(X) := \bigcup_{Y \in X} \mathrm{supp}_{n-1}(Y) \quad (X \in \mathcal{P}_*^{(n)}(V),\ n \geq 2).$$

Then $\mathrm{supp}_n(\varepsilon)$ is the underlying base-vertex set "mentioned" by the nested object ε.

(B→A: edge-nesting to supervertices). Given $\mathsf{H}_B = (V, \mathbb{E})$, define

$$V_A := \mathbb{E} \ \subseteq \ \mathcal{P}_*^{(n)}(V), \qquad E_A := \{\ \varepsilon^\star \ \mid\ \varepsilon \in \mathbb{E}\ \}, \qquad \varepsilon^\star := \{\varepsilon\} \in \mathcal{P}(V_A) \setminus \{\varnothing\}.$$

Thus $\mathsf{H}_A := (V_A, E_A)$ is a Model A SuperHyperGraph whose supervertices are precisely the nested edges of Model B. If one needs an incidence-like representation on the base set, it is recovered via supp_n.

(A→B: supervertices to edge-nesting). Conversely, suppose $\mathsf{H}_A = (V, E)$ with $V \subseteq \mathcal{P}^n(V_0)$. If we identify the base vertex set with V_0 and restrict to nonempty objects, we may set

$$\mathbb{E} := V \ \subseteq \ \mathcal{P}_*^{(n)}(V_0),$$

viewing each n-supervertex as a nested superhyperedge; base-level incidence is again read through supp_n. Under this identification, "supervertex-based" constructions and "nested-edge-based" constructions describe the same higher-order objects, but with the higher-order layer assigned to vertices (Model A) or edges (Model B).

Equivalence conditions and chapter usage. The two models are interchangeable provided we:

(i) fix a base set (either V_0 for Model A or V for Model B) and consistently exclude $\varnothing$ when required;

(ii) interpret any nested object ε by its support $\mathrm{supp}_n(\varepsilon) \subseteq V$ when translating incidence, disjointness, or distance-based notions to the base level;

(iii) state explicitly (when necessary) whether an invariant is computed on the supervertex layer or on the support layer.

In this book, Chapter 2 (foundations, flattening/support operators, and embeddings from nested hyperedges) uses Model A as the standard set-theoretic typing formalism, while certain constructions in Chapter 4 (e.g. matchings and Hosoya-type indices for nested superhyperedges) adopt Model B for convenience. Whenever a definition depends on the chosen representation (for instance, distance-based indices), we will specify the layer (supervertex vs. support) on which the computation is performed.

The following definition is recorded for later use, whenever needed.

Definition 2.1.10 (Pair-incidence multiplicity)**.** Let $H = (V, \mathcal{E})$ be a hypergraph. For distinct $u, v \in V$, define

$$\mu_H(u,v) \;:=\; |\{\, e \in \mathcal{E} : \; \{u,v\} \subseteq e \,\}|.$$

Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a SuperHyperGraph. For distinct $A, B \in \mathbb{V}$, define

$$\mu_{\mathbb{H}}(A,B) \;:=\; |\{\, f \in \mathbb{E} : \; \{A,B\} \subseteq f \,\}|.$$

2.2 Relationship between Nested Hyperedges and n-SuperHyperGraphs

As a concept related to SuperHyperGraphs, *nested hyperedges* are also known. The idea of nested hyperedges is likewise a highly important notion. In this section, we investigate the relationship between nested hyperedges and n-SuperHyperGraphs.

Definition 2.2.1 (Nested hyperedges)**.** Let $H = (V, \mathcal{E})$ be a hypergraph. Two distinct hyperedges $e, f \in \mathcal{E}$ are said to be *nested* if $e \subsetneq f$. We say that H is a *hypergraph with nested hyperedges* if there exist $e, f \in \mathcal{E}$ with $e \subsetneq f$. More generally, a *nesting chain* is a sequence $(e_0, e_1, \ldots, e_t) \subseteq \mathcal{E}$ such that

$$e_0 \subsetneq e_1 \subsetneq \cdots \subsetneq e_t.$$

Definition 2.2.2 (n-fold singleton lift)**.** Fix a base set V_0 and $n \geq 1$. Define recursively the maps

$$\mathrm{lift}_0 : V_0 \to \mathcal{P}^0(V_0) = V_0, \qquad \mathrm{lift}_{t+1}(x) := \{\mathrm{lift}_t(x)\} \quad (t \geq 0).$$

Thus $\mathrm{lift}_{n-1}(x) \in \mathcal{P}^{n-1}(V_0)$ is the $(n-1)$-times iterated singleton of x. For a subset $e \subseteq V_0$, define its *n-lift* by

$$\widehat{e}^{(n)} \;:=\; \{\mathrm{lift}_{n-1}(v) : v \in e\} \;\in\; \mathcal{P}\big(\mathcal{P}^{n-1}(V_0)\big) = \mathcal{P}^n(V_0).$$

Theorem 2.2.3 (Nested-hyperedge hypergraphs embed into n-SuperHyperGraphs)**.** *Let $H = (V_0, \mathcal{E}_0)$ be a finite hypergraph (possibly with nested hyperedges), and fix $n \geq 2$. Define a supervertex set*

$$V \;:=\; \{\mathrm{lift}_{n-1}(v) : v \in V_0\} \;\cup\; \{\widehat{e}^{(n)} : e \in \mathcal{E}_0\} \;\subseteq\; \mathcal{P}^n(V_0).$$

Define a superhyperedge family $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ by

$$E \;:=\; \{\varepsilon_e : \; e \in \mathcal{E}_0\}, \qquad \varepsilon_e \;:=\; \{\widehat{e}^{(n)}\} \;\cup\; \{\mathrm{lift}_{n-1}(v) : v \in e\}.$$

Then $\mathrm{SHG}^{(n)} := (V, E)$ is an n-SuperHyperGraph (in the powerset-hierarchy sense), and:

(i) *(*Incidence recovery*) For every $v \in V_0$ and $e \in \mathcal{E}_0$,*

$$v \in e \quad \iff \quad \mathrm{lift}_{n-1}(v) \in \widehat{e}^{(n)} \quad \iff \quad \mathrm{lift}_{n-1}(v) \in \varepsilon_e.$$

(ii) *(*Nestedness preservation*) For any* $e, f \in \mathcal{E}_0$*,*

$$e \subseteq f \quad \Longleftrightarrow \quad \widehat{e}^{(n)} \subseteq \widehat{f}^{(n)}.$$

In particular, if $e \subsetneq f$ *in* H*, then the corresponding supervertices satisfy* $\widehat{e}^{(n)} \subsetneq \widehat{f}^{(n)}$ *in* $\mathrm{SHG}^{(n)}$.

Proof. By construction, $\mathrm{lift}_{n-1}(v) \in \mathcal{P}^{n-1}(V_0)$ for all $v \in V_0$, hence $\{\mathrm{lift}_{n-1}(v) : v \in V_0\} \subseteq \mathcal{P}^{n}(V_0)$. Also, for each $e \subseteq V_0$, the set $\widehat{e}^{(n)}$ is a subset of $\mathcal{P}^{n-1}(V_0)$, so $\widehat{e}^{(n)} \in \mathcal{P}^{n}(V_0)$. Therefore $V \subseteq \mathcal{P}^{n}(V_0)$.

Next, for each $e \in \mathcal{E}_0$, the superhyperedge $\varepsilon_e = \{\widehat{e}^{(n)}\} \cup \{\mathrm{lift}_{n-1}(v) : v \in e\}$ is a nonempty subset of V, so $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$. Hence (V, E) is a well-defined superhypergraph on a powerset-hierarchy vertex domain, i.e., an n-SuperHyperGraph.

For (i), observe that $\widehat{e}^{(n)} = \{\mathrm{lift}_{n-1}(u) : u \in e\}$, so $\mathrm{lift}_{n-1}(v) \in \widehat{e}^{(n)}$ holds exactly when $v \in e$. Since $\widehat{e}^{(n)} \in \varepsilon_e$ and all $\mathrm{lift}_{n-1}(v)$ with $v \in e$ are included in ε_e by definition, the final equivalence follows.

For (ii), suppose $e \subseteq f$. Then every $v \in e$ also lies in f, hence $\mathrm{lift}_{n-1}(v) \in \widehat{f}^{(n)}$ whenever $\mathrm{lift}_{n-1}(v) \in \widehat{e}^{(n)}$, so $\widehat{e}^{(n)} \subseteq \widehat{f}^{(n)}$. Conversely, if $\widehat{e}^{(n)} \subseteq \widehat{f}^{(n)}$, then for every $v \in e$ we have $\mathrm{lift}_{n-1}(v) \in \widehat{e}^{(n)} \subseteq \widehat{f}^{(n)}$, hence $v \in f$ by (i), so $e \subseteq f$. □

Remark 2.2.4 (Why the converse fails)**.** The construction in Theorem 2.2.3 produces a restricted subclass of n-SuperHyperGraphs: every supervertex representing an original hyperedge has the special form $\widehat{e}^{(n)} = \{\mathrm{lift}_{n-1}(v) : v \in e\}$, i.e., it is a set of $(n-1)$-fold singletons. A general n-SuperHyperGraph may contain supervertices that do *not* have this form, so it need not arise from any ordinary hypergraph by this embedding.

For example, let $V_0 = \{a, b, c\}$ and $n = 2$. Consider the 2-level supervertex

$$X := \{\{a, b\}\} \in \mathcal{P}^2(V_0),$$

whose unique inner set $\{a, b\}$ is not a singleton. No subset $e \subseteq V_0$ satisfies $\widehat{e}^{(2)} = \{\{v\} : v \in e\} = X$. Thus any 2-SuperHyperGraph that uses X as a supervertex lies outside the image of the embedding above.

Chapter 3

Chemical Graph Class

In this chapter, we briefly review chemical graphs and related concepts.

3.1 Chemical SuperHyperGraphs

Chemical structure and reactivity are naturally multiscale. Atoms combine into bonds; bonds form functional groups; functional groups assemble into larger motifs and molecules; and, at an even higher level, molecules participate in assemblies and reaction networks. To model such nested organization in a single combinatorial object, we use *chemical superhypergraphs*, which allow successive layers of set-valued entities and may carry quantitative annotations (e.g., bond strengths, interaction energies, or reaction rates).

Definition 3.1.1 (Chemical graph)**.** [63] Let $\mathcal{A}$ be a set of atom labels (for instance, element symbols with optional tags), and let $\mathcal{B}$ be a set of bond labels (for instance, single/double/triple/aromatic, or a bond order). A *chemical graph* is a labeled undirected graph

$$G_{\text{chem}} = (V, E, \lambda_V, \lambda_E),$$

where:

- (V, E) is a finite simple undirected graph (unless specified otherwise);
- $\lambda_V : V \to \mathcal{A}$ assigns an atom label to each vertex (each $v \in V$ represents an atom);
- $\lambda_E : E \to \mathcal{B}$ assigns a bond label to each edge (each $e \in E$ represents a chemical bond).

Definition 3.1.2 (Chemical hypergraph)**.** [35,36,64] A *chemical hypergraph* describing a chemical system is a multilevel hypergraph

$$H_{\text{chem}} = \big(V_0, E_S, E_N, E_D\big),$$

where:

- V_0 is a finite set of *atomic nodes* (each $v \in V_0$ represents an atom);
- $E_S \subseteq \mathcal{P}(V_0) \setminus \{\emptyset\}$ is a family of *simple hyperedges* (e.g., bonds or molecular substructures), so each $e_S \in E_S$ is a nonempty subset of V_0;
- $E_N \subseteq \mathcal{P}(E_S) \setminus \{\emptyset\}$ is a family of *nesting hyperedges* (molecules), where each $e_N \in E_N$ is a nonempty subset of E_S indicating which bonds/substructures constitute that molecule;
- $E_D \subseteq E_N \times E_N$ is a set of *directed hyperedges* (reactions), where $(e_{N,r}, e_{N,p}) \in E_D$ indicates that the reactant molecule-hyperedge $e_{N,r}$ yields the product molecule-hyperedge $e_{N,p}$.

Hence H_{chem} represents atoms at level 0, bonds/substructures at level 1, molecules as collections of level-1 units, and reactions as directed connections between molecule-level objects.

Definition 3.1.3 (Chemical SuperHyperGraph)**.** Fix integers $m \geq 1$ and $n \geq 0$. A *chemical superhypergraph* is an m-level weighted structure

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

satisfying:

- 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 formed 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 attribute at level ℓ (e.g., bond strength, interaction energy, or reaction rate). The intended meaning of w_ℓ depends on the modeling context.

Example 3.1.4 (A chemical hypergraph for a simple reaction)**.** We illustrate Definition 3.1.2 using the hydrogenation

$$\mathrm{H_2} + \mathrm{Cl_2} \longrightarrow 2\,\mathrm{HCl}.$$

Let the atomic node set be

$$V_0 = \{H_1, H_2, Cl_1, Cl_2\},$$

where H_1, H_2 are the two hydrogen atoms and Cl_1, Cl_2 are the two chlorine atoms.

Level-1 simple hyperedges (bonds). Let

$$E_S = \left\{\, e_{\mathrm{H_2}}, e_{\mathrm{Cl_2}}, e^{(1)}_{\mathrm{HCl}}, e^{(2)}_{\mathrm{HCl}} \,\right\},$$

where

$$e_{\mathrm{H}_2} = \{H_1, H_2\}, \qquad e_{\mathrm{Cl}_2} = \{Cl_1, Cl_2\}, \qquad e^{(1)}_{\mathrm{HCl}} = \{H_1, Cl_1\}, \qquad e^{(2)}_{\mathrm{HCl}} = \{H_2, Cl_2\}.$$

Level-2 nesting hyperedges (molecules). Let

$$E_N = \{\, M_{\mathrm{H}_2}, M_{\mathrm{Cl}_2}, M^{(1)}_{\mathrm{HCl}}, M^{(2)}_{\mathrm{HCl}} \,\} \subseteq \mathcal{P}(E_S) \setminus \{\emptyset\},$$

with

$$M_{\mathrm{H}_2} = \{e_{\mathrm{H}_2}\}, \quad M_{\mathrm{Cl}_2} = \{e_{\mathrm{Cl}_2}\}, \quad M^{(1)}_{\mathrm{HCl}} = \{e^{(1)}_{\mathrm{HCl}}\}, \quad M^{(2)}_{\mathrm{HCl}} = \{e^{(2)}_{\mathrm{HCl}}\}.$$

Directed hyperedges (reaction). Let

$$E_D = \{\, (M_{\mathrm{H}_2} \cup M_{\mathrm{Cl}_2},\ M^{(1)}_{\mathrm{HCl}} \cup M^{(2)}_{\mathrm{HCl}}) \,\} \ \subseteq\ E_N \times E_N.$$

Then $H_{\mathrm{chem}} = (V_0, E_S, E_N, E_D)$ is a chemical hypergraph encoding atoms, bonds, molecules, and the directed reaction.

Example 3.1.5 (A small chemical SuperHyperGraph with weights)**.** We illustrate Definition 3.1.3 with $m = 2$ and $n = 0$ (so $\mathcal{P}^0(V_0) = V_0$), using a toy molecule with three atoms and two bonds.

Let

$$V_0 = \{O, H_1, H_2\}$$

(think of a water-like structure with one oxygen and two hydrogens).

Level 1: first-level units (bonds). Let

$$E_1 = \{\, b_1, b_2 \,\} \subseteq \mathcal{P}^0(V_0) \setminus \{\emptyset\} = \mathcal{P}(V_0) \setminus \{\emptyset\}, \qquad b_1 = \{O, H_1\}, \quad b_2 = \{O, H_2\}.$$

Define a bond-strength weight $w_1 : E_1 \to \mathbb{R}_{\geq 0}$ by

$$w_1(b_1) = 1.00, \qquad w_1(b_2) = 0.95.$$

Level 2: aggregates (the molecule). Let

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

Define an aggregate-level weight $w_2 : E_2 \to \mathbb{R}_{\geq 0}$ by

$$w_2(M) = w_1(b_1) + w_1(b_2) = 1.95,$$

interpretable, for instance, as a simplified total interaction energy.

Therefore,

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

is a chemical SuperHyperGraph with explicit level-wise weights.

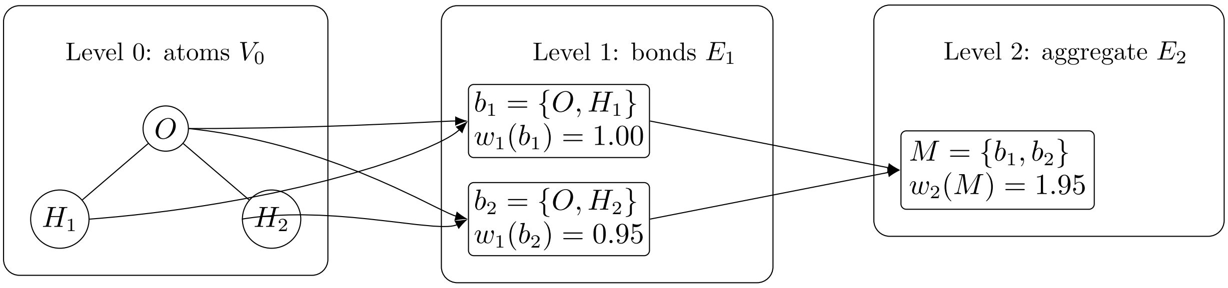

Figure 3.1: A small chemical SuperHyperGraph $\mathcal{CSH}^{(2,0)} = (V_0, E_1, E_2, w_1, w_2)$: atoms (Level 0) form bonds (Level 1) with weights w_1, and bonds aggregate into a molecule object (Level 2) with weight w_2.

3.2 Chemical SuperHyperTree

A chemical tree is a connected acyclic molecular graph whose vertex degrees model valence and are bounded by four typically [65–67]. A chemical hypertree is a hypergraph whose incidence graph is a tree, with maximum vertex degrees constrained by four globally [68]. A chemical superhypertree is an n-superhypergraph whose incidence graph is a tree and whose supervertex degrees are at most four.

Definition 3.2.1 (Tree)**.** A graph $T = (V, E)$ is a *tree* if it is connected and acyclic. Equivalently, T is connected and $|E| = |V| - 1$.

Definition 3.2.2 (Chemical tree)**.** A *chemical tree* is a tree T with maximum degree

$$\Delta(T) \le 4.$$

Definition 3.2.3 (Vertex degree in a hypergraph)**.** For a hypergraph $H = (V, E)$ and $v \in V$, the (hypergraph) degree is

$$\deg_H(v) := |\{ e \in E : \ v \in e \}|,$$

and the maximum degree is $\Delta(H) := \max_{v \in V} \deg_H(v)$.

Definition 3.2.4 (Incidence graph)**.** Let $H = (V, E)$ be a hypergraph. Its (bipartite) incidence graph is

$$\mathrm{Inc}(H) := (V \sqcup E, \ I), \qquad I := \big\{\{v, e\} : v \in V, \ e \in E, \ v \in e\big\}.$$

Definition 3.2.5 (HyperTree (Berge-tree / incidence-tree))**.** [69, 70] A hypergraph H is a *HyperTree* (or *hypertree* in the incidence sense) if $\mathrm{Inc}(H)$ is a (graph-theoretic) tree. Equivalently, $\mathrm{Inc}(H)$ is connected and acyclic.

Definition 3.2.6 (Chemical HyperTree)**.** A *Chemical HyperTree* is a HyperTree H with

$$\Delta(H) \le 4.$$

Example 3.2.7 (A chemical hypertree)**.** Let

$$V = \{C, O, H_1, H_2, H_3, H_4\}$$

be a set of atomic nodes (one carbon, one oxygen, and four hydrogens). Define a hyperedge family

$$\mathcal{E} = \{\, e_1, e_2, e_3, e_4, e_5 \,\},$$

where

$$e_1 = \{C, H_1\}, \quad e_2 = \{C, H_2\}, \quad e_3 = \{C, H_3\}, \quad e_4 = \{C, O\}, \quad e_5 = \{O, H_4\}.$$

Then the incidence graph $\mathrm{Inc}(H)$ has bipartition $V \sqcup \mathcal{E}$ and edges $\{v, e_i\}$ whenever $v \in e_i$. It is connected and has

$$|V| + |\mathcal{E}| = 6 + 5 = 11 \quad \text{vertices and} \quad \sum_{i=1}^{5} |e_i| = (2 + 2 + 2 + 2 + 2) = 10 \quad \text{edges},$$

so $|\mathrm{E}(\mathrm{Inc}(H))| = |\mathrm{V}(\mathrm{Inc}(H))| - 1$ and hence $\mathrm{Inc}(H)$ is a tree. Therefore $H = (V, \mathcal{E})$ is a hypertree.

Moreover, the hypergraph degrees are

$$d_H(C) = 4, \qquad d_H(O) = 2, \qquad d_H(H_i) = 1 \ (i = 1, 2, 3, 4),$$

so

$$\Delta(H) = \max_{v \in V} d_H(v) = 4 \leq 4.$$

Thus H is a *chemical hypertree*.

Remark 3.2.8 (k-uniform hypertrees used in parts of chemical hypergraph theory)**.** A *k-uniform* hypergraph satisfies $|e| = k$ for all $e \in E$. One common (and widely used) construction of a k-uniform hypertree is the so-called *k-th power of an ordinary tree*: start from a tree T and "expand" each edge into a k-set by adjoining $k - 2$ new vertices specific to that edge, yielding a connected k-uniform hypergraph with incidence graph a tree.

Definition 3.2.9 (Degree in an n-SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be an n-SuperHyperGraph. For $\gtrapprox \in \mathbb{V}$, define

$$\deg_{\mathbb{H}}(\gtrapprox) := \bigl|\{\ \in \mathbb{E} : \ \gtrapprox \in \ \}\bigr|, \qquad \Delta(\mathbb{H}) := \max_{\gtrapprox \in \mathbb{V}} \deg_{\mathbb{H}}(\gtrapprox).$$

Definition 3.2.10 (Incidence graph of an n-SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$. Its incidence graph is

$$\mathrm{Inc}(\mathbb{H}) := (\mathbb{V} \sqcup \mathbb{E},\ \mathbb{I}), \qquad \mathbb{I} := \bigl\{\{\gtrapprox, \ \} : \ \gtrapprox \in \mathbb{V}, \ \ \in \mathbb{E}, \ \gtrapprox \in \ \bigr\}.$$

Definition 3.2.11 (SuperHyperTree)**.** [14] An n-SuperHyperGraph $\mathbb{H}$ is an *n-SuperHyperTree* (or *SuperHyperTree* when n is fixed) if $\mathrm{Inc}(\mathbb{H})$ is a (graph-theoretic) tree.

Definition 3.2.12 (Chemical SuperHyperTree)**.** A *Chemical SuperHyperTree* is an n-SuperHyperTree $\mathbb{H}$ satisfying

$$\Delta(\mathbb{H}) \leq 4.$$

Example 3.2.13 (A chemical SuperHyperTree)**.** Fix $n = 1$ and let the base set of atoms be

$$V_0 = \{C, O, H_1, H_2, H_3, H_4\}.$$

Define the 1-supervertex set (a subset of $\mathcal{P}(V_0)$) by

$$\mathbb{V} = \{\{C\}, \{O\}, \{H_1\}, \{H_2\}, \{H_3\}, \{H_4\}\}.$$

Define the superhyperedge family

$$\mathbb{E} = \{ f_1, f_2, f_3, f_4, f_5 \},$$

where

$$f_1 = \{\{C\}, \{H_1\}\}, \quad f_2 = \{\{C\}, \{H_2\}\}, \quad f_3 = \{\{C\}, \{H_3\}\}, \quad f_4 = \{\{C\}, \{O\}\}, \quad f_5 = \{\{O\}, \{H_4\}\}.$$

Then $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ is a 1-SuperHyperGraph.

Incidence graph. The incidence graph $\mathrm{Inc}(\mathbb{H})$ has bipartition $\mathbb{V} \sqcup \mathbb{E}$ and an edge $\{X, f_i\}$ whenever $X \in f_i$. Hence

$$|\mathrm{V}(\mathrm{Inc}(\mathbb{H}))| = |\mathbb{V}| + |\mathbb{E}| = 6 + 5 = 11, \qquad |\mathrm{E}(\mathrm{Inc}(\mathbb{H}))| = \sum_{i=1}^{5} |f_i| = 2 + 2 + 2 + 2 + 2 = 10.$$

Moreover, $\mathrm{Inc}(\mathbb{H})$ is connected (every f_i is incident to $\{C\}$ or $\{O\}$), so $|\mathrm{E}| = |\mathrm{V}| - 1$ implies that $\mathrm{Inc}(\mathbb{H})$ is a tree. Therefore $\mathbb{H}$ is a *SuperHyperTree*.

Maximum superdegree. The superdegrees are

$$d_{\mathbb{H}}(\{C\}) = 4, \qquad d_{\mathbb{H}}(\{O\}) = 2, \qquad d_{\mathbb{H}}(\{H_i\}) = 1 \ (i = 1, 2, 3, 4),$$

so

$$\Delta(\mathbb{H}) = \max_{X \in \mathbb{V}} d_{\mathbb{H}}(X) = 4 \leq 4.$$

Hence $\mathbb{H}$ is a *chemical SuperHyperTree*.

3.3 Chemical Reaction SuperHyperGraph

Chemical Reaction Graph is a directed graph where vertices are molecules and edges represent reactant-to-product transformations induced by each chemical reaction [71, 72]. Chemical Reaction SuperHyperGraph is a hierarchical directed structure using iterated powersets; nodes are nested molecule-sets, and edges encode reactions between higher-order reactant/product supervertices.

Definition 3.3.1 (Chemical Reaction HyperGraph)**.** [71–73] Let V_1 be a finite set of *molecule-nodes* (each node represents one molecule, reactant or product). A *Chemical Reaction HyperGraph* is a directed hypergraph

$$\mathcal{R} = (V_1, E_D),$$

where

$$E_D \subseteq \big(\mathcal{P}(V_1) \setminus \{\emptyset\}\big) \times \big(\mathcal{P}(V_1) \setminus \{\emptyset\}\big).$$

Each element $(R, P) \in E_D$, usually written $R \to P$, is called a *reaction hyperedge*, where $R \subseteq V_1$ is the nonempty reactant set and $P \subseteq V_1$ is the nonempty product set.

Definition 3.3.2 (Directed cycle in a reaction hypergraph)**.** Let $\mathcal{R} = (V_1, E_D)$ be a Chemical Reaction HyperGraph. A *directed cycle* is a sequence

$$v_0, (R_1 \to P_1), v_1, (R_2 \to P_2), \ldots, (R_k \to P_k), v_k$$

with $k \geq 1$, $v_0 = v_k$, $v_i \in V_1$, and $(R_i \to P_i) \in E_D$ such that

$$v_{i-1} \in R_i \quad \text{and} \quad v_i \in P_i \qquad (i = 1, \ldots, k).$$

We call $\mathcal{R}$ *acyclic* if it has no directed cycle.

Definition 3.3.3 (Chemical Reaction Graph (graph projection of a reaction hypergraph))**.** Let $\mathcal{R} = (V_1, E_D)$ be a Chemical Reaction HyperGraph. The *Chemical Reaction Graph* induced by $\mathcal{R}$ is the directed (simple) graph

$$G(\mathcal{R}) \;=\; (V_1, A),$$

whose arc set $A \subseteq V_1 \times V_1$ is defined by

$$(u, v) \in A \quad \Longleftrightarrow \quad \exists\, (R \to P) \in E_D \text{ such that } u \in R,\ v \in P,\ u \neq v.$$

Thus each reaction hyperedge $R \to P$ induces all arcs from every reactant $u \in R$ to every product $v \in P$.

Remark 3.3.4 (Singleton reactions recover a directed graph)**.** If every reaction hyperedge satisfies $|R| = |P| = 1$, then $\mathcal{R}$ is essentially a directed graph on V_1, and $G(\mathcal{R})$ is that directed graph.

Definition 3.3.5 (Chemical Reaction SuperHyperGraph)**.** Let V_1 be the finite set of molecule-nodes and fix an integer $n \geq 1$. A *Chemical Reaction SuperHyperGraph of level* n is a directed n-superhypergraph

$$\mathrm{CRSH}(n) \;=\; \big(V^{(n)}, E_R^{(n)}\big),$$

where

$$V^{(n)} := \mathcal{P}^n(V_1), \qquad E_R^{(n)} \;\subseteq\; V^{(n)} \times V^{(n)}.$$

Each $(R', P') \in E_R^{(n)}$ is called an *n-superreaction*, encoding a transformation from the n-supervertex R' (reactants) to the n-supervertex P' (products).

Remark 3.3.6 (Canonical embedding of reaction hypergraphs into reaction superhypergraphs)**.** Define the nesting map $\iota_n : \mathcal{P}(V_1) \setminus \{\emptyset\} \to \mathcal{P}^n(V_1)$ recursively by

$$\iota_1(S) = S, \qquad \iota_{k+1}(S) = \{\iota_k(S)\} \quad (k \geq 1).$$

Then each reaction hyperedge $(R \to P) \in E_D$ can be lifted to the n-superreaction

$$\big(\iota_n(R),\ \iota_n(P)\big) \in V^{(n)} \times V^{(n)},$$

so a Chemical Reaction HyperGraph embeds naturally as a directed sub-superhypergraph of $\mathrm{CRSH}(n)$.

Example 3.3.7 (A level-2 Chemical Reaction SuperHyperGraph)**.** Consider the reaction

$$H_2 + Cl_2 \longrightarrow 2\,HCl.$$

Let the molecule-node set be

$$V_1 = \{H_2, Cl_2, HCl\}.$$

Fix $n = 2$. Then

$$V^{(2)} = \mathcal{P}^2(V_1) = \mathcal{P}(\mathcal{P}(V_1)).$$

Define the (level-2) superreactant and superproduct nodes by

$$R' := \big\{\{H_2\}, \{Cl_2\}\big\} \in \mathcal{P}(\mathcal{P}(V_1)), \qquad P' := \big\{\{HCl\}\big\} \in \mathcal{P}(\mathcal{P}(V_1)).$$

(Here R' encodes the set of two reactant species, while P' encodes the product species; multiplicity "2" can be recorded separately if desired, e.g. as a stoichiometric weight on the superreaction.)

Let the directed superreaction set be

$$E_R^{(2)} = \{(R', P')\} \subseteq V^{(2)} \times V^{(2)}.$$

Then

$$\mathrm{CRSH}(2) = \big(V^{(2)}, E_R^{(2)}\big)$$

is a level-2 Chemical Reaction SuperHyperGraph in the sense of Definition 3.3.5, with a single 2-superreaction (R', P') representing $H_2 + Cl_2 \to 2\,HCl$.

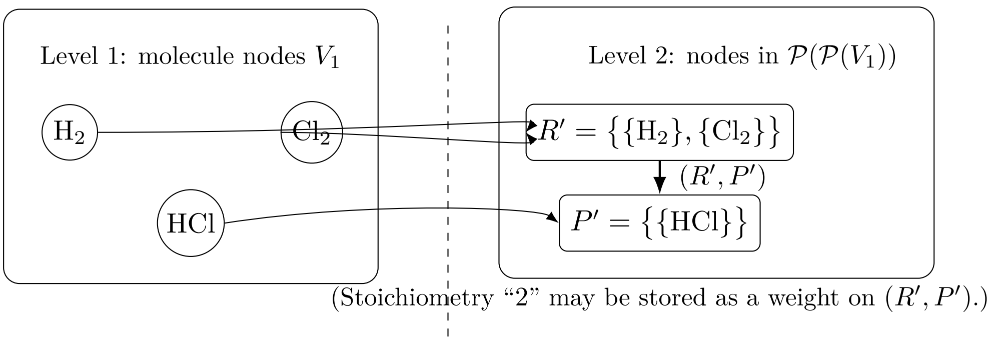

Figure 3.2: A level-2 Chemical Reaction SuperHyperGraph $\mathrm{CRSH}(2) = (V^{(2)}, E_R^{(2)})$ for $H_2 + Cl_2 \to 2\,HCl$, represented by a single directed 2-superreaction (R', P').

Chapter 4

Topological Indices in SuperHyperGraphs

A topological index is a numerical invariant derived from a graph's structure, summarizing connectivity, degrees, or distances in order to compare systems quantitatively. In this chapter, we introduce a range of concepts related to topological indices in SuperHyperGraphs. At present, substantial room remains for further mathematical analysis in this area. We hope that this chapter will serve as an encyclopedic reference for researchers and practitioners.

4.1 Sombor Index and Related Concepts

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 [74–76]. Subsequent work has investigated numerous extensions and applications, including chemical graphs [77, 78], fuzzy graphs [40, 79], and neutrosophic graphs [41, 80]. Several related degree-based indices are also widely studied, such as modified Sombor indices [81–83], Zagreb-type indices [46, 84–87], and the ABC and GA indices [42, 43, 88, 89].

4.1.1 Sombor Index of SuperHyperGraphs

For hypergraphs, one natural generalization aggregates squared vertex degrees inside each hyperedge and then sums the resulting Euclidean norms over all hyperedges [90]. 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 4.1.1 (Sombor index of a hypergraph)**.** [90] 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 4.1.2 (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

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

Definition 4.1.3 (Sombor index of an n-SuperHyperGraph)**.** [1,4] Let $\mathrm{SHG}^{(n)} = (V, E)$ be an n-SuperHyperGraph and let $d_{\mathrm{SHG}^{(n)}}(\cdot)$ be as in Definition 4.1.2. The *Sombor index* of $\mathrm{SHG}^{(n)}$ is defined by

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

Remark 4.1.4. 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 4.1.3 coincides with Definition 4.1.1.

Example 4.1.5 (Sombor index of a 1-SuperHyperGraph)**.** Let $V_0 = \{1, 2, 3\}$ and consider the 1-SuperHyperGraph $\mathrm{SHG}^{(1)} = (V, E)$ defined by

$$V = \bigl\{\{1\}, \{2\}, \{3\}, \{1, 2\}\bigr\} \subseteq \mathcal{P}(V_0), \qquad E = \{e_1, e_2\},$$

where

$$e_1 = \bigl\{\{1\}, \{2\}, \{1, 2\}\bigr\}, \qquad e_2 = \bigl\{\{2\}, \{3\}\bigr\}.$$

The (super)degrees are

$$d(\{1\}) = 1, \qquad d(\{2\}) = 2, \qquad d(\{3\}) = 1, \qquad d(\{1, 2\}) = 1,$$

because $\{2\}$ belongs to both e_1 and e_2, while the other supervertices belong to exactly one superedge.

Contribution of e_1.

$$\sqrt{\sum_{x \in e_1} d(x)^2} = \sqrt{d(\{1\})^2 + d(\{2\})^2 + d(\{1, 2\})^2} = \sqrt{1^2 + 2^2 + 1^2} = \sqrt{6}.$$

Contribution of e_2.

$$\sqrt{\sum_{x \in e_2} d(x)^2} = \sqrt{d(\{2\})^2 + d(\{3\})^2} = \sqrt{2^2 + 1^2} = \sqrt{5}.$$

Therefore, by Definition 4.1.3,

$$SO\bigl(\mathrm{SHG}^{(1)}\bigr) = \sqrt{6} + \sqrt{5}.$$

4.1.2 Shifted (general) Sombor index

Shifted (general) Sombor index sums, over edges, the Euclidean norm of endpoint degree-pairs after shifting each degree by a.

Definition 4.1.6 (Shifted (general) Sombor index)**.** For a real parameter $a \in \mathbb{R}$, the *shifted (general) Sombor index* is

$$\mathrm{SO}_a(G) \;:=\; \sum_{uv \in E(G)} \sqrt{(d(u)-a)^2 + (d(v)-a)^2}.$$

Remark 4.1.7 (Geometric interpretation)**.** For each edge $uv \in E(G)$, the quantity

$$\sqrt{(d(u)-a)^2 + (d(v)-a)^2} \;=\; \big\|(d(u), d(v)) - (a,a)\big\|_2$$

is the Euclidean distance from $(d(u), d(v))$ to the reference point (a, a) in $\mathbb{R}^2$. Hence $\mathrm{SO}_a(G)$ aggregates such distances over all edges.

Proposition 4.1.8 (Standard specializations)**.** *The following identities hold:*

$$\mathrm{SO}_0(G) = \mathrm{SO}(G), \qquad \mathrm{SO}_1(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$

and

$$\mathrm{SO}_{\bar{d}}(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-\bar{d})^2 + (d(v)-\bar{d})^2}.$$

Proof. These are immediate from Definition 4.1.6 by substituting $a = 0$, $a = 1$, and $a = \bar{d}$, respectively. □

Definition 4.1.9 (Shifted (general) Sombor index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. For a real parameter $a \in \mathbb{R}$, the *shifted (general) Sombor index* of H is defined by

$$\mathrm{SO}_a(H) \;:=\; \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \sqrt{(d_H(u)-a)^2 + (d_H(v)-a)^2}\,,$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.1.10 (Shifted (general) Sombor index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. For a real parameter $a \in \mathbb{R}$, the *shifted (general) Sombor index* of $\mathbb{H}$ is defined by

$$\mathrm{SO}_a(\mathbb{H}) \;:=\; \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \sqrt{(d_{\mathbb{H}}(A)-a)^2 + (d_{\mathbb{H}}(B)-a)^2}\,,$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.1.11 (Shifted Sombor index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{\, f_1, f_2 \,\}, \qquad f_1 = \{A, B\}, \quad f_2 = \{B, C\}.$$

Then the (super)degrees are

$$d_{\mathbb{H}}(A) = 1, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 1.$$

Fix the shift parameter $a = 1$. Since each superhyperedge has size 2, each inner sum has one term:

$$\mathrm{SO}_1(\mathbb{H}) = \sqrt{(d_{\mathbb{H}}(A) - 1)^2 + (d_{\mathbb{H}}(B) - 1)^2} + \sqrt{(d_{\mathbb{H}}(B) - 1)^2 + (d_{\mathbb{H}}(C) - 1)^2}.$$

Substituting the degrees yields

$$\mathrm{SO}_1(\mathbb{H}) = \sqrt{(1-1)^2 + (2-1)^2} + \sqrt{(2-1)^2 + (1-1)^2} = \sqrt{1} + \sqrt{1} = 2.$$

Theorem 4.1.12 (SuperHyperGraph shifted Sombor index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then for every $a \in \mathbb{R}$,*

$$\mathrm{SO}_a(\mathbb{G}) = \mathrm{SO}_a(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then for every $a \in \mathbb{R}$,*

$$\mathrm{SO}_a(\mathbb{H}_0) = \mathrm{SO}_a(H).$$

Consequently, Definition 4.1.10 strictly extends the shifted (general) Sombor indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.1.10 contains exactly one term per f, namely

$$\sqrt{(d_{\mathbb{G}}(u) - a)^2 + (d_{\mathbb{G}}(v) - a)^2}.$$

Since $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Thus each $f = \{u, v\}$ contributes $\sqrt{(d_G(u) - a)^2 + (d_G(v) - a)^2}$, which is exactly the contribution of the edge uv to $\mathrm{SO}_a(G)$. Summing over all edges yields $\mathrm{SO}_a(\mathbb{G}) = \mathrm{SO}_a(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Hence, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.1.10 coincides term-by-term with that in Definition 4.1.9. Summing over all $e \in \mathcal{E}$ yields $\mathrm{SO}_a(\mathbb{H}_0) = \mathrm{SO}_a(H)$. □

4.1.3 p-Sombor Index

The p-Sombor index sums over edges the L^p-norm of endpoint degree pairs: $\big(d(u)^p + d(v)^p\big)^{1/p}$ [74, 91, 92].

Definition 4.1.13 (p-Sombor index)**.** Let $p \in \mathbb{R} \setminus \{0\}$. The *$p$-Sombor index* of G is

$$\mathrm{SO}_p(G) \;:=\; \sum_{uv \in E(G)} \big(d(u)^p + d(v)^p\big)^{1/p}.$$

Remark 4.1.14 (Well-definedness for negative p)**.** If $p < 0$, then $d(u)^p$ and $d(v)^p$ require $d(u), d(v) > 0$. This holds automatically for endpoints of edges, since $uv \in E(G)$ implies $d(u) \geq 1$ and $d(v) \geq 1$.

Proposition 4.1.15 (Key special cases)**.** *Let G be a finite simple graph. Then:*

1. $\mathrm{SO}_2(G) = \mathrm{SO}(G)$.

2. $\mathrm{SO}_1(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big) = \sum_{v \in V(G)} d(v)^2$. *In particular,* $\mathrm{SO}_1(G)$ *coincides with the first Zagreb index* $M_1(G)$.

3. $\mathrm{SO}_{-1}(G) = \sum_{uv \in E(G)} \dfrac{d(u)d(v)}{d(u) + d(v)}$. *Consequently, the inverse sum indeg index*

$$\mathrm{ISI}(G) \;:=\; \sum_{uv \in E(G)} \frac{2d(u)d(v)}{d(u) + d(v)}$$

satisfies $\mathrm{ISI}(G) = 2\,\mathrm{SO}_{-1}(G)$.

Proof. (1) Substituting $p = 2$ into Definition 4.1.13 gives

$$\mathrm{SO}_2(G) = \sum_{uv \in E(G)} \big(d(u)^2 + d(v)^2\big)^{1/2} = \mathrm{SO}(G).$$

(2) For $p = 1$,

$$\mathrm{SO}_1(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big).$$

To show $\sum_{uv \in E}(d(u) + d(v)) = \sum_{v \in V} d(v)^2$, observe that each vertex v appears in exactly $d(v)$ edges, and in each incident edge it contributes $d(v)$ once. Hence the total contribution of v equals $d(v) \cdot d(v) = d(v)^2$.

(3) For $p = -1$, Definition 4.1.13 yields

$$\big(d(u)^{-1} + d(v)^{-1}\big)^{-1} = \left(\frac{d(u) + d(v)}{d(u)d(v)}\right)^{-1} = \frac{d(u)d(v)}{d(u) + d(v)},$$

and the displayed identity follows by summing over $E(G)$. The relation with $\mathrm{ISI}(G)$ is then immediate. □

Definition 4.1.16 (p-Sombor index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. Let $p \in \mathbb{R} \setminus \{0\}$. The *p-Sombor index* of H is defined by

$$\mathrm{SO}_p(H) \ := \sum_{e\in\mathcal{E}} \sum_{\substack{u,v\in e \\ u<v}} \big(d_H(u)^p + d_H(v)^p\big)^{1/p},$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.1.17 (p-Sombor index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. Let $p \in \mathbb{R} \setminus \{0\}$. The *p-Sombor index* of $\mathbb{H}$ is defined by

$$\mathrm{SO}_p(\mathbb{H}) \ := \sum_{f\in\mathbb{E}} \sum_{\substack{A,B\in f \\ A<B}} \big(d_{\mathbb{H}}(A)^p + d_{\mathbb{H}}(B)^p\big)^{1/p},$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.1.18 (A concrete computation of the p–Sombor index)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f_1, f_2\},$$

where

$$f_1 = \{A, B\}, \qquad f_2 = \{A, B, C\}.$$

Fix the total order $A < B < C$. Then the superdegrees are

$$d_{\mathbb{H}}(A) = 2, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 1,$$

because A and B belong to both f_1 and f_2, whereas C belongs only to f_2.

Take $p = 1$. Then each unordered pair $\{X, Y\}$ contributes

$$\big(d_{\mathbb{H}}(X)^1 + d_{\mathbb{H}}(Y)^1\big)^1 = d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y).$$

Contribution of f_1. The only pair in $f_1 = \{A, B\}$ is $\{A, B\}$, hence

$$\sum_{\substack{X,Y\in f_1 \\ X<Y}} \big(d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y)\big) = d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B) = 2 + 2 = 4.$$

Contribution of f_2. The unordered pairs in $f_2 = \{A, B, C\}$ are $\{A, B\}, \{A, C\}, \{B, C\}$. Thus

$$\sum_{\substack{X,Y\in f_2 \\ X<Y}} \big(d_{\mathbb{H}}(X)+d_{\mathbb{H}}(Y)\big) = (d_{\mathbb{H}}(A)+d_{\mathbb{H}}(B))+(d_{\mathbb{H}}(A)+d_{\mathbb{H}}(C))+(d_{\mathbb{H}}(B)+d_{\mathbb{H}}(C)) = (2+2)+(2+1)+(2+1) = 10.$$

Therefore,

$$\mathrm{SO}_1(\mathbb{H}) = 4 + 10 = 14.$$

Same superhypergraph with $p = 2$ (classical Sombor-type). If $p = 2$, then the pair contribution becomes $\sqrt{d_{\mathbb{H}}(X)^2 + d_{\mathbb{H}}(Y)^2}$, and one obtains

$$\mathrm{SO}_2(\mathbb{H}) = \underbrace{\sqrt{2^2 + 2^2}}_{f_1:\{A,B\}} + \underbrace{\Big(\sqrt{2^2 + 2^2} + \sqrt{2^2 + 1^2} + \sqrt{2^2 + 1^2}\Big)}_{f_2:\{A,B\},\{A,C\},\{B,C\}} = 2\sqrt{2} + \sqrt{8} + 2\sqrt{5} = 4\sqrt{2} + 2\sqrt{5}.$$

Theorem 4.1.19 (SuperHyperGraph p-Sombor index generalizes the graph and hypergraph cases)**.** *Let $p \in \mathbb{R} \setminus \{0\}$. Then:*

1. *If $G = (V, E)$ is a finite simple undirected graph and $\mathbb{G} := (V, E)$ is the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges), then*

$$\mathrm{SO}_p(\mathbb{G}) = \mathrm{SO}_p(G).$$

2. *If $H = (V, \mathcal{E})$ is a finite hypergraph and $\mathbb{H}_0 := (V, \mathcal{E})$ is the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges), then*

$$\mathrm{SO}_p(\mathbb{H}_0) = \mathrm{SO}_p(H).$$

Consequently, Definition 4.1.17 strictly extends the p-Sombor indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.1.17 contains exactly one term per f, namely

$$\big(d_{\mathbb{G}}(u)^p + d_{\mathbb{G}}(v)^p\big)^{1/p}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Thus the contribution of f equals $(d_G(u)^p + d_G(v)^p)^{1/p}$, which is precisely the contribution of the edge uv to $\mathrm{SO}_p(G)$. Summing over all $f \in E$ yields $\mathrm{SO}_p(\mathbb{G}) = \mathrm{SO}_p(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Hence, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.1.17 coincides term-by-term with that in Definition 4.1.16. Summing over all $e \in \mathcal{E}$ yields $\mathrm{SO}_p(\mathbb{H}_0) = \mathrm{SO}_p(H)$. □

4.1.4 Unified View: Sombor-type and (a, p)-Sombor

The (a, p)-Sombor index sums over edges the L^p-norm of shifted degrees: $\big(|d(u) - a|^p + |d(v) - a|^p\big)^{1/p}$.

Definition 4.1.20 (Sombor-type degree descriptor)**.** Let $F : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ be a symmetric function, i.e., $F(x, y) = F(y, x)$. The associated *Sombor-type degree index* is

$$\mathrm{TI}_F(G) := \sum_{uv \in E(G)} F\big(d(u), d(v)\big).$$

Remark 4.1.21. Many degree-based topological indices can be written in the Sombor-type form TI_F for a suitable choice of F. For instance,

$$F(x,y)=\sqrt{x^2+y^2} \quad\Rightarrow\quad \mathrm{TI}_F(G)=\mathrm{SO}(G),$$

and

$$F(x,y)=x+y \quad\Rightarrow\quad \mathrm{TI}_F(G)=\mathrm{SO}_1(G)=M_1(G).$$

Definition 4.1.22 ((a,p)-Sombor index)**.** Let $a\in\mathbb{R}$ and let $p\in\mathbb{R}\setminus\{0\}$. Define

$$\mathrm{SO}_{a,p}(G) \;:=\; \sum_{uv\in E(G)} \Big(\,|d(u)-a|^p+|d(v)-a|^p\Big)^{1/p}.$$

Proposition 4.1.23 (Containment of the main variants)**.** *Let G be a finite simple graph.*

1. $\mathrm{SO}_{0,2}(G)=\mathrm{SO}(G)$.

2. $\mathrm{SO}_{1,2}(G)=\mathrm{SO}_1(G)$ *(the shifted index with $a=1$).*

3. $\mathrm{SO}_{\bar d,2}(G)=\mathrm{SO}_{\bar d}(G)$ *(the shifted index with $a=\bar d$).*

4. $\mathrm{SO}_{0,p}(G)=\mathrm{SO}_p(G)$ *for every $p\neq 0$.*

Proof. Each identity is obtained by direct substitution into Definition 4.1.22. When $p=2$, the absolute values are immaterial because $(x-a)^2=|x-a|^2$. □

Definition 4.1.24 ((a,p)-Sombor index of a hypergraph)**.** Let $H=(V,\mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v\in V$. Let $a\in\mathbb{R}$ and $p\in\mathbb{R}\setminus\{0\}$. The (a,p)-*Sombor index* of H is defined by

$$\mathrm{SO}_{a,p}(H) \;:=\; \sum_{e\in\mathcal{E}} \sum_{\substack{u,v\in e\\ u<v}} \Big(\,|d_H(u)-a|^p+|d_H(v)-a|^p\Big)^{1/p},$$

where $u<v$ indicates that the inner sum ranges over unordered distinct pairs $\{u,v\}\subseteq e$.

Definition 4.1.25 ((a,p)-Sombor index of a SuperHyperGraph)**.** Let $\mathbb{H}=(\mathbb{V},\mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X\in\mathbb{V}$. Let $a\in\mathbb{R}$ and $p\in\mathbb{R}\setminus\{0\}$. The (a,p)-*Sombor index* of $\mathbb{H}$ is defined by

$$\mathrm{SO}_{a,p}(\mathbb{H}) \;:=\; \sum_{f\in\mathbb{E}} \sum_{\substack{A,B\in f\\ A<B}} \Big(\,|d_{\mathbb{H}}(A)-a|^p+|d_{\mathbb{H}}(B)-a|^p\Big)^{1/p},$$

where $A<B$ indicates that the inner sum ranges over unordered distinct pairs $\{A,B\}\subseteq f$.

Example 4.1.26 (A concrete computation of the (a,p)–Sombor index)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f_1, f_2\},$$

where

$$f_1 = \{A, B\}, \qquad f_2 = \{A, B, C\}.$$

Fix the total order $A < B < C$. Then the superdegrees are

$$d_{\mathbb{H}}(A) = 2, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 1,$$

because A and B belong to both f_1 and f_2, whereas C belongs only to f_2.

Choose parameters $a = 1$ and $p = 2$. Then for a pair $\{X, Y\}$ the summand becomes

$$\Big(|d_{\mathbb{H}}(X) - 1|^2 + |d_{\mathbb{H}}(Y) - 1|^2\Big)^{1/2}.$$

Contribution of f_1. The only unordered pair in $f_1 = \{A, B\}$ is $\{A, B\}$, so

$$\sum_{\substack{X,Y \in f_1 \\ X<Y}} \Big(|d_{\mathbb{H}}(X) - 1|^2 + |d_{\mathbb{H}}(Y) - 1|^2\Big)^{1/2} = \Big(|2-1|^2 + |2-1|^2\Big)^{1/2} = \sqrt{2}.$$

Contribution of f_2. The unordered pairs in $f_2 = \{A, B, C\}$ are $\{A, B\}, \{A, C\}, \{B, C\}$. Hence

$$\sum_{\substack{X,Y \in f_2 \\ X<Y}} \Big(|d_{\mathbb{H}}(X)-1|^2+|d_{\mathbb{H}}(Y)-1|^2\Big)^{1/2} = \sqrt{2}+\Big(|2-1|^2+|1-1|^2\Big)^{1/2}+\Big(|2-1|^2+|1-1|^2\Big)^{1/2} = \sqrt{2}+2.$$

Therefore,

$$\mathrm{SO}_{1,2}(\mathbb{H}) = \big(\sqrt{2}\big) + \big(\sqrt{2} + 2\big) = 2\sqrt{2} + 2 \approx 4.8284.$$

Same example with a different exponent. If we keep $a = 1$ but take $p = 1$, then each pair contributes

$$|d_{\mathbb{H}}(X) - 1| + |d_{\mathbb{H}}(Y) - 1|,$$

and the value becomes

$$\begin{aligned} \mathrm{SO}_{1,1}(\mathbb{H}) &= \underbrace{(|2-1| + |2-1|)}_{f_1:\{A,B\}} \\ &+ \underbrace{\big[(|2-1| + |2-1|) + (|2-1| + |1-1|) + (|2-1| + |1-1|)\big]}_{f_2:\{A,B\},\{A,C\},\{B,C\}} \\ &= 2 + (2 + 1 + 1) = 6. \end{aligned}$$

Theorem 4.1.27 (SuperHyperGraph (a,p)-Sombor index generalizes the graph and hypergraph cases)**.** *Let $a \in \mathbb{R}$ and $p \in \mathbb{R} \setminus \{0\}$. Then:*

1. *If $G = (V, E)$ is a finite simple undirected graph and $\mathbb{G} := (V, E)$ is the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges), then*

$$\mathrm{SO}_{a,p}(\mathbb{G}) = \mathrm{SO}_{a,p}(G).$$

2. *If $H = (V, \mathcal{E})$ is a finite hypergraph and $\mathbb{H}_0 := (V, \mathcal{E})$ is the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges), then*

$$\mathrm{SO}_{a,p}(\mathbb{H}_0) = \mathrm{SO}_{a,p}(H).$$

Consequently, Definition 4.1.25 strictly extends the (a, p)-Sombor indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.1.25 contains exactly one term per f, namely

$$\Big(|d_{\mathbb{G}}(u) - a|^p + |d_{\mathbb{G}}(v) - a|^p \Big)^{1/p}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Thus each $f = \{u, v\}$ contributes

$$\Big(|d_G(u) - a|^p + |d_G(v) - a|^p \Big)^{1/p},$$

which is precisely the contribution of the edge uv to $\mathrm{SO}_{a,p}(G)$. Summing over all $f \in E$ yields $\mathrm{SO}_{a,p}(\mathbb{G}) = \mathrm{SO}_{a,p}(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Hence, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.1.25 coincides term-by-term with that in Definition 4.1.24. Summing over all $e \in \mathcal{E}$ yields $\mathrm{SO}_{a,p}(\mathbb{H}_0) = \mathrm{SO}_{a,p}(H)$. □

4.1.5 Euler-Sombor and Cross-term Variants of a SuperHyperGraph

The Euler-Sombor index sums over edges $\sqrt{d(u)^2 + d(v)^2 + d(u)d(v)}$, combining degree norms with a cross-term [93–97].

Definition 4.1.28 (Euler-Sombor index)**.** The *Euler-Sombor index* of G is

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

Definition 4.1.29 (Parameterized cross-term Sombor index)**.** For a real parameter $\lambda \in \mathbb{R}$, define

$$\mathrm{EUS}_\lambda(G) := \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + \lambda\, d(u)d(v)}.$$

Definition 4.1.30 (Euler-Sombor index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. The *Euler-Sombor index* of H is defined by

$$\mathrm{EUS}(H) := \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \sqrt{d_H(u)^2 + d_H(v)^2 + d_H(u)d_H(v)}\,,$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.1.31 (Euler-Sombor index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. The *Euler-Sombor index* of $\mathbb{H}$ is defined by

$$\mathrm{EUS}(\mathbb{H}) := \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \sqrt{d_{\mathbb{H}}(A)^2 + d_{\mathbb{H}}(B)^2 + d_{\mathbb{H}}(A)d_{\mathbb{H}}(B)}\,,$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.1.32 (A concrete computation of the Euler–Sombor index)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f_1, f_2\},$$

where

$$f_1 = \{A, B\}, \qquad f_2 = \{A, B, C\}.$$

Fix the total order $A < B < C$. Then the superdegrees are

$$d_{\mathbb{H}}(A) = 2, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 1,$$

because A and B belong to both f_1 and f_2, while C belongs only to f_2.

By Definition 4.1.31, the contribution of f_1 is the single pair $\{A, B\}$:

$$\sum_{\substack{X,Y \in f_1 \\ X<Y}} \sqrt{d_{\mathbb{H}}(X)^2 + d_{\mathbb{H}}(Y)^2 + d_{\mathbb{H}}(X)d_{\mathbb{H}}(Y)} = \sqrt{2^2 + 2^2 + 2 \cdot 2} = \sqrt{12} = 2\sqrt{3}.$$

For f_2, the unordered pairs are $\{A, B\}, \{A, C\}, \{B, C\}$, hence

$$\sum_{\substack{X,Y \in f_2 \\ X<Y}} \sqrt{d_{\mathbb{H}}(X)^2 + d_{\mathbb{H}}(Y)^2 + d_{\mathbb{H}}(X)d_{\mathbb{H}}(Y)} = \sqrt{12} + \sqrt{2^2 + 1^2 + 2 \cdot 1} + \sqrt{2^2 + 1^2 + 2 \cdot 1} = 2\sqrt{3} + 2\sqrt{7}.$$

Therefore,

$$\mathrm{EUS}(\mathbb{H}) = (2\sqrt{3}) + (2\sqrt{3} + 2\sqrt{7}) = 4\sqrt{3} + 2\sqrt{7} \approx 12.2195.$$

Theorem 4.1.33 (SuperHyperGraph Euler-Sombor index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\mathrm{EUS}(\mathbb{G}) = \mathrm{EUS}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\mathrm{EUS}(\mathbb{H}_0) = \mathrm{EUS}(H).$$

Consequently, Definition 4.1.31 strictly extends the Euler-Sombor indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.1.31 contains exactly one term per f, namely

$$\sqrt{d_{\mathbb{G}}(u)^2 + d_{\mathbb{G}}(v)^2 + d_{\mathbb{G}}(u)d_{\mathbb{G}}(v)}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Hence the contribution of f equals

$$\sqrt{d_G(u)^2 + d_G(v)^2 + d_G(u)d_G(v)},$$

which is precisely the contribution of the edge uv to $\mathrm{EUS}(G)$. Summing over all $f \in E$ yields $\mathrm{EUS}(\mathbb{G}) = \mathrm{EUS}(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Thus, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.1.31 coincides term-by-term with the inner pair-sum in Definition 4.1.30. Summing over all $e \in \mathcal{E}$ yields $\mathrm{EUS}(\mathbb{H}_0) = \mathrm{EUS}(H)$. □

4.1.6 Complex Sombor Index of a SuperHyperGraph

The complex Sombor index sums, over edges, the principal square-root of squared complex degrees $(d + i\tau)$ of endpoints.

Definition 4.1.34 (Complex Sombor index)**.** Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of a vertex $v \in V$. Fix an auxiliary vertex attribute (a real-valued weight)

$$\tau : V \to \mathbb{R}_{\geq 0}.$$

Define the *complex degree* of v by

$$\delta_\tau(v) := d_G(v) + i\,\tau(v) \qquad (v \in V),$$

where $i^2 = -1$. The *complex Sombor index* of G (with respect to τ) is the complex number

$$\mathrm{CSO}_\tau(G) := \sum_{uv \in E} \sqrt{\delta_\tau(u)^2 + \delta_\tau(v)^2}\ ,$$

where $\sqrt{\cdot}$ denotes the principal branch of the complex square root.

Remark 4.1.35 (Canonical choice of τ)**.** A natural choice is $\tau(v) = \varepsilon_G(v)$ (vertex eccentricity), yielding a degree-eccentricity complexification:

$$\mathrm{CSO}_\varepsilon(G) \;=\; \sum_{uv\in E} \sqrt{\big(d_G(u) + i\varepsilon_G(u)\big)^2 + \big(d_G(v) + i\varepsilon_G(v)\big)^2}\,.$$

Proposition 4.1.36 (Reduction to the classical Sombor index)**.** *If $\tau \equiv 0$, then $\mathrm{CSO}_\tau(G)$ coincides with the classical Sombor index:*

$$\mathrm{CSO}_0(G) \;=\; \sum_{uv\in E} \sqrt{d_G(u)^2 + d_G(v)^2} \;=\; \mathrm{SO}(G).$$

Proof. If $\tau \equiv 0$, then $\delta_\tau(v) = d_G(v)$ is real and nonnegative for every $v \in V$. Hence, for each edge $uv \in E$,

$$\sqrt{\delta_\tau(u)^2 + \delta_\tau(v)^2} = \sqrt{d_G(u)^2 + d_G(v)^2},$$

and summing over all edges yields the claim. □

Definition 4.1.37 (Complex Sombor index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. Fix an auxiliary vertex attribute (a real-valued weight)

$$\tau :\; V \to \mathbb{R}_{\geq 0}.$$

Define the *complex degree* of $v \in V$ by

$$\delta_\tau(v) \;:=\; d_H(v) \;+\; i\,\tau(v) \qquad (v \in V),$$

where $i^2 = -1$. The *complex Sombor index* of H (with respect to τ) is the complex number

$$\mathrm{CSO}_\tau(H) \;:=\; \sum_{e\in\mathcal{E}} \sum_{\substack{u,v\in e\\ u<v}} \sqrt{\;\delta_\tau(u)^2 + \delta_\tau(v)^2\;}\;,$$

where $\sqrt{\cdot}$ denotes the principal branch of the complex square root and $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.1.38 (Complex Sombor index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. Fix an auxiliary supervertex attribute (a real-valued weight)

$$\tau :\; \mathbb{V} \to \mathbb{R}_{\geq 0}.$$

Define the *complex degree* of $X \in \mathbb{V}$ by

$$\delta_\tau(X) \;:=\; d_{\mathbb{H}}(X) \;+\; i\,\tau(X) \qquad (X \in \mathbb{V}),$$

where $i^2 = -1$. The *complex Sombor index* of $\mathbb{H}$ (with respect to τ) is the complex number

$$\mathrm{CSO}_\tau(\mathbb{H}) \;:=\; \sum_{f\in\mathbb{E}} \sum_{\substack{A,B\in f\\ A<B}} \sqrt{\;\delta_\tau(A)^2 + \delta_\tau(B)^2\;}\;,$$

where $\sqrt{\cdot}$ denotes the principal branch of the complex square root and $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.1.39 (A concrete computation of the complex Sombor index)**.** Let the SuperHyperGraph be

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f\}, \qquad f = \{A, B, C\}.$$

Fix the total order $A < B < C$. Since each supervertex belongs to exactly one superhyperedge,

$$d_{\mathbb{H}}(A) = d_{\mathbb{H}}(B) = d_{\mathbb{H}}(C) = 1.$$

Choose an auxiliary attribute $\tau : \mathbb{V} \to \mathbb{R}_{\geq 0}$ by

$$\tau(A) = 0, \qquad \tau(B) = 1, \qquad \tau(C) = 2.$$

Hence the complex degrees are

$$\delta_\tau(A) = 1, \qquad \delta_\tau(B) = 1 + i, \qquad \delta_\tau(C) = 1 + 2i,$$

and therefore

$$\delta_\tau(A)^2 = 1, \qquad \delta_\tau(B)^2 = (1+i)^2 = 2i, \qquad \delta_\tau(C)^2 = (1+2i)^2 = -3 + 4i.$$

Because $\mathbb{E} = \{f\}$ and $f = \{A, B, C\}$, Definition 4.1.38 gives

$$\mathrm{CSO}_\tau(\mathbb{H}) = \sum_{\substack{X,Y \in f \\ X<Y}} \sqrt{\delta_\tau(X)^2 + \delta_\tau(Y)^2} = \sqrt{1+2i} + \sqrt{-2+4i} + \sqrt{-3+6i},$$

where $\sqrt{\cdot}$ denotes the principal complex square root.

Using the standard principal-square-root formula

$$\sqrt{a+bi} = \sqrt{\frac{r+a}{2}} \; + \; i\,\mathrm{sgn}(b)\sqrt{\frac{r-a}{2}}, \qquad r = \sqrt{a^2+b^2},$$

we obtain the explicit closed forms

$$\sqrt{1+2i} = \sqrt{\frac{\sqrt{5}+1}{2}} \; + \; i\sqrt{\frac{\sqrt{5}-1}{2}},$$

$$\sqrt{-2+4i} = \sqrt{\sqrt{5}-1} \; + \; i\sqrt{\sqrt{5}+1},$$

$$\sqrt{-3+6i} = \sqrt{\frac{3(\sqrt{5}-1)}{2}} \; + \; i\sqrt{\frac{3(\sqrt{5}+1)}{2}}.$$

Hence

$$\mathrm{CSO}_\tau(\mathbb{H}) = \left(\sqrt{\frac{\sqrt{5}+1}{2}} + \sqrt{\sqrt{5}-1} + \sqrt{\frac{3(\sqrt{5}-1)}{2}}\right) + i\left(\sqrt{\frac{\sqrt{5}-1}{2}} + \sqrt{\sqrt{5}+1} + \sqrt{\frac{3(\sqrt{5}+1)}{2}}\right).$$

Numerically,

$$\mathrm{CSO}_\tau(\mathbb{H}) \approx (4.4136) + i(4.3378).$$

Theorem 4.1.40 (SuperHyperGraph complex Sombor index generalizes the graph and hypergraph cases)**.** *Fix τ on the relevant vertex/supervertex set.*

1. *Let $G = (V, E)$ be a finite simple undirected graph and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Identify $\tau : V \to \mathbb{R}_{\geq 0}$ with the same map on $\mathbb{V} = V$. Then*

$$\mathrm{CSO}_\tau(\mathbb{G}) = \mathrm{CSO}_\tau(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges). Identify $\tau : V \to \mathbb{R}_{\geq 0}$ with the same map on $\mathbb{V} = V$. Then*

$$\mathrm{CSO}_\tau(\mathbb{H}_0) = \mathrm{CSO}_\tau(H).$$

Consequently, Definition 4.1.38 strictly extends the complex Sombor indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ every superhyperedge has size 2, say $f = \{u, v\}$. Hence the inner sum in Definition 4.1.38 contains exactly one term per f, namely

$$\sqrt{\delta_\tau(u)^2 + \delta_\tau(v)^2}.$$

Moreover, because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$, and τ is the same function on V. Therefore $\delta_\tau(u) = d_G(u) + i\tau(u)$ and $\delta_\tau(v) = d_G(v) + i\tau(v)$ agree with the complex degrees used in the graph definition of $\mathrm{CSO}_\tau(G)$. Thus each $f = \{u, v\}$ contributes the same summand as the edge uv in $\mathrm{CSO}_\tau(G)$, and summing over all edges yields $\mathrm{CSO}_\tau(\mathbb{G}) = \mathrm{CSO}_\tau(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Also, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

With the same τ on V, we have $\delta_\tau(v) = d_H(v) + i\tau(v)$ in both settings. Hence, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.1.38 coincides term-by-term with that in Definition 4.1.37, and summing over all $e \in \mathcal{E}$ yields $\mathrm{CSO}_\tau(\mathbb{H}_0) = \mathrm{CSO}_\tau(H)$. □

4.2 Wiener Index of a SuperHyperGraph

The *Wiener index of a graph* is the sum of shortest-path distances $d(u, v)$ over all unordered vertex pairs $\{u, v\}$ [98–100]. Related notions are also well studied, including the Wiener index of chemical graphs [101–103], the Wiener index of fuzzy graphs [104–106], and the Wiener index of neutrosophic graphs [80, 107, 108].

4.2.1 Wiener index of a SuperHyperGraph

The *Wiener index of a superhypergraph* sums shortest distances between base vertices in the induced superhypergraph metric, extending graphs.

Let $G = (V(G), E(G))$ be a finite, simple, connected (undirected) graph. For $u, v \in V(G)$, let $d_G(u, v)$ denote the usual shortest-path distance (the minimum number of edges in a u-v path).

Definition 4.2.1 (Wiener index of a graph)**.** [98–100] The *Wiener index* of G is

$$W(G) \ := \sum_{\{u,v\}\subseteq V(G)} d_G(u, v) \ = \ \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} d_G(u, v).$$

We use the standard (Berge-type) notion of path and distance: a u-v path is an alternating sequence

$$(v_0, e_1, v_1, \dots, e_p, v_p)$$

with $v_0 = u$, $v_p = v$, all v_i distinct, all e_i distinct, and $v_{i-1}, v_i \in e_i$ for each i; its length is p. The distance $d_H(u, v)$ is the minimum length of a u-v path (and $d_H(u, u) = 0$). If every vertex pair is joined by a path, then H is connected.

Definition 4.2.2 (Wiener index of a hypergraph)**.** Let H be a finite connected hypergraph. Its *Wiener index* is

$$W(H) \ := \sum_{\{u,v\}\subseteq V(H)} d_H(u, v) \ = \ \frac{1}{2} \sum_{u\in V(H)} \sum_{v\in V(H)} d_H(u, v),$$

i.e., the sum of distances over all unordered vertex pairs.

To encode nested or hierarchical "vertices," we adopt a powerset-based universe. Let X be a nonempty finite base set and let $\mathcal{P}^0(X) := X$, $\mathcal{P}^{i+1}(X) := \mathcal{P}(\mathcal{P}^i(X))$. Fix an integer $r \geq 0$ and set

$$\mathcal{U}_r(X) \ := \ \bigcup_{i=0}^{r} (\mathcal{P}^i(X) \setminus \{\emptyset\}).$$

Definition 4.2.3 (Superpath, distance, and Wiener index of a superhypergraph)**.** Let $\mathbb{H}$ be a SuperHyperGraph. A *superpath* from A to B (with $A, B \in V(\mathbb{H})$) is an alternating sequence

$$(A_0, f_1, A_1, \dots, f_p, A_p)$$

where $A_0 = A$, $A_p = B$, the A_i are distinct supervertices, the f_i are distinct superhyperedges, and $A_{i-1}, A_i \in f_i$ for each i. Its length is p. If such a superpath exists for every pair of supervertices, we call $\mathbb{H}$ *connected.*

For connected $\mathbb{H}$, define the *distance* $d_{\mathbb{H}}(A, B)$ as the minimum length of an A-B superpath, and define the *Wiener index* by

$$W(\mathbb{H}) \ := \sum_{\{A,B\}\subseteq V(\mathbb{H})} d_{\mathbb{H}}(A, B) \ = \ \frac{1}{2} \sum_{A\in V(\mathbb{H})} \sum_{B\in V(\mathbb{H})} d_{\mathbb{H}}(A, B).$$

4.2.2 Hyper-Wiener index

The hyper-Wiener index is a distance-based topological index summing, over all unordered vertex pairs, half of $d + d^2$ [109–112].

Definition 4.2.4 (Hyper-Wiener index)**.** Let $G = (V, E)$ be a finite simple connected graph. For $u, v \in V$, let $d_G(u, v)$ denote the usual shortest-path distance between u and v. The Wiener index of G is

$$W(G) \;:=\; \sum_{\{u,v\}\subseteq V} d_G(u, v).$$

The *hyper-Wiener index* of G is defined by

$$WW(G) \;:=\; \frac{1}{2} \sum_{\{u,v\}\subseteq V} \Big(d_G(u, v) + d_G(u, v)^2\Big).$$

Equivalently,

$$WW(G) \;=\; \frac{1}{2}\,W(G) \;+\; \frac{1}{2} \sum_{\{u,v\}\subseteq V} d_G(u, v)^2.$$

Definition 4.2.5 (Hyper-Wiener index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $d_H(\cdot, \cdot)$ be the distance. The *hyper-Wiener index* of H is defined by

$$WW(H) \;:=\; \frac{1}{2} \sum_{\{u,v\}\subseteq V} \Big(d_H(u, v) + d_H(u, v)^2\Big).$$

Equivalently,

$$WW(H) \;=\; \frac{1}{4} \sum_{u\in V} \sum_{v\in V} \Big(d_H(u, v) + d_H(u, v)^2\Big),$$

since $d_H(u, u) = 0$ and the distance is symmetric.

Definition 4.2.6 ((Recall) Superpath and distance in a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph (in particular, $\mathbb{V}$ is a finite set of supervertices and $\mathbb{E} \subseteq \mathcal{P}(\mathbb{V}) \setminus \{\emptyset\}$ is a finite family of superhyperedges). A *superpath* of length $p \geq 1$ from A to B is an alternating sequence

$$(A_0,\; f_1,\; A_1,\; f_2,\; \ldots,\; f_p,\; A_p),$$

where $A_0 = A$, $A_p = B$, the supervertices $A_0, \ldots, A_p \in \mathbb{V}$ are pairwise distinct, the superhyperedges $f_1, \ldots, f_p \in \mathbb{E}$ are pairwise distinct, and $\{A_{i-1}, A_i\} \subseteq f_i$ for all $i = 1, \ldots, p$. If $A = B$, we take the length-0 superpath (A).

The *superdistance* $d_{\mathbb{H}}(A, B)$ is the minimum length of a superpath from A to B (and $d_{\mathbb{H}}(A, A) = 0$). We call $\mathbb{H}$ *connected* if $d_{\mathbb{H}}(A, B) < \infty$ for all $A, B \in \mathbb{V}$.

Definition 4.2.7 (Hyper-Wiener index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot, \cdot)$ be the superdistance from Definition 4.2.6. The *hyper-Wiener index* of $\mathbb{H}$ is defined by

$$WW(\mathbb{H}) \;:=\; \frac{1}{2} \sum_{\{A,B\}\subseteq \mathbb{V}} \Big(d_{\mathbb{H}}(A, B) + d_{\mathbb{H}}(A, B)^2\Big).$$

Equivalently,

$$WW(\mathbb{H}) \;=\; \frac{1}{4} \sum_{A\in \mathbb{V}} \sum_{B\in \mathbb{V}} \Big(d_{\mathbb{H}}(A, B) + d_{\mathbb{H}}(A, B)^2\Big).$$

Theorem 4.2.8 (SuperHyperGraph hyper-Wiener index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple connected graph and let*

$$\mathbb{G} \;:=\; (V,\; E)$$

be the SuperHyperGraph whose supervertex set is V and whose superhyperedge family is the set of 2-subsets $E \subseteq \binom{V}{2}$. Then for all $u, v \in V$,

$$d_{\mathbb{G}}(u, v) = d_G(u, v),$$

and consequently

$$WW(\mathbb{G}) = WW(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph and let*

$$\mathbb{H} \;:=\; (V,\; \mathcal{E})$$

be the SuperHyperGraph with the same vertex set and the same edge family (viewed as superhyperedges). Then for all $u, v \in V$,

$$d_{\mathbb{H}}(u, v) = d_H(u, v),$$

and consequently

$$WW(\mathbb{H}) = WW(H).$$

In particular, Definition 4.2.7 strictly extends both the classical hyper-Wiener index of graphs and the hyper-Wiener index of hypergraphs (Definition 4.2.5).

Proof. (1) In $\mathbb{G}$, a superpath from u to v is precisely an alternating sequence

$$(u = v_0,\; e_1,\; v_1,\; e_2, \ldots, e_p,\; v_p = v)$$

with $e_i = \{v_{i-1}, v_i\} \in E$ for each i, i.e., an ordinary (simple) graph path in G. Hence the minimum possible length over such sequences equals the usual shortest-path distance in G, so $d_{\mathbb{G}}(u, v) = d_G(u, v)$ for all $u, v \in V$. Substituting this equality into Definition 4.2.7 yields $WW(\mathbb{G}) = WW(G)$.

(2) In $\mathbb{H} = (V, \mathcal{E})$, a superpath is exactly a Berge path in the hypergraph H, because the incidence condition $\{x_{i-1}, x_i\} \subseteq e_i$ is identical in both settings. Therefore the minimum length of a u-v superpath equals the minimum length of a u-v Berge path, i.e., $d_{\mathbb{H}}(u, v) = d_H(u, v)$ for all $u, v \in V$. Again substituting into Definition 4.2.7 gives $WW(\mathbb{H}) = WW(H)$. □

4.2.3 Steiner Wiener index of Graph

The Steiner k-Wiener index sums, over all k-vertex subsets, the minimum size of a connected subgraph spanning them [99, 113–115].

Definition 4.2.9 (Steiner distance)**.** Let $G = (V, E)$ be a connected graph and let $S \subseteq V$ with $|S| \geq 2$. The *Steiner distance* of S in G is

$$d_G(S) \;:=\; \min\{\, |E(H)| :\; H \text{ is a connected subgraph of } G \text{ and } S \subseteq V(H)\,\}.$$

Equivalently,

$$d_G(S) \;=\; \min\{\, |E(T)| :\; T \text{ is a subtree of } G \text{ and } S \subseteq V(T)\,\}.$$

In particular, if $S = \{u, v\}$, then $d_G(\{u, v\}) = d_G(u, v)$ coincides with the usual shortest-path distance.

Definition 4.2.10 (k-th Steiner Wiener index)**.** Let $G = (V, E)$ be a connected graph of order n and let k be an integer with $2 \leq k \leq n$. The *k-th Steiner Wiener index* (also called the *Steiner k-Wiener index*) of G is

$$SW_k(G) \;:=\; \sum_{\substack{S \subseteq V \\ |S| = k}} d_G(S).$$

For $k = 2$, one has $SW_2(G) = \sum_{\{u,v\} \subseteq V} d_G(u, v) = W(G)$, i.e., it reduces to the ordinary Wiener index.

Definition 4.2.11 (Steiner distance in a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $S \subseteq V$ with $|S| \geq 2$. For any nonempty $F \subseteq \mathcal{E}$, write

$$V(F) \;:=\; \bigcup_{e \in F} e, \qquad H[F] \;:=\; \bigl(V(F),\, F\bigr),$$

viewed as a subhypergraph of H. We say that $H[F]$ is *connected* if every pair of vertices in $V(F)$ is joined by a Berge path using only hyperedges from F (equivalently, the hypergraph distance in $H[F]$ is finite for all pairs).

The *Steiner distance* of S in H is

$$d_H(S) \;:=\; \min\bigl\{\, |F| :\; \emptyset \neq F \subseteq \mathcal{E},\; S \subseteq V(F),\; \text{and } H[F] \text{ is connected}\,\bigr\}.$$

Definition 4.2.12 (k-th Steiner Wiener index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph of order $n = |V|$, and let k be an integer with $2 \leq k \leq n$. The *k-th Steiner Wiener index* of H is

$$SW_k(H) \;:=\; \sum_{\substack{S \subseteq V \\ |S| = k}} d_H(S),$$

where $d_H(S)$ is the Steiner distance from Definition 4.2.11.

Definition 4.2.13 (Steiner distance in a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $\mathcal{S} \subseteq \mathbb{V}$ with $|\mathcal{S}| \geq 2$. For any nonempty $\mathbb{F} \subseteq \mathbb{E}$, write

$$\mathbb{V}(\mathbb{F}) := \bigcup_{f \in \mathbb{F}} f, \qquad \mathbb{H}[\mathbb{F}] := (\mathbb{V}(\mathbb{F}), \mathbb{F}),$$

viewed as a sub-SuperHyperGraph of $\mathbb{H}$. We say that $\mathbb{H}[\mathbb{F}]$ is *connected* if every pair of supervertices in $\mathbb{V}(\mathbb{F})$ is joined by a superpath using only superhyperedges from $\mathbb{F}$ (equivalently, the superdistance in $\mathbb{H}[\mathbb{F}]$ is finite for all pairs).

The *Steiner distance* of $\mathcal{S}$ in $\mathbb{H}$ is

$$d_{\mathbb{H}}(\mathcal{S}) := \min\{ |\mathbb{F}| : \emptyset \neq \mathbb{F} \subseteq \mathbb{E}, \ \mathcal{S} \subseteq \mathbb{V}(\mathbb{F}), \ \text{and } \mathbb{H}[\mathbb{F}] \text{ is connected} \}.$$

Definition 4.2.14 (k-th Steiner Wiener index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph of order $N = |\mathbb{V}|$, and let k be an integer with $2 \leq k \leq N$. The *k-th Steiner Wiener index* of $\mathbb{H}$ is

$$SW_k(\mathbb{H}) := \sum_{\substack{\mathcal{S} \subseteq \mathbb{V} \\ |\mathcal{S}| = k}} d_{\mathbb{H}}(\mathcal{S}),$$

where $d_{\mathbb{H}}(\mathcal{S})$ is as in Definition 4.2.13.

Theorem 4.2.15 (Steiner Wiener index of SuperHyperGraphs generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple connected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then for every $S \subseteq V$ with $|S| \geq 2$ one has*

$$d_{\mathbb{G}}(S) = d_G(S),$$

and hence for every k with $2 \leq k \leq |V|$,

$$SW_k(\mathbb{G}) = SW_k(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing the hyperedges as superhyperedges. Then for every $S \subseteq V$ with $|S| \geq 2$ one has*

$$d_{\mathbb{H}_0}(S) = d_H(S),$$

and hence for every k with $2 \leq k \leq |V|$,

$$SW_k(\mathbb{H}_0) = SW_k(H).$$

Consequently, Definition 4.2.14 strictly extends the Steiner Wiener indices of graphs and hypergraphs.

Proof. (1) Fix $S \subseteq V$ with $|S| \geq 2$. Any nonempty edge set $F \subseteq E$ determines a graph subgraph $G[F]$ and, simultaneously, a sub-SuperHyperGraph $\mathbb{G}[F]$ with the same edge set F and vertex set $V(F) = \bigcup_{e \in F} e$. Because each edge $e \in E$ is a 2-set, connectivity of $G[F]$ is equivalent to connectivity of $\mathbb{G}[F]$ (both are characterized by existence of usual paths/superpaths using edges in F). Moreover, $S \subseteq V(F)$ is the same condition in both settings. Therefore the minimization problems defining $d_G(S)$ (previously defined) and $d_{\mathbb{G}}(S)$ (Definition 4.2.13) range over the same family of feasible edge sets F and use the same objective $|F|$, so $d_{\mathbb{G}}(S) = d_G(S)$. Summing over all k-subsets S yields $SW_k(\mathbb{G}) = SW_k(G)$.

(2) Fix $S \subseteq V$ with $|S| \geq 2$ and consider any nonempty $\mathbb{F} \subseteq \mathcal{E}$. By construction, the sub-SuperHyperGraph $\mathbb{H}_0[\mathbb{F}]$ equals the subhypergraph $H[\mathbb{F}]$ as a set system: they have the same edge family $\mathbb{F}$ and the same vertex set $V(\mathbb{F}) = \bigcup_{e \in \mathbb{F}} e$. A Berge path in $H[\mathbb{F}]$ is exactly a superpath in $\mathbb{H}_0[\mathbb{F}]$ (the incidence condition $\{x_{i-1}, x_i\} \subseteq e_i$ is identical), hence $H[\mathbb{F}]$ is connected if and only if $\mathbb{H}_0[\mathbb{F}]$ is connected. Again, the feasibility condition $S \subseteq V(\mathbb{F})$ and the objective $|\mathbb{F}|$ coincide. Thus the minima defining $d_H(S)$ (Definition 4.2.11) and $d_{\mathbb{H}_0}(S)$ (Definition 4.2.13) are equal, i.e., $d_{\mathbb{H}_0}(S) = d_H(S)$. Summing over all k-subsets S yields $SW_k(\mathbb{H}_0) = SW_k(H)$. □

4.2.4 Complex Wiener index

The complex Wiener index sums complexified pairwise distances $d + i|\tau(u) - \tau(v)|$, combining shortest-path length with attribute-difference magnitude.

Definition 4.2.16 (Complex distance induced by a vertex attribute)**.** Let (X, d) be a finite set equipped with a symmetric distance function $d : X \times X \to \mathbb{R}_{\geq 0}$ with $d(x, x) = 0$. Fix a (real-valued) vertex attribute $\tau : X \to \mathbb{R}_{\geq 0}$. Define the *complex distance* by

$$d_\tau^{\mathbb{C}}(x, y) \;:=\; d(x, y) \;+\; i\,|\tau(x) - \tau(y)| \qquad (x, y \in X),$$

where $i^2 = -1$.

Definition 4.2.17 (Complex Wiener index of a graph)**.** Let $G = (V, E)$ be a finite connected graph with usual distance $d_G(\cdot, \cdot)$. Fix $\tau : V \to \mathbb{R}_{\geq 0}$ and define $d_\tau^{\mathbb{C}}$ on V by Definition 4.2.16 with $d = d_G$. The *complex Wiener index* of G (with respect to τ) is the complex number

$$\mathrm{CW}_\tau(G) \;:=\; \sum_{\{u,v\} \subseteq V} d_\tau^{\mathbb{C}}(u, v) \;=\; \sum_{\{u,v\} \subseteq V} \Big(d_G(u, v) + i\,|\tau(u) - \tau(v)| \Big).$$

Definition 4.2.18 (Complex Wiener index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph with the fixed hypergraph distance $d_H(\cdot, \cdot)$ (e.g., Berge-type). Fix $\tau : V \to \mathbb{R}_{\geq 0}$ and define $d_\tau^{\mathbb{C}}$ on V by Definition 4.2.16 with $d = d_H$. The *complex Wiener index* of H (with respect to τ) is

$$\mathrm{CW}_\tau(H) \;:=\; \sum_{\{u,v\} \subseteq V} d_\tau^{\mathbb{C}}(u, v) \;=\; \sum_{\{u,v\} \subseteq V} \Big(d_H(u, v) + i\,|\tau(u) - \tau(v)| \Big).$$

Definition 4.2.19 (Complex Wiener index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph with the fixed superdistance $d_{\mathbb{H}}(\cdot,\cdot)$ on $\mathbb{V}$. Fix $\tau : \mathbb{V} \to \mathbb{R}_{\geq 0}$ and define $d_\tau^{\mathbb{C}}$ on $\mathbb{V}$ by Definition 4.2.16 with $d = d_{\mathbb{H}}$. The *complex Wiener index* of $\mathbb{H}$ (with respect to τ) is

$$\mathrm{CW}_\tau(\mathbb{H}) \;:=\; \sum_{\{A,B\}\subseteq\mathbb{V}} d_\tau^{\mathbb{C}}(A,B) \;=\; \sum_{\{A,B\}\subseteq\mathbb{V}} \Big(d_{\mathbb{H}}(A,B) + i\,|\tau(A)-\tau(B)|\Big).$$

Proposition 4.2.20 (Reduction to the classical Wiener index)**.** *If τ is constant (in particular, if $\tau \equiv 0$), then the complex Wiener index reduces to the usual Wiener index:*

$$\mathrm{CW}_\tau(G) = W(G), \qquad \mathrm{CW}_\tau(H) = W(H), \qquad \mathrm{CW}_\tau(\mathbb{H}) = W(\mathbb{H}).$$

Proof. If τ is constant, then $|\tau(x)-\tau(y)| = 0$ for all x, y. Hence $d_\tau^{\mathbb{C}}(x,y) = d(x,y)$ in each setting, and summing over unordered pairs yields the corresponding Wiener index. □

4.3 Hosoya index of a SuperHyperGraph

The *Hosoya index of a graph* counts all matchings in G, i.e., independent edge-sets, including the empty matching [116–119]. Related notions such as the Hosoya index of a chemical graph are also known [120]. The *Hosoya index of a superhypergraph* counts all pairwise disjoint superhyperedges, generalizing graph matchings and hence Hosoya index.

Definition 4.3.1 (Matching in a graph)**.** (cf. [121]) Let $G = (V, E)$ be a finite (simple, undirected) graph. A *matching* in G is a subset $M \subseteq E$ such that no two distinct edges in M share a common endpoint. For $s \in \mathbb{Z}_{\geq 0}$, an *s-matching* is a matching M with $|M| = s$. We write $m(G; s)$ for the number of s-matchings of G, and adopt the convention $m(G; 0) = 1$ (the empty matching).

Definition 4.3.2 (Hosoya index of a graph)**.** [116–119] Let G be a finite graph. The *Hosoya index* of G, denoted by $Z(G)$ (or $z(G)$), is defined as the total number of matchings in G:

$$Z(G) \;:=\; \sum_{s=0}^{\lfloor |V(G)|/2 \rfloor} m(G; s).$$

Equivalently, $Z(G)$ counts all subsets of $E(G)$ whose edges are pairwise vertex-disjoint (including the empty set).

Definition 4.3.3 (Iterated powerset universe)**.** Let V be a nonempty finite set (the *base-vertex* set). Define recursively

$$\mathcal{P}^{(0)}(V) := V, \qquad \mathcal{P}^{(k+1)}(V) := \mathcal{P}(\mathcal{P}^{(k)}(V)) \setminus \{\emptyset\} \quad (k \geq 0),$$

where $\mathcal{P}(\cdot)$ is the usual powerset. Elements of $\mathcal{P}^{(k)}(V)$ may be viewed as *objects of depth k* built from V.

Definition 4.3.4 (Finite SuperHyperGraph). A *(finite) SuperHyperGraph* is a pair $\mathbb{S} = (V, \mathcal{E})$ where V is a finite base-vertex set and $\mathcal{E}$ is a finite set of *superhyperedges* such that there exists $L \geq 1$ with

$$\mathcal{E} \subseteq \bigcup_{k=1}^{L} \mathcal{P}^{(k)}(V).$$

Thus each $E \in \mathcal{E}$ is a nonempty nested set-object ultimately constructed from elements of V.

Definition 4.3.5 (Base-support (flattening) map). Define supp : $\bigcup_{k\geq 0} \mathcal{P}^{(k)}(V) \to \mathcal{P}(V)$ recursively by

$$\mathrm{supp}(v) := \{v\} \quad (v \in V), \qquad \mathrm{supp}(X) := \bigcup_{x \in X} \mathrm{supp}(x) \quad (X \in \mathcal{P}^{(k)}(V),\ k \geq 1).$$

For a superhyperedge $E \in \mathcal{E}$, the set $\mathrm{supp}(E) \subseteq V$ is the collection of base-vertices that occur in E after fully "flattening" the nested structure.

Definition 4.3.6 (Supermatching). Let $\mathbb{S} = (V, \mathcal{E})$ be a SuperHyperGraph. A *supermatching* is a subset $M \subseteq \mathcal{E}$ such that for any two distinct $E, F \in M$ one has

$$\mathrm{supp}(E) \cap \mathrm{supp}(F) = \emptyset.$$

For $s \in \mathbb{Z}_{\geq 0}$, an *s-supermatching* is a supermatching M with $|M| = s$. Let $m(\mathbb{S}; s)$ denote the number of s-supermatchings of $\mathbb{S}$, and set $m(\mathbb{S}; 0) = 1$.

Definition 4.3.7 (Hosoya index of a SuperHyperGraph). Let $\mathbb{S} = (V, \mathcal{E})$ be a finite SuperHyperGraph. Its *Hosoya index* is the total number of supermatchings:

$$Z(\mathbb{S}) := \sum_{s=0}^{|\mathcal{E}|} m(\mathbb{S}; s).$$

4.4 Randić index of a SuperHyperGraph

The *Randić index of a graph* is $R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$, measuring branching via inverse degree products [31,45,122,123]. The *Randić index of a superhypergraph* sums analogous inverse square-roots of endpoint superdegrees over superhyperedges, extending $R(G)$ consistently.

Definition 4.4.1 (General Randić index of a graph). [31, 45, 122, 123] Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of $v \in V$. For a real parameter $\alpha \in \mathbb{R}$, the *general Randić index* of G is

$$R_\alpha(G) := \sum_{uv \in E} \big(d_G(u)\, d_G(v)\big)^{\alpha}.$$

The classical *Randić (connectivity) index* is the special case

$$R(G) := R_{-1/2}(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_G(u)\, d_G(v)}}.$$

Definition 4.4.2 ((Recall) r-SuperHyperGraph, incidence, and degree)**.** An *r-SuperHyperGraph* is a pair $\mathbb{S} = (V, \mathcal{E})$ where V is a finite base vertex set and $\mathcal{E} \subseteq \mathcal{P}^r(V)$ is a finite family of *superhyperedges.* A base vertex $v \in V$ is *incident* with a superhyperedge $E \in \mathcal{E}$ if $v \in \mathrm{Flat}_r(E)$.

The (base) degree of $v \in V$ in $\mathbb{S}$ is

$$d_{\mathbb{S}}(v) \;:=\; \bigl|\{E \in \mathcal{E} : v \in \mathrm{Flat}_r(E)\}\bigr|.$$

Definition 4.4.3 (General Randić index of a SuperHyperGraph)**.** Let $\mathbb{S} = (V, \mathcal{E})$ be an r-SuperHyperGraph and let $\alpha \in \mathbb{R}$. The *general Randić index* of $\mathbb{S}$ is defined by

$$R_\alpha(\mathbb{S}) \;:=\; \sum_{E \in \mathcal{E}} \; \sum_{\{u,v\} \subseteq \mathrm{Flat}_r(E)} \bigl(d_{\mathbb{S}}(u)\, d_{\mathbb{S}}(v)\bigr)^{\alpha},$$

where the inner sum ranges over all unordered *distinct* pairs $\{u, v\}$ contained in $\mathrm{Flat}_r(E)$. The *Randić index* of $\mathbb{S}$ is $R(\mathbb{S}) := R_{-1/2}(\mathbb{S})$.

4.5 Zagreb indices of a SuperHyperGraph

The *Zagreb indices of a graph* are $M_1(G) = \sum_{v \in V(G)} d(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ [124–128]. Related notions such as hyper-Zagreb indices [46, 47, 129], Zagreb indices in fuzzy graphs [130, 131], Zagreb indices in Chemical graphs [132–135], and Zagreb indices in neutrosophic graphs [136, 137] are also known.

4.5.1 Zagreb indices of a superhypergraph

The *Zagreb indices of a superhypergraph* analogously sum squared superdegrees and products over superhyperedges using an appropriate incidence-based degree notion.

Definition 4.5.1 (First and second Zagreb indices of a graph)**.** [124–126] Let $G = (V(G), E(G))$ be a (simple) graph. For each $v \in V(G)$, let $d_G(v)$ denote the degree of v. The *first Zagreb index* and *second Zagreb index* of G are defined by

$$M_1(G) \;:=\; \sum_{v \in V(G)} d_G(v)^2, \qquad M_2(G) \;:=\; \sum_{\{u,v\} \in E(G)} d_G(u)\, d_G(v).$$

Definition 4.5.2 (Degree and pair-incidence multiplicity)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a SuperHyperGraph. For $X \in \mathbb{V}$, define the *degree* of X by

$$d_{\mathbb{H}}(X) \;:=\; \bigl|\{\, e \in \mathbb{E} : X \in e \,\}\bigr|.$$

For distinct $X, Y \in \mathbb{V}$, define the *pair-incidence multiplicity* by

$$\mu_{\mathbb{H}}(X, Y) \;:=\; \bigl|\{\, e \in \mathbb{E} : \{X, Y\} \subseteq e \,\}\bigr|.$$

(Thus, $\mu_{\mathbb{H}}(X, Y) \geq 1$ exactly when X and Y co-occur in at least one superhyperedge.)

Definition 4.5.3 (First and second Zagreb indices of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a SuperHyperGraph. Define

$$M_1(\mathbb{H}) := \sum_{X \in \mathbb{V}} d_{\mathbb{H}}(X)^2, \qquad M_2(\mathbb{H}) := \sum_{\{X,Y\} \subseteq \mathbb{V}} \mu_{\mathbb{H}}(X,Y)\, d_{\mathbb{H}}(X)\, d_{\mathbb{H}}(Y),$$

where the second sum ranges over all 2-element subsets $\{X, Y\}$ of $\mathbb{V}$.

Remark 4.5.4. If $\mathbb{H}$ has the property that each unordered pair $\{X, Y\}$ is contained in *at most one* superhyperedge, then $\mu_{\mathbb{H}}(X, Y) \in \{0, 1\}$ and

$$M_2(\mathbb{H}) = \sum_{\substack{\{X,Y\} \subseteq \mathbb{V} \\ \mu_{\mathbb{H}}(X,Y)=1}} d_{\mathbb{H}}(X)\, d_{\mathbb{H}}(Y),$$

i.e., the sum runs over adjacent pairs.

4.5.2 Hyper-Zagreb indices

Hyper-Zagreb indices are degree-based measures summing, over edges, squared degree sums (HM1) and squared degree products (HM2) [46, 47, 138–141].

Definition 4.5.5 (Hyper-Zagreb indices)**.** Let $G = (V(G), E(G))$ be a finite simple connected graph, and let $d_G(v)$ denote the (usual) degree of $v \in V(G)$.

First hyper-Zagreb index. The *first hyper-Zagreb index* of G is

$$\mathrm{HM}_1(G) := \sum_{uv \in E(G)} \big(d_G(u) + d_G(v)\big)^2.$$

Second hyper-Zagreb index (vertex-degree product convention). The *second hyper-Zagreb index* of G (in the vertex-degree product convention) is

$$\mathrm{HM}_2(G) := \sum_{uv \in E(G)} \big(d_G(u)\, d_G(v)\big)^2.$$

Definition 4.5.6 (Hyper-Zagreb indices of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. The *first hyper-Zagreb index* of H is defined by

$$\mathrm{HM}_1(H) := \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \big(d_H(u) + d_H(v)\big)^2,$$

and the *second hyper-Zagreb index* (vertex-degree product convention) is defined by

$$\mathrm{HM}_2(H) := \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \big(d_H(u)\, d_H(v)\big)^2,$$

where $u < v$ indicates that each inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.5.7 (Hyper-Zagreb indices of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. The *first hyper-Zagreb index* of $\mathbb{H}$ is defined by

$$\mathrm{HM}_1(\mathbb{H}) := \sum_{f\in\mathbb{E}} \sum_{\substack{A,B\in f\\ A<B}} \big(d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B)\big)^2,$$

and the *second hyper-Zagreb index* (vertex-degree product convention) is defined by

$$\mathrm{HM}_2(\mathbb{H}) := \sum_{f\in\mathbb{E}} \sum_{\substack{A,B\in f\\ A<B}} \big(d_{\mathbb{H}}(A)\, d_{\mathbb{H}}(B)\big)^2,$$

where $A < B$ indicates that each inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Theorem 4.5.8 (SuperHyperGraph hyper-Zagreb indices generalize the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\mathrm{HM}_1(\mathbb{G}) = \mathrm{HM}_1(G), \qquad \mathrm{HM}_2(\mathbb{G}) = \mathrm{HM}_2(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\mathrm{HM}_1(\mathbb{H}_0) = \mathrm{HM}_1(H), \qquad \mathrm{HM}_2(\mathbb{H}_0) = \mathrm{HM}_2(H).$$

Consequently, Definition 4.5.7 strictly extends the hyper-Zagreb indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so each inner sum in Definition 4.5.7 contains exactly one term per f. Since $\mathbb{G}$ is G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Therefore the contribution of $f = \{u, v\}$ to $\mathrm{HM}_1(\mathbb{G})$ equals $(d_G(u) + d_G(v))^2$, and its contribution to $\mathrm{HM}_2(\mathbb{G})$ equals $(d_G(u)d_G(v))^2$, i.e., the corresponding edge contributions in $\mathrm{HM}_1(G)$ and $\mathrm{HM}_2(G)$. Summing over all $f \in E$ yields $\mathrm{HM}_1(\mathbb{G}) = \mathrm{HM}_1(G)$ and $\mathrm{HM}_2(\mathbb{G}) = \mathrm{HM}_2(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are exactly the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Hence, for each $e \in \mathcal{E}$, the inner pair-sums defining $\mathrm{HM}_1(\mathbb{H}_0)$ and $\mathrm{HM}_2(\mathbb{H}_0)$ coincide term-by-term with those defining $\mathrm{HM}_1(H)$ and $\mathrm{HM}_2(H)$, respectively. Summing over all $e \in \mathcal{E}$ yields $\mathrm{HM}_1(\mathbb{H}_0) = \mathrm{HM}_1(H)$ and $\mathrm{HM}_2(\mathbb{H}_0) = \mathrm{HM}_2(H)$. □

4.5.3 Augmented Zagreb index (AZI)

The Augmented Zagreb index (AZI) is a degree-based topological descriptor summing, over edges, the cubed ratio $d(u)d(v)/(d(u)+d(v)-2)$, used to predict molecular properties [142–145].

Definition 4.5.9 (Augmented Zagreb index of a graph)**.** Let $G=(V,E)$ be a finite simple graph, and let $d_G(\cdot)$ be the usual degree. Assume $d_G(u)+d_G(v)>2$ for every edge $uv\in E$ (equivalently, no edge joins two degree-1 vertices). The *augmented Zagreb index* of G is

$$\mathrm{AZI}(G) := \sum_{uv\in E}\left(\frac{d_G(u)\,d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

Definition 4.5.10 (Augmented Zagreb index of a hypergraph)**.** Let $H=(V,\mathcal{E})$ be a finite hypergraph, and let $d_H(\cdot)$ be the hypergraph degree. Assume $d_H(u)+d_H(v)>2$ for every pair $\{u,v\}$ counted below. Define

$$\mathrm{AZI}(H) := \sum_{e\in\mathcal{E}}\sum_{\substack{u,v\in e\\ u<v}}\left(\frac{d_H(u)\,d_H(v)}{d_H(u)+d_H(v)-2}\right)^3.$$

Definition 4.5.11 (Augmented Zagreb index of a SuperHyperGraph)**.** Let $\mathbb{H}=(\mathbb{V},\mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot)$ be the superdegree. Assume $d_{\mathbb{H}}(A)+d_{\mathbb{H}}(B)>2$ for every pair $\{A,B\}$ counted below. Define

$$\mathrm{AZI}(\mathbb{H}) := \sum_{f\in\mathbb{E}}\sum_{\substack{A,B\in f\\ A<B}}\left(\frac{d_{\mathbb{H}}(A)\,d_{\mathbb{H}}(B)}{d_{\mathbb{H}}(A)+d_{\mathbb{H}}(B)-2}\right)^3.$$

Example 4.5.12 (Augmented Zagreb index of a small SuperHyperGraph)**.** Let $\mathbb{H}=(\mathbb{V},\mathbb{E})$ be the finite SuperHyperGraph with

$$\mathbb{V}=\{A,B,C\},\qquad \mathbb{E}=\{f_1,f_2,f_3\},$$

where the superedges are

$$f_1=\{A,B,C\},\qquad f_2=\{A,B\},\qquad f_3=\{A,C\}.$$

The superdegrees (incidence counts) are

$$d_{\mathbb{H}}(A)=3,\qquad d_{\mathbb{H}}(B)=2,\qquad d_{\mathbb{H}}(C)=2,$$

so that $d_{\mathbb{H}}(X)+d_{\mathbb{H}}(Y)>2$ for every pair $\{X,Y\}$ that appears below.

We compute $\mathrm{AZI}(\mathbb{H})$ by summing, for each superedge, over all unordered pairs of distinct supervertices contained in it.

Contribution of $f_1=\{A,B,C\}$. The pairs are $\{A,B\}$, $\{A,C\}$, and $\{B,C\}$:

$$\left(\frac{d(A)d(B)}{d(A)+d(B)-2}\right)^3=\left(\frac{3\cdot 2}{3+2-2}\right)^3=\left(\frac{6}{3}\right)^3=8,$$

$$\left(\frac{d(A)d(C)}{d(A)+d(C)-2}\right)^3 = \left(\frac{3\cdot 2}{3+2-2}\right)^3 = 8,$$

$$\left(\frac{d(B)d(C)}{d(B)+d(C)-2}\right)^3 = \left(\frac{2\cdot 2}{2+2-2}\right)^3 = \left(\frac{4}{2}\right)^3 = 8.$$

Hence the total from f_1 equals $8+8+8=24$.

Contribution of $f_2 = \{A, B\}$. Only the pair $\{A, B\}$ occurs, contributing 8.

Contribution of $f_3 = \{A, C\}$. Only the pair $\{A, C\}$ occurs, contributing 8.

Total. Therefore,

$$\mathrm{AZI}(\mathbb{H}) = \sum_{f\in\mathbb{E}} \sum_{\substack{X,Y\in f\\ X<Y}} \left(\frac{d_{\mathbb{H}}(X)\, d_{\mathbb{H}}(Y)}{d_{\mathbb{H}}(X)+d_{\mathbb{H}}(Y)-2}\right)^3 = 24+8+8 = 40.$$

4.6 Gutman index of a SuperHyperGraph

The *Gutman index of a graph* is $\sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)\,\mathrm{dist}_G(u,v)$, combining degrees with pairwise shortest-path distances [146–149]. The Gutman index of fuzzy graphs [150] among related topics, have also been widely studied. The *Gutman index of a superhypergraph* extends this by using superhypergraph degrees and shortest superincidence distances between supervertices in pairs.

Definition 4.6.1 (Gutman index of a graph)**.** [146, 147] The *Gutman index* of G is

$$\mathrm{Gut}(G) := \sum_{\{u,v\}\subseteq V(G)} \deg_G(u)\deg_G(v)\, d_G(u,v) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} \deg_G(u)\deg_G(v)\, d_G(u,v).$$

Definition 4.6.2 (Adjacency, degree)**.** Let $\mathcal{S} = (\mathcal{V}, \mathcal{E})$ be an n-SuperHyperGraph. Distinct supervertices $x, y \in \mathcal{V}$ are *adjacent* if there exists $e \in \mathcal{E}$ with $\{x, y\} \subseteq e$. The *degree* of $x \in \mathcal{V}$ is

$$\deg_{\mathcal{S}}(x) := |\{\, e \in \mathcal{E} : x \in e \,\}|.$$

Definition 4.6.3 (Berge path and distance)**.** A *(Berge) path* of length $p \geq 1$ from x to y in $\mathcal{S}$ is a sequence

$$(x = v_0,\ e_1,\ v_1,\ e_2,\ \ldots,\ e_p,\ v_p = y),$$

where $v_0, \ldots, v_p \in \mathcal{V}$ are pairwise distinct, $e_1, \ldots, e_p \in \mathcal{E}$ are pairwise distinct, and $\{v_{i-1}, v_i\} \subseteq e_i$ for all $i = 1, \ldots, p$. If such a path exists for every ordered pair of distinct vertices, $\mathcal{S}$ is called *connected*. For a connected $\mathcal{S}$, the *distance* $D_{\mathcal{S}}(x, y)$ is the minimum length of a path from x to y (and $D_{\mathcal{S}}(x, x) = 0$).

Definition 4.6.4 (Gutman index of a SuperHyperGraph)**.** Let $\mathcal{S} = (\mathcal{V}, \mathcal{E})$ be a finite connected n-SuperHyperGraph. Its *Gutman index* is

$$\mathrm{Gut}(\mathcal{S}) \;:=\; \sum_{\{x,y\}\subseteq\mathcal{V}} \deg_{\mathcal{S}}(x)\deg_{\mathcal{S}}(y)\,D_{\mathcal{S}}(x,y) \;=\; \frac{1}{2}\sum_{x\in\mathcal{V}}\sum_{y\in\mathcal{V}} \deg_{\mathcal{S}}(x)\deg_{\mathcal{S}}(y)\,D_{\mathcal{S}}(x,y).$$

Example 4.6.5 (Gutman index of a small 1-SuperHyperGraph)**.** Let $V_0 = \{1,2,3,4\}$ and consider the 1-SuperHyperGraph

$$\mathcal{S} = (\mathcal{V}, \mathcal{E}), \qquad \mathcal{V} = \{A, B, C, D\} \subseteq \mathcal{P}(V_0),$$

with 1-supervertices

$$A = \{1,2\}, \quad B = \{2,3\}, \quad C = \{3,4\}, \quad D = \{1,4\},$$

and superedges

$$\mathcal{E} = \{e_1, e_2, e_3\}, \qquad e_1 = \{A, B, C\}, \quad e_2 = \{A, D\}, \quad e_3 = \{C, D\}.$$

This $\mathcal{S}$ is connected.

Degrees. By definition, $\deg_{\mathcal{S}}(X) = |\{e \in \mathcal{E} : X \in e\}|$, hence

$$\deg_{\mathcal{S}}(A) = 2, \qquad \deg_{\mathcal{S}}(B) = 1, \qquad \deg_{\mathcal{S}}(C) = 2, \qquad \deg_{\mathcal{S}}(D) = 2.$$

Distances. Let $D_{\mathcal{S}}(X, Y)$ be the shortest-path distance in the *2-section* graph of $\mathcal{S}$, where distinct supervertices are adjacent if they occur together in some superedge. Then the adjacencies are AB, AC, BC (from e_1), AD (from e_2), and CD (from e_3), so

$$D_{\mathcal{S}}(A,B) = D_{\mathcal{S}}(A,C) = D_{\mathcal{S}}(A,D) = D_{\mathcal{S}}(B,C) = D_{\mathcal{S}}(C,D) = 1, \qquad D_{\mathcal{S}}(B,D) = 2.$$

Gutman index. Therefore,

$$\begin{aligned}
\mathrm{Gut}(\mathcal{S}) &= \sum_{\{X,Y\}\subseteq\mathcal{V}} \deg_{\mathcal{S}}(X)\deg_{\mathcal{S}}(Y)\,D_{\mathcal{S}}(X,Y) \\
&= (2\cdot 1)\cdot 1 + (2\cdot 2)\cdot 1 + (2\cdot 2)\cdot 1 + (1\cdot 2)\cdot 1 + (1\cdot 2)\cdot 2 + (2\cdot 2)\cdot 1 \\
&= 2 + 4 + 4 + 2 + 4 + 4 \;=\; 20.
\end{aligned}$$

Hence the Gutman index of $\mathcal{S}$ equals 20.

4.7 Atom-Bond Connectivity (ABC) index

The Atom-Bond Connectivity (ABC) index sums, over edges, square roots of $\big(d(u) + d(v) - 2\big)/\big(d(u)d(v)\big)$, correlating with molecular properties [151–154].

Definition 4.7.1 (Atom-Bond Connectivity (ABC) index)**.** [152] Let $G = (V(G), E(G))$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of a vertex $v \in V(G)$. The *atom-bond connectivity index* (ABC index) of G is defined by

$$\mathrm{ABC}(G) \;:=\; \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)\, d_G(v)}}\,.$$

Remark 4.7.2. In the original introduction of the ABC index, some authors included an additional constant factor $\sqrt{2}$; the current standard convention is to omit this factor.

Definition 4.7.3 (Atom-Bond Connectivity (ABC) index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and for each vertex $v \in V$ let

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

be its (hypergraph) degree. The *atom-bond connectivity (ABC) index* of H is defined by

$$\mathrm{ABC}(H) \;:=\; \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \sqrt{\frac{d_H(u) + d_H(v) - 2}{d_H(u)\, d_H(v)}}\,,$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.7.4 (Atom-Bond Connectivity (ABC) index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and for each supervertex $X \in \mathbb{V}$ let

$$d_{\mathbb{H}}(X) \;:=\; |\{\, f \in \mathbb{E} \mid X \in f \,\}|$$

be its (super)degree. The *atom-bond connectivity (ABC) index* of $\mathbb{H}$ is defined by

$$\mathrm{ABC}(\mathbb{H}) \;:=\; \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \sqrt{\frac{d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B) - 2}{d_{\mathbb{H}}(A)\, d_{\mathbb{H}}(B)}}\,,$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.7.5 (ABC index of a small SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the finite SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f_1, f_2, f_3\},$$

where the superedges are

$$f_1 = \{A, B, C\}, \qquad f_2 = \{A, B\}, \qquad f_3 = \{A, C\}.$$

The (super)degrees are incidence counts:

$$d_{\mathbb{H}}(A) = |\{f \in \mathbb{E} : A \in f\}| = 3, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 2.$$

We compute $\mathrm{ABC}(\mathbb{H})$ using Definition 4.7.4.

Contribution of $f_1 = \{A, B, C\}$. The unordered pairs are $\{A, B\}, \{A, C\}, \{B, C\}$:

$$\sqrt{\frac{d(A) + d(B) - 2}{d(A)d(B)}} = \sqrt{\frac{3 + 2 - 2}{3 \cdot 2}} = \sqrt{\frac{3}{6}} = \frac{1}{\sqrt{2}},$$

$$\sqrt{\frac{d(A) + d(C) - 2}{d(A)d(C)}} = \sqrt{\frac{3 + 2 - 2}{3 \cdot 2}} = \frac{1}{\sqrt{2}},$$

$$\sqrt{\frac{d(B) + d(C) - 2}{d(B)d(C)}} = \sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} = \sqrt{\frac{2}{4}} = \frac{1}{\sqrt{2}}.$$

Hence the total from f_1 is $3 \cdot \frac{1}{\sqrt{2}} = \frac{3}{\sqrt{2}}$.

Contribution of $f_2 = \{A, B\}$. Only the pair $\{A, B\}$ occurs, contributing $\frac{1}{\sqrt{2}}$.

Contribution of $f_3 = \{A, C\}$. Only the pair $\{A, C\}$ occurs, contributing $\frac{1}{\sqrt{2}}$.

Total. Therefore,

$$\mathrm{ABC}(\mathbb{H}) = \sum_{f \in \mathbb{E}} \sum_{\substack{X, Y \in f \\ X < Y}} \sqrt{\frac{d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y) - 2}{d_{\mathbb{H}}(X)\, d_{\mathbb{H}}(Y)}} = \frac{3}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} = \frac{5}{\sqrt{2}}.$$

Theorem 4.7.6 (SuperHyperGraph ABC index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\mathrm{ABC}(\mathbb{G}) = \mathrm{ABC}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\mathrm{ABC}(\mathbb{H}_0) = \mathrm{ABC}(H).$$

Consequently, Definition 4.7.4 strictly extends the atom-bond connectivity indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge is a 2-set $f = \{u, v\}$. Hence the inner sum in Definition 4.7.4 contains exactly one term per f, namely

$$\sqrt{\frac{d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v) - 2}{d_{\mathbb{G}}(u)\, d_{\mathbb{G}}(v)}}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Therefore each $f = \{u, v\}$ contributes

$$\sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)\, d_G(v)}},$$

which is exactly the contribution of the edge uv to $\mathrm{ABC}(G)$. Summing over all $f \in E$ yields $\mathrm{ABC}(\mathbb{G}) = \mathrm{ABC}(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are exactly the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Thus, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.7.4 coincides term-by-term with the inner pair-sum in Definition 4.7.3. Summing over all $e \in \mathcal{E}$ yields $\mathrm{ABC}(\mathbb{H}_0) = \mathrm{ABC}(H)$. □

4.8 Estrada index

Estrada index sums exponentials of adjacency eigenvalues, equivalently trace of matrix exponential, measuring weighted closed-walk counts and network centrality [155–159].

Definition 4.8.1 (Estrada index)**.** [155–157] Let $G = (V, E)$ be a finite simple (undirected) graph on n vertices, and let $A(G) = (a_{ij})_{1\le i,j\le n}$ be its adjacency matrix. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of $A(G)$ (counted with algebraic multiplicity). The *Estrada index* of G is defined by

$$EE(G) \;:=\; \sum_{i=1}^{n} e^{\lambda_i}.$$

Equivalently, using the matrix exponential,

$$EE(G) \;=\; \mathrm{tr}\!\left(e^{A(G)}\right) \;=\; \sum_{k=0}^{\infty} \frac{\mathrm{tr}\!\left(A(G)^k\right)}{k!}.$$

Remark 4.8.2 (Spectral moments and closed walks)**.** For each integer $k \ge 0$, the k-th spectral moment of G is

$$M_k(G) \;:=\; \sum_{i=1}^{n} \lambda_i^k \;=\; \mathrm{tr}\!\left(A(G)^k\right).$$

Moreover, $\mathrm{tr}(A(G)^k)$ equals the number of closed walks of length k in G. Hence

$$EE(G) \;=\; \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}.$$

Definition 4.8.3 (Adjacency matrix of a hypergraph (clique-expansion, normalized))**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph with $|V| = n$. Define the symmetric $n \times n$ matrix $A(H) = (a_{uv})_{u,v\in V}$ by

$$a_{uu} \;:=\; 0 \quad (u \in V), \qquad a_{uv} \;:=\; \sum_{\substack{e\in\mathcal{E}\\ \{u,v\}\subseteq e}} \frac{1}{|e|-1} \quad (u \ne v).$$

Definition 4.8.4 (Estrada index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $A(H)$ be as in Definition 4.8.3. Let $\lambda_1(H), \ldots, \lambda_n(H)$ be the eigenvalues of $A(H)$ (counted with algebraic multiplicity). The *Estrada index* of H is

$$EE(H) \;:=\; \sum_{i=1}^{n} e^{\lambda_i(H)} \;=\; \operatorname{tr}\bigl(e^{A(H)}\bigr).$$

Definition 4.8.5 (Adjacency matrix of a SuperHyperGraph (clique-expansion, normalized))**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $|\mathbb{V}| = N$. Define the symmetric $N \times N$ matrix $A(\mathbb{H}) = (a_{XY})_{X,Y \in \mathbb{V}}$ by

$$a_{XX} \;:=\; 0 \quad (X \in \mathbb{V}), \qquad a_{XY} \;:=\; \sum_{\substack{f \in \mathbb{E} \\ \{X,Y\} \subseteq f}} \frac{1}{|f| - 1} \quad (X \neq Y).$$

Definition 4.8.6 (Estrada index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph and let $A(\mathbb{H})$ be as in Definition 4.8.5. Let $\lambda_1(\mathbb{H}), \ldots, \lambda_N(\mathbb{H})$ be the eigenvalues of $A(\mathbb{H})$. The *Estrada index* of $\mathbb{H}$ is

$$EE(\mathbb{H}) \;:=\; \sum_{i=1}^{N} e^{\lambda_i(\mathbb{H})} \;=\; \operatorname{tr}\bigl(e^{A(\mathbb{H})}\bigr).$$

Example 4.8.7 (A minimal nontrivial example)**.** Consider the SuperHyperGraph $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{\, f \,\}, \qquad f = \{A, B, C\}.$$

Since $|f| = 3$, Definition 4.8.5 gives, for distinct $X, Y \in \mathbb{V}$,

$$a_{XY} = \sum_{\substack{g \in \mathbb{E} \\ \{X,Y\} \subseteq g}} \frac{1}{|g| - 1} = \frac{1}{|f| - 1} = \frac{1}{2}, \qquad a_{XX} = 0.$$

Hence

$$A(\mathbb{H}) = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} = \frac{1}{2}\,(J_3 - I_3),$$

where J_3 is the 3×3 all-ones matrix. It follows that the eigenvalues of $A(\mathbb{H})$ are

$$\lambda_1(\mathbb{H}) = 1, \qquad \lambda_2(\mathbb{H}) = \lambda_3(\mathbb{H}) = -\frac{1}{2}.$$

Therefore, by Definition 4.8.6,

$$EE(\mathbb{H}) = \sum_{i=1}^{3} e^{\lambda_i(\mathbb{H})} = e^1 + 2e^{-1/2}.$$

Theorem 4.8.8 (SuperHyperGraph Estrada index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple (undirected) graph and let $\mathbb{G} := (V, E)$ be the SuperHyperGraph obtained by viewing each edge $\{u, v\} \in E$ as a 2-element superhyperedge. Then*

$$A(\mathbb{G}) = A(G), \qquad \textit{and hence} \qquad EE(\mathbb{G}) = EE(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing each hyperedge $e \in \mathcal{E}$ as a superhyperedge. Then*

$$A(\mathbb{H}_0) = A(H), \qquad \textit{and hence} \qquad EE(\mathbb{H}_0) = EE(H).$$

Consequently, the Estrada index of SuperHyperGraphs in Definition 4.8.6 strictly extends (i) the classical Estrada index of graphs and (ii) the Estrada index of hypergraphs in Definition 4.8.4.

Proof. (1) Fix distinct $u, v \in V$. In $\mathbb{G} = (V, E)$, every superhyperedge has size 2, so for $u \neq v$ we have

$$a_{uv}(\mathbb{G}) = \sum_{\substack{f \in E \\ \{u,v\} \subseteq f}} \frac{1}{|f| - 1} = \begin{cases} \frac{1}{2-1} = 1, & \text{if } \{u, v\} \in E, \\ 0, & \text{otherwise,} \end{cases}$$

which equals the (u, v)-entry of the usual adjacency matrix $A(G)$. Also $a_{uu}(\mathbb{G}) = 0 = a_{uu}(G)$. Hence $A(\mathbb{G}) = A(G)$ entrywise, and therefore

$$EE(\mathbb{G}) = \operatorname{tr}\bigl(e^{A(\mathbb{G})}\bigr) = \operatorname{tr}\bigl(e^{A(G)}\bigr) = EE(G).$$

(2) Fix distinct $u, v \in V$. By construction, $\mathbb{H}_0 = (V, \mathcal{E})$ has the same edge family as H, hence for $u \neq v$,

$$a_{uv}(\mathbb{H}_0) = \sum_{\substack{f \in \mathcal{E} \\ \{u,v\} \subseteq f}} \frac{1}{|f| - 1} = a_{uv}(H), \qquad a_{uu}(\mathbb{H}_0) = 0 = a_{uu}(H).$$

Thus $A(\mathbb{H}_0) = A(H)$ entrywise, and consequently

$$EE(\mathbb{H}_0) = \operatorname{tr}\bigl(e^{A(\mathbb{H}_0)}\bigr) = \operatorname{tr}\bigl(e^{A(H)}\bigr) = EE(H).$$

□

4.9 Szeged index

Szeged index sums, over edges, products of counts of vertices closer to each endpoint than the other, generalizing Wiener index [160–163]. We extend this concept using the SuperHyperGraph framework.

Definition 4.9.1 (Szeged index)**.** [160,161] Let $G = (V, E)$ be a finite simple connected graph, and let $d_G(\cdot, \cdot)$ denote the usual shortest-path distance in G. For an edge $e = uv \in E$, define the vertex sets

$$N_u(e) := \{\, x \in V \mid d_G(x, u) < d_G(x, v) \,\}, \qquad N_v(e) := \{\, x \in V \mid d_G(x, v) < d_G(x, u) \,\},$$

and set

$$n_u(e) := |N_u(e)|, \qquad n_v(e) := |N_v(e)|.$$

The *Szeged index* of G is

$$\mathrm{Sz}(G) := \sum_{uv \in E} n_u(uv)\, n_v(uv).$$

Remark 4.9.2 (Equidistant vertices and the revised Szeged index)**.** For $e = uv \in E$, the set of vertices equidistant from u and v is

$$N_0(e) \ := \ \{ \, x \in V \mid d_G(x,u) = d_G(x,v) \, \}.$$

The classical Szeged index ignores $N_0(e)$ (it uses strict inequalities above). A commonly used variant is the *revised Szeged index*

$$\mathrm{Sz}^*(G) \ := \ \sum_{uv \in E} \Big(n_u(uv) + \tfrac{1}{2}|N_0(uv)| \Big) \Big(n_v(uv) + \tfrac{1}{2}|N_0(uv)| \Big).$$

Definition 4.9.3 (Szeged index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $d_H(\cdot,\cdot)$ denote the hypergraph distance already fixed (Berge-type).

For a hyperedge $e \in \mathcal{E}$ and a vertex $u \in e$, define

$$N_u(e) \ := \ \big\{ \, x \in V \mid d_H(x,u) < \min_{v \in e \setminus \{u\}} d_H(x,v) \, \big\}, \qquad n_u(e) \ := \ |N_u(e)|.$$

The *Szeged index* of H is defined by

$$\mathrm{Sz}(H) \ := \ \sum_{e \in \mathcal{E}} \ \sum_{\substack{u,v \in e \\ u<v}} n_u(e)\, n_v(e),$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.9.4 (Szeged index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot,\cdot)$ denote the superdistance already fixed.

For a superhyperedge $f \in \mathbb{E}$ and a supervertex $A \in f$, define

$$\mathbb{N}_A(f) \ := \ \big\{ \, X \in \mathbb{V} \mid d_{\mathbb{H}}(X,A) < \min_{B \in f \setminus \{A\}} d_{\mathbb{H}}(X,B) \, \big\}, \qquad \ltimes_A(f) \ := \ |\mathbb{N}_A(f)|.$$

The *Szeged index* of $\mathbb{H}$ is defined by

$$\mathrm{Sz}(\mathbb{H}) \ := \ \sum_{f \in \mathbb{E}} \ \sum_{\substack{A,B \in f \\ A<B}} \ltimes_A(f) \ltimes_B(f),$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.9.5 (Szeged index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{ \, f_1, f_2 \, \}, \qquad f_1 = \{A, B\}, \ \ f_2 = \{B, C\}.$$

This is the path A–B–C viewed as a SuperHyperGraph, hence the superdistance is

$$d_{\mathbb{H}}(A,B) = d_{\mathbb{H}}(B,C) = 1, \qquad d_{\mathbb{H}}(A,C) = 2.$$

Edge $f_1 = \{A, B\}$. Since $f_1 \setminus \{A\} = \{B\}$ and $f_1 \setminus \{B\} = \{A\}$,

$$\mathbb{N}_A(f_1) = \{X \in \mathbb{V} : d_{\mathbb{H}}(X,A) < d_{\mathbb{H}}(X,B)\} = \{A\}, \quad \ltimes_A(f_1) = 1,$$

$$\mathbb{N}_B(f_1) = \{X \in \mathbb{V} : d_{\mathbb{H}}(X, B) < d_{\mathbb{H}}(X, A)\} = \{B, C\}, \quad \ltimes_B(f_1) = 2.$$

Thus the contribution of f_1 to $\mathrm{Sz}(\mathbb{H})$ is $\ltimes_A(f_1)\ltimes_B(f_1) = 1 \cdot 2 = 2$.

Edge $f_2 = \{B, C\}$. Similarly,

$$\mathbb{N}_B(f_2) = \{X \in \mathbb{V} : d_{\mathbb{H}}(X, B) < d_{\mathbb{H}}(X, C)\} = \{A, B\}, \quad \ltimes_B(f_2) = 2,$$

$$\mathbb{N}_C(f_2) = \{X \in \mathbb{V} : d_{\mathbb{H}}(X, C) < d_{\mathbb{H}}(X, B)\} = \{C\}, \quad \ltimes_C(f_2) = 1.$$

Hence the contribution of f_2 is $\ltimes_B(f_2)\ltimes_C(f_2) = 2 \cdot 1 = 2$.

Therefore,

$$\mathrm{Sz}(\mathbb{H}) = 2 + 2 = 4.$$

Theorem 4.9.6 (SuperHyperGraph Szeged index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple connected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\mathrm{Sz}(\mathbb{G}) = \mathrm{Sz}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\mathrm{Sz}(\mathbb{H}_0) = \mathrm{Sz}(H).$$

Consequently, Definition 4.9.4 strictly extends both the classical Szeged index of graphs and the Szeged index of hypergraphs (Definition 4.9.3).

Proof. (1) In $\mathbb{G} = (V, E)$, every superhyperedge $f \in E$ has the form $f = \{u, v\}$ with $u \neq v$. Fix such an edge $f = \{u, v\}$. Because $f \setminus \{u\} = \{v\}$, the defining inequality in Definition 4.9.4 becomes

$$d_{\mathbb{G}}(x, u) < \min_{B \in \{v\}} d_{\mathbb{G}}(x, B) \iff d_{\mathbb{G}}(x, u) < d_{\mathbb{G}}(x, v).$$

By the previously established identification $d_{\mathbb{G}}(\cdot, \cdot) = d_G(\cdot, \cdot)$ (for graph-as-SuperHyperGraph), we obtain $\mathbb{N}_u(f) = N_u(uv)$ and hence $\ltimes_u(f) = n_u(uv)$, and similarly $\ltimes_v(f) = n_v(uv)$. Moreover, the inner sum over unordered pairs in $f = \{u, v\}$ contains exactly one term, so the contribution of f to $\mathrm{Sz}(\mathbb{G})$ equals $n_u(uv)\, n_v(uv)$. Summing over all $f \in E$ yields $\mathrm{Sz}(\mathbb{G}) = \mathrm{Sz}(G)$.

(2) Consider $\mathbb{H}_0 = (V, \mathcal{E})$. Here the supervertices are exactly the vertices of H, and the superdistance equals the hypergraph distance: $d_{\mathbb{H}_0} = d_H$ (as previously fixed for the hypergraph-as-SuperHyperGraph embedding). Fix $e \in \mathcal{E}$ and $u \in e$. Then Definition 4.9.4 gives

$$\mathbb{N}_u(e) = \{\, x \in V :\ d_{\mathbb{H}_0}(x, u) < \min_{v \in e \setminus \{u\}} d_{\mathbb{H}_0}(x, v) \,\} = \{\, x \in V :\ d_H(x, u) < \min_{v \in e \setminus \{u\}} d_H(x, v) \,\} = N_u(e),$$

and hence $\ltimes_u(e) = n_u(e)$ for all $u \in e$. Therefore, for each $e \in \mathcal{E}$, the inner pair-sum in $\mathrm{Sz}(\mathbb{H}_0)$ equals the inner pair-sum in $\mathrm{Sz}(H)$, and summing over $e \in \mathcal{E}$ yields $\mathrm{Sz}(\mathbb{H}_0) = \mathrm{Sz}(H)$. □

4.10 Padmakar-Ivan (PI) index

Padmakar–Ivan (PI) index sums, over edges, counts of other edges closer to one endpoint than the other, excluding ties [164–167]. We extend this concept using the SuperHyperGraph framework.

Definition 4.10.1 (Padmakar-Ivan (PI) index)**.** [164–167] Let $G = (V, E)$ be a finite simple connected graph, and let $d_G(\cdot,\cdot)$ denote the usual shortest-path distance in G.

Distance from a vertex to an edge. For a vertex $x \in V$ and an edge $f = ab \in E$, define

$$d_G(x, f) \;:=\; \min\{\, d_G(x, a),\, d_G(x, b)\,\}.$$

Edge partition induced by an edge $e = uv$. For $e = uv \in E$, define

$$E_u(e) \;:=\; \{\, f \in E \mid d_G(u, f) < d_G(v, f)\,\}, \qquad E_v(e) \;:=\; \{\, f \in E \mid d_G(v, f) < d_G(u, f)\,\},$$

and set

$$n_{eu}(e) \;:=\; |E_u(e)|, \qquad n_{ev}(e) \;:=\; |E_v(e)|.$$

(Edges f with $d_G(u, f) = d_G(v, f)$ are *equidistant* from u and v and are not counted by either $n_{eu}(e)$ or $n_{ev}(e)$.)

PI index. The *Padmakar-Ivan index* of G is

$$\mathrm{PI}(G) \;:=\; \sum_{e=uv\in E} \big(n_{eu}(e) + n_{ev}(e)\big).$$

Remark 4.10.2 (Equivalent form via equidistant edges)**.** For $e = uv \in E$, let

$$E_0(e) \;:=\; \{\, f \in E \mid d_G(u, f) = d_G(v, f)\,\}, \qquad n_{e0}(e) := |E_0(e)|.$$

Then E is the disjoint union $E_u(e) \,\dot\cup\, E_v(e) \,\dot\cup\, E_0(e)$, so

$$n_{eu}(e) + n_{ev}(e) = |E| - n_{e0}(e), \qquad \text{and hence} \qquad \mathrm{PI}(G) = \sum_{e\in E} \big(|E| - n_{e0}(e)\big).$$

Definition 4.10.3 (Distance from a vertex to a hyperedge)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $d_H(\cdot,\cdot)$ be the fixed hypergraph distance on V. For a vertex $x \in V$ and a hyperedge $e \in \mathcal{E}$, define

$$d_H(x, e) \;:=\; \min_{y\in e} d_H(x, y).$$

Definition 4.10.4 (Padmakar-Ivan index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph. For a hyperedge $e \in \mathcal{E}$ and for $u \in e$, define

$$\mathcal{E}_u(e) \;:=\; \Big\{\, f \in \mathcal{E} \;\Big|\; d_H(u, f) \;<\; \min_{v\in e\setminus\{u\}} d_H(v, f)\,\Big\}, \qquad n_{eu}(e) \;:=\; |\mathcal{E}_u(e)|.$$

The *Padmakar-Ivan (PI) index* of H is defined by

$$\mathrm{PI}(H) \;:=\; \sum_{e\in\mathcal{E}} \sum_{\substack{u,v\in e\\ u<v}} \big(n_{eu}(e) + n_{ev}(e)\big),$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.10.5 (Distance from a supervertex to a superhyperedge)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot, \cdot)$ be the fixed superdistance on $\mathbb{V}$. For a supervertex $X \in \mathbb{V}$ and a superhyperedge $f \in \mathbb{E}$, define

$$d_{\mathbb{H}}(X, f) \ := \ \min_{Y \in f} d_{\mathbb{H}}(X, Y).$$

Definition 4.10.6 (Padmakar-Ivan index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph. For a superhyperedge $f \in \mathbb{E}$ and for $A \in f$, define

$$\mathbb{E}_A(f) \ := \ \Big\{ g \in \mathbb{E} \ \Big| \ d_{\mathbb{H}}(A, g) \ < \min_{B \in f \setminus \{A\}} d_{\mathbb{H}}(B, g) \Big\}, \qquad \ltimes_{eA}(f) \ := \ |\mathbb{E}_A(f)|.$$

The *Padmakar-Ivan (PI) index* of $\mathbb{H}$ is defined by

$$\mathrm{PI}(\mathbb{H}) \ := \sum_{f \in \mathbb{E}} \sum_{\substack{A, B \in f \\ A < B}} \big(\ltimes_{eA}(f) + \ltimes_{eB}(f) \big),$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.10.7 (Padmakar–Ivan index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{ f_1, f_2 \}, \qquad f_1 = \{A, B\}, \ \ f_2 = \{B, C\}.$$

This is the path A–B–C viewed as a SuperHyperGraph, so the superdistances are

$$d_{\mathbb{H}}(A, B) = d_{\mathbb{H}}(B, C) = 1, \qquad d_{\mathbb{H}}(A, C) = 2.$$

For a supervertex X and a superhyperedge f, recall

$$d_{\mathbb{H}}(X, f) = \min_{Y \in f} d_{\mathbb{H}}(X, Y).$$

Step 1: edge $f_1 = \{A, B\}$. We compute $\mathbb{E}_A(f_1)$ and $\mathbb{E}_B(f_1)$.

For $g = f_1$, we have $d_{\mathbb{H}}(A, f_1) = 0$ and $d_{\mathbb{H}}(B, f_1) = 0$, so $0 < 0$ is false; thus $f_1 \notin \mathbb{E}_A(f_1)$ and $f_1 \notin \mathbb{E}_B(f_1)$.

For $g = f_2$, we have

$$d_{\mathbb{H}}(A, f_2) = \min\{d_{\mathbb{H}}(A, B), d_{\mathbb{H}}(A, C)\} = \min\{1, 2\} = 1,$$

$$d_{\mathbb{H}}(B, f_2) = \min\{d_{\mathbb{H}}(B, B), d_{\mathbb{H}}(B, C)\} = \min\{0, 1\} = 0.$$

Hence $d_{\mathbb{H}}(A, f_2) < d_{\mathbb{H}}(B, f_2)$ is $1 < 0$, false, while $d_{\mathbb{H}}(B, f_2) < d_{\mathbb{H}}(A, f_2)$ is $0 < 1$, true. Therefore,

$$\mathbb{E}_A(f_1) = \emptyset, \quad \ltimes_{eA}(f_1) = 0, \qquad \mathbb{E}_B(f_1) = \{f_2\}, \quad \ltimes_{eB}(f_1) = 1.$$

Thus the contribution of f_1 to $\mathrm{PI}(\mathbb{H})$ is $\ltimes_{eA}(f_1) + \ltimes_{eB}(f_1) = 0 + 1 = 1$.

Step 2: edge $f_2 = \{B, C\}$. Similarly, for $g = f_1$ we compute

$$d_{\mathbb{H}}(B, f_1) = 0, \qquad d_{\mathbb{H}}(C, f_1) = \min\{d_{\mathbb{H}}(C, A), d_{\mathbb{H}}(C, B)\} = \min\{2, 1\} = 1.$$

Hence $d_{\mathbb{H}}(B, f_1) < d_{\mathbb{H}}(C, f_1)$ is $0 < 1$, true, and $d_{\mathbb{H}}(C, f_1) < d_{\mathbb{H}}(B, f_1)$ is $1 < 0$, false. Also $g = f_2$ is equidistant ($0 < 0$ fails) for both endpoints. Therefore,

$$\mathbb{E}_B(f_2) = \{f_1\}, \quad \ltimes_{eB}(f_2) = 1, \qquad \mathbb{E}_C(f_2) = \emptyset, \quad \ltimes_{eC}(f_2) = 0.$$

So the contribution of f_2 is $\ltimes_{eB}(f_2) + \ltimes_{eC}(f_2) = 1 + 0 = 1$.

Conclusion. Summing contributions over f_1 and f_2 yields

$$\mathrm{PI}(\mathbb{H}) = 1 + 1 = 2.$$

Theorem 4.10.8 (SuperHyperGraph PI index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple connected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*
$$\mathrm{PI}(\mathbb{G}) = \mathrm{PI}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*
$$\mathrm{PI}(\mathbb{H}_0) = \mathrm{PI}(H).$$

Consequently, Definition 4.10.6 strictly extends the Padmakar-Ivan indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ every superhyperedge has size 2, say $f = \{u, v\}$. Fix $u \in f$ and consider any $g \in E$. By Definition 4.10.5,

$$d_{\mathbb{G}}(u, g) = \min_{x \in g} d_{\mathbb{G}}(u, x).$$

Since $g = \{a, b\}$ is an ordinary edge and $d_{\mathbb{G}}(\cdot, \cdot) = d_G(\cdot, \cdot)$ for the graph-as-SuperHyperGraph embedding, we have

$$d_{\mathbb{G}}(u, g) = \min\{d_G(u, a), d_G(u, b)\} = d_G(u, g),$$

which is exactly the vertex-to-edge distance used in the classical PI index. Moreover, because $f \setminus \{u\} = \{v\}$, the defining inequality in $\mathbb{E}_u(f)$ becomes

$$d_{\mathbb{G}}(u, g) < \min_{B \in \{v\}} d_{\mathbb{G}}(B, g) \iff d_G(u, g) < d_G(v, g),$$

so $\mathbb{E}_u(f) = E_u(uv)$ and hence $\ltimes_{eu}(f) = n_{eu}(uv)$ (and similarly for v). Finally, for a 2-edge $f = \{u, v\}$ the inner pair-sum in Definition 4.10.6 has exactly one term, so the contribution of f equals $n_{eu}(uv) + n_{ev}(uv)$. Summing over all $f \in E$ yields $\mathrm{PI}(\mathbb{G}) = \mathrm{PI}(G)$.

(2) Consider $\mathbb{H}_0 = (V, \mathcal{E})$. Here the supervertices are precisely the vertices of H, the superdistance equals the hypergraph distance ($d_{\mathbb{H}_0} = d_H$), and the superedge family equals $\mathcal{E}$. Fix $e \in \mathcal{E}$, $u \in e$, and $f \in \mathcal{E}$. By Definition 4.10.5,

$$d_{\mathbb{H}_0}(u, f) = \min_{x \in f} d_{\mathbb{H}_0}(u, x) = \min_{x \in f} d_H(u, x) = d_H(u, f),$$

which coincides with Definition 4.10.3. Therefore,

$$f \in \mathbb{E}_u(e) \iff d_{\mathbb{H}_0}(u, f) < \min_{v \in e \setminus \{u\}} d_{\mathbb{H}_0}(v, f) \iff d_H(u, f) < \min_{v \in e \setminus \{u\}} d_H(v, f) \iff f \in \mathcal{E}_u(e),$$

so $\mathbb{E}_u(e) = \mathcal{E}_u(e)$ and hence $\ltimes_{eu}(e) = n_{eu}(e)$ for all $u \in e$. Consequently, for each $e \in \mathcal{E}$ the inner pair-sum defining $\mathrm{PI}(\mathbb{H}_0)$ equals that defining $\mathrm{PI}(H)$, and summing over $e \in \mathcal{E}$ yields $\mathrm{PI}(\mathbb{H}_0) = \mathrm{PI}(H)$. □

4.11 Harmonic index

Harmonic index sums, over edges, 2 divided by endpoint degree sum, emphasizing low-degree connections and graph branching in complex networks [168–171]. We extend this concept using the SuperHyperGraph framework.

Definition 4.11.1 (Harmonic index). [168–171] Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of a vertex $v \in V$. The *harmonic index* of G is defined by

$$H(G) := \sum_{uv \in E} \frac{2}{d_G(u) + d_G(v)}.$$

Remark 4.11.2 (Harmonic polynomial). A commonly used generating polynomial associated with the harmonic index is

$$H(G, x) := \sum_{uv \in E} x^{d_G(u)+d_G(v)-1}.$$

It satisfies

$$H(G) = 2 \int_0^1 H(G, x)\, dx.$$

Definition 4.11.3 (Harmonic index of a hypergraph). Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $d_H(v)$ denote the (hypergraph) degree of $v \in V$. The *harmonic index* of H is defined by

$$H(H) := \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \frac{2}{d_H(u) + d_H(v)},$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.11.4 (Harmonic index of a SuperHyperGraph). Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and let $d_{\mathbb{H}}(X)$ denote the (super)degree of a supervertex $X \in \mathbb{V}$. The *harmonic index* of $\mathbb{H}$ is defined by

$$H(\mathbb{H}) := \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \frac{2}{d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B)},$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.11.5 (Harmonic index of a simple SuperHyperGraph). Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{ f_1, f_2 \}, \qquad f_1 = \{A, B\}, \quad f_2 = \{B, C\}.$$

Thus $\mathbb{H}$ is the path A–B–C viewed as a SuperHyperGraph. The (super)degrees are

$$d_{\mathbb{H}}(A) = 1, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 1.$$

For $f_1 = \{A, B\}$ the inner sum has one term, giving

$$\frac{2}{d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B)} = \frac{2}{1+2} = \frac{2}{3}.$$

For $f_2 = \{B, C\}$ we similarly obtain

$$\frac{2}{d_{\mathbb{H}}(B) + d_{\mathbb{H}}(C)} = \frac{2}{2+1} = \frac{2}{3}.$$

Therefore,

$$H(\mathbb{H}) = \frac{2}{3} + \frac{2}{3} = \frac{4}{3}.$$

Theorem 4.11.6 (SuperHyperGraph harmonic index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$H(\mathbb{G}) = H(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$H(\mathbb{H}_0) = H(H).$$

Consequently, Definition 4.12.5 strictly extends the harmonic indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.12.5 contains exactly one term per f, namely

$$\frac{2}{d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v)}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Hence the contribution of f equals $\frac{2}{d_G(u)+d_G(v)}$, which is precisely the contribution of the edge uv to $H(G)$. Summing over all $f \in E$ yields $H(\mathbb{G}) = H(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Thus, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.12.5 coincides term-by-term with that in Definition 4.12.4. Summing over all $e \in \mathcal{E}$ gives $H(\mathbb{H}_0) = H(H)$. □

4.12 Albertson (irregularity) index

Albertson irregularity index sums absolute degree differences across edges, quantifying how far a graph deviates from regularity in a network [172–174]. We extend this concept using the SuperHyperGraph framework.

Definition 4.12.1 (Albertson (irregularity) index)**.** [172–174] Let $G = (V, E)$ be a finite simple undirected graph, and let $\deg_G(v)$ denote the (usual) degree of a vertex $v \in V$. For an edge $e = uv \in E$, define its *imbalance* by

$$\mathrm{imb}(e) \;:=\; \bigl|\deg_G(u) - \deg_G(v)\bigr|.$$

The *Albertson index* (also called the *irregularity* of G) is

$$\mathrm{Alb}(G) \;:=\; \sum_{uv \in E} \bigl|\deg_G(u) - \deg_G(v)\bigr|.$$

Remark 4.12.2. A graph G is regular if and only if $\mathrm{Alb}(G) = 0$.

Remark 4.12.3 (p-Albertson index (a common generalization))**.** For a real parameter $p \geq 1$, one often defines the *p-Albertson index* by

$$A_p(G) \;:=\; \left(\sum_{uv \in E} \bigl|\deg_G(u) - \deg_G(v)\bigr|^p \right)^{1/p},$$

which reduces to the classical Albertson index when $p = 1$.

Definition 4.12.4 (Harmonic index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph. For each vertex $v \in V$, let

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

be its (hypergraph) degree. The *harmonic index* of H is defined by

$$H(H) \;:=\; \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \frac{2}{d_H(u) + d_H(v)},$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.12.5 (Harmonic index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph. For each supervertex $X \in \mathbb{V}$, let

$$d_{\mathbb{H}}(X) \;:=\; |\{\, f \in \mathbb{E} \mid X \in f \,\}|$$

be its (super)degree. The *harmonic index* of $\mathbb{H}$ is defined by

$$H(\mathbb{H}) \;:=\; \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \frac{2}{d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B)},$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.12.6 (Harmonic index of a 3-uniform SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C, D\}, \qquad \mathbb{E} = \{\, f_1, f_2 \,\}, \qquad f_1 = \{A, B, C\}, \quad f_2 = \{B, C, D\}.$$

Then the (super)degrees are

$$d_{\mathbb{H}}(A) = 1, \quad d_{\mathbb{H}}(B) = 2, \quad d_{\mathbb{H}}(C) = 2, \quad d_{\mathbb{H}}(D) = 1.$$

Contribution of $f_1 = \{A, B, C\}$. The unordered pairs in f_1 are $\{A, B\}$, $\{A, C\}$, and $\{B, C\}$, hence

$$\sum_{\substack{X,Y \in f_1 \\ X<Y}} \frac{2}{d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y)} = \frac{2}{1+2} + \frac{2}{1+2} + \frac{2}{2+2} = \frac{2}{3} + \frac{2}{3} + \frac{1}{2} = \frac{11}{6}.$$

Contribution of $f_2 = \{B, C, D\}$. The unordered pairs in f_2 are $\{B, C\}$, $\{B, D\}$, and $\{C, D\}$, hence

$$\sum_{\substack{X,Y \in f_2 \\ X<Y}} \frac{2}{d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y)} = \frac{2}{2+2} + \frac{2}{2+1} + \frac{2}{2+1} = \frac{1}{2} + \frac{2}{3} + \frac{2}{3} = \frac{11}{6}.$$

Therefore,

$$H(\mathbb{H}) = \frac{11}{6} + \frac{11}{6} = \frac{11}{3}.$$

Theorem 4.12.7 (SuperHyperGraph harmonic index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$H(\mathbb{G}) = H(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$H(\mathbb{H}_0) = H(H).$$

Consequently, Definition 4.12.5 strictly extends the harmonic indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$. For such f, the inner sum in Definition 4.12.5 contains exactly one term, namely

$$\frac{2}{d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v)}.$$

Because $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Hence the contribution of f is $\frac{2}{d_G(u)+d_G(v)}$. Summing over all $f \in E$ yields $H(\mathbb{G}) = H(G)$.

(2) Consider $\mathbb{H}_0 = (V, \mathcal{E})$. Here the supervertices are precisely the vertices of H, the superedges are exactly the hyperedges, and for every vertex $v \in V$ the superdegree equals the hypergraph degree:

$$d_{\mathbb{H}_0}(v) = |\{ e \in \mathcal{E} \mid v \in e \}| = d_H(v).$$

Thus, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.12.5 coincides with the inner pair-sum in Definition 4.12.4. Summing over all $e \in \mathcal{E}$ gives $H(\mathbb{H}_0) = H(H)$. □

4.13 Sum-connectivity index

Sum-connectivity index sums, over all edges, the inverse square root of endpoint degree sums, measuring branching and connectivity overall structure [175–179]. We extend this concept using the SuperHyperGraph framework.

Definition 4.13.1 (Sum-connectivity index)**.** [175–177] Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of a vertex $v \in V$. The *sum-connectivity index* of G (also denoted by $R^+(G)$ in the literature) is defined by

$$\chi(G) \;:=\; R^+(G) \;:=\; \sum_{uv \in E(G)} \bigl(d_G(u) + d_G(v)\bigr)^{-1/2}.$$

Definition 4.13.2 (Sum-connectivity index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph, and for each vertex $v \in V$ let

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

be its (hypergraph) degree. The *sum-connectivity index* of H is defined by

$$\chi(H) \;:=\; \sum_{e \in \mathcal{E}} \sum_{\substack{u,v \in e \\ u<v}} \bigl(d_H(u) + d_H(v)\bigr)^{-1/2},$$

where $u < v$ indicates that the inner sum ranges over unordered distinct pairs $\{u, v\} \subseteq e$.

Definition 4.13.3 (Sum-connectivity index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph, and for each supervertex $X \in \mathbb{V}$ let

$$d_{\mathbb{H}}(X) \;:=\; |\{ f \in \mathbb{E} \mid X \in f \}|$$

be its (super)degree. The *sum-connectivity index* of $\mathbb{H}$ is defined by

$$\chi(\mathbb{H}) \;:=\; \sum_{f \in \mathbb{E}} \sum_{\substack{A,B \in f \\ A<B}} \bigl(d_{\mathbb{H}}(A) + d_{\mathbb{H}}(B)\bigr)^{-1/2},$$

where $A < B$ indicates that the inner sum ranges over unordered distinct pairs $\{A, B\} \subseteq f$.

Example 4.13.4 (Sum-connectivity index of a small SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the finite SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f_1, f_2, f_3\},$$

where the superedges are

$$f_1 = \{A, B, C\}, \qquad f_2 = \{A, B\}, \qquad f_3 = \{A, C\}.$$

The (super)degrees are incidence counts:

$$d_{\mathbb{H}}(A) = |\{f \in \mathbb{E} : A \in f\}| = 3, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 2.$$

We compute $\chi(\mathbb{H})$ using Definition 4.13.3.

Contribution of $f_1 = \{A, B, C\}$. The unordered pairs are $\{A, B\}, \{A, C\}, \{B, C\}$, hence

$$(d(A) + d(B))^{-1/2} = (3 + 2)^{-1/2} = \frac{1}{\sqrt{5}}, \qquad (d(A) + d(C))^{-1/2} = (3 + 2)^{-1/2} = \frac{1}{\sqrt{5}},$$

$$(d(B) + d(C))^{-1/2} = (2 + 2)^{-1/2} = \frac{1}{\sqrt{4}} = \frac{1}{2}.$$

Therefore the total from f_1 equals

$$\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{5}} + \frac{1}{2} = \frac{2}{\sqrt{5}} + \frac{1}{2}.$$

Contribution of $f_2 = \{A, B\}$. Only the pair $\{A, B\}$ occurs, contributing $\frac{1}{\sqrt{5}}$.

Contribution of $f_3 = \{A, C\}$. Only the pair $\{A, C\}$ occurs, contributing $\frac{1}{\sqrt{5}}$.

Total. Hence,

$$\chi(\mathbb{H}) = \sum_{f \in \mathbb{E}} \sum_{\substack{X, Y \in f \\ X < Y}} \big(d_{\mathbb{H}}(X) + d_{\mathbb{H}}(Y)\big)^{-1/2} = \left(\frac{2}{\sqrt{5}} + \frac{1}{2}\right) + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{5}} = \frac{4}{\sqrt{5}} + \frac{1}{2}.$$

Theorem 4.13.5 (SuperHyperGraph sum-connectivity index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\chi(\mathbb{G}) = \chi(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\chi(\mathbb{H}_0) = \chi(H).$$

Consequently, Definition 4.13.3 strictly extends the sum-connectivity indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has the form $f = \{u, v\}$, so the inner sum in Definition 4.13.3 contains exactly one term per f, namely

$$\big(d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v)\big)^{-1/2}.$$

Since $\mathbb{G}$ is just G viewed as a SuperHyperGraph, the superdegree equals the usual graph degree: $d_{\mathbb{G}}(u) = d_G(u)$ and $d_{\mathbb{G}}(v) = d_G(v)$. Thus each edge contributes $(d_G(u) + d_G(v))^{-1/2}$, and summing over all edges gives $\chi(\mathbb{G}) = \chi(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertices are the vertices of H and the superedges are exactly the hyperedges. Moreover, for every $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{\, e \in \mathcal{E} \mid v \in e \,\}| = d_H(v).$$

Hence, for each $e \in \mathcal{E}$, the inner pair-sum in Definition 4.13.3 coincides term-by-term with that in Definition 4.13.2. Summing over all $e \in \mathcal{E}$ yields $\chi(\mathbb{H}_0) = \chi(H)$. □

4.14 Merrifield-Simmons index

Merrifield–Simmons index counts all independent vertex sets in a graph, including the empty set; equivalently, the independence polynomial at 1 [180–183]. We extend this concept using the SuperHyperGraph framework.

Definition 4.14.1 (First geometric-arithmetic index (GA index))**.** [184] Let $G = (V, E)$ be a finite simple connected graph, and let $d_G(u)$ denote the (usual) degree of a vertex $u \in V$. The *first geometric-arithmetic index* of G (often called simply the *geometric-arithmetic index*) is

$$\mathrm{GA}(G) \;:=\; \mathrm{GA}_1(G) \;:=\; \sum_{uv \in E} \frac{2\sqrt{d_G(u)\, d_G(v)}}{d_G(u) + d_G(v)}.$$

Equivalently,

$$\mathrm{GA}_1(G) \;=\; \sum_{uv \in E} \frac{\sqrt{d_G(u)\, d_G(v)}}{\frac{1}{2}\,(d_G(u) + d_G(v))}.$$

Definition 4.14.2 (Merrifield-Simmons index)**.** Let $G = (V, E)$ be a finite simple graph. A set $S \subseteq V$ is called *independent* if no two distinct vertices of S are adjacent in G. The *Merrifield-Simmons index* of G, denoted by $\sigma(G)$, is the number of independent vertex sets of G (including the empty set), i.e.,

$$\sigma(G) \;:=\; \big|\{\, S \subseteq V : \; S \text{ is independent in } G \,\}\big|.$$

Remark 4.14.3 (Independence polynomial viewpoint)**.** Define the independence polynomial

$$I(G; x) \;:=\; \sum_{k \geq 0} i_k(G)\, x^k,$$

where $i_k(G)$ is the number of independent vertex sets of size k. Then $\sigma(G) = I(G; 1)$.

Definition 4.14.4 (Merrifield-Simmons index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph. A set $S \subseteq V$ is called *independent in* H if it contains no hyperedge, i.e.,

$$\forall\, e \in \mathcal{E}, \quad e \nsubseteq S.$$

Equivalently, S is independent iff for every $e \in \mathcal{E}$ one has $|S \cap e| \le |e| - 1$. The *Merrifield-Simmons index* of H is the number of independent vertex sets:

$$\sigma(H) \;:=\; \big|\{\, S \subseteq V :\; S \text{ is independent in } H \,\}\big|.$$

Definition 4.14.5 (Merrifield-Simmons index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph. A set $\mathcal{S} \subseteq \mathbb{V}$ is called *independent in* $\mathbb{H}$ if it contains no superhyperedge, i.e.,

$$\forall\, f \in \mathbb{E}, \quad f \nsubseteq \mathcal{S}.$$

The *Merrifield-Simmons index* of $\mathbb{H}$ is the number of independent supervertex sets:

$$\sigma(\mathbb{H}) \;:=\; \big|\{\, \mathcal{S} \subseteq \mathbb{V} :\; \mathcal{S} \text{ is independent in } \mathbb{H} \,\}\big|.$$

Example 4.14.6 (Merrifield–Simmons index of a small SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the finite SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f\}, \qquad f = \{A, B, C\}.$$

Thus $\mathbb{H}$ has a single superhyperedge containing all three supervertices.

A set $\mathcal{S} \subseteq \mathbb{V}$ is independent in $\mathbb{H}$ if and only if it does *not* contain the whole superhyperedge f, i.e., $f \nsubseteq \mathcal{S}$. Since $f = \mathbb{V}$, the only subset that violates independence is $\mathcal{S} = \mathbb{V}$ itself. Therefore every proper subset of $\mathbb{V}$ is independent.

Hence the Merrifield–Simmons index equals the number of all subsets of $\mathbb{V}$ minus the one forbidden subset:

$$\sigma(\mathbb{H}) = \big|\mathcal{P}(\mathbb{V})\big| - 1 = 2^{|\mathbb{V}|} - 1 = 2^3 - 1 = 7.$$

Equivalently, the independent sets are

$$\emptyset,\ \{A\},\ \{B\},\ \{C\},\ \{A, B\},\ \{A, C\},\ \{B, C\}.$$

Theorem 4.14.7 (SuperHyperGraph Merrifield-Simmons index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\sigma(\mathbb{G}) = \sigma(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\sigma(\mathbb{H}_0) = \sigma(H).$$

Consequently, Definition 4.14.5 strictly extends the Merrifield-Simmons indices of graphs and hypergraphs.

Proof. (1) A subset $\mathcal{S} \subseteq V$ is independent in the SuperHyperGraph $\mathbb{G} = (V, E)$ (in the sense of Definition 4.14.5) iff it contains no superhyperedge $f \in E$ as a subset, i.e., iff there is no edge $\{u, v\} \in E$ with $\{u, v\} \subseteq \mathcal{S}$. This holds exactly when $\mathcal{S}$ contains no adjacent pair of vertices in G, i.e., when $\mathcal{S}$ is an independent vertex set in the ordinary graph-theoretic sense. Hence the collections of independent sets in $\mathbb{G}$ and in G coincide, and therefore $\sigma(\mathbb{G}) = \sigma(G)$.

(2) In $\mathbb{H}_0 = (V, \mathcal{E})$, the supervertex set equals V and the superhyperedge family equals $\mathcal{E}$. A set $\mathcal{S} \subseteq V$ is independent in $\mathbb{H}_0$ iff for all $e \in \mathcal{E}$ one has $e \nsubseteq \mathcal{S}$, which is precisely the definition of independence in the hypergraph H given in Definition 4.14.4. Hence the families of independent sets coincide, and therefore $\sigma(\mathbb{H}_0) = \sigma(H)$. □

4.15 Total eccentricity index

Total eccentricity index is the sum, over all vertices, of each vertex's eccentricity: its maximum shortest-path distance to any vertex [185–187].

Definition 4.15.1 (Eccentricity and total eccentricity index)**.** [185–187] Let $G = (V(G), E(G))$ be a finite simple connected graph, and let $d_G(u, v)$ denote the usual shortest-path distance between vertices $u, v \in V(G)$.

For a vertex $v \in V(G)$, the *eccentricity* of v is

$$\varepsilon_G(v) \ := \ \max\{\, d_G(v, u) \mid u \in V(G) \,\}.$$

The *total eccentricity index* (or *total eccentricity*) of G is

$$\zeta(G) \ := \sum_{v \in V(G)} \varepsilon_G(v).$$

Remark 4.15.2 (Average eccentricity)**.** The *average eccentricity* is the arithmetic mean of vertex eccentricities:

$$\operatorname{avec}(G) \ := \ \frac{1}{|V(G)|} \sum_{v \in V(G)} \varepsilon_G(v) \ = \ \frac{\zeta(G)}{|V(G)|}.$$

Definition 4.15.3 (Eccentricity and total eccentricity index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $d_H(\cdot, \cdot)$ be the fixed hypergraph distance on V. For a vertex $v \in V$, the *eccentricity* of v in H is

$$\varepsilon_H(v) \ := \ \max\{\, d_H(v, u) \mid u \in V \,\}.$$

The *total eccentricity index* of H is

$$\zeta(H) \ := \sum_{v \in V} \varepsilon_H(v).$$

Definition 4.15.4 (Eccentricity and total eccentricity index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot, \cdot)$ be the fixed superdistance on $\mathbb{V}$. For a supervertex $X \in \mathbb{V}$, the *eccentricity* of X in $\mathbb{H}$ is

$$\varepsilon_{\mathbb{H}}(X) \ := \ \max\{\, d_{\mathbb{H}}(X, Y) \mid Y \in \mathbb{V} \,\}.$$

The *total eccentricity index* of $\mathbb{H}$ is

$$\zeta(\mathbb{H}) \ := \ \sum_{X \in \mathbb{V}} \varepsilon_{\mathbb{H}}(X).$$

Example 4.15.5 (Total eccentricity index of a small SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the finite connected SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{e_1, e_2\}, \qquad e_1 = \{A, B\}, \ \ e_2 = \{B, C\}.$$

Assume the superdistance $d_{\mathbb{H}}(\cdot, \cdot)$ is the standard shortest-path distance in the 2-section graph of $\mathbb{H}$ (i.e., two distinct supervertices are adjacent if they appear together in some superhyperedge). Then the 2-section is the path $A - B - C$, hence

$$d_{\mathbb{H}}(A, B) = 1, \quad d_{\mathbb{H}}(B, C) = 1, \quad d_{\mathbb{H}}(A, C) = 2,$$

and $d_{\mathbb{H}}(X, X) = 0$ for all $X \in \mathbb{V}$.

Therefore the eccentricities are

$$\varepsilon_{\mathbb{H}}(A) = \max\{0, 1, 2\} = 2, \qquad \varepsilon_{\mathbb{H}}(B) = \max\{1, 0, 1\} = 1, \qquad \varepsilon_{\mathbb{H}}(C) = \max\{2, 1, 0\} = 2.$$

Consequently, the total eccentricity index equals

$$\zeta(\mathbb{H}) = \sum_{X \in \mathbb{V}} \varepsilon_{\mathbb{H}}(X) = 2 + 1 + 2 = 5.$$

Theorem 4.15.6 (SuperHyperGraph total eccentricity index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple connected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$\zeta(\mathbb{G}) = \zeta(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the SuperHyperGraph obtained by viewing hyperedges as superhyperedges. Then*

$$\zeta(\mathbb{H}_0) = \zeta(H).$$

Consequently, Definition 4.15.4 strictly extends the total eccentricity indices of graphs and hypergraphs.

Proof. (1) For the graph-as-SuperHyperGraph $\mathbb{G} = (V, E)$, the superdistance agrees with the usual graph distance: $d_{\mathbb{G}}(u, v) = d_G(u, v)$ for all $u, v \in V$ (as established earlier for this embedding). Therefore, for each $v \in V$,

$$\varepsilon_{\mathbb{G}}(v) = \max_{u \in V} d_{\mathbb{G}}(v, u) = \max_{u \in V} d_G(v, u) = \varepsilon_G(v).$$

Summing over all $v \in V$ yields

$$\zeta(\mathbb{G}) = \sum_{v \in V} \varepsilon_{\mathbb{G}}(v) = \sum_{v \in V} \varepsilon_G(v) = \zeta(G).$$

(2) For the hypergraph-as-SuperHyperGraph $\mathbb{H}_0 = (V, \mathcal{E})$, the superdistance agrees with the hypergraph distance: $d_{\mathbb{H}_0}(u, v) = d_H(u, v)$ for all $u, v \in V$ (as established earlier for this embedding). Hence, for each $v \in V$,

$$\varepsilon_{\mathbb{H}_0}(v) = \max_{u \in V} d_{\mathbb{H}_0}(v, u) = \max_{u \in V} d_H(v, u) = \varepsilon_H(v).$$

Summing over $v \in V$ yields $\zeta(\mathbb{H}_0) = \zeta(H)$. □

4.16 Harary index of a SuperHyperGraph

Harary index of a graph sums reciprocals of shortest-path distances over all unordered vertex pairs, emphasizing closeness: nearby vertices contribute more than distant ones [188–191].

Definition 4.16.1 (Harary index of a graph)**.** Let $G = (V, E)$ be a finite connected graph, and let $d_G(\cdot, \cdot)$ denote the usual shortest-path distance on V. The *Harary index* of G is

$$\mathrm{Har}(G) \;:=\; \sum_{\{u,v\} \subseteq V} \frac{1}{d_G(u, v)}.$$

Definition 4.16.2 (Harary index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite connected hypergraph, and let $d_H(\cdot, \cdot)$ denote the fixed hypergraph distance on V (e.g., Berge-type distance). The *Harary index* of H is

$$\mathrm{Har}(H) \;:=\; \sum_{\{u,v\} \subseteq V} \frac{1}{d_H(u, v)}.$$

Definition 4.16.3 (Harary index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite connected SuperHyperGraph, and let $d_{\mathbb{H}}(\cdot, \cdot)$ denote the fixed superdistance on $\mathbb{V}$. The *Harary index* of $\mathbb{H}$ is

$$\mathrm{Har}(\mathbb{H}) \;:=\; \sum_{\{A,B\} \subseteq \mathbb{V}} \frac{1}{d_{\mathbb{H}}(A, B)}.$$

Example 4.16.4 (Harary index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C, D\}, \qquad \mathbb{E} = \{\, f_1, f_2 \,\}, \qquad f_1 = \{A, B, C\}, \;\; f_2 = \{C, D\}.$$

Thus A, B, C form a 3-uniform superhyperedge and C is linked to D by a 2-edge.

Using the standard superdistance (minimum superpath length), the pairwise distances are:

$$d_{\mathbb{H}}(A, B) = d_{\mathbb{H}}(A, C) = d_{\mathbb{H}}(B, C) = 1,$$
$$d_{\mathbb{H}}(C, D) = 1, \qquad d_{\mathbb{H}}(A, D) = d_{\mathbb{H}}(B, D) = 2.$$

Therefore, the Harary index is

$$\begin{aligned}\mathrm{Har}(\mathbb{H}) &= \frac{1}{d_{\mathbb{H}}(A,B)} + \frac{1}{d_{\mathbb{H}}(A,C)} + \frac{1}{d_{\mathbb{H}}(A,D)} + \frac{1}{d_{\mathbb{H}}(B,C)} + \frac{1}{d_{\mathbb{H}}(B,D)} + \frac{1}{d_{\mathbb{H}}(C,D)} \\ &= 1 + 1 + \frac{1}{2} + 1 + \frac{1}{2} + 1 \;=\; 5.\end{aligned}$$

Remark 4.16.5 (Well-definedness)**.** Because G, H, and $\mathbb{H}$ are assumed connected, one has $d_G(u, v) \geq 1$, $d_H(u, v) \geq 1$, and $d_{\mathbb{H}}(A, B) \geq 1$ for all distinct pairs; hence every summand is well-defined.

Theorem 4.16.6 (SuperHyperGraph Harary index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite connected graph and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$d_{\mathbb{G}}(u, v) = d_G(u, v) \quad \textit{for all } u, v \in V, \qquad \textit{and consequently} \qquad \mathrm{Har}(\mathbb{G}) = \mathrm{Har}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite connected hypergraph and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges). Then*

$$d_{\mathbb{H}_0}(u, v) = d_H(u, v) \quad \textit{for all } u, v \in V, \qquad \textit{and consequently} \qquad \mathrm{Har}(\mathbb{H}_0) = \mathrm{Har}(H).$$

In particular, Definition 4.16.3 strictly extends the Harary indices of graphs (Definition 4.16.1) and hypergraphs (Definition 4.16.2).

Proof. (1) In $\mathbb{G} = (V, E)$, a superpath is exactly an ordinary graph path in G (each superhyperedge is a 2-set), so the minimal superpath length between u and v equals the usual shortest-path distance: $d_{\mathbb{G}}(u, v) = d_G(u, v)$. Substituting into Definition 4.16.3 yields

$$\mathrm{Har}(\mathbb{G}) = \sum_{\{u,v\} \subseteq V} \frac{1}{d_{\mathbb{G}}(u, v)} = \sum_{\{u,v\} \subseteq V} \frac{1}{d_G(u, v)} = \mathrm{Har}(G).$$

(2) In $\mathbb{H}_0 = (V, \mathcal{E})$, a superpath is precisely a Berge path in H (the incidence condition is identical), hence $d_{\mathbb{H}_0}(u, v) = d_H(u, v)$ for all $u, v \in V$. Therefore,

$$\mathrm{Har}(\mathbb{H}_0) = \sum_{\{u,v\} \subseteq V} \frac{1}{d_{\mathbb{H}_0}(u, v)} = \sum_{\{u,v\} \subseteq V} \frac{1}{d_H(u, v)} = \mathrm{Har}(H).$$

□

4.17 Kirchhoff index of a SuperHyperGraph

Kirchhoff index equals the sum of effective resistances over all vertex pairs, equivalently n times the Laplacian pseudoinverse trace, measuring global connectivity [192–195].

Definition 4.17.1 (Kirchhoff index of a graph)**.** Let $G = (V, E)$ be a finite connected simple graph on $n = |V|$ vertices. Let $A(G)$ be its adjacency matrix and $D(G) = \mathrm{diag}(d_G(v))_{v\in V}$ its degree matrix. The (combinatorial) Laplacian is

$$L(G) \;:=\; D(G) - A(G).$$

Let $L(G)^+$ denote the Moore–Penrose pseudoinverse of $L(G)$. The *Kirchhoff index* of G is

$$\mathrm{Kf}(G) \;:=\; n\,\mathrm{tr}\big(L(G)^+\big) \;=\; n\sum_{i=2}^{n} \frac{1}{\lambda_i(L(G))},$$

where $0 = \lambda_1(L(G)) < \lambda_2(L(G)) \le \cdots \le \lambda_n(L(G))$ are the eigenvalues of $L(G)$.

Remark 4.17.2 (Equivalent effective-resistance form)**.** For $u, v \in V$, define the effective resistance

$$R^G_{\mathrm{eff}}(u, v) \;:=\; (e_u - e_v)^{\mathsf{T}} L(G)^+ (e_u - e_v),$$

where e_u is the standard basis vector of $\mathbb{R}^V$ at u. Then $\mathrm{Kf}(G) = \sum_{\{u,v\}\subseteq V} R^G_{\mathrm{eff}}(u, v)$.

Definition 4.17.3 (Clique-expansion adjacency and Laplacian of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph with $n = |V|$. Define the symmetric matrix $A(H) = (a_{uv})_{u,v\in V}$ by

$$a_{uu} \;:=\; 0 \quad (u \in V), \qquad a_{uv} \;:=\; \sum_{\substack{e\in\mathcal{E}\\ \{u,v\}\subseteq e}} \frac{1}{|e| - 1} \quad (u \ne v).$$

Let $D(H) = \mathrm{diag}\big(\delta_H(u)\big)_{u\in V}$, where

$$\delta_H(u) \;:=\; \sum_{v\in V} a_{uv},$$

and define the (weighted) Laplacian of H by

$$L(H) \;:=\; D(H) - A(H).$$

Definition 4.17.4 (Kirchhoff index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph on $n = |V|$ vertices such that the Laplacian $L(H)$ (from Definition 4.17.3) has a one-dimensional kernel (equivalently, the weighted graph with adjacency $A(H)$ is connected). Let $L(H)^+$ be the Moore–Penrose pseudoinverse. The *Kirchhoff index* of H is

$$\mathrm{Kf}(H) \;:=\; n\,\mathrm{tr}\big(L(H)^+\big) \;=\; n\sum_{i=2}^{n} \frac{1}{\lambda_i(L(H))},$$

where $0 = \lambda_1(L(H)) < \lambda_2(L(H)) \le \cdots \le \lambda_n(L(H))$ are the eigenvalues of $L(H)$.

Definition 4.17.5 (Clique-expansion adjacency and Laplacian of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $N = |\mathbb{V}|$. Define the symmetric matrix $A(\mathbb{H}) = (a_{AB})_{A,B\in\mathbb{V}}$ by

$$a_{AA} := 0 \quad (A \in \mathbb{V}), \qquad a_{AB} := \sum_{\substack{f\in\mathbb{E} \\ \{A,B\}\subseteq f}} \frac{1}{|f|-1} \quad (A \neq B).$$

Let $D(\mathbb{H}) = \operatorname{diag}\big(\delta_{\mathbb{H}}(A)\big)_{A\in\mathbb{V}}$, where

$$\delta_{\mathbb{H}}(A) := \sum_{B\in\mathbb{V}} a_{AB},$$

and define the (weighted) Laplacian of $\mathbb{H}$ by

$$L(\mathbb{H}) := D(\mathbb{H}) - A(\mathbb{H}).$$

Definition 4.17.6 (Kirchhoff index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph on $N = |\mathbb{V}|$ supervertices such that the Laplacian $L(\mathbb{H})$ (Definition 4.17.5) has a one-dimensional kernel (equivalently, the weighted graph with adjacency $A(\mathbb{H})$ is connected). Let $L(\mathbb{H})^+$ be the Moore–Penrose pseudoinverse. The *Kirchhoff index* of $\mathbb{H}$ is

$$\mathrm{Kf}(\mathbb{H}) := N \operatorname{tr}\!\big(L(\mathbb{H})^+\big) = N \sum_{i=2}^{N} \frac{1}{\lambda_i(L(\mathbb{H}))},$$

where $0 = \lambda_1(L(\mathbb{H})) < \lambda_2(L(\mathbb{H})) \le \cdots \le \lambda_N(L(\mathbb{H}))$.

Example 4.17.7 (Kirchhoff index of a minimal nontrivial SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f\}, \qquad f = \{A, B, C\}.$$

Using the clique-expansion adjacency from Definition 4.17.5, for $X \neq Y$ we have

$$a_{XY} = \sum_{\substack{g\in\mathbb{E} \\ \{X,Y\}\subseteq g}} \frac{1}{|g|-1} = \frac{1}{|f|-1} = \frac{1}{2}, \qquad a_{XX} = 0.$$

Hence

$$A(\mathbb{H}) = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

The weighted degree of each supervertex is $\delta_{\mathbb{H}}(A) = \delta_{\mathbb{H}}(B) = \delta_{\mathbb{H}}(C) = 1$, so

$$D(\mathbb{H}) = \operatorname{diag}(1,1,1), \qquad L(\mathbb{H}) = D(\mathbb{H}) - A(\mathbb{H}) = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}.$$

Since $A(\mathbb{H}) = \frac{1}{2}(J_3 - I_3)$, we have

$$L(\mathbb{H}) = \frac{3}{2} I_3 - \frac{1}{2} J_3,$$

so the eigenvalues of $L(\mathbb{H})$ are

$$\lambda_1(L(\mathbb{H})) = 0, \qquad \lambda_2(L(\mathbb{H})) = \lambda_3(L(\mathbb{H})) = \frac{3}{2}.$$

Therefore, by Definition 4.17.6 with $N = |\mathbb{V}| = 3$,

$$\mathrm{Kf}(\mathbb{H}) = 3\left(\frac{1}{3/2} + \frac{1}{3/2}\right) = 3\left(\frac{2}{3} + \frac{2}{3}\right) = 4.$$

Theorem 4.17.8 (SuperHyperGraph Kirchhoff index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite connected simple graph and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$A(\mathbb{G}) = A(G), \qquad L(\mathbb{G}) = L(G), \qquad \textit{and hence} \qquad \mathrm{Kf}(\mathbb{G}) = \mathrm{Kf}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges). Then*

$$A(\mathbb{H}_0) = A(H), \qquad L(\mathbb{H}_0) = L(H), \qquad \textit{and hence} \qquad \mathrm{Kf}(\mathbb{H}_0) = \mathrm{Kf}(H).$$

Consequently, the Kirchhoff index of SuperHyperGraphs in Definition 4.17.6 strictly extends the Kirchhoff indices of graphs and hypergraphs.

Proof. (1) For $\mathbb{G} = (V, E)$, every superhyperedge has size 2. Hence, for distinct $u, v \in V$,

$$a_{uv}(\mathbb{G}) = \sum_{\substack{f \in E \\ \{u,v\} \subseteq f}} \frac{1}{|f| - 1} = \begin{cases} 1, & \{u, v\} \in E, \\ 0, & \text{otherwise,} \end{cases}$$

so $A(\mathbb{G}) = A(G)$ entrywise and therefore $L(\mathbb{G}) = D(\mathbb{G}) - A(\mathbb{G}) = D(G) - A(G) = L(G)$. Taking Moore–Penrose pseudoinverses gives $L(\mathbb{G})^+ = L(G)^+$, whence

$$\mathrm{Kf}(\mathbb{G}) = |V| \operatorname{tr}\big(L(\mathbb{G})^+\big) = |V| \operatorname{tr}\big(L(G)^+\big) = \mathrm{Kf}(G).$$

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$, the superedge family equals $\mathcal{E}$. Thus the defining formula for clique-expansion adjacency gives, for all $u, v \in V$,

$$a_{uv}(\mathbb{H}_0) = \sum_{\substack{f \in \mathcal{E} \\ \{u,v\} \subseteq f}} \frac{1}{|f| - 1} = a_{uv}(H),$$

so $A(\mathbb{H}_0) = A(H)$ and hence $L(\mathbb{H}_0) = L(H)$. Therefore $L(\mathbb{H}_0)^+ = L(H)^+$ and

$$\mathrm{Kf}(\mathbb{H}_0) = |V| \operatorname{tr}\big(L(\mathbb{H}_0)^+\big) = |V| \operatorname{tr}\big(L(H)^+\big) = \mathrm{Kf}(H).$$

□

4.18 Balaban index of a SuperHyperGraph

Balaban index normalizes a sum over edges of reciprocal square roots of endpoint transmissions, measuring global branching via distance-based vertex centralities and cyclomatic correction [196–199].

Definition 4.18.1 (Transmission)**.** Let X be a finite set and let $d : X \times X \to \mathbb{R}_{\geq 0}$ be a symmetric function with $d(x, x) = 0$. Assume (X, d) is connected in the sense that $d(x, y) > 0$ for all distinct $x, y \in X$ (e.g., d is a graph/hypergraph distance). For $x \in X$, the *transmission* of x is

$$w_{(X,d)}(x) \; := \; \sum_{y \in X} d(x, y).$$

Definition 4.18.2 (Balaban index of a graph)**.** [196–199] Let $G = (V, E)$ be a finite connected simple graph with $n = |V|$ and $m = |E|$. Let d_G be the usual graph distance and let

$$w_G(v) \; := \; \sum_{u \in V} d_G(v, u)$$

be the transmission of v (Definition 4.18.1). Define the cyclomatic number

$$\mu(G) \; := \; m - n + 1.$$

The *Balaban index* (Balaban J index) of G is

$$\mathrm{J}(G) \; := \; \frac{m}{\mu(G) + 1} \sum_{uv \in E} \frac{1}{\sqrt{w_G(u)\, w_G(v)}}.$$

Definition 4.18.3 (Balaban index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph on $n = |V|$ vertices. Let d_H be the fixed hypergraph distance on V (e.g., Berge-type distance), and define transmissions

$$w_H(v) \; := \; \sum_{u \in V} d_H(v, u) \qquad (v \in V).$$

For distinct $u, v \in V$, let $\mu_H(u, v)$ be the pair-incidence multiplicity (the number of hyperedges containing $\{u, v\}$). Define the *pair-incidence edge count*

$$m_2(H) \; := \; \sum_{\{u,v\} \subseteq V} \mu_H(u, v),$$

and the associated cyclomatic-type parameter

$$\mu_2(H) \; := \; m_2(H) - n + 1.$$

Assume $\mu_2(H) \geq 0$ and $w_H(v) > 0$ for all $v \in V$ (in particular, the distance structure is connected). The *Balaban index* of H is

$$\mathrm{J}(H) \; := \; \frac{m_2(H)}{\mu_2(H) + 1} \sum_{\{u,v\} \subseteq V} \frac{\mu_H(u, v)}{\sqrt{w_H(u)\, w_H(v)}}.$$

Definition 4.18.4 (Balaban index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph on $N = |\mathbb{V}|$ supervertices. Let $d_{\mathbb{H}}$ be the fixed superdistance on $\mathbb{V}$ and define transmissions

$$w_{\mathbb{H}}(A) \; := \; \sum_{B \in \mathbb{V}} d_{\mathbb{H}}(A, B) \qquad (A \in \mathbb{V}).$$

For distinct $A, B \in \mathbb{V}$, let $\mu_{\mathbb{H}}(A, B)$ be the pair-incidence multiplicity (the number of superhyperedges containing $\{A, B\}$). Define

$$m_2(\mathbb{H}) \; := \; \sum_{\{A,B\} \subseteq \mathbb{V}} \mu_{\mathbb{H}}(A, B), \qquad \mu_2(\mathbb{H}) \; := \; m_2(\mathbb{H}) - N + 1.$$

Assume $\mu_2(\mathbb{H}) \geq 0$ and $w_{\mathbb{H}}(A) > 0$ for all $A \in \mathbb{V}$. The *Balaban index* of $\mathbb{H}$ is

$$\mathrm{J}(\mathbb{H}) \; := \; \frac{m_2(\mathbb{H})}{\mu_2(\mathbb{H}) + 1} \sum_{\{A,B\} \subseteq \mathbb{V}} \frac{\mu_{\mathbb{H}}(A, B)}{\sqrt{w_{\mathbb{H}}(A)\, w_{\mathbb{H}}(B)}}.$$

Example 4.18.5 (Balaban index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{\, f_1, f_2 \,\}, \qquad f_1 = \{A, B\}, \;\; f_2 = \{B, C\}.$$

Thus $\mathbb{H}$ is the path A–B–C viewed as a SuperHyperGraph. The superdistances are

$$d_{\mathbb{H}}(A, B) = d_{\mathbb{H}}(B, C) = 1, \qquad d_{\mathbb{H}}(A, C) = 2.$$

Step 1: transmissions. By definition,

$$w_{\mathbb{H}}(A) = d(A, A) + d(A, B) + d(A, C) = 0 + 1 + 2 = 3,$$

$$w_{\mathbb{H}}(B) = d(B, A) + d(B, B) + d(B, C) = 1 + 0 + 1 = 2,$$
$$w_{\mathbb{H}}(C) = d(C, A) + d(C, B) + d(C, C) = 2 + 1 + 0 = 3.$$

Step 2: pair-incidence multiplicities. The unordered pairs are $\{A, B\}, \{A, C\}, \{B, C\}$. Since $f_1 = \{A, B\}$ and $f_2 = \{B, C\}$,

$$\mu_{\mathbb{H}}(A, B) = 1, \qquad \mu_{\mathbb{H}}(B, C) = 1, \qquad \mu_{\mathbb{H}}(A, C) = 0.$$

Hence

$$m_2(\mathbb{H}) = \sum_{\{X,Y\} \subseteq \mathbb{V}} \mu_{\mathbb{H}}(X, Y) = 1 + 0 + 1 = 2, \qquad \mu_2(\mathbb{H}) = m_2(\mathbb{H}) - |\mathbb{V}| + 1 = 2 - 3 + 1 = 0.$$

Step 3: Balaban index. Using Definition 4.18.4,

$$\begin{aligned}
\mathrm{J}(\mathbb{H}) &= \frac{m_2(\mathbb{H})}{\mu_2(\mathbb{H}) + 1} \sum_{\{X,Y\} \subseteq \mathbb{V}} \frac{\mu_{\mathbb{H}}(X, Y)}{\sqrt{w_{\mathbb{H}}(X)\, w_{\mathbb{H}}(Y)}} \\
&= \frac{2}{1} \left(\frac{1}{\sqrt{w_{\mathbb{H}}(A)\, w_{\mathbb{H}}(B)}} + \frac{1}{\sqrt{w_{\mathbb{H}}(B)\, w_{\mathbb{H}}(C)}} \right) \\
&= 2 \left(\frac{1}{\sqrt{3 \cdot 2}} + \frac{1}{\sqrt{2 \cdot 3}} \right) = \frac{4}{\sqrt{6}}.
\end{aligned}$$

Theorem 4.18.6 (SuperHyperGraph Balaban index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite connected simple graph and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Assume the superdistance on $\mathbb{G}$ coincides with the usual graph distance (as fixed earlier). Then*

$$m_2(\mathbb{G}) = m, \qquad \mu_2(\mathbb{G}) = \mu(G), \qquad w_{\mathbb{G}}(v) = w_G(v) \;\; (v \in V),$$

and consequently

$$\mathrm{J}(\mathbb{G}) = \mathrm{J}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges). Assume the superdistance on $\mathbb{H}_0$ coincides with the chosen hypergraph distance d_H. Then*

$$m_2(\mathbb{H}_0) = m_2(H), \qquad \mu_2(\mathbb{H}_0) = \mu_2(H), \qquad w_{\mathbb{H}_0}(v) = w_H(v) \quad (v \in V),$$

and consequently

$$\mathrm{J}(\mathbb{H}_0) = \mathrm{J}(H).$$

Hence Definition 4.18.4 strictly extends the Balaban indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$ each superhyperedge has size 2, so for distinct $u, v \in V$,

$$\mu_{\mathbb{G}}(u, v) = \begin{cases} 1, & \{u, v\} \in E, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore

$$m_2(\mathbb{G}) = \sum_{\{u,v\} \subseteq V} \mu_{\mathbb{G}}(u, v) = |E| = m, \qquad \mu_2(\mathbb{G}) = m - n + 1 = \mu(G).$$

Moreover, by the assumed equality of distances, $d_{\mathbb{G}} = d_G$, hence transmissions coincide: $w_{\mathbb{G}}(v) = \sum_{u \in V} d_{\mathbb{G}}(v, u) = \sum_{u \in V} d_G(v, u) = w_G(v)$. Substituting these identities into Definition 4.18.4 yields exactly Definition 4.18.2, i.e., $\mathrm{J}(\mathbb{G}) = \mathrm{J}(G)$.

(2) For $\mathbb{H}_0 = (V, \mathcal{E})$ the superedge family equals $\mathcal{E}$, hence $\mu_{\mathbb{H}_0}(u, v) = \mu_H(u, v)$ for all distinct $u, v \in V$. Consequently $m_2(\mathbb{H}_0) = m_2(H)$ and $\mu_2(\mathbb{H}_0) = \mu_2(H)$. By the assumed equality of distances, $d_{\mathbb{H}_0} = d_H$, so $w_{\mathbb{H}_0}(v) = w_H(v)$ for all $v \in V$. Substituting into Definition 4.18.4 yields Definition 4.18.3, i.e., $\mathrm{J}(\mathbb{H}_0) = \mathrm{J}(H)$. □

4.19 Forgotten index of a SuperHyperGraph

Forgotten index is the sum over all vertices of the cube of their degrees, emphasizing high-degree vertices and capturing overall branching intensity [200–205].

Definition 4.19.1 (Forgotten index of a graph)**.** [200, 201] Let $G = (V, E)$ be a finite simple undirected graph. For $v \in V$, let $d_G(v) := |\{ u \in V : \{u, v\} \in E \}|$ be the (usual) degree of v. The *forgotten index* (or *F-index*) of G is

$$\mathrm{F}(G) := \sum_{v \in V} d_G(v)^3.$$

Definition 4.19.2 (Forgotten index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph. For $v \in V$, let $d_H(v) := |\{ e \in \mathcal{E} : v \in e \}|$ be the (hypergraph) degree of v. The *forgotten index* of H is

$$\mathrm{F}(H) := \sum_{v \in V} d_H(v)^3.$$

Definition 4.19.3 (Forgotten index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph. For $A \in \mathbb{V}$, let $d_{\mathbb{H}}(A) := |\{ f \in \mathbb{E} : A \in f \}|$ be the (super)degree of A. The *forgotten index* of $\mathbb{H}$ is

$$\mathrm{F}(\mathbb{H}) \;:=\; \sum_{A \in \mathbb{V}} d_{\mathbb{H}}(A)^3.$$

Example 4.19.4 (Forgotten index of a simple SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph with

$$\mathbb{V} = \{A, B, C, D\}, \qquad \mathbb{E} = \{ f_1, f_2, f_3 \}, \qquad f_1 = \{A, B, C\}, \;\; f_2 = \{B, C, D\}, \;\; f_3 = \{C, D\}.$$

The (super)degrees are

$$d_{\mathbb{H}}(A) = 1, \qquad d_{\mathbb{H}}(B) = 2, \qquad d_{\mathbb{H}}(C) = 2, \qquad d_{\mathbb{H}}(D) = 2.$$

Therefore, by Definition 4.19.3,

$$\mathrm{F}(\mathbb{H}) = \sum_{X \in \{A,B,C,D\}} d_{\mathbb{H}}(X)^3 = 1^3 + 2^3 + 2^3 + 2^3 = 1 + 8 + 8 + 8 = 25.$$

Theorem 4.19.5 (SuperHyperGraph forgotten index generalizes the graph and hypergraph cases)**.**

1. *Let $G = (V, E)$ be a finite simple undirected graph, and let $\mathbb{G} := (V, E)$ be the associated SuperHyperGraph (vertices as supervertices, edges as 2-element superhyperedges). Then*

$$d_{\mathbb{G}}(v) = d_G(v) \quad (v \in V), \qquad \textit{and consequently} \qquad \mathrm{F}(\mathbb{G}) = \mathrm{F}(G).$$

2. *Let $H = (V, \mathcal{E})$ be a finite hypergraph, and let $\mathbb{H}_0 := (V, \mathcal{E})$ be the associated SuperHyperGraph (obtained by viewing hyperedges as superhyperedges). Then*

$$d_{\mathbb{H}_0}(v) = d_H(v) \quad (v \in V), \qquad \textit{and consequently} \qquad \mathrm{F}(\mathbb{H}_0) = \mathrm{F}(H).$$

Hence Definition 4.19.3 strictly extends the forgotten indices of graphs and hypergraphs.

Proof. (1) In $\mathbb{G} = (V, E)$, the superedge family equals the edge set E, so

$$d_{\mathbb{G}}(v) = |\{ f \in E : v \in f \}| = |\{ \{u, v\} \in E \}| = d_G(v).$$

Substituting into Definition 4.19.3 gives

$$\mathrm{F}(\mathbb{G}) = \sum_{v \in V} d_{\mathbb{G}}(v)^3 = \sum_{v \in V} d_G(v)^3 = \mathrm{F}(G).$$

(2) In $\mathbb{H}_0 = (V, \mathcal{E})$, the superedge family equals $\mathcal{E}$, so for each $v \in V$,

$$d_{\mathbb{H}_0}(v) = |\{ f \in \mathcal{E} : v \in f \}| = d_H(v).$$

Hence

$$\mathrm{F}(\mathbb{H}_0) = \sum_{v \in V} d_{\mathbb{H}_0}(v)^3 = \sum_{v \in V} d_H(v)^3 = \mathrm{F}(H).$$

□

Chapter 5

Spectral SuperHyperGraph

Spectral graph theory studies graphs via the eigenvalues and eigenvectors of associated matrices (such as the adjacency and Laplacian matrices), thereby linking structural properties to connectivity, expansion, random walks, and dynamical behavior. These ideas are also closely related to applications in chemistry. In this chapter, we investigate spectral aspects of SuperHyperGraphs.

5.1 Graph Eigenvalues

Graph eigenvalues are the eigenvalues of a graph's adjacency (or Laplacian) matrix; they form the spectrum, encoding global structural properties: connectivity, expansion, dynamics, and symmetry [206–209].

Definition 5.1.1 (Eigenvalues of a matrix)**.** Let $A \in \mathbb{R}^{n\times n}$. A scalar $\lambda \in \mathbb{C}$ is an *eigenvalue* of A if there exists a nonzero vector $x \in \mathbb{C}^n$ such that

$$Ax = \lambda x.$$

When A is real symmetric (as in the graph matrices below), all eigenvalues are real and one may take $x \in \mathbb{R}^n$.

Definition 5.1.2 (Adjacency and Laplacian matrices of a graph)**.** Let $G = (V, E)$ be a finite simple undirected graph with $V = \{1, \dots, n\}$. The *adjacency matrix* of G is $A(G) = (a_{ij}) \in \{0, 1\}^{n\times n}$ defined by

$$a_{ij} = \begin{cases} 1, & \{i, j\} \in E, \\ 0, & \text{otherwise.} \end{cases}$$

Let $d_i := |\{j \in V : \{i, j\} \in E\}|$ be the degree of vertex i, and let $D(G) := \mathrm{diag}(d_1, \dots, d_n)$. The *(combinatorial) Laplacian matrix* and *signless Laplacian matrix* are

$$L(G) := D(G) - A(G), \qquad Q(G) := D(G) + A(G).$$

Definition 5.1.3 (Graph eigenvalues and spectra)**.** The *adjacency eigenvalues* (resp. *Laplacian eigenvalues*, *signless Laplacian eigenvalues*) of G are the eigenvalues of $A(G)$ (resp. $L(G)$, $Q(G)$), counted with algebraic multiplicity. Their multisets are denoted by $\operatorname{spec}(A(G))$, $\operatorname{spec}(L(G))$, and $\operatorname{spec}(Q(G))$, respectively. The *spectral radius* of G is $\rho(G) := \max \operatorname{spec}(A(G))$.

Definition 5.1.4 (Tensor–vector products)**.** Let $\mathcal{T} = (t_{i_1 \cdots i_k})$ be a real tensor of order $k \geq 2$ and dimension n. For $x \in \mathbb{R}^n$, define $\mathcal{T}x^{k-1} \in \mathbb{R}^n$ componentwise by

$$\left(\mathcal{T}x^{k-1}\right)_i := \sum_{i_2,\ldots,i_k=1}^{n} t_{i\, i_2 \cdots i_k}\, x_{i_2} \cdots x_{i_k} \qquad (i = 1, \ldots, n).$$

Also write $x^{[k-1]} \in \mathbb{R}^n$ for the vector with entries $\left(x^{[k-1]}\right)_i := x_i^{k-1}$.

Definition 5.1.5 (H-eigenvalues of a tensor)**.** Let $\mathcal{T}$ be a real tensor of order $k \geq 2$ and dimension n, and let $\mathcal{I}$ be the identity tensor (with entries $i_{i_1 \cdots i_k} = 1$ if $i_1 = \cdots = i_k$ and 0 otherwise). A real number $\lambda \in \mathbb{R}$ is an *H-eigenvalue* of $\mathcal{T}$ if there exists a nonzero vector $x \in \mathbb{R}^n$ such that

$$(\lambda \mathcal{I} - \mathcal{T})x^{k-1} = 0, \quad \text{equivalently} \quad \mathcal{T}x^{k-1} = \lambda x^{[k-1]}.$$

Such an x is called an *H-eigenvector* associated with λ.

Definition 5.1.6 (Adjacency and Laplacian tensors of a k-uniform hypergraph)**.** Let $H = (V, E)$ be a finite simple k-uniform hypergraph ($k \geq 3$) on $V = \{1, \ldots, n\}$. Its *adjacency tensor* is the order-k, dimension-n tensor $\mathcal{A}(H) = (a_{i_1 \cdots i_k})$ given by

$$a_{i_1 \cdots i_k} := \begin{cases} \dfrac{1}{(k-1)!}, & \{i_1, \ldots, i_k\} \in E, \\ 0, & \text{otherwise.} \end{cases}$$

Let $d_i := |\{e \in E : i \in e\}|$ be the degree of vertex i, and let $\mathcal{D}(H)$ be the diagonal order-k tensor whose diagonal entry $d_{i \cdots i}$ equals d_i. The *Laplacian tensor* and *signless Laplacian tensor* are

$$\mathcal{L}(H) := \mathcal{D}(H) - \mathcal{A}(H), \qquad \mathcal{Q}(H) := \mathcal{D}(H) + \mathcal{A}(H).$$

Definition 5.1.7 (Hypergraph eigenvalues (tensor-based))**.** For a k-uniform hypergraph H, the *adjacency H-eigenvalues* (resp. *Laplacian H-eigenvalues*, *signless Laplacian H-eigenvalues*) are the H-eigenvalues of $\mathcal{A}(H)$ (resp. $\mathcal{L}(H)$, $\mathcal{Q}(H)$), counted with multiplicity. Their multisets are denoted by $\operatorname{spec}_H(\mathcal{A}(H))$, $\operatorname{spec}_H(\mathcal{L}(H))$, and $\operatorname{spec}_H(\mathcal{Q}(H))$, respectively.

Remark 5.1.8 (Consistency with graphs)**.** When $k = 2$, the above tensor definitions reduce to the usual matrix definitions: $\mathcal{A}(H)$ becomes the adjacency matrix and $\mathcal{L}(H)$ becomes the graph Laplacian matrix, and Definition 5.1.5 becomes $Ax = \lambda x$.

Definition 5.1.9 (Adjacency tensor of a k-uniform n-SuperHyperGraph)**.** Let $\mathbb{H} = (V, E)$ be a finite k-uniform n-SuperHyperGraph with $|V| = N$ and a fixed labeling $V = \{X_1, \ldots, X_N\}$. Its *adjacency tensor* is the order-k, dimension-N symmetric tensor $\mathcal{A}(\mathbb{H}) = (a_{i_1 \cdots i_k})$ defined by

$$a_{i_1 \cdots i_k} := \begin{cases} \dfrac{1}{(k-1)!}, & \{X_{i_1}, \ldots, X_{i_k}\} \in E, \\ 0, & \text{otherwise.} \end{cases}$$

For each supervertex X_i, its (hyper)degree is $d_i := |\{\varepsilon \in E : X_i \in \varepsilon\}|$. Let $\mathcal{D}(\mathbb{H})$ be the diagonal order-k tensor with diagonal entries $d_{i\cdots i} = d_i$. Define the *Laplacian tensor* and *signless Laplacian tensor* by

$$\mathcal{L}(\mathbb{H}) := \mathcal{D}(\mathbb{H}) - \mathcal{A}(\mathbb{H}), \qquad \mathcal{Q}(\mathbb{H}) := \mathcal{D}(\mathbb{H}) + \mathcal{A}(\mathbb{H}).$$

Definition 5.1.10 (H-eigenvalues of a tensor)**.** Let $\mathcal{T}$ be a real tensor of order $k \geq 2$ and dimension N. For $x \in \mathbb{R}^N$, define $\mathcal{T}x^{k-1} \in \mathbb{R}^N$ by

$$\left(\mathcal{T}x^{k-1}\right)_i := \sum_{i_2,\ldots,i_k=1}^{N} t_{i\,i_2\cdots i_k}\, x_{i_2} \cdots x_{i_k}, \qquad x^{[k-1]} := (x_1^{k-1}, \ldots, x_N^{k-1}).$$

A scalar $\lambda \in \mathbb{R}$ is an *H-eigenvalue* of $\mathcal{T}$ if there exists $x \in \mathbb{R}^N \setminus \{0\}$ such that

$$\mathcal{T}x^{k-1} = \lambda\, x^{[k-1]}.$$

Definition 5.1.11 (SuperHyperGraph eigenvalues and spectra)**.** Let $\mathbb{H}$ be a finite k-uniform n-SuperHyperGraph. The *adjacency eigenvalues* of $\mathbb{H}$ are the H-eigenvalues of $\mathcal{A}(\mathbb{H})$. Similarly, the *Laplacian eigenvalues* and *signless Laplacian eigenvalues* of $\mathbb{H}$ are the H-eigenvalues of $\mathcal{L}(\mathbb{H})$ and $\mathcal{Q}(\mathbb{H})$, respectively. We denote these multisets (with multiplicity) by

$$\mathrm{spec}_H\big(\mathcal{A}(\mathbb{H})\big), \quad \mathrm{spec}_H\big(\mathcal{L}(\mathbb{H})\big), \quad \mathrm{spec}_H\big(\mathcal{Q}(\mathbb{H})\big).$$

Example 5.1.12 (A 3-uniform 1-SuperHyperGraph with explicit H-spectra)**.** Let $V_0 = \{a, b, c\}$ and $n = 1$. Define the 1-supervertex set

$$\mathbb{V} = \{X_1, X_2, X_3\} \quad \text{with} \quad X_1 = \{a\},\ X_2 = \{b\},\ X_3 = \{c\}.$$

Let $\mathbb{E} = \{f\}$ with the unique 3-superedge

$$f = \{X_1, X_2, X_3\}.$$

Then $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ is k-uniform with $k = 3$ (every superedge has size 3).

Adjacency tensor. By Definition 5.1.9 (with $k = 3$), the adjacency tensor $\mathcal{A}(\mathbb{H}) = (a_{i_1 i_2 i_3})$ has entries

$$a_{i_1 i_2 i_3} = \begin{cases} \frac{1}{(3-1)!} = \frac{1}{2}, & \{i_1, i_2, i_3\} = \{1, 2, 3\}, \\ 0, & \text{otherwise.} \end{cases}$$

Hence, for $x = (x_1, x_2, x_3)^\mathsf{T} \in \mathbb{R}^3$, Definition 5.1.4 gives

$$\big(\mathcal{A}(\mathbb{H})x^2\big)_1 = x_2 x_3, \qquad \big(\mathcal{A}(\mathbb{H})x^2\big)_2 = x_1 x_3, \qquad \big(\mathcal{A}(\mathbb{H})x^2\big)_3 = x_1 x_2.$$

The H-eigenvalue equation (Definition 5.1.10) becomes

$$x_2 x_3 = \lambda x_1^2, \qquad x_1 x_3 = \lambda x_2^2, \qquad x_1 x_2 = \lambda x_3^2.$$

If $x_1 x_2 x_3 \neq 0$, multiplying the three equations yields $\lambda^3 = 1$, so (for real λ) one has $\lambda = 1$; then the ratio relations force $x_1 = x_2 = x_3$, so $x = (1, 1, 1)^\mathsf{T}$ is an H-eigenvector for $\lambda = 1$. If x has at least two zero coordinates (e.g., $x = (1, 0, 0)^\mathsf{T}$), then $\mathcal{A}(\mathbb{H})x^2 = 0$, so $\lambda = 0$ is also an H-eigenvalue. Therefore the (real) H-spectrum is

$$\mathrm{spec}_H\big(\mathcal{A}(\mathbb{H})\big) = \{\, 1,\, 0 \,\}.$$

Laplacian and signless Laplacian tensors. Each supervertex lies in exactly one superedge, so the degrees are $d_1 = d_2 = d_3 = 1$, and $\mathcal{D}(\mathbb{H})$ is the diagonal order-3 tensor with diagonal entries 1. Thus $\mathcal{L}(\mathbb{H}) = \mathcal{D}(\mathbb{H}) - \mathcal{A}(\mathbb{H})$ and $\mathcal{Q}(\mathbb{H}) = \mathcal{D}(\mathbb{H}) + \mathcal{A}(\mathbb{H})$ satisfy

$$\big(\mathcal{L}(\mathbb{H})x^2\big)_1 = x_1^2 - x_2x_3, \quad \big(\mathcal{L}(\mathbb{H})x^2\big)_2 = x_2^2 - x_1x_3, \quad \big(\mathcal{L}(\mathbb{H})x^2\big)_3 = x_3^2 - x_1x_2,$$

$$\big(\mathcal{Q}(\mathbb{H})x^2\big)_1 = x_1^2 + x_2x_3, \quad \big(\mathcal{Q}(\mathbb{H})x^2\big)_2 = x_2^2 + x_1x_3, \quad \big(\mathcal{Q}(\mathbb{H})x^2\big)_3 = x_3^2 + x_1x_2.$$

For $x = (1,1,1)^\mathsf{T}$,

$$\mathcal{L}(\mathbb{H})x^2 = 0 \cdot x^{[2]}, \qquad \mathcal{Q}(\mathbb{H})x^2 = 2 \cdot x^{[2]},$$

so $0 \in \mathrm{spec}_H(\mathcal{L}(\mathbb{H}))$ and $2 \in \mathrm{spec}_H(\mathcal{Q}(\mathbb{H}))$. For $x = (1,0,0)^\mathsf{T}$,

$$\mathcal{L}(\mathbb{H})x^2 = 1 \cdot x^{[2]}, \qquad \mathcal{Q}(\mathbb{H})x^2 = 1 \cdot x^{[2]},$$

so 1 is an H-eigenvalue of both $\mathcal{L}(\mathbb{H})$ and $\mathcal{Q}(\mathbb{H})$. In fact, as above one checks that these are the only real H-eigenvalues, hence

$$\mathrm{spec}_H\big(\mathcal{L}(\mathbb{H})\big) = \{\,0,\,1\,\}, \qquad \mathrm{spec}_H\big(\mathcal{Q}(\mathbb{H})\big) = \{\,1,\,2\,\}.$$

Theorem 5.1.13 (Hypergraph eigenvalues are a special case of n-SuperHyperGraph eigenvalues)**.** *Let $H = (V_0, \mathcal{E}_0)$ be a finite simple k-uniform hypergraph, and let $\mathbb{H}^{(n)}$ be its canonical k-uniform n-SuperHyperGraph embedding. Then, after identifying vertices via the bijection $\varphi = \mathrm{lift}_{n-1}$,*

$$\mathrm{spec}_H\big(\mathcal{A}(H)\big) = \mathrm{spec}_H\big(\mathcal{A}(\mathbb{H}^{(n)})\big), \quad \mathrm{spec}_H\big(\mathcal{L}(H)\big) = \mathrm{spec}_H\big(\mathcal{L}(\mathbb{H}^{(n)})\big), \quad \mathrm{spec}_H\big(\mathcal{Q}(H)\big) = \mathrm{spec}_H\big(\mathcal{Q}(\mathbb{H}^{(n)})\big).$$

In particular, adjacency/Laplacian/signless-Laplacian eigenpairs correspond under coordinate relabeling.

Proof. Fix an ordering $V_0 = \{v_1, \dots, v_N\}$ and label $V = \{\varphi(v_1), \dots, \varphi(v_N)\}$. We have

$$\{v_{i_1}, \dots, v_{i_k}\} \in \mathcal{E}_0 \quad \Longleftrightarrow \quad \{\varphi(v_{i_1}), \dots, \varphi(v_{i_k})\} \in E.$$

Comparing Definition 5.1.9 with the standard adjacency-tensor definition for k-uniform hypergraphs (on the vertex list $v_1, \dots, v_N$), we see that the tensors $\mathcal{A}(H)$ and $\mathcal{A}(\mathbb{H}^{(n)})$ have identical entries under this identification; hence they are the same tensor up to the chosen labeling. The same holds for degree tensors $\mathcal{D}$, because degrees are preserved by the edge correspondence, and therefore also for $\mathcal{L} = \mathcal{D} - \mathcal{A}$ and $\mathcal{Q} = \mathcal{D} + \mathcal{A}$.

Consequently, the polynomial eigen-equation $\mathcal{T}x^{k-1} = \lambda x^{[k-1]}$ (Definition 5.1.10) is identical for H and $\mathbb{H}^{(n)}$ after relabeling coordinates, so the eigenvalues (with multiplicity) coincide, and eigenvectors correspond by the same relabeling. □

Theorem 5.1.14 (Graph eigenvalues are a further special case)**.** *Let $G = (V_0, E_0)$ be a finite simple undirected graph. View G as a 2-uniform hypergraph $H = (V_0, \mathcal{E}_0)$ with $\mathcal{E}_0 = \{\{u,v\} : uv \in E_0\}$. Let $\mathbb{H}^{(n)}$ be its 2-uniform n-SuperHyperGraph embedding. Then the adjacency H-eigenvalue equation for $\mathbb{H}^{(n)}$ reduces to the matrix eigenvalue equation for G, and*

$$\mathrm{spec}\big(A(G)\big) = \mathrm{spec}_H\big(\mathcal{A}(\mathbb{H}^{(n)})\big), \qquad \mathrm{spec}\big(L(G)\big) = \mathrm{spec}_H\big(\mathcal{L}(\mathbb{H}^{(n)})\big), \qquad \mathrm{spec}\big(Q(G)\big) = \mathrm{spec}_H\big(\mathcal{Q}(\mathbb{H}^{(n)})\big).$$

Proof. When $k = 2$, an order-2 tensor is just an $N \times N$ matrix. Moreover, for $k = 2$, the tensor eigen-equation $\mathcal{A}x^{k-1} = \lambda x^{[k-1]}$ becomes

$$Ax = \lambda x,$$

because $x^{k-1} = x$ and $x^{[k-1]} = x$. Thus the H-eigenvalues of $\mathcal{A}(\mathbb{H}^{(n)})$ coincide with the ordinary matrix eigenvalues of $A(G)$. The same reduction applies to $\mathcal{L}$ and $\mathcal{Q}$, yielding the Laplacian and signless Laplacian spectra. □

Remark 5.1.15 (Non-uniform superhypergraphs)**.** If $\mathbb{H} = (V, E)$ is not k-uniform (edge sizes vary), tensor spectra are no longer canonical without an additional choice (uniformization or operator model). In that setting one often defines eigenvalues via a chosen Laplacian/operator $L : \mathbb{R}^{|V|} \to \mathbb{R}^{|V|}$ and the equation $L(x) = \lambda x$, or via matrix models such as incidence-based operators. The uniform case above is the cleanest setting in which the tensor notion simultaneously generalizes hypergraph and graph eigenvalues without extra conventions.

5.2 HL-index of Graph

The *HL-index* (HOMO/LUMO index) of a graph [210–213] is a spectral descriptor: take the adjacency eigenvalues near the middle of the spectrum and set

$$R(G) = \max\{|\lambda_H|, |\lambda_L|\}.$$

Definition 5.2.1 (HL-index of a graph)**.** Let $G = (V, E)$ be a finite simple undirected graph on $n := |V|$ vertices, and let $A(G) \in \mathbb{R}^{n\times n}$ be its adjacency matrix. Let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

be the (real) eigenvalues of $A(G)$, listed with algebraic multiplicity. Define the *HOMO/LUMO indices* H, L by

$$(H, L) := \begin{cases} \left(\frac{n}{2},\ \frac{n}{2} + 1\right), & \text{if } n \text{ is even,} \\ \left(\frac{n+1}{2},\ \frac{n+1}{2}\right), & \text{if } n \text{ is odd.} \end{cases}$$

The *HL-index* of G is

$$R(G) \ := \ \max\{\, |\lambda_H|,\ |\lambda_L|\, \}.$$

Definition 5.2.2 (Clique-expansion adjacency matrix of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph with $V = \{1, \ldots, n\}$ and $\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$. Define the symmetric matrix $A(H) = (a_{ij}) \in \mathbb{R}^{n\times n}$ by

$$a_{ii} := 0, \qquad a_{ij} := \sum_{\substack{e\in\mathcal{E} \\ \{i,j\}\subseteq e}} \frac{1}{|e| - 1} \quad (i \neq j).$$

Definition 5.2.3 (HL-index of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph with $n := |V|$, and let $A(H)$ be as in Definition 5.2.2. Let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

be the (real) eigenvalues of $A(H)$, listed with algebraic multiplicity. With H, L defined from n exactly as in Definition 5.2.1, the *HL-index* of the hypergraph H is

$$R(H) \ := \ \max\{\, |\lambda_H|,\ |\lambda_L|\, \}.$$

Theorem 5.2.4 (Graphs are a special case)**.** *Let $G = (V, E)$ be a finite simple graph on $V = \{1, \ldots, n\}$, and view it as the 2-uniform hypergraph $H_G = (V, \mathcal{E})$ with $\mathcal{E} := \{\{i, j\} : \{i, j\} \in E\}$. Then $A(H_G) = A(G)$. Consequently,*

$$R(H_G) = R(G).$$

Proof. If $i \neq j$, then by Definition 5.2.2,

$$a_{ij}(H_G) = \sum_{\substack{e \in \mathcal{E} \\ \{i,j\} \subseteq e}} \frac{1}{|e| - 1}.$$

In a 2-uniform hypergraph, $\{i, j\} \subseteq e$ holds iff $e = \{i, j\}$, and then $|e| - 1 = 1$. Hence $a_{ij}(H_G) = 1$ exactly when $\{i, j\} \in E$, and $a_{ij}(H_G) = 0$ otherwise; also $a_{ii}(H_G) = 0$. Therefore $A(H_G)$ is exactly the adjacency matrix $A(G)$, so their eigenvalues coincide, and thus $R(H_G) = R(G)$ by Definitions 5.2.1 and 5.2.3. □

Definition 5.2.5 (Clique-expansion adjacency matrix of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $N := |\mathbb{V}|$. Fix an ordering $\mathbb{V} = \{X_1, \ldots, X_N\}$. Define the symmetric matrix $A(\mathbb{H}) = (a_{ij}) \in \mathbb{R}^{N \times N}$ by

$$a_{ii} := 0, \qquad a_{ij} := \sum_{\substack{f \in \mathbb{E} \\ \{X_i, X_j\} \subseteq f}} \frac{1}{|f| - 1} \quad (i \neq j).$$

We call $A(\mathbb{H})$ the *(normalized) clique-expansion adjacency matrix* of $\mathbb{H}$.

Definition 5.2.6 (HL-indices H, L (HOMO/LUMO positions))**.** Let $N \in \mathbb{N}$ and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ be a real sequence. Define indices $H, L \in \{1, \ldots, N\}$ by

$$(H, L) := \begin{cases} \left(\frac{N}{2}, \frac{N}{2} + 1\right), & \text{if } N \text{ is even}, \\ \left(\frac{N+1}{2}, \frac{N+1}{2}\right), & \text{if } N \text{ is odd}. \end{cases}$$

Definition 5.2.7 (HL-index of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $N := |\mathbb{V}|$. Let $A(\mathbb{H})$ be the matrix from Definition 5.2.5, and let

$$\lambda_1(\mathbb{H}) \geq \lambda_2(\mathbb{H}) \geq \cdots \geq \lambda_N(\mathbb{H})$$

be the eigenvalues of $A(\mathbb{H})$, listed with algebraic multiplicity. Let (H, L) be as in Definition 5.2.6 applied to N. The *HL-index* of $\mathbb{H}$ is

$$R(\mathbb{H}) \; := \; \max\{\, |\lambda_H(\mathbb{H})|, \; |\lambda_L(\mathbb{H})| \,\}.$$

Remark 5.2.8 (Well-definedness)**.** The matrix $A(\mathbb{H})$ is real symmetric, hence all eigenvalues are real and the ordering above is valid.

Example 5.2.9 (HL-index of a small SuperHyperGraph)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{f\}, \quad f = \{A, B, C\}.$$

Use the normalized clique-expansion adjacency matrix $A(\mathbb{H})$ from Definition 5.2.5. Since the unique superhyperedge has size $|f| = 3$, each distinct pair $\{X, Y\} \subseteq f$ contributes $\frac{1}{|f|-1} = \frac{1}{2}$. Hence, in the ordering (A, B, C),

$$A(\mathbb{H}) = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} = \frac{1}{2}(J_3 - I_3),$$

where J_3 is the 3×3 all-ones matrix.

The eigenvalues of $J_3 - I_3$ are $2, -1, -1$, hence

$$\lambda_1(\mathbb{H}) = 1, \qquad \lambda_2(\mathbb{H}) = \lambda_3(\mathbb{H}) = -\tfrac{1}{2}.$$

Here $N = 3$ is odd, so Definition 5.2.6 gives $(H, L) = \left(\frac{3+1}{2}, \frac{3+1}{2}\right) = (2, 2)$. Therefore, by Definition 5.2.7,

$$R(\mathbb{H}) = \max\{|\lambda_2(\mathbb{H})|, |\lambda_2(\mathbb{H})|\} = |\lambda_2(\mathbb{H})| = \frac{1}{2}.$$

Theorem 5.2.10 (HL-index of SuperHyperGraphs generalizes the hypergraph HL-index)**.** *Let $H = (V, \mathcal{E})$ be a finite hypergraph with $n := |V|$. Let $\mathbb{H}_0 = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph obtained by viewing H as a SuperHyperGraph:*

$$\mathbb{V} := V, \qquad \mathbb{E} := \mathcal{E}.$$

Let $A(H)$ be the clique-expansion adjacency matrix of the hypergraph H, i.e.,

$$A(H) = (b_{ij}), \qquad b_{ii} := 0, \qquad b_{ij} := \sum_{\substack{e \in \mathcal{E} \\ \{v_i, v_j\} \subseteq e}} \frac{1}{|e| - 1} \quad (i \neq j),$$

for a fixed ordering $V = \{v_1, \ldots, v_n\}$. Then

$$A(\mathbb{H}_0) = A(H).$$

Consequently, the eigenvalues (with multiplicity) coincide and

$$R(\mathbb{H}_0) = R(H),$$

where $R(H)$ denotes the HL-index of the hypergraph defined from $A(H)$ by the same HOMO/LUMO rule.

Proof. Fix an ordering $V = \{v_1, \ldots, v_n\}$ and identify $\mathbb{V} = V$ via $X_i := v_i$. For $i \neq j$, Definition 5.2.5 yields

$$a_{ij}(\mathbb{H}_0) = \sum_{\substack{f \in \mathbb{E} \\ \{X_i, X_j\} \subseteq f}} \frac{1}{|f| - 1} = \sum_{\substack{e \in \mathcal{E} \\ \{v_i, v_j\} \subseteq e}} \frac{1}{|e| - 1} = b_{ij}(H),$$

and also $a_{ii}(\mathbb{H}_0) = 0 = b_{ii}(H)$. Hence $A(\mathbb{H}_0) = A(H)$ entrywise, so their spectra coincide:

$$\lambda_k(\mathbb{H}_0) = \lambda_k(H) \qquad (k = 1, \ldots, n).$$

The HOMO/LUMO indices (H, L) depend only on n, so the same indices are used for both objects. Therefore,

$$R(\mathbb{H}_0) = \max\{|\lambda_H(\mathbb{H}_0)|, |\lambda_L(\mathbb{H}_0)|\} = \max\{|\lambda_H(H)|, |\lambda_L(H)|\} = R(H).$$

□

5.3 Singular graphs

A *singular graph* [214, 215] is a graph whose adjacency matrix is singular:

$$\det A(G) = 0, \quad \text{equivalently} \quad 0 \in \operatorname{spec}(A(G)).$$

Its *nullity* is $\eta(G) := \dim \ker A(G)$.

Definition 5.3.1 (Singular graph and nullity)**.** Let $G = (V, E)$ be a finite simple undirected graph on $n := |V|$ vertices, and let $A(G) \in \mathbb{R}^{n \times n}$ be its adjacency matrix. We say that G is *singular* if $A(G)$ is singular, i.e.,

$$\det A(G) = 0 \iff 0 \in \operatorname{spec}(A(G)).$$

The *nullity* of G is

$$\eta(G) \;:=\; \dim \ker A(G),$$

equivalently the (algebraic = geometric) multiplicity of the eigenvalue 0 in $\operatorname{spec}(A(G))$. A nonzero vector $x \in \ker A(G)$ is called a *kernel eigenvector* (a 0-eigenvector).

Definition 5.3.2 (Adjacency matrix of a hypergraph)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph of order $n := |V|$, where $\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ and $|e| \geq 2$ for all $e \in \mathcal{E}$. Fix an ordering $V = \{v_1, \ldots, v_n\}$. The *adjacency matrix* of H is the symmetric matrix $A(H) = (a_{ij}) \in \mathbb{R}^{n \times n}$ defined by

$$a_{ii} := 0, \qquad a_{ij} := \bigl|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\bigr| \quad (i \neq j).$$

Definition 5.3.3 (Singular hypergraph and nullity)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph and let $A(H)$ be its adjacency matrix (Definition 5.3.2). We say that H is *singular* if

$$\det A(H) = 0 \iff 0 \in \operatorname{spec}(A(H)).$$

The *nullity* of H is

$$\eta(H) \;:=\; \dim \ker A(H),$$

equivalently the multiplicity of 0 as an eigenvalue of $A(H)$.

Proposition 5.3.4 (Consistency with graphs)**.** *Let $G = (V, E)$ be a finite simple graph and view it as the 2-uniform hypergraph $H_G = (V, \mathcal{E})$ with $\mathcal{E} := \{\{u, v\} : \{u, v\} \in E\}$. Then $A(H_G) = A(G)$. In particular,*

$$G \text{ is singular} \iff H_G \text{ is singular}, \qquad \text{and} \qquad \eta(G) = \eta(H_G).$$

Proof. For $i \neq j$, Definition 5.3.2 gives

$$a_{ij}(H_G) = \bigl|\{e \in \mathcal{E} : \{v_i, v_j\} \subseteq e\}\bigr|.$$

Since every $e \in \mathcal{E}$ has size 2, we have $\{v_i, v_j\} \subseteq e$ if and only if $e = \{v_i, v_j\}$, so $a_{ij}(H_G) = 1$ exactly when $\{v_i, v_j\} \in E$, and $a_{ij}(H_G) = 0$ otherwise; also $a_{ii}(H_G) = 0$. Hence $A(H_G) = A(G)$, and the statements follow from Definitions 5.3.1 and 5.3.3. □

Definition 5.3.5 (Adjacency matrix of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $|\mathbb{V}| = N$, where $\mathbb{E} \subseteq \mathcal{P}(\mathbb{V}) \setminus \{\emptyset\}$. Fix an ordering $\mathbb{V} = \{X_1, \dots, X_N\}$. The *adjacency matrix* of $\mathbb{H}$ is the symmetric matrix $A(\mathbb{H}) = (a_{ij}) \in \mathbb{R}^{N \times N}$ defined by

$$a_{ii} := 0, \qquad a_{ij} := \big|\{\, f \in \mathbb{E} : \ \{X_i, X_j\} \subseteq f \,\}\big| \quad (i \neq j).$$

Definition 5.3.6 (Singular SuperHyperGraph and nullity)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph and let $A(\mathbb{H})$ be its adjacency matrix (Definition 5.3.5). We say that $\mathbb{H}$ is *singular* if $A(\mathbb{H})$ is singular, i.e.,

$$\det A(\mathbb{H}) = 0 \quad \Longleftrightarrow \quad 0 \in \operatorname{spec}(A(\mathbb{H})).$$

The *nullity* of $\mathbb{H}$ is

$$\eta(\mathbb{H}) \ := \ \dim \ker A(\mathbb{H}),$$

equivalently the multiplicity of the eigenvalue 0 in $\operatorname{spec}(A(\mathbb{H}))$.

Remark 5.3.7 (Model choice)**.** The adjacency matrix in Definition 5.3.5 is the natural pair-cooccurrence model: it counts how many superhyperedges contain a given unordered pair of distinct supervertices. Other matrix/tensor representations exist, but this one is the most direct extension of the standard hypergraph pair-incidence adjacency matrix.

Example 5.3.8 (A singular SuperHyperGraph with nullity 1)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \big\{f_1, f_2\big\},$$

where

$$f_1 = \{A, B\}, \qquad f_2 = \{B, C\}.$$

Using the pair-cooccurrence adjacency matrix (Definition 5.3.5), the unordered pairs $\{A, B\}$ and $\{B, C\}$ occur in exactly one superhyperedge each, while $\{A, C\}$ occurs in none. Hence, in the ordering (A, B, C),

$$A(\mathbb{H}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

A direct calculation gives

$$\det A(\mathbb{H}) = 0,$$

so $\mathbb{H}$ is *singular*. In fact, the eigenvalues are

$$\operatorname{spec}(A(\mathbb{H})) = \{\sqrt{2},\ 0,\ -\sqrt{2}\},$$

so $0 \in \operatorname{spec}(A(\mathbb{H}))$ with multiplicity 1. Therefore the nullity is

$$\eta(\mathbb{H}) = \dim \ker A(\mathbb{H}) = 1.$$

One nonzero kernel eigenvector is

$$x = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \qquad \text{since} \qquad A(\mathbb{H})\, x = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Theorem 5.3.9 (Singular SuperHyperGraphs generalize singular hypergraphs)**.** *Let $H = (V, \mathcal{E})$ be a finite hypergraph with $|V| = n$, and let $\mathbb{H}_0 = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph obtained by viewing H as a SuperHyperGraph:*

$$\mathbb{V} := V, \qquad \mathbb{E} := \mathcal{E}.$$

Let $A(H)$ be the hypergraph adjacency matrix

$$A(H) = (b_{ij}), \qquad b_{ii} := 0, \quad b_{ij} := \big|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\big| \ (i \neq j),$$

for a fixed ordering $V = \{v_1, \ldots, v_n\}$. Then

$$A(\mathbb{H}_0) = A(H).$$

Consequently,

$$H \text{ is singular} \iff \mathbb{H}_0 \text{ is singular}, \qquad \text{and} \qquad \eta(H) = \eta(\mathbb{H}_0).$$

Proof. Fix an ordering $V = \{v_1, \ldots, v_n\}$ and identify $\mathbb{V} = V$ via $X_i := v_i$. For $i \neq j$, by Definition 5.3.5,

$$a_{ij}(\mathbb{H}_0) = \big|\{\, f \in \mathbb{E} : \ \{X_i, X_j\} \subseteq f \,\}\big| = \big|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\big| = b_{ij}(H).$$

Also $a_{ii}(\mathbb{H}_0) = 0 = b_{ii}(H)$. Hence $A(\mathbb{H}_0) = A(H)$ entrywise. Therefore $\det A(\mathbb{H}_0) = \det A(H)$, the spectra coincide, and the nullities $\dim\ker A(\mathbb{H}_0) = \dim\ker A(H)$ coincide as well, proving the claims. □

5.4 Graph Energy

The *energy* of a graph G [216–218] is the sum of absolute values of its adjacency eigenvalues:

$$\mathcal{E}(G) \ = \ \sum_{i=1}^{n} \big|\lambda_i(A(G))\big|.$$

The energy of fuzzy graphs, neutrosophic graphs, and hypergraphs has also been studied in the literature [219–223].

Definition 5.4.1 (Graph energy)**.** Let $G = (V, E)$ be a finite simple undirected graph with $|V| = n$, and let $A(G) \in \mathbb{R}^{n\times n}$ be its adjacency matrix. Let

$$\lambda_1, \lambda_2, \ldots, \lambda_n$$

be the (real) eigenvalues of $A(G)$, counted with algebraic multiplicity. The *energy* of G is

$$\mathcal{E}(G) \ := \ \sum_{i=1}^{n} |\lambda_i|.$$

Remark 5.4.2 (Matrix viewpoint)**.** For any real matrix M, the *energy* (also called the *trace norm*) is defined by

$$\mathcal{E}(M) \ := \ \sum_{i} s_i(M),$$

where $s_i(M)$ are the singular values of M. If M is real symmetric, then $s_i(M) = |\lambda_i(M)|$, hence $\mathcal{E}(M) = \sum_i |\lambda_i(M)|$. In particular, $\mathcal{E}(G) = \mathcal{E}(A(G))$.

Definition 5.4.3 (Hypergraph adjacency matrix)**.** Let $H = (V, \mathcal{E})$ be a finite (simple) hypergraph with $V = \{v_1, \ldots, v_n\}$ and $\mathcal{E} \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$, where $|e| \geq 2$ for all $e \in \mathcal{E}$. Its *adjacency matrix* is the symmetric matrix $A(H) = (a_{ij}) \in \mathbb{R}^{n \times n}$ defined by

$$a_{ii} := 0, \qquad a_{ij} := \big|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\big| \quad (i \neq j).$$

Definition 5.4.4 (Adjacency energy of a hypergraph)**.** [224] Let H be a hypergraph on n vertices and let $A(H)$ be its adjacency matrix (Definition 5.4.3). Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $A(H)$, counted with algebraic multiplicity. The *(adjacency) energy* of H is

$$\mathcal{E}(H) \ := \ \sum_{i=1}^{n} |\lambda_i| \ = \ \|A(H)\|_*.$$

Proposition 5.4.5 (Graphs as a special case)**.** *Let $G = (V, E)$ be a finite simple graph on $V = \{v_1, \ldots, v_n\}$, and view it as the 2-uniform hypergraph $H_G = (V, \mathcal{E})$ with $\mathcal{E} := \{\{u, v\} : \{u, v\} \in E\}$. Then $A(H_G) = A(G)$. Consequently,*

$$\mathcal{E}(H_G) = \mathcal{E}(G).$$

Proof. For $i \neq j$,

$$a_{ij}(H_G) = \big|\{\, e \in \mathcal{E} : \{v_i, v_j\} \subseteq e \,\}\big|.$$

Since every $e \in \mathcal{E}$ has size 2, the condition $\{v_i, v_j\} \subseteq e$ holds if and only if $e = \{v_i, v_j\}$, hence $a_{ij}(H_G) = 1$ exactly when $\{v_i, v_j\} \in E$, and 0 otherwise; also $a_{ii}(H_G) = 0$. Thus $A(H_G) = A(G)$, so the eigenvalues (with multiplicity) coincide, and therefore the energies coincide. □

Definition 5.4.6 (Adjacency matrix of a SuperHyperGraph)**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $\mathbb{E} \subseteq \mathcal{P}(\mathbb{V}) \setminus \{\emptyset\}$ and $|\mathbb{V}| = N$. Fix an ordering $\mathbb{V} = \{X_1, \ldots, X_N\}$. The *adjacency matrix* of $\mathbb{H}$ is the symmetric matrix $A(\mathbb{H}) = (a_{ij}) \in \mathbb{R}^{N \times N}$ defined by

$$a_{ii} := 0, \qquad a_{ij} := \big|\{\, f \in \mathbb{E} : \ \{X_i, X_j\} \subseteq f \,\}\big| \quad (i \neq j).$$

Definition 5.4.7 (Energy of a SuperHyperGraph)**.** Let $\mathbb{H}$ be a finite SuperHyperGraph and let $A(\mathbb{H})$ be as in Definition 5.4.6. Let $\lambda_1, \ldots, \lambda_N$ be the eigenvalues of $A(\mathbb{H})$, counted with algebraic multiplicity. The *(adjacency) energy* of $\mathbb{H}$ is

$$\mathcal{E}(\mathbb{H}) \ := \ \sum_{i=1}^{N} |\lambda_i| \ = \ \|A(\mathbb{H})\|_*,$$

where $\| \cdot \|_*$ denotes the trace norm (sum of singular values).

Remark 5.4.8. Since $A(\mathbb{H})$ is real symmetric, its singular values equal $|\lambda_i|$, so $\mathcal{E}(\mathbb{H}) = \sum_i |\lambda_i|$ is well-defined and real.

Example 5.4.9 (Energy of a small SuperHyperGraph)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{A, B, C\}, \qquad \mathbb{E} = \{\, f \,\}, \quad f = \{A, B, C\}.$$

Using the pair-cooccurrence adjacency matrix (Definition 5.4.6), each unordered pair $\{A, B\}, \{A, C\}, \{B, C\}$ is contained in exactly one superhyperedge f. Hence, with the ordering (A, B, C),

$$A(\mathbb{H}) = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

which is the adjacency matrix of K_3. Its eigenvalues are

$$\lambda_1 = 2, \qquad \lambda_2 = \lambda_3 = -1.$$

Therefore, by Definition 5.4.7,

$$\mathcal{E}(\mathbb{H}) = \sum_{i=1}^{3} |\lambda_i| = |2| + |-1| + |-1| = 4.$$

Theorem 5.4.10 (SuperHyperGraph energy generalizes hypergraph energy)**.** *Let $H = (V, \mathcal{E})$ be a finite hypergraph with $|V| = n$, and let $\mathbb{H}_0 = (\mathbb{V}, \mathbb{E})$ be the SuperHyperGraph obtained by viewing H as a SuperHyperGraph, i.e.,*

$$\mathbb{V} := V, \qquad \mathbb{E} := \mathcal{E}.$$

Let $A(H)$ be the hypergraph adjacency matrix defined by

$$A(H) = (b_{ij}), \qquad b_{ii} := 0, \quad b_{ij} := \big|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\big| \ (i \neq j),$$

for a fixed ordering $V = \{v_1, \ldots, v_n\}$. Then

$$A(\mathbb{H}_0) = A(H), \qquad \textit{and hence} \qquad \mathcal{E}(\mathbb{H}_0) = \mathcal{E}(H).$$

Consequently, Definition 5.4.7 strictly extends the (adjacency) energy of hypergraphs.

Proof. Fix an ordering $V = \{v_1, \ldots, v_n\}$ and identify $\mathbb{V} = V$ via $X_i := v_i$. For $i \neq j$, by Definition 5.4.6 we have

$$a_{ij}(\mathbb{H}_0) = \big|\{\, f \in \mathbb{E} : \ \{X_i, X_j\} \subseteq f \,\}\big| = \big|\{\, e \in \mathcal{E} : \ \{v_i, v_j\} \subseteq e \,\}\big| = b_{ij}(H),$$

and also $a_{ii}(\mathbb{H}_0) = 0 = b_{ii}(H)$. Hence $A(\mathbb{H}_0) = A(H)$ entrywise, so the eigenvalues (with multiplicity) coincide. Therefore,

$$\mathcal{E}(\mathbb{H}_0) = \sum_{i=1}^{n} \big|\lambda_i(A(\mathbb{H}_0))\big| = \sum_{i=1}^{n} \big|\lambda_i(A(H))\big| = \mathcal{E}(H),$$

as claimed. □

5.5 Periodic graph

A *periodic graph* [225–227] is one that repeats under a fixed shift (e.g., time-layer translation), or, in the quantum-walk sense, admits $\tau \neq 0$ with

$$\exp(i\tau A(G)) \text{ diagonal (equivalently each vertex returns up to phase).}$$

Definition 5.5.1 (Dynamic/periodic graph induced by a static graph)**.** Let $G_0 = (V_0, E_0, T)$ be a finite directed graph with vertex set $V_0 = \{1, \dots, n\}$, edge set $E_0 \subseteq V_0 \times V_0$, and an integer *transit-time* function $T : E_0 \to \mathbb{Z}$, written $T(u, v) = t_{uv}$. The *dynamic (periodic) graph* induced by G_0 is the (locally finite) infinite directed graph $G^\infty = (V^\infty, E^\infty)$ defined by

$$V^\infty := \{ v^p : v \in V_0, \ p \in \mathbb{Z} \}, \qquad E^\infty := \{ (u^p, v^{p+t_{uv}}) : (u, v) \in E_0, \ p \in \mathbb{Z} \}.$$

Equivalently, G^∞ satisfies the *periodicity property*

$$(u^p, v^q) \in E^\infty \iff (u^{p+1}, v^{q+1}) \in E^\infty,$$

i.e., shifting all time-indices by $+1$ preserves adjacency.

Remark 5.5.2 (Period q)**.** More generally, one may say that an infinite graph $G^\infty = (V^\infty, E^\infty)$ with $V^\infty = \{v^p : v \in V_0, \ p \in \mathbb{Z}\}$ is *periodic with period* $q \in \mathbb{N}$ if

$$(u^p, v^r) \in E^\infty \iff (u^{p+q}, v^{r+q}) \in E^\infty.$$

Definition 5.5.3 (Continuous-time quantum walk on a graph)**.** Let X be a finite simple undirected graph on n vertices with adjacency matrix $A \in \mathbb{R}^{n \times n}$. Define the unitary matrix-valued function

$$H(t) := \exp(itA) \qquad (t \in \mathbb{R}),$$

where $i = \sqrt{-1}$.

Definition 5.5.4 (Periodicity (quantum-walk sense))**.** Let X and $H(t)$ be as in Definition 5.5.3.

(i) X is *periodic with respect to a vector* $z \in \mathbb{C}^n \setminus \{0\}$ if there exist $\tau \in \mathbb{R}$ and $\gamma \in \mathbb{C}$ with $|\gamma| = 1$ such that

$$H(\tau)z = \gamma z.$$

(ii) X is *periodic at a vertex* u if it is periodic with respect to the standard basis vector e_u; equivalently, there exists $\tau \in \mathbb{R}$ such that

$$|H(\tau)_{u,u}| = 1.$$

(iii) X is *periodic* if there exists $\tau \in \mathbb{R}$ such that $H(\tau)$ is diagonal (equivalently, each vertex is periodic, possibly with different phases).

Definition 5.5.5 (Dynamic/periodic hypergraph (time-expansion model))**.** Let $H_0 = (V_0, \mathcal{E}_0)$ be a finite (undirected) hypergraph. Fix an *offset signature* δ that assigns an integer $\delta_{v,e} \in \mathbb{Z}$ to each incidence $v \in e$. Define the infinite vertex set

$$V^\infty := \{ v^p : v \in V_0, \ p \in \mathbb{Z} \}.$$

For each $e \in \mathcal{E}_0$ and $p \in \mathbb{Z}$, define the time-shifted hyperedge

$$e^p := \{ v^{p+\delta_{v,e}} : v \in e \} \subseteq V^\infty.$$

Set

$$\mathcal{E}^\infty := \{ e^p : e \in \mathcal{E}_0, \ p \in \mathbb{Z} \}.$$

Then $H^\infty := (V^\infty, \mathcal{E}^\infty)$ is called a *dynamic (periodic) hypergraph* induced by (H_0, δ). It is periodic (of period 1) in the sense that shifting all time-indices by $+1$ maps $\mathcal{E}^\infty$ to itself. If $\delta_{v,e} = 0$ for all $v \in e$, then each hyperedge lies within a single time-layer p.

Definition 5.5.6 (Periodic hypergraph in a quantum-walk sense)**.** Let $H = (V, \mathcal{E})$ be a finite hypergraph on $|V| = n$ vertices, and fix a symmetric matrix representation $M(H) \in \mathbb{R}^{n \times n}$ (e.g., a chosen adjacency or Laplacian matrix model). Define

$$U_H(t) := \exp\bigl(it\, M(H)\bigr) \qquad (t \in \mathbb{R}).$$

We say that H is *periodic at vertex* u if there exists $\tau \in \mathbb{R}$ such that

$$\bigl|U_H(\tau)_{u,u}\bigr| = 1,$$

and H is *periodic* if there exists $\tau \in \mathbb{R}$ such that $U_H(\tau)$ is diagonal.

Definition 5.5.7 (Dynamic/periodic SuperHyperGraph (time-expansion model))**.** Let $\mathbb{H}_0 = (\mathbb{V}_0, \mathbb{E}_0)$ be a finite (undirected) SuperHyperGraph, where $\mathbb{E}_0 \subseteq \mathcal{P}(\mathbb{V}_0) \setminus \{\emptyset\}$. Fix an *offset signature* δ assigning an integer $\delta_{X,f} \in \mathbb{Z}$ to each incidence $X \in f$ with $X \in \mathbb{V}_0$ and $f \in \mathbb{E}_0$.

Define the infinite supervertex set

$$\mathbb{V}^\infty := \{ X^p : X \in \mathbb{V}_0, \ p \in \mathbb{Z} \}.$$

For each $f \in \mathbb{E}_0$ and $p \in \mathbb{Z}$, define the time-shifted superhyperedge

$$f^p := \{ X^{p+\delta_{X,f}} : X \in f \} \subseteq \mathbb{V}^\infty.$$

Set

$$\mathbb{E}^\infty := \{ f^p : f \in \mathbb{E}_0, \ p \in \mathbb{Z} \}, \qquad \mathbb{H}^\infty := (\mathbb{V}^\infty, \mathbb{E}^\infty).$$

We call $\mathbb{H}^\infty$ the *dynamic (periodic) SuperHyperGraph* induced by $(\mathbb{H}_0, \delta)$.

Definition 5.5.8 (Period q (shift periodicity))**.** Let $\mathbb{H}^\infty = (\mathbb{V}^\infty, \mathbb{E}^\infty)$ be as in Definition 5.5.7. For $q \in \mathbb{N}$, define the shift map $S_q : \mathbb{V}^\infty \to \mathbb{V}^\infty$ by

$$S_q(X^p) := X^{p+q}.$$

We say that $\mathbb{H}^\infty$ is *periodic with period* q if S_q is an automorphism, i.e.,

$$f \in \mathbb{E}^\infty \iff S_q(f) \in \mathbb{E}^\infty, \qquad S_q(f) := \{ S_q(Y) : Y \in f \}.$$

Equivalently, shifting all time-indices by $+q$ preserves the superedge family.

Definition 5.5.9 (Periodic SuperHyperGraph (quantum-walk/operator sense))**.** Let $\mathbb{H} = (\mathbb{V}, \mathbb{E})$ be a finite SuperHyperGraph with $|\mathbb{V}| = N$. Fix a symmetric matrix representation $M(\mathbb{H}) \in \mathbb{R}^{N\times N}$ (e.g., a clique-expansion adjacency or Laplacian model). Define the unitary matrix-valued function

$$U_{\mathbb{H}}(t) \;:=\; \exp\bigl(i\,t\,M(\mathbb{H})\bigr) \qquad (t \in \mathbb{R}).$$

We say that $\mathbb{H}$ is *periodic at a supervertex* $X \in \mathbb{V}$ if there exists $\tau \in \mathbb{R} \setminus \{0\}$ such that

$$\bigl|U_{\mathbb{H}}(\tau)_{X,X}\bigr| = 1,$$

and $\mathbb{H}$ is *periodic* if there exists $\tau \in \mathbb{R} \setminus \{0\}$ such that $U_{\mathbb{H}}(\tau)$ is diagonal (equivalently, each supervertex returns to itself up to a phase).

Example 5.5.10 (A periodic SuperHyperGraph in the quantum-walk sense)**.** Let

$$\mathbb{H} = (\mathbb{V}, \mathbb{E}), \qquad \mathbb{V} = \{X_1, X_2\}, \qquad \mathbb{E} = \bigl\{\{X_1, X_2\}\bigr\}.$$

Choose the symmetric operator model $M(\mathbb{H})$ to be the (clique-expansion) adjacency matrix

$$M(\mathbb{H}) = A(\mathbb{H}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Since $A(\mathbb{H})^2 = I_2$, the matrix exponential admits the closed form

$$U_{\mathbb{H}}(t) = \exp\bigl(itA(\mathbb{H})\bigr) = \cos(t)\, I_2 + i\sin(t)\, A(\mathbb{H}) = \begin{pmatrix} \cos t & i\sin t \\ i\sin t & \cos t \end{pmatrix}.$$

At time $\tau = \pi$ we obtain

$$U_{\mathbb{H}}(\pi) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -I_2,$$

which is diagonal. Hence $\mathbb{H}$ is *periodic* in the sense of Definition 5.5.9. Moreover, $\bigl|U_{\mathbb{H}}(\pi)_{X_1,X_1}\bigr| = \bigl|U_{\mathbb{H}}(\pi)_{X_2,X_2}\bigr| = 1$, so $\mathbb{H}$ is periodic at each supervertex. (Indeed, $U_{\mathbb{H}}(2\pi) = I_2$, so 2π is a full return time.)

Theorem 5.5.11 (Periodic hypergraphs are a special case of periodic SuperHyperGraphs)**.** *Let $H_0 = (V_0, \mathcal{E}_0)$ be a finite (undirected) hypergraph.*

(i) ***(Time-expansion model).*** *View H_0 as the SuperHyperGraph $\mathbb{H}_0 = (\mathbb{V}_0, \mathbb{E}_0)$ by setting*

$$\mathbb{V}_0 := V_0, \qquad \mathbb{E}_0 := \mathcal{E}_0.$$

Fix any offset signature $\delta_{v,e} \in \mathbb{Z}$ for incidences $v \in e$. Then the dynamic hypergraph H^∞ induced by (H_0, δ) (Definition of dynamic/periodic hypergraph) coincides (as a set system) with the dynamic SuperHyperGraph $\mathbb{H}^\infty$ induced by $(\mathbb{H}_0, \delta)$ (Definition 5.5.7). In particular, H^∞ is periodic of period q iff $\mathbb{H}^\infty$ is periodic of period q (Definition 5.5.8).

(ii) ***(Quantum-walk/operator model).*** *Let $M(H)$ be the chosen symmetric matrix representation for hypergraphs (e.g., the clique-expansion adjacency matrix), and define $M(\mathbb{H})$ by the same formula on $\mathbb{V} = V$ and $\mathbb{E} = \mathcal{E}$. Then $M(\mathbb{H}) = M(H)$, hence*

$$U_{\mathbb{H}}(t) = \exp\bigl(it\,M(\mathbb{H})\bigr) = \exp\bigl(it\,M(H)\bigr) = U_H(t).$$

Therefore, H is periodic (or periodic at a vertex) in the hypergraph sense iff $\mathbb{H}$ is periodic (or periodic at the corresponding supervertex) in the SuperHyperGraph sense (Definition 5.5.9).

Consequently, the notion of periodic SuperHyperGraph *strictly generalizes the notion of* periodic hypergraph *under either standard periodicity model above.*

Proof. **(i)** By construction, $\mathbb{V}^\infty = \{v^p : v \in V_0,\ p \in \mathbb{Z}\} = V^\infty$. For each $e \in \mathcal{E}_0$ and $p \in \mathbb{Z}$, the time-shifted edge in the hypergraph model is $e^p = \{v^{p+\delta_{v,e}} : v \in e\}$. In the SuperHyperGraph model, the corresponding time-shifted superedge is $e^p = \{X^{p+\delta_{X,e}} : X \in e\}$, which is identical after identifying X with v. Hence $\mathbb{E}^\infty = \mathcal{E}^\infty$ and $\mathbb{H}^\infty = H^\infty$. The period-$q$ condition is therefore the same statement in both languages: the shift map $S_q(v^p) = v^{p+q}$ preserves the edge family.

(ii) Under the identification $\mathbb{V} = V$ and $\mathbb{E} = \mathcal{E}$, the matrix model is defined by the same entrywise formula, so $M(\mathbb{H}) = M(H)$. Taking matrix exponentials yields $U_{\mathbb{H}}(t) = U_H(t)$ for all t. Thus the periodicity conditions (diagonality at some τ, or return at a specified vertex) coincide. □

Chapter 6

Proposed Concepts for Topological Indices

With respect to the structure of topological indices, we consider whether it is possible to investigate notions such as the *topological index of a hierarchical superhypergraph* and the *topological hyperindex of a graph.*

6.1 Topological Index of Hierarchical SuperHyperGraph

A hierarchical superhypergraph is a superhypergraph whose vertices live across multiple powerset levels, with edges allowed to join mixed-level supervertices, while maintaining downward-closure coherence.

Definition 6.1.1 (Hierarchical SuperHyperGraph of height r)**.** Let V_0 be a finite, nonempty base set. For $k \geq 0$ define iterated powersets

$$\mathcal{P}^0(V_0) := V_0, \qquad \mathcal{P}^{k+1}(V_0) := \mathcal{P}\big(\mathcal{P}^k(V_0)\big),$$

and fix an integer $r \geq 0$. Set the *hierarchical universe*

$$\mathcal{U}_r(V_0) \;:=\; \bigcup_{k=0}^{r} \Big(\mathcal{P}^k(V_0) \setminus \{\emptyset\}\Big).$$

For $x \in \mathcal{U}_r(V_0)$, define its *level*

$$\ell(x) \;:=\; \min\{\, k \in \{0, 1, \ldots, r\} : x \in \mathcal{P}^k(V_0)\,\}.$$

A *hierarchical superhypergraph of height* r on V_0 is a pair

$$\mathbb{H}^{\langle r \rangle} = (V, E)$$

such that

(H1) (*Hierarchical vertex set*) V is a finite nonempty set with

$$V \subseteq \mathcal{U}_r(V_0).$$

Elements of V are called *hierarchical supervertices.*

(H2) (*Cross-level edges*) E is a finite family of nonempty subsets of V:

$$E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}.$$

Elements of E are called *hierarchical superhyperedges.* In particular, a superhyperedge may contain supervertices of *different* levels.

(H3) (*Coherence / downward closure*) If $X \in V$ and $\ell(X) \geq 1$, then

$$X \subseteq V.$$

Equivalently, whenever a higher-level supervertex is present, all its immediate constituents are also present as supervertices.

For each $k \in \{0, \dots, r\}$ we define the *k-th layer* by

$$V_k \;:=\; \{\, x \in V : \; \ell(x) = k \,\}, \qquad \text{so that} \qquad V = \dot{\bigcup}_{k=0}^{r} V_k.$$

Definition 6.1.2 (Hierarchical topologization)**.** Fix a height $r \geq 0$. A *hierarchical topologization* is an assignment

$$\mathfrak{T}^{\langle r \rangle} : \; \{\text{hierarchical superhypergraphs of height } r\} \longrightarrow \{\text{topologies}\}$$

such that for each hierarchical superhypergraph $\mathbb{H}^{\langle r \rangle} = (V, E)$, the object $\mathfrak{T}^{\langle r \rangle}(\mathbb{H}^{\langle r \rangle})$ is a topology on the underlying hierarchical supervertex set V, and the assignment is *isomorphism-covariant*: if $\varphi : \mathbb{H}^{\langle r \rangle} \to \mathbb{H}'^{\langle r \rangle}$ is an isomorphism of hierarchical superhypergraphs (a bijection $\varphi : V \to V'$ preserving superhyperedges), then

$$\mathfrak{T}^{\langle r \rangle}(\mathbb{H}'^{\langle r \rangle}) = \{\, \varphi(U) \mid U \in \mathfrak{T}^{\langle r \rangle}(\mathbb{H}^{\langle r \rangle}) \,\}.$$

Equivalently, $\varphi : (V, \mathfrak{T}^{\langle r \rangle}(\mathbb{H}^{\langle r \rangle})) \to (V', \mathfrak{T}^{\langle r \rangle}(\mathbb{H}'^{\langle r \rangle}))$ is a homeomorphism.

Definition 6.1.3 (Topological invariant functional)**.** A functional

$$\Phi : \; \{(X, \tau) : \tau \text{ a topology on } X\} \longrightarrow \mathbb{R}$$

is called a *topological invariant* if $\Phi(X, \tau) = \Phi(Y, \sigma)$ whenever (X, τ) and (Y, σ) are homeomorphic.

Definition 6.1.4 (Topological index of a hierarchical SuperHyperGraph)**.** Fix a height $r \geq 0$, a hierarchical topologization $\mathfrak{T}^{\langle r \rangle}$, and a topological invariant Φ. For a hierarchical superhypergraph $\mathbb{H}^{\langle r \rangle} = (V, E)$, its *topological index* (with respect to Φ and $\mathfrak{T}^{\langle r \rangle}$) is

$$\mathrm{HTI}_{\Phi, \mathfrak{T}^{\langle r \rangle}}\big(\mathbb{H}^{\langle r \rangle}\big) \;:=\; \Phi\Big(V, \; \mathfrak{T}^{\langle r \rangle}\big(\mathbb{H}^{\langle r \rangle}\big)\Big).$$

Theorem 6.1.5 (Isomorphism invariance)**.** *Under the assumptions of Definition 6.1.4,* $\mathrm{HTI}_{\Phi, \mathfrak{T}^{\langle r \rangle}}$ *is an invariant of hierarchical superhypergraphs: if* $\mathbb{H}^{\langle r \rangle} \cong \mathbb{H}'^{\langle r \rangle}$*, then*

$$\mathrm{HTI}_{\Phi, \mathfrak{T}^{\langle r \rangle}}\big(\mathbb{H}^{\langle r \rangle}\big) = \mathrm{HTI}_{\Phi, \mathfrak{T}^{\langle r \rangle}}\big(\mathbb{H}'^{\langle r \rangle}\big).$$

Proof. Let $\varphi : \mathbb{H}^{\langle r\rangle} \to \mathbb{H}'^{\langle r\rangle}$ be an isomorphism. By isomorphism-covariance of $\mathfrak{T}^{\langle r\rangle}$ (Definition 6.1.2), φ is a homeomorphism between the induced topological spaces on the hierarchical supervertex sets. Since Φ is a topological invariant (Definition 6.1.3), the values coincide, giving the claim. □

Definition 6.1.6 (Support (flattening) of a hierarchical supervertex)**.** Let $\mathbb{H}^{\langle r\rangle} = (V, E)$ be a hierarchical superhypergraph on a base set V_0. Define the *support* map $\mathrm{Supp} : V \to \mathcal{P}(V_0) \setminus \{\emptyset\}$ recursively by

$$\mathrm{Supp}(x) \;:=\; \{x\} \quad (x \in V_0), \qquad \mathrm{Supp}(X) \;:=\; \bigcup_{y\in X} \mathrm{Supp}(y) \quad (X \in V \setminus V_0).$$

Definition 6.1.7 (Hierarchical incidence degree)**.** Let $\mathbb{H}^{\langle r\rangle} = (V, E)$ be a hierarchical superhypergraph. For $v \in V_0$, define its *hierarchical incidence degree* by

$$d_{\mathrm{inc}}(v) \;:=\; \big|\{\, e \in E : \; \exists\, X \in e \text{ with } v \in \mathrm{Supp}(X) \,\}\big|.$$

(Thus, a base vertex v is counted once per hierarchical superhyperedge that contains at least one supervertex whose support contains v.)

Definition 6.1.8 (Sombor index of a hierarchical SuperHyperGraph)**.** Let $\mathbb{H}^{\langle r\rangle} = (V, E)$ be a hierarchical superhypergraph, and let $d_{\mathrm{inc}}(\cdot)$ be as in Definition 6.1.7. Define the *Sombor index* of $\mathbb{H}^{\langle r\rangle}$ by

$$\mathrm{HSO}\big(\mathbb{H}^{\langle r\rangle}\big) \;:=\; \sum_{e\in E} \sum_{\substack{X,Y\in e\\ X<Y}} \sqrt{d_{\mathrm{inc}}\big(\mathrm{Supp}(X)\big)^2 + d_{\mathrm{inc}}\big(\mathrm{Supp}(Y)\big)^2}\,.$$

Here, for a nonempty subset $S \subseteq V_0$, we use the shorthand

$$d_{\mathrm{inc}}(S) \;:=\; \sum_{v\in S} d_{\mathrm{inc}}(v),$$

and $X < Y$ indicates that the inner sum ranges over unordered distinct pairs $\{X, Y\} \subseteq e$.

6.2 Topological HyperIndex and SuperHyperIndex of Graph

6.2.1 Basic Framework

Topological HyperIndex is a set-valued graph invariant: it maps each graph, via an induced topology, to a nonempty set of topological-invariant values. Its significance is that it models uncertainty, parameter ranges, or multiple admissible constructions without collapsing results to a single number. Topological SuperHyperIndex is a higher-order set-valued invariant: it maps each graph to an iterated nonempty powerset of invariant values, reflecting layered constructions. Its significance is that it encodes multi-level or hierarchical uncertainty and enables structured aggregation and comparison across different topological layers.

Definition 6.2.1 (Nonempty iterated powerset)**.** Let S be a nonempty set and write $\mathcal{P}_+(S) := \mathcal{P}(S) \setminus \{\emptyset\}$. Define recursively

$$\mathcal{P}_+^0(S) := S, \qquad \mathcal{P}_+^{m+1}(S) := \mathcal{P}\big(\mathcal{P}_+^m(S)\big) \setminus \{\emptyset\} \quad (m \geq 0).$$

Definition 6.2.2 (Hyper-valued and superhyper-valued topological invariants)**.** Let S be a nonempty set. A map

$$\Phi : \{(X,\tau) : \tau \text{ a topology on } X\} \longrightarrow \mathcal{P}_+(S)$$

is called a *hyper-valued topological invariant* if $\Phi(X,\tau) = \Phi(Y,\sigma)$ whenever (X,τ) and (Y,σ) are homeomorphic.

More generally, for $m \geq 1$, a map

$$\Phi^{(m)} : \{(X,\tau)\} \longrightarrow \mathcal{P}_+^m(S)$$

is called a *superhyper-valued topological invariant* if it is constant on homeomorphism classes.

Definition 6.2.3 (Topological HyperIndex of a graph)**.** Fix $n \geq 0$ and assume we are given an isomorphism-covariant n-level topologization $G \mapsto \mathfrak{T}^{(n)}(G)$ on the underlying set $\mathcal{P}_n(V(G))$. Let Φ be a hyper-valued topological invariant with codomain $\mathcal{P}_+(S)$.

For a graph $G = (V, E)$, the *topological hyperindex* is defined by

$$\mathrm{TopHI}_{\Phi,\mathfrak{T}^{(n)}}(G) \;:=\; \Phi\big(\mathcal{P}_n(V),\, \mathfrak{T}^{(n)}(G)\big) \;\in\; \mathcal{P}_+(S).$$

Definition 6.2.4 (Topological SuperHyperIndex of a graph)**.** Fix $n \geq 0$ and $m \geq 1$. Let $\mathfrak{T}^{(n)}$ be an isomorphism-covariant n-level topologization, and let $\Phi^{(m)}$ be a superhyper-valued topological invariant with codomain $\mathcal{P}_+^m(S)$.

For a graph $G = (V, E)$, the *topological superhyperindex* is defined by

$$\mathrm{TopSHI}^{(m)}_{\Phi^{(m)},\mathfrak{T}^{(n)}}(G) \;:=\; \Phi^{(m)}\big(\mathcal{P}_n(V),\, \mathfrak{T}^{(n)}(G)\big) \;\in\; \mathcal{P}_+^m(S).$$

Theorem 6.2.5 (Graph-isomorphism invariance)**.** *Let $n \geq 0$ and assume $\mathfrak{T}^{(n)}$ is isomorphism-covariant.*

1. *If Φ is a hyper-valued topological invariant, then* $\mathrm{TopHI}_{\Phi,\mathfrak{T}^{(n)}}$ *is a graph invariant.*

2. *If $\Phi^{(m)}$ is a superhyper-valued topological invariant, then* $\mathrm{TopSHI}^{(m)}_{\Phi^{(m)},\mathfrak{T}^{(n)}}$ *is a graph invariant.*

Proof. Let $\varphi : G \to G'$ be a graph isomorphism. By isomorphism-covariance of $\mathfrak{T}^{(n)}$, the induced bijection $\varphi^{(n)} : \mathcal{P}_n(V(G)) \to \mathcal{P}_n(V(G'))$ is a homeomorphism between

$$\big(\mathcal{P}_n(V(G)), \mathfrak{T}^{(n)}(G)\big) \quad \text{and} \quad \big(\mathcal{P}_n(V(G')), \mathfrak{T}^{(n)}(G')\big).$$

Since Φ (resp. $\Phi^{(m)}$) is constant on homeomorphism classes, the corresponding values agree, yielding $\mathrm{TopHI}_{\Phi,\mathfrak{T}^{(n)}}(G) = \mathrm{TopHI}_{\Phi,\mathfrak{T}^{(n)}}(G')$ (resp. the analogous equality for TopSHI). □

Theorem 6.2.6 (Reduction to the classical (single-valued) topological index)**.** *Assume that a hyper-valued invariant Φ is* singleton-valued*, i.e., $|\Phi(X,\tau)| = 1$ for all (X,τ). Define the associated real-valued invariant $\widehat{\Phi}(X,\tau)$ as the unique element of $\Phi(X,\tau)$. Then*

$$\mathrm{TopHI}_{\Phi,\mathfrak{T}^{(n)}}(G) \;=\; \{\; \widehat{\Phi}(\mathcal{P}_n(V(G)), \mathfrak{T}^{(n)}(G)) \;\},$$

so TopHI *collapses to the usual single-valued topological index.*

Proof. Immediate from the definition of singleton-valuedness. □

6.2.2 Sombor HyperIndex and SuperHyperIndex

The Sombor HyperIndex maps a graph to the set $\{\mathrm{SO}_a(G) : a \in A\}$, capturing multiple shifted Sombor values simultaneously. The Sombor SuperHyperIndex maps a graph to an iterated family of such sets over admissible parameter-sets, encoding hierarchical uncertainty about shifts.

Definition 6.2.7 (Sombor HyperIndex of a graph)**.** Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ denote the (usual) degree of $v \in V$. Fix a nonempty parameter set $A \subseteq \mathbb{R}$. The *Sombor HyperIndex* of G with respect to A is the nonempty subset of $\mathbb{R}_{\geq 0}$ given by

$$\mathrm{SOHI}_A(G) \;:=\; \Big\{\, \mathrm{SO}_a(G) \;\Big|\; a \in A \,\Big\},$$

where $\mathrm{SO}_a(G)$ is the shifted (general) Sombor index

$$\mathrm{SO}_a(G) \;=\; \sum_{uv \in E} \sqrt{(d_G(u) - a)^2 + (d_G(v) - a)^2}.$$

Definition 6.2.8 (Sombor SuperHyperIndex of a graph)**.** Let $G = (V, E)$ be a finite simple undirected graph, and let $d_G(v)$ be the vertex degree. Fix integers $m \geq 1$ and nonempty parameter sets $A_1, \ldots, A_m \subseteq \mathbb{R}$. Define recursively

$$\mathrm{SOSHI}^{(1)}_{A_1}(G) \;:=\; \mathrm{SOHI}_{A_1}(G), \qquad \mathrm{SOSHI}^{(k+1)}_{A_1,\ldots,A_{k+1}}(G) \;:=\; \Big\{\, \mathrm{SOSHI}^{(k)}_{A_1,\ldots,A_k}(G) \;\Big|\; A_k \in A_{k+1} \,\Big\},$$

provided A_{k+1} is a nonempty family of nonempty subsets of $\mathbb{R}$ for each k. More explicitly, if $A_{k+1} \subseteq \mathcal{P}(\mathbb{R}) \setminus \{\emptyset\}$, then

$$\mathrm{SOSHI}^{(k+1)}_{A_1,\ldots,A_{k+1}}(G) \;\subseteq\; \mathcal{P}^{\,k}(\mathbb{R}) \setminus \{\emptyset\}.$$

We call $\mathrm{SOSHI}^{(m)}_{A_1,\ldots,A_m}(G)$ the *Sombor SuperHyperIndex* of G (of depth m).

Remark 6.2.9 (A clean two-level specification)**.** A common choice is to take $A_1 \subseteq \mathbb{R}$ (possible shifts) and $A_2 \subseteq \mathcal{P}(\mathbb{R}) \setminus \{\emptyset\}$ (admissible shift-sets). Then

$$\mathrm{SOSHI}^{(2)}_{A_1,A_2}(G) = \Big\{\, \mathrm{SOHI}_B(G) \;\Big|\; B \in A_2 \,\Big\} = \Big\{\, \{\, \mathrm{SO}_a(G) : a \in B \,\} \;\Big|\; B \in A_2 \,\Big\},$$

which is an element of $\mathcal{P}(\mathcal{P}(\mathbb{R})) \setminus \{\emptyset\}$ and captures "uncertainty about the uncertainty" (a hierarchy of admissible parameter-sets).

Proposition 6.2.10 (Reduction to a single Sombor index)**.** *If $A = \{a_0\}$ is a singleton, then $\mathrm{SOHI}_A(G) = \{\mathrm{SO}_{a_0}(G)\}$, i.e., the hyperindex collapses to one value.*

Proof. Immediate from Definition 6.2.7. ☐

Chapter 7

Conclusion

In this book, we introduced and formalized a variety of Chemical SuperHyperGraphs and numerous topological indices on SuperHyperGraphs. In future work, we expect further progress on extensions developed within uncertainty-aware frameworks, including Fuzzy Graphs [228, 229], Intuitionistic Fuzzy Graphs [230, 231], Neutrosophic Graphs [232–236], and Plithogenic Graphs [2, 237].

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Data Availability

This research is purely theoretical, involving no data collection or analysis. We encourage future researchers to pursue empirical investigations to further develop and validate the concepts introduced here.

Ethical Approval

As this research is entirely theoretical in nature and does not involve human participants or animal subjects, no ethical approval is required.

Use of Generative AI and AI-Assisted Tools

The authors used generative AI and AI-assisted tools for limited language support (e.g., English grammar and style checking). These tools were not used to generate original scientific content, results, or proofs, and they were employed in a manner consistent with applicable ethical standards and publication policies. All technical content was reviewed and validated by the authors.

Conflicts of Interest

The authors confirm that there are no conflicts of interest related to the research or its publication.

Disclaimer

This work presents theoretical concepts that have not yet undergone practical testing or validation. Future researchers are encouraged to apply and assess these ideas in empirical contexts. While every effort has been made to ensure accuracy and appropriate referencing, unintentional errors or omissions may still exist. Readers are advised to verify referenced materials on their own. The views and conclusions expressed here are the authors' own and do not necessarily reflect those of their affiliated organizations.

Appendix (List of Tables)

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Hypergraphs extend traditional graph theory by allowing edges to connect arbitrary non-empty subsets of a vertex set. By recursively applying the powerset construction, we derive nested, higher-order objects known as SuperHyperGraphs. In this framework, both vertices and edges possess multi-layered, set-valued structures, offering unparalleled expressive capacity for modeling complex systems. Topological indices serve as critical numerical invariants that translate structural features—such as degree sequences, distance metrics, and connectivity—into quantitative data used to analyze and compare network properties. Despite the potential of SuperHyperGraphs, a systematic theory of their structural parameters remains underdeveloped. This volume extends a diverse range of topological indices from classical graph and hypergraph settings to the SuperHyperGraph domain. Expanding upon the research foundation established in previous works, we investigate how these indices characterize the intrinsic properties of higher-order nested networks.

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