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Hierarchical Signaling Networks through SuperHypergraphs

Takaaki Fujita^{1*} 

¹ Independent Researcher, Tokyo, Japan; Takaaki.fujita060@gmail.com.

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Abstract

Graph theory studies mathematical structures of vertices and edges to model relationships and connectivity. Hypergraphs extend traditional graphs by allowing *hyperedges* that connect any number of vertices simultaneously. Superhypergraphs further generalize this idea through iterated powerset layers, enabling hierarchical and self-referential connections among hyperedges. Graph theory is also extensively used in biology, biochemistry, and related fields. A *Signaling Graph* is a directed graph in which vertices represent entities and edges denote activation or inhibition of targets. A *Signaling Hypergraph* generalizes signaling graphs by using hyperedges that link sets of regulators to sets of targets in reactions. In this paper, we define the *Signaling n-SuperHypergraph*, which extends these concepts using superhypergraphs, and we briefly examine its properties. Although this work is purely theoretical, we hope that future research will further advance hierarchical modeling in complex systems.

Keywords: Superhypergraph, Hypergraph, Signaling Graph, Signaling Hypergraph

1 | Preliminaries

This section fixes the basic notation and recalls the core set-theoretic constructions used throughout the paper. Unless explicitly stated otherwise, every set considered below is finite.

1.1 | Power Set and n -th Power Set

We define the usual powerset operator and its iterated (higher-order) variants, which later serve as the ambient domains for SuperHyperGraph constructions.

Definition 1 (Power Set). [1] The *power set* of S , denoted by $\mathcal{P}(S)$, is the family of all subsets of S :

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

 **Corresponding Author:** takaaki.fujita060@gmail.com

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Definition 2 (*n*-th Power Set). [2, 3] Define, for $n \geq 1$, the *n*-th power set of S recursively by

$$\mathcal{P}^{(1)}(S) = \mathcal{P}(S), \quad \mathcal{P}^{(n+1)}(S) = \mathcal{P}(\mathcal{P}^{(n)}(S)).$$

Likewise, the *n*-th nonempty power set of S is defined by

$$\mathcal{P}^{*(1)}(S) = \mathcal{P}(S) \setminus \{\emptyset\}, \quad \mathcal{P}^{*(n+1)}(S) = \mathcal{P}(\mathcal{P}^{*(n)}(S)) \setminus \{\emptyset\}.$$

1.2 | SuperHyperGraph

A hypergraph generalizes an ordinary graph by allowing an edge, called a *hyperedge*, to be incident with an arbitrary number of vertices, thereby representing higher-order interactions [4, 5, 6, 7]. Related concepts, including fuzzy hypergraphs [8, 9, 10], are also well known. A *SuperHyperGraph* further generalizes this viewpoint by embedding such incidence structures into iterated powerset layers. This framework has been introduced and further developed in recent studies [11, 12, 13, 14].

Definition 3 (Hypergraph). [15, 16] A *hypergraph* is a pair $H = (V(H), E(H))$ where:

- $V(H)$ is a nonempty set of *vertices*;
- $E(H)$ is a set of *hyperedges*, each hyperedge being a nonempty subset of $V(H)$.

Thus, unlike a standard graph, a single hyperedge may join more than two vertices. In this paper, we work in the finite setting, i.e., both $V(H)$ and $E(H)$ are finite.

Definition 4 (*n*-SuperHyperGraph). [11]

Let V_0 be a finite nonempty set of basic vertices. For each integer $k \geq 0$, define the iterated powerset levels by

$$\mathcal{P}^0(V_0) = V_0, \quad \mathcal{P}^{k+1}(V_0) = \mathcal{P}(\mathcal{P}^k(V_0)),$$

where $\mathcal{P}(X)$ denotes the usual power set of X .

An *n-SuperHyperGraph* is an ordered pair

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

satisfying

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

Elements of V are called *n-supervertices*, and elements of E are called *n-superedges*.

1.3 | Signaling Hypergraph

A *signaling hypergraph* is a directed hypergraph model for biochemical reaction and regulatory events: each directed hyperedge specifies a set of required reactant/regulator hypernodes (the tail) and a set of product hypernodes (the head). A hypernode is called a *leaf* if it is incident to exactly one signaling hyperedge (e.g., it appears in the tail or head of exactly one hyperedge). We recall this formalism, which is widely used in pathway and signaling-network modeling [17, 18, 19].

Definition 5 (Hypernode). Let V be a finite set of *molecular entities* (e.g., proteins, complexes, small molecules). A *hypernode* is any nonempty subset $X \subseteq V$. Let

$$\mathcal{V} \subseteq 2^V \setminus \{\emptyset\}$$

be the collection of hypernodes under consideration. An element $X \in \mathcal{V}$ represents a single molecule when $|X| = 1$ and a molecular complex when $|X| \geq 2$.

Definition 6 (Signaling Hyperedge). (cf. [17, 18]) A *signaling hyperedge* is a directed hyperedge

$$e = (T(e), H(e)),$$

where the *tail* $T(e)$ and the *head* $H(e)$ are nonempty subsets of $\mathcal{V}$:

$$\emptyset \neq T(e) \subseteq \mathcal{V}, \quad \emptyset \neq H(e) \subseteq \mathcal{V}.$$

Conceptually, $T(e)$ collects the reactant and positive-regulator hypernodes that must be simultaneously present for event e to occur, while $H(e)$ is the set of product hypernodes produced by e .

Definition 7 (Signaling Hypergraph). (cf. [17, 18]) A *signaling hypergraph* is a triple

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

where:

- V is a finite set of molecular entities;
- $\mathcal{V} \subseteq 2^V \setminus \{\emptyset\}$ is a specified set of hypernodes (molecules or complexes);
- E is a finite set of signaling hyperedges $e = (T(e), H(e))$ with

$$\emptyset \neq T(e) \subseteq \mathcal{V}, \quad \emptyset \neq H(e) \subseteq \mathcal{V}.$$

We also assume that every molecular entity appears in at least one hypernode:

$$\bigcup_{X \in \mathcal{V}} X = V.$$

Definition 8 (Backward Star). Let $\mathcal{H} = (V, \mathcal{V}, E)$ be a signaling hypergraph and let $X \in \mathcal{V}$. The *backward star* of X is the set of hyperedges that produce X :

$$\text{BS}(X) = \{e \in E \mid X \in H(e)\}.$$

Definition 9 (B-Connection). Fix a *source hypernode* $s \in \mathcal{V}$. A hypernode $X \in \mathcal{V}$ is said to be *B-connected* to s if X belongs to the smallest subset $B \subseteq \mathcal{V}$ such that

$$s \in B \quad \text{and} \quad (T(e) \subseteq B) \implies (H(e) \subseteq B) \quad \text{for all } e \in E.$$

We denote this least such set by $B_{\mathcal{H}}(s)$ and write $X \in B_{\mathcal{H}}(s)$. Equivalently, $X \in B_{\mathcal{H}}(s)$ if either $X = s$, or there exists $e \in E$ with $X \in H(e)$ and every element of $T(e)$ is B-connected to s .

Definition 10 (Acyclicity and B-Hyperpath). Let $\mathcal{H} = (V, \mathcal{V}, E)$ be a signaling hypergraph and let $s, t \in \mathcal{V}$. An *acyclic B-hyperpath* from s to t is a sub-hypergraph

$$\Pi(s, t) = (\mathcal{V}_{\Pi}, E_{\Pi}), \quad \mathcal{V}_{\Pi} \subseteq \mathcal{V}, \quad E_{\Pi} \subseteq E,$$

such that $s, t \in \mathcal{V}_{\Pi}$ and, for every $e \in E_{\Pi}$,

$$T(e) \cup H(e) \subseteq \mathcal{V}_{\Pi},$$

and the following conditions hold:

- (1) *Terminal connectivity*: $t \in B_{\Pi}(s)$, where $B_{\Pi}(s)$ denotes the B-connected set computed using only $\mathcal{V}_{\Pi}$ and E_{Π} .
- (2) *Minimality*: No proper sub-hypergraph of $\Pi(s, t)$ (obtained by deleting any hypernode and/or any hyperedge) still satisfies $t \in B_{\Pi}(s)$.
- (3) *Acyclicity*: $\Pi(s, t)$ admits no directed cycle. Equivalently, there exists an *ordering* function $o : \mathcal{V}_{\Pi} \rightarrow \mathbb{R}$ such that for every $e = (T(e), H(e)) \in E_{\Pi}$ and every $X \in T(e)$ and $Y \in H(e)$,

$$o(X) < o(Y).$$

2 | Result: Signaling n -SuperHypergraphs

We now introduce a directed signaling analogue of an n -SuperHyperGraph. The essential point is that a signaling superhyperedge must retain its orientation; therefore, it is represented by an ordered pair consisting of a nonempty tail and a nonempty head, rather than merely by their union.

For a set X , write

$$\mathcal{P}_*(X) := \mathcal{P}(X) \setminus \{\emptyset\}.$$

Definition 11 (Signaling n -SuperHypergraph). Let $n \geq 1$, let V_0 be a finite nonempty base set, and define

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

A *signaling n -SuperHypergraph* over V_0 is a pair

$$\text{SNHT}^{(n)} = (V_n, E_n),$$

satisfying the following conditions:

(1)

$$\emptyset \neq V_n \subseteq \mathcal{P}^n(V_0).$$

The elements of V_n are called *n -supervertices* or *n -level signaling nodes*.

(2)

$$E_n \subseteq \mathcal{P}_*(V_n) \times \mathcal{P}_*(V_n).$$

Thus every signaling n -superhyperedge is an ordered pair

$$e = (T_e, H_e),$$

where

$$\emptyset \neq T_e \subseteq V_n, \quad \emptyset \neq H_e \subseteq V_n.$$

The sets T_e and H_e are called the *tail* and *head* of e , respectively. We also write

$$T(e) := T_e, \quad H(e) := H_e.$$

The *support* of e is the nonempty subset

$$\text{supp}(e) := T(e) \cup H(e) \subseteq V_n.$$

Since $V_n \subseteq \mathcal{P}^n(V_0)$, it follows that

$$\text{supp}(e) \in \mathcal{P}(V_n) \subseteq \mathcal{P}^{n+1}(V_0).$$

The signaling n -SuperHypergraph is called *proper* if

$$T(e) \cap H(e) = \emptyset \quad \text{for every } e \in E_n.$$

Remark 12 (Why the ordered-pair representation is necessary). A *directed signaling superhyperedge* must be represented by the ordered pair

$$e = (T(e), H(e)),$$

not merely by the support $T(e) \cup H(e)$. Indeed, the directed superhyperedges

$$(T, H) \quad \text{and} \quad (H, T)$$

have the same support $T \cup H$, but generally represent opposite signaling directions.

More generally, two distinct directed superhyperedges may have the same support while having different tail-head decompositions. Representing an edge only by $T(e) \cup H(e)$ would therefore lose essential signaling information.

Remark 13 (Indexing convention). The index n refers to the powerset level of the supervertices:

$$V_n \subseteq \mathcal{P}^n(V_0).$$

Consequently, the support of a signaling n -superhyperedge belongs to the next powerset level,

$$\text{supp}(e) \in \mathcal{P}^{n+1}(V_0).$$

Under this convention, an ordinary signaling hypergraph is recovered when $n = 1$, because its hypernodes are nonempty subsets of V_0 . If one instead indexes the structure by the powerset level of its edge supports, then the same ordinary signaling hypergraph may be called a *level-2 signaling structure*. These two indexing conventions should not be mixed.

Theorem 14 (Underlying n -SuperHyperGraph). *Let*

$$\text{SNHT}^{(n)} = (V_n, E_n)$$

be a signaling n -SuperHypergraph. Define

$$\underline{E}_n := \{\text{supp}(e) \mid e \in E_n\} = \{T(e) \cup H(e) \mid e \in E_n\}.$$

Then

$$\underline{\text{SNHT}}^{(n)} := (V_n, \underline{E}_n)$$

is an n -SuperHyperGraph.

The structure $\underline{\text{SNHT}}^{(n)}$ is called the underlying undirected n -SuperHyperGraph of $\text{SNHT}^{(n)}$.

Proof: For every $e \in E_n$,

$$\emptyset \neq T(e) \subseteq V_n, \quad \emptyset \neq H(e) \subseteq V_n.$$

Therefore

$$\emptyset \neq T(e) \cup H(e) \subseteq V_n,$$

and hence

$$\text{supp}(e) \in \mathcal{P}(V_n) \setminus \{\emptyset\}.$$

It follows that

$$\underline{E}_n \subseteq \mathcal{P}(V_n) \setminus \{\emptyset\}.$$

Since

$$V_n \subseteq \mathcal{P}^n(V_0),$$

the pair

$$(V_n, \underline{E}_n)$$

satisfies the defining conditions of an n -SuperHyperGraph. □

Remark 15. *The passage from E_n to $\underline{E}_n$ forgets the directions of the signaling superhyperedges. Moreover, if two distinct directed superhyperedges $e, f \in E_n$ satisfy*

$$\text{supp}(e) = \text{supp}(f),$$

then they correspond to a single edge of the underlying undirected SuperHyperGraph.

Theorem 16 (Recovery of classical signaling hypergraphs). *Let*

$$\mathcal{H} = (V_0, \mathcal{V}, E)$$

be a classical signaling hypergraph, where

$$\emptyset \neq \mathcal{V} \subseteq \mathcal{P}(V_0) \setminus \{\emptyset\}$$

and

$$E \subseteq \mathcal{P}_*(\mathcal{V}) \times \mathcal{P}_*(\mathcal{V}).$$

Then

$$\text{SNHT}^{(1)} := (\mathcal{V}, E)$$

is a signaling 1-SuperHypergraph over V_0 .

Conversely, every signaling 1-SuperHypergraph over V_0 determines a classical signaling hypergraph on the same base set. Hence classical signaling hypergraphs and signaling 1-SuperHypergraphs are equivalent under the present indexing convention.

Proof: Because

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

the set $\mathcal{V}$ is a valid set of 1-supervertices. Furthermore, every $e \in E$ is an ordered pair

$$e = (T(e), H(e))$$

with

$$\emptyset \neq T(e) \subseteq \mathcal{V}, \quad \emptyset \neq H(e) \subseteq \mathcal{V}.$$

Thus

$$E \subseteq \mathcal{P}_*(\mathcal{V}) \times \mathcal{P}_*(\mathcal{V}),$$

and therefore $(\mathcal{V}, E)$ is a signaling 1-SuperHypergraph.

The converse follows immediately by reversing the same construction. $\square$

Example 17 (T-cell receptor signaling as a 2-SuperHypergraph). Consider the finite base set

$$V_0 = \{\text{TCR}, \text{pMHC}, \text{CD3}, \text{ZAP70}\}.$$

Define the first-level molecular objects

$$X_1 := \{\text{TCR}, \text{pMHC}\}, \quad X_2 := \{\text{CD3}\}, \quad X_3 := \{\text{CD3}, \text{ZAP70}\}.$$

Then

$$X_1, X_2, X_3 \in \mathcal{P}(V_0).$$

Define two second-level supervertices by

$$U_a := \{X_1, X_2\} = \{\{\text{TCR}, \text{pMHC}\}, \{\text{CD3}\}\},$$

and

$$U_b := \{X_3\} = \{\{\text{CD3}, \text{ZAP70}\}\}.$$

Since U_a and U_b are sets of subsets of V_0 ,

$$U_a, U_b \in \mathcal{P}^2(V_0).$$

Set

$$V_2 := \{U_a, U_b\} \subseteq \mathcal{P}^2(V_0),$$

and define the signaling 2-superhyperedge

$$e := (\{U_a\}, \{U_b\}).$$

Equivalently,

$$T(e) = \{U_a\}, \quad H(e) = \{U_b\}.$$

Thus

$$E_2 := \{e\} \subseteq \mathcal{P}_*(V_2) \times \mathcal{P}_*(V_2).$$

Consequently,

$$\text{SNHT}^{(2)} = (V_2, E_2)$$

is a signaling 2-SuperHypergraph.

Its underlying undirected superhyperedge is

$$\text{supp}(e) = T(e) \cup H(e) = \{U_a, U_b\}.$$

Because

$$\{U_a, U_b\} \in \mathcal{P}(\mathcal{P}^2(V_0)) = \mathcal{P}^3(V_0),$$

the support of e is a third-level powerset object, although its incident supervertices are second-level objects.

Biologically, U_a represents a receptor/co-receptor assembly, whereas U_b represents a downstream CD3–ZAP70 assembly. The directed superhyperedge e represents the signaling transition

$$U_a \longrightarrow U_b.$$

Example 18 (Transcription initiation as a 2-SuperHypergraph). Let

$$V_0 = \{\text{TF}, \text{P}, \text{M}, \text{R}\},$$

where TF denotes a transcription factor, P a promoter region, M the Mediator complex, and R RNA Polymerase II.

Define

$$Y_1 := \{\text{TF}, \text{P}\}, \quad Y_2 := \{\text{M}\},$$

and

$$Y_3 := \{\text{P}, \text{M}\}, \quad Y_4 := \{\text{R}\}.$$

Then

$$Y_1, Y_2, Y_3, Y_4 \in \mathcal{P}(V_0).$$

Define

$$U_a := \{Y_1, Y_2\} = \{\{\text{TF}, \text{P}\}, \{\text{M}\}\},$$

and

$$U_b := \{Y_3, Y_4\} = \{\{\text{P}, \text{M}\}, \{\text{R}\}\}.$$

Hence

$$U_a, U_b \in \mathcal{P}^2(V_0).$$

Set

$$V_2 := \{U_a, U_b\}$$

and

$$e := (\{U_a\}, \{U_b\}).$$

Then

$$E_2 := \{e\} \subseteq \mathcal{P}_*(V_2) \times \mathcal{P}_*(V_2),$$

and therefore

$$\text{SNHT}^{(2)} = (V_2, E_2)$$

is a signaling 2-SuperHypergraph.

The tail U_a represents a pre-initiation assembly involving a transcription factor, a promoter, and Mediator, whereas the head U_b represents a downstream assembly containing promoter-associated Mediator and RNA Polymerase II. Thus the directed superhyperedge models the hierarchical transition

$$U_a \longrightarrow U_b.$$

Definition 19 (Underlying directed graph). Let

$$\text{SNHT}^{(n)} = (V_n, E_n)$$

be a signaling n -SuperHypergraph. Its *underlying directed graph* is

$$\mathcal{D}(\text{SNHT}^{(n)}) := (V_n, A_n),$$

where

$$A_n := \bigcup_{e \in E_n} (T(e) \times H(e)).$$

Equivalently,

$$(U, W) \in A_n \iff \exists e \in E_n \text{ such that } U \in T(e) \text{ and } W \in H(e).$$

If $T(e) \cap H(e) \neq \emptyset$, then A_n contains a loop (U, U) for every

$$U \in T(e) \cap H(e).$$

Definition 20 (Acyclic signaling n -SuperHypergraph). A signaling n -SuperHypergraph

$$\text{SNHT}^{(n)} = (V_n, E_n)$$

is called *acyclic* if its underlying directed graph

$$\mathcal{D}(\text{SNHT}^{(n)})$$

contains no directed cycle. In this definition, a directed loop (U, U) is regarded as a directed cycle of length 1.

Consequently, every acyclic signaling n -SuperHypergraph satisfies

$$T(e) \cap H(e) = \emptyset \quad \text{for all } e \in E_n.$$

Theorem 21 (Equivalent characterizations of acyclicity). *Let*

$$\text{SNHT}^{(n)} = (V_n, E_n)$$

be a finite signaling n -SuperHypergraph. The following statements are equivalent:

(a) $\text{SNHT}^{(n)}$ is acyclic.

(b) There exists a function

$$o : V_n \longrightarrow \mathbb{R}$$

such that

$$o(U) < o(W)$$

for every $e \in E_n$, every $U \in T(e)$, and every $W \in H(e)$.

(c) The elements of V_n can be enumerated as

$$V_n = \{U_1, U_2, \dots, U_m\}$$

in such a way that, whenever

$$U_i \in T(e) \quad \text{and} \quad U_j \in H(e)$$

for some $e \in E_n$, one has

$$i < j.$$

Proof: (a) $\Rightarrow$ (b). If $\text{SNHT}^{(n)}$ is acyclic, then its underlying directed graph

$$\mathcal{D}(\text{SNHT}^{(n)})$$

is a finite directed acyclic graph. Hence it admits a topological ordering. Assign to each $U \in V_n$ its position $o(U)$ in such an ordering. For every arc $U \rightarrow W$, one then has

$$o(U) < o(W).$$

In particular, this inequality holds whenever

$$U \in T(e) \quad \text{and} \quad W \in H(e)$$

for some $e \in E_n$.

(b) $\Rightarrow$ (c). Since V_n is finite, arrange its elements in nondecreasing order of their o -values, breaking ties arbitrarily. If

$$U_i \in T(e) \quad \text{and} \quad U_j \in H(e),$$

then $o(U_i) < o(U_j)$, and therefore $i < j$.

(c) $\Rightarrow$ (a). Suppose, to the contrary, that the underlying directed graph contains a directed cycle

$$U_{i_1} \longrightarrow U_{i_2} \longrightarrow \dots \longrightarrow U_{i_k} \longrightarrow U_{i_1}.$$

Condition (c) would imply

$$i_1 < i_2 < \dots < i_k < i_1,$$

which is impossible. Therefore the underlying directed graph contains no directed cycle, and $\text{SNHT}^{(n)}$ is acyclic. $\square$

3 | Conclusion

In this paper, we introduced the notion of a *signaling n-SuperHypergraph*, extending the classical signaling-hypergraph framework to the superhypergraph setting through iterated powerset structures. We established its relationship with ordinary signaling hypergraphs, described the underlying hypergraph and directed-graph structures, and presented basic results concerning reduction, representation, and acyclicity. The illustrative examples involving T-cell receptor signaling and transcription initiation demonstrated how the proposed framework can represent hierarchical collections of molecular entities, complexes, and directed signaling events.

Although the present study is purely theoretical, the proposed model may provide a foundation for more detailed mathematical and computational analyses of hierarchical signaling systems. Future work may investigate signaling reachability, B-connectivity, superhyperpaths, centrality measures, incidence matrices, algorithms for detecting signaling cascades, and applications to biological pathway analysis. It will also be worthwhile to develop uncertainty-aware extensions based on fuzzy graphs [20, 21], neutrosophic graphs [22, 23, 24], uncertain graphs [25], and plithogenic graphs [26, 27].

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Data Availability

The datasets generated during and/or analyzed during the current study are not publicly available due to the privacy-preserving nature of the data but are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that there is no conflict of interest in the research.

Ethical Approval

This article does not contain any studies with human participants or animals performed by any of the authors.

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