# Molecular Line HyperGraphs and SuperHyperGraphs

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**Abstract**. Hypergraphs extend classical graphs by allowing *hyperedges* to connect any nonempty subset of vertices, thereby capturing complex group-level relationships. Superhypergraphs advance this framework by introducing recursively nested powerset layers, which represent hierarchical and self-referential connections among hyperedges. A *line graph* encodes edge adjacencies of a given graph by turning each edge into a vertex and joining two such vertices when the corresponding edges share an endpoint. An *iterated line graph* applies this construction repeatedly, each time to the result of the previous step. Within chemistry, molecular and chemical graphs are well established, and hypergraphs, line graphs, and superhypergraphs have also been explored in this setting. In this paper, we introduce *Molecular Line SuperHyperGraphs* and *Molecular Iterated Line SuperHyperGraphs*, provide formal definitions, and discuss potential applications. We expect that these frameworks will enable clearer and more faithful representations of hierarchical molecular structure in chemistry.

**Keywords:** SuperHyperGraph, HyperGraph, Line Graph, Molecular Graph, Iterated Line Graph

## 1. Preliminaries

This section outlines the fundamental notions and notation adopted in the present work. Throughout, all graphs and hypergraphs under consideration are assumed to be finite.

### 1.1. *Hypergraphs and Superhypergraphs*

A *hypergraph* extends the standard graph model by permitting each edge, termed a *hyperedge*, to link any nonempty subset of the vertex set, thereby enabling the modeling of interactions among more than two vertices [1–4]. A *superhypergraph* builds upon this concept by repeatedly applying powerset operations to the hypergraph structure, producing hierarchically nested layers of hyperedge connections [5–7]. This enhanced structural model has been the focus of several recent studies [8–10]. Given its high descriptive capacity for hierarchical modeling, the superhypergraph framework is anticipated to support a broadening scope of applications [11–14], and it is expected to assume an even more prominent role in the future.

**Definition 1.1** (Base Set). Let $S$ be a nonempty set, called the *base set*. All higher-order objects, such as powersets and supervertices, are constructed from $S$:

$$S = \{\, x \mid x \text{ is an element of the domain}\,\}.$$

**Definition 1.2** (Powerset). [15] For any set $S$, its *powerset* $\text{POWS}(S)$ is the collection of all subsets of $S$, including $\emptyset$ and $S$ itself:

$$\text{POWS}(S) = \{\, A \mid A \subseteq S \,\}.$$

**Definition 1.3** ($n$-th Powerset). [16]. Let $H$ be a set. The *n-th powerset* $\text{POWS}^n(H)$ is defined recursively by

$$\text{POWS}^0(H) = H, \qquad \text{POWS}^{k+1}(H) = \text{POWS}\big(\text{POWS}^k(H)\big), \quad k \geq 0.$$

The *nonempty n-th powerset* $\text{POWS}^{*n}(H)$ is defined similarly but removes the empty set at each stage:

$$\text{POWS}^{*0}(H) = H, \qquad \text{POWS}^{*(k+1)}(H) = \text{POWS}^*\big(\text{POWS}^{*k}(H)\big),$$

where $\text{POWS}^*(X) = \text{POWS}(X) \setminus \{\emptyset\}$

**Example 1.4** ($n$-th powerset in biochemistry: amino-acid subsets and collections of subsets (with concrete uses)). Let $H = \{\text{Ala}, \text{Gly}, \text{Ser}\}$ be a set of three amino acids ($|H| = 3$). Then

$$\text{POWS}^1(H) = \text{POWS}(H) = \big\{\emptyset, \{\text{Ala}\}, \{\text{Gly}\}, \{\text{Ser}\}, \{\text{Ala}, \text{Gly}\}, \{\text{Ala}, \text{Ser}\}, \{\text{Gly}, \text{Ser}\}, H\big\},$$

so $|\text{POWS}^1(H)| = 2^3 = 8$. The second powerset $\text{POWS}^2(H) = \text{POWS}(\text{POWS}(H))$ consists of *collections of amino-acid subsets*. For instance,

$$\big\{\emptyset, \{\text{Ala}\}\big\}, \qquad \big\{\{\text{Ala}, \text{Gly}\}, \{\text{Ser}\}\big\}, \qquad \text{POWS}^1(H) \in \text{POWS}^2(H).$$

Since $|\text{POWS}^1(H)| = 8$, we have $|\text{POWS}^2(H)| = 2^8 = 256$. Likewise, the nonempty versions $\text{POWS}^{*1}(H) = \text{POWS}(H) \setminus \{\emptyset\}$ and $\text{POWS}^{*2}(H) = \text{POWS}(\text{POWS}^{*1}(H)) \setminus \{\emptyset\}$ remove $\emptyset$ at each level.

**Concrete biochemical uses.**

(a) *Alternative binding-site compositions across conditions.* Suppose three experimentally observed microstates of a pocket have residue sets

$$S_1 = \{\text{Ala}, \text{Gly}\}, \quad S_2 = \{\text{Gly}, \text{Ser}\}, \quad S_3 = \{\text{Ala}, \text{Ser}\},$$

occurring with frequencies $p_1 = 0.5$, $p_2 = 0.3$, $p_3 = 0.2$ (with $p_1 + p_2 + p_3 = 1$). The *ensemble of observed compositions* is $X = \{S_1, S_2, S_3\} \in \text{POWS}^2(H)$. From $X$ and $\mathbf{p}$, we obtain explicit, decision-relevant quantities:

$$\mathbb{P}(\text{Ala present}) = p_1 + p_3 = 0.7, \qquad \mathbb{P}(\text{Gly present}) = p_1 + p_2 = 0.8,$$

$$\mathbb{P}(\text{Ser present}) = p_2 + p_3 = 0.5, \qquad \mathbb{E}[\|S\|] = \sum_{i=1}^{3} p_i \, |S_i| = 2.0.$$

Conservation and variability are summarized by

$$\text{consensus core} = \bigcap X = \emptyset, \qquad \text{coverage} = \bigcup X = H, \qquad s(X) := \frac{|\cap X|}{|\cup X|} = \frac{0}{3} = 0,$$

while focusing on the "Gly-including" subensemble $X' = \{S_1, S_2\}$ yields $\cap X' = \{\text{Gly}\}$, $\cup X' = \{\text{Ala}, \text{Gly}, \text{Ser}\}$, and $s(X') = 1/3$. Thus $\text{POWS}^2(H)$ encodes concrete microstate ensembles supporting probabilistic pocket design (e.g., prioritizing Gly-compatible ligands).

(b) *Peptide-motif library specification.* A position-tolerant motif can be declared as a *set of allowed residue sets*. For example, the repertoire

$$\mathcal{R} = \big\{\{\text{Ala}\}, \{\text{Gly}\}, \{\text{Ala}, \text{Gly}\}\big\} \in \text{POWS}^2(H)$$

precisely states which single-residue choices (and their allowable variability) the library will synthesize at that position. Quantities such as the minimum/maximum diversity and a consensus choice are computed directly:

$$\cap\mathcal{R} = \emptyset, \qquad \cup\mathcal{R} = \{\text{Ala}, \text{Gly}\}, \qquad \text{effective alphabet size} = |\cup\mathcal{R}| = 2.$$

**Definition 1.5** (HyperGraph)**.** [17] A finite *HyperGraph* $H = (V, E)$ is specified by:

- A nonempty vertex set $V$.
- A collection $E$ of hyperedges, where each $e \in E$ is a nonempty subset of $V$.

HyperGraphs generalize ordinary graphs by permitting edges to join any number of vertices, making them ideal for modeling higher-order relationships. In this work, we assume both $V$ and $E$ are finite.

**Example 1.6** (Biochemical HyperGraph: a small metabolic fragment)**.** (cf. [18]) Let the vertex set list metabolites

$$V = \{\text{Glc}, \text{ATP}, \text{G6P}, \text{ADP}, \text{F6P}, \text{Pi}\}.$$

Define three hyperedges representing (undirected) participation sets of reactions:

$$e_1 = \{\text{Glc}, \text{ATP}, \text{G6P}, \text{ADP}\} \qquad\qquad \text{(hexokinase step)},$$

$$e_2 = \{\text{G6P}, \text{F6P}\} \qquad\qquad \text{(phosphoglucose isomerase)},$$

$$e_3 = \{\text{ATP}, \text{ADP}, \text{Pi}\} \qquad \text{(ATP hydrolysis / phosphate transfer pool)}.$$

Then $\mathcal{H} = (V, E)$ with $E = \{e_1, e_2, e_3\}$ is a molecular hypergraph capturing multi-metabolite participation. With row order $(\text{Glc}, \text{ATP}, \text{G6P}, \text{ADP}, \text{F6P}, \text{Pi})$ and column order $(e_1, e_2, e_3)$, the incidence matrix is

$$\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

where $H_{v,e} = 1$ iff metabolite $v$ participates in reaction-hyperedge $e$. This representation natively accommodates multi-substrate/multi-product chemistry.

**Definition 1.7** (Level-$n$ SuperHyperGraph (incidence form)). (cf. [19]) Fix a finite base set $V_0$ and an integer $n \geq 0$. Let $V_n \subseteq \text{POWS}^n(V_0)$ be a finite set, whose elements are called *n-supervertices*. A *level-n SuperHyperGraph* is a pair

$$\mathcal{H}^{(n)} = (V_n, \mathcal{E}), \quad \text{with} \quad \emptyset \neq \mathcal{E} \subseteq \text{POWS}(V_n) \setminus \{\emptyset\}.$$

Thus each *n-superedge* $E \in \mathcal{E}$ is a nonempty subset of the vertex set $V_n$. (When $n = 0$, this is an ordinary finite hypergraph; when, additionally, every $E \in \mathcal{E}$ has size 2, it is an ordinary graph.)

**Notation 1** (Stars). *For $\mathcal{H}^{(n)} = (V_n, \mathcal{E})$ and $v \in V_n$, the* star *of $v$ is*

$$\mathsf{Star}_{\mathcal{H}}(v) := \{E \in \mathcal{E} : v \in E\} \subseteq \mathcal{E}.$$

*We also write $\mathcal{E}^{\neq \emptyset}(v) := \mathsf{Star}_{\mathcal{H}}(v)$ and $\mathcal{E}^{(\geq 2)}(v) := \{E \in \mathcal{E} : v \in E \text{ and } |E| \geq 2\}$ when we wish to exclude size-1 edges in the star.*

**Example        1.8        (Level-1        Molecular SuperHyperGraph: signaling modules along EGFR–MAPK).** (cf. [20]) Let the base set $V_0$ collect reaction/bond identifiers

$$V_0 = \{r_{\text{EGF:EGFR}}, \; r_{\text{EGFR}\rightarrow\text{RAS}}, \; r_{\text{RAF}\rightarrow\text{MEK}}, \; r_{\text{MEK}\rightarrow\text{ERK}}\}.$$

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Form three 1-supervertices (subsets of $V_0$) corresponding to functional modules:

$$M_{\text{EGFR}} = \{\, r_{\text{EGF:EGFR}},\ r_{\text{EGFR}\to\text{RAS}} \,\},$$

$$M_{\text{Bridge}} = \{\, r_{\text{EGFR}\to\text{RAS}},\ r_{\text{RAF}\to\text{MEK}} \,\},$$

$$M_{\text{MAPK}} = \{\, r_{\text{RAF}\to\text{MEK}},\ r_{\text{MEK}\to\text{ERK}} \,\}.$$

Set $V_1 = \{M_{\text{EGFR}}, M_{\text{Bridge}}, M_{\text{MAPK}}\} \subseteq \text{POWS}^1(V_0)$. Define 1-superedges (nonempty subsets of $V_1$) to encode immediate module couplings:

$$E_A = \{M_{\text{EGFR}}, M_{\text{Bridge}}\}, \qquad E_B = \{M_{\text{Bridge}}, M_{\text{MAPK}}\}.$$

Then the level-1 SuperHyperGraph is

$$\mathcal{H}^{(1)} = (V_1,\ \mathcal{E}), \qquad \mathcal{E} = \{E_A, E_B\} \subseteq \text{POWS}(V_1) \setminus \{\emptyset\}.$$

**Concrete "lift" from reactions to modules.**
Order the reactions as $(r_{\text{EGF:EGFR}},\ r_{\text{EGFR}\to\text{RAS}},\ r_{\text{RAF}\to\text{MEK}},\ r_{\text{MEK}\to\text{ERK}})$ and the modules as $(M_{\text{EGFR}},\ M_{\text{Bridge}},\ M_{\text{MAPK}})$. The *module-membership incidence matrix* $B \in \{0,1\}^{4\times 3}$, with $B_{r,M} = 1 \iff r \in M$, is

$$B = \begin{array}{c} \begin{matrix} M_{\text{EGFR}} & M_{\text{Bridge}} & M_{\text{MAPK}} \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \end{array} \qquad \text{(rows in the reaction order above).}$$

From $B$ we obtain the *module-overlap matrix*

$$O := B^\top B = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}, \qquad O_{ij} = |\, M_i \cap M_j \,|.$$

The "lift" is now explicit: we place a 1-superedge between modules $M_i$ and $M_j$ *iff* they share at least one reaction, i.e. $O_{ij} \geq 1$ for $i \neq j$. Thus the superedge set $\mathcal{E} = \{E_A, E_B\}$ is precisely the set of pairs with $O_{ij} \geq 1$:

$$E_A = \{M_{\text{EGFR}}, M_{\text{Bridge}}\} \text{ (since } O_{12} = 1), \qquad E_B = \{M_{\text{Bridge}}, M_{\text{MAPK}}\} \text{ (since } O_{23} = 1),$$

and there is no superedge between $M_{\text{EGFR}}$ and $M_{\text{MAPK}}$ because $O_{13} = 0$.
Equivalently, the *module-coupling adjacency* is the thresholded matrix

$$A_{\text{mod}} = \mathbf{1}\{\, O_{ij} \geq 1,\ i \neq j \,\} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

which encodes exactly the two superedges above. The 1-superedge incidence (rows $M$, columns $E_A, E_B$) is

$$S = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{bmatrix}, \qquad \deg_{\mathcal{H}^{(1)}}(M_{\text{EGFR}}) = 1, \quad \deg_{\mathcal{H}^{(1)}}(M_{\text{Bridge}}) = 2, \quad \deg_{\mathcal{H}^{(1)}}(M_{\text{MAPK}}) = 1.$$

Hence, (i) embed modules as subsets $V_1 \subseteq \text{POWS}(V_0)$; (ii) compute overlaps $O = B^\top B$ to obtain a *deterministic* coupling rule $(M_i, M_j) \in \mathcal{E} \iff O_{ij} \geq 1$; and (iii) represent the resulting module–module couplings by $A_{\text{mod}}$ or $S$. This makes the passage from reaction-level incidence to module-level connectivity explicit, algorithmic, and checkable, and it extends verbatim to deeper levels $n > 1$ by replacing $B$ with the corresponding level-$n$ membership matrix.

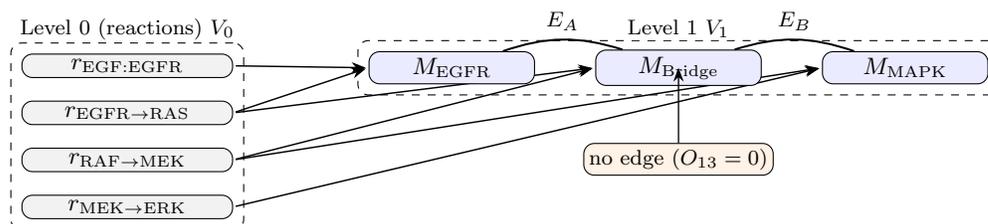Figure 1 illustrates the graph for this concrete example.



FIGURE 1. Level-1 Molecular SuperHyperGraph (EGFR–MAPK): reactions (level 0) lift to modules (level 1), and module couplings form 1-superedges $E_A, E_B$.

**Example 1.9** (Biochemical 2-SuperHyperGraph: EGFR–MAPK signaling programs). (cf. [21]) We build a concrete level-2 SuperHyperGraph that organizes biochemical reactions $\rightarrow$ modules $\rightarrow$ programs.

Level 0 (base set of reactions). Let the base set $V_0$ collect reaction/interaction identifiers

$$V_0 = \big\{ r_{\text{EGF:EGFR}}, \ r_{\text{EGFR}\rightarrow\text{RAS}}, \ r_{\text{RAF}\rightarrow\text{MEK}}, \ r_{\text{MEK}\rightarrow\text{ERK}} \big\}.$$

Level 1 (modules as subsets of $V_0$). Define three 1-supervertices (functional modules)

$$M_{\text{EGFR}} := \{ r_{\text{EGF:EGFR}}, \ r_{\text{EGFR}\rightarrow\text{RAS}} \},$$

$$M_{\text{Bridge}} := \{ r_{\text{EGFR}\rightarrow\text{RAS}}, \ r_{\text{RAF}\rightarrow\text{MEK}} \},$$

$$M_{\text{MAPK}} := \{ r_{\text{RAF}\rightarrow\text{MEK}}, \ r_{\text{MEK}\rightarrow\text{ERK}} \},$$

and set $V_1 := \{M_{\text{EGFR}}, M_{\text{Bridge}}, M_{\text{MAPK}}\} \subseteq \text{POWS}^1(V_0)$.

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Level 2 (programs as subsets of modules). Form 2-supervertices (programs) by grouping modules:

$$P_1 := \{\, M_{\mathrm{EGFR}}, M_{\mathrm{Bridge}} \,\}, \qquad P_2 := \{\, M_{\mathrm{Bridge}}, M_{\mathrm{MAPK}} \,\}, \qquad P_3 := \{\, M_{\mathrm{EGFR}}, M_{\mathrm{Bridge}}, M_{\mathrm{MAPK}} \,\}.$$

Each $P_i$ is a subset of $V_1$, hence an element of $\mathrm{POWS}(V_1) = \mathrm{POWS}^2(V_0)$. Set the level-2 vertex set

$$V_2 := \{P_1, P_2, P_3\} \subseteq \mathrm{POWS}^2(V_0).$$

Level 2 superedges (coupled programs). Define nonempty 2-superedges as subsets of $V_2$ that capture jointly active programs:

$$F_1 := \{P_1, P_2\}, \qquad F_2 := \{P_2, P_3\}.$$

Let $\mathcal{E}_2 := \{F_1, F_2\} \subseteq \mathrm{POWS}(V_2) \setminus \{\emptyset\}$.

Resulting 2-SuperHyperGraph. The biochemical level-2 SuperHyperGraph is

$$\mathcal{H}^{(2)} := \big(V_2,\ \mathcal{E}_2\big),$$

where:

- $V_2$ consists of 2-supervertices $P_i$, each a *set of modules* (i.e., a set of sets of reactions).
- $\mathcal{E}_2$ consists of 2-superedges $F_j$, each a nonempty set of such programs indicating co-activation/coupling.

By construction $V_2 \subseteq \mathrm{POWS}^2(V_0)$ (each $P_i \subseteq V_1 \subseteq \mathrm{POWS}^1(V_0)$), and $\mathcal{E}_2 \subseteq \mathrm{POWS}(V_2) \setminus \{\emptyset\}$. Hence $\mathcal{H}^{(2)}$ satisfies the definition of a finite level-2 SuperHyperGraph.

### 1.2. *Line Graph*

A line graph represents edges of a graph as vertices, linking them if the original edges share a common endpoint (cf. [22–24]).

**Definition 1.10** (Line graph). (cf. [22–24]) Let $G = (V(G), E(G))$ be a (loopless) undirected simple graph. The *line graph* $L(G)$ is the (simple) graph defined by

$$V\big(L(G)\big) = E(G), \qquad \{e, f\} \in E\big(L(G)\big) \iff e \cap f \neq \emptyset,$$

i.e., two vertices of $L(G)$ are adjacent exactly when the corresponding two edges of $G$ share an endpoint.

**Example 1.11** (Line Graph in chemical physics: linear triatomic O=C=O). Model the molecule by the simple graph $G = (V, E)$ with

$$V = \{O_{\mathrm{L}}, C, O_{\mathrm{R}}\}, \qquad E = \{e_{\mathrm{C-O_L}} = \{C, O_{\mathrm{L}}\},\ e_{\mathrm{C-O_R}} = \{C, O_{\mathrm{R}}\}\}.$$

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The line graph $L(G)$ has vertex set $V' := E = \{e_{\text{C--O}_\text{L}}, e_{\text{C--O}_\text{R}}\}$. Since the two bonds share the common atom C, they are adjacent in $L(G)$:

$$E' = \{\, \{\, e_{\text{C--O}_\text{L}},\ e_{\text{C--O}_\text{R}} \,\} \,\}.$$

Thus $L(G) \cong K_2$. Physically, $L(G)$ encodes bond–bond adjacency (useful for building bond-coupling models in vibrational or electronic Hamiltonians).

A line hypergraph transforms each hyperedge into a vertex and encodes how these vertices (interaction terms) meet at original vertices; it is thus a higher-order analogue of the line graph (cf. [25–29]).

**Definition 1.12** (Clique of rank $r$). Let $X$ be a finite set and let $r$ be an integer with $0 \leq r \leq |X|$. The *clique of rank $r$* on $X$ is the (simple) $r$-uniform hypergraph

$$\mathsf{K}^{(r)}(X) := \left(X,\ \binom{X}{r}\right).$$

In particular, rank 2 yields the complete graph on $X$; rank 1 yields the hypergraph with singleton hyperedges; rank 0 yields the hypergraph with empty hyperedge family (all vertices isolated).

**Definition 1.13** (Line hypergraph (multi-valued)). (cf. [25–28]) Let $H = (V, \mathcal{E})$ be a hypergraph without isolated vertices, and list $V = \{v_1, \ldots, v_n\}$. For each $v \in V$, write

$$\mathcal{E}_H(v) := \{\, e \in \mathcal{E} :\ v \in e \,\} \qquad \text{and} \qquad \deg_H(v) := |\mathcal{E}_H(v)|.$$

Define two integer vectors

$$\mathbf{1}_H = (\deg_H(v_1), \ldots, \deg_H(v_n)), \qquad \mathbf{0}_H = (0_{v_i})_{i=1}^n \ \text{with}\ 0_{v_i} = \begin{cases} 0, & \deg_H(v_i) = 1, \\ 2, & \deg_H(v_i) \geq 2. \end{cases}$$

Let $\mathcal{D}_H := \{D = (d_{v_i})_{i=1}^n :\ \mathbf{0}_H \leq D \leq \mathbf{1}_H \text{ componentwise}\}$. For any $D \in \mathcal{D}_H$, define the (single-valued) line hypergraph

$$L_D(H) := \left(\ \mathcal{E},\ \bigcup_{v \in V} \binom{\mathcal{E}_H(v)}{d_v} \ \right),$$

i.e., the vertex set is $\mathcal{E}$ (original hyperedges), and for each $v \in V$ we add the rank-$d_v$ clique on $\mathcal{E}_H(v)$. The (multi-valued) *line hypergraph* of $H$ is the set

$$L(H) := \{\, L_D(H) : D \in \mathcal{D}_H \,\}.$$

**Remark 1.14** (Two standard specializations). Within the family $L(H)$, two choices are particularly common:

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(i) (Pairwise adjacency / line graph analogue) Choosing $d_v = 2$ for all $v$ with $\deg_H(v) \geq 2$ produces a 2-uniform line hypergraph (a simple graph) that connects two hyperedges whenever they share at least one original vertex.

(ii) (Star hyperedges) Choosing $d_v = \deg_H(v)$ produces one hyperedge $\mathcal{E}_H(v)$ per $v$, i.e., the "star" of $v$. This yields a natural higher-order grouping of interaction terms.

**Example 1.15** (Line hypergraph in chemical physics: four-atom cluster with two three-body terms)**.** Let the atom set be $V = \{A, B, C, D\}$. Include three pair interactions and two three-body (angular) interactions:

$$\mathcal{E} = \{e_{AB} = \{A, B\}, \ e_{BC} = \{B, C\}, \ e_{CD} = \{C, D\}, \ e_{ABC} = \{A, B, C\}, \ e_{BCD} = \{B, C, D\}\}.$$

Set $\mathcal{H} := (V, \mathcal{E})$. For each atom $v \in V$, the incident-hyperedge set (star) is

$$\mathcal{E}_{\mathcal{H}}(v) := \{\, e \in \mathcal{E} : \ v \in e \,\}.$$

Concretely,

$$\mathcal{E}_{\mathcal{H}}(A) = \{e_{AB}, e_{ABC}\},$$
$$\mathcal{E}_{\mathcal{H}}(B) = \{e_{AB}, e_{BC}, e_{ABC}, e_{BCD}\},$$
$$\mathcal{E}_{\mathcal{H}}(C) = \{e_{BC}, e_{CD}, e_{ABC}, e_{BCD}\},$$
$$\mathcal{E}_{\mathcal{H}}(D) = \{e_{CD}, e_{BCD}\}.$$

Now choose the maximal parameter vector $D^{\max} \in \mathcal{D}_{\mathcal{H}}$ defined by $d_v := \deg_{\mathcal{H}}(v) = |\mathcal{E}_{\mathcal{H}}(v)|$ for all $v \in V$. Then $\binom{\mathcal{E}_{\mathcal{H}}(v)}{d_v} = \{\mathcal{E}_{\mathcal{H}}(v)\}$, hence

$$L_{D^{\max}}(\mathcal{H}) = \Big( \ \mathcal{E}, \ \{\mathcal{E}_{\mathcal{H}}(A), \mathcal{E}_{\mathcal{H}}(B), \mathcal{E}_{\mathcal{H}}(C), \mathcal{E}_{\mathcal{H}}(D)\} \ \Big).$$

Interpretation: each vertex represents an interaction term (pair or three-body), and each hyperedge groups all interaction terms that meet at a common atom—an organization useful for many-body potential assembly in chemical-physics simulations.

A line superhypergraph maps each superedge to a vertex, linking them through superedges containing a common supervertex in the original structure [30].

**Definition 1.16** (Line SuperHyperGraph)**.** [30] Let $\mathcal{H}^{(n)} = (V_n, \mathcal{E})$ be a level-$n$ SuperHyperGraph. Its *line SuperHyperGraph* is the pair

$$\mathsf{L}^{(n)}(\mathcal{H}) \ = \ \big(V'_{n+1}, \ \mathcal{E}'_{n+1}\big)$$

defined by

$$V'_{n+1} \ := \ \mathcal{E} \qquad \text{and} \qquad \mathcal{E}'_{n+1} \ := \ \{\, \mathsf{Star}_{\mathcal{H}}(v) \subseteq \mathcal{E} \ : \ v \in V_n, \ \mathsf{Star}_{\mathcal{H}}(v) \neq \emptyset \,\}.$$

Intuitively, $\mathsf{L}^{(n)}(\mathcal{H})$ has one vertex for each superedge of $\mathcal{H}$; for every supervertex $v \in V_n$, we add a (hyper)edge collecting *all* superedges that contain $v$.

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**Example 1.17** (Line SuperHyperGraph in chemical physics: conjugated fragment couplings).
Let $V_0 = \{b_{12}, b_{23}, b_{34}\}$ denote bond identifiers along a short conjugated chain $C_1-C_2-C_3-C_4$.
Form a level-1 molecular SuperHyperGraph $\mathcal{H}^{(1)} = (V_1, \mathcal{E})$ by grouping bonds into chemically
meaningful fragments (supervertices):

$$T_{\text{left}} = \{b_{12}, b_{23}\}, \quad T_{\text{right}} = \{b_{23}, b_{34}\}, \quad T_{\text{cap}} = \{b_{12}\}.$$

Set

$$V_1 = \{T_{\text{left}}, T_{\text{right}}, T_{\text{cap}}\}, \qquad \mathcal{E} = \big\{ E_1 = \{T_{\text{left}}, T_{\text{right}}\}, \quad E_2 = \{T_{\text{left}}, T_{\text{cap}}\} \big\},$$

where $E_1$ encodes $\pi$-conjugation across the central region and $E_2$ encodes local coupling at
the chain end. The *line SuperHyperGraph* $\mathbf{L}(\mathcal{H}^{(1)}) = (V_2', \mathcal{E}_2')$ has

$$V_2' := \mathcal{E} = \{E_1, E_2\},$$

and, for each $T \in V_1$, the hyperedge $\mathsf{Star}_{\mathcal{H}^{(1)}}(T) = \{E \in \mathcal{E} : T \in E\}$. Explicitly,

$$\mathsf{Star}(T_{\text{left}}) = \{E_1, E_2\}, \qquad \mathsf{Star}(T_{\text{right}}) = \{E_1\}, \qquad \mathsf{Star}(T_{\text{cap}}) = \{E_2\}.$$

Therefore

$$\mathcal{E}_2' = \big\{ \{E_1, E_2\}, \{E_1\}, \{E_2\} \big\}.$$

Here, vertices of $\mathbf{L}(\mathcal{H}^{(1)})$ represent fragment–fragment coupling channels $(E_1, E_2)$, while its
hyperedges record which channels meet at the same fragment—an arrangement aligning with
fragment-based Hamiltonian partitioning and energy-transfer analyses in chemical physics.

### 1.3. *Iterated line graphs*

An iterated line graph is formed by repeatedly applying the line graph transformation to a
graph, using each result as the next input [31–36].

**Definition 1.18** (Iterated line graphs). (cf. [31–36]) Define $L^0(G) := G$. For each integer
$n \geq 1$, the *n-th iterated line graph* of $G$ is defined recursively by

$$L^n(G) := L\big(L^{n-1}(G)\big).$$

Equivalently, many authors write $L_1(G) = L(G)$ and $L_n(G) = L\big(L_{n-1}(G)\big)$ for $n \geq 2$.

**Example 1.19** (Iterated Line Graph: a peptide backbone fragment). Consider a linear
four–residue peptide fragment with $C_\alpha$ atoms

$$V = \{R_1, R_2, R_3, R_4\}, \qquad E = \{e_{12} = \{R_1, R_2\}, \ e_{23} = \{R_2, R_3\}, \ e_{34} = \{R_3, R_4\}\}.$$

This graph models covalent backbone connectivity (edges = peptide bonds). The line graph
$L(G)$ has

$$V' = E = \{e_{12}, e_{23}, e_{34}\}, \qquad E' = \{\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}\},$$

so $L(G) \cong P_3$ (a path on three vertices), encoding *bond–bond adjacency.* Iterating once more,

$$L^2(G) = L(P_3) = P_2,$$

and then $L^3(G) = L(P_2) = P_1$ (a single vertex). In general for a chain $P_n$ (e.g., an unbranched peptide segment),

$$L(P_n) = P_{n-1} \quad (n \geq 2), \qquad L^k(P_n) = P_{n-k} \text{ while defined.}$$

This illustrates how repeated line transforms propagate from atom–atom bonds to adjacency between bonds, then to adjacency between those adjacencies, and so on.

An iterated line hypergraph applies the line hypergraph construction repeatedly to a hypergraph, capturing higher-order adjacency of hyperedges over iterations [30].

**Definition 1.20** (Iterated line hypergraphs). [30] Define $L^0(H) := H$ and, for each $n \geq 1$, set

$$L^n(H) := L\big(L^{n-1}(H)\big).$$

**Example 1.21** (Iterated line hypergraph: a phosphate–transfer micro-network). (cf. [37]) Let metabolites be

$$V = \{\text{ATP, ADP, Pi}\},$$

and define a hypergraph $\mathcal{H} = (V, \mathcal{E})$ whose hyperedges encode participation sets of elementary processes:

$$e_0 = \{\text{ATP}, \text{ADP}, \text{Pi}\} \text{ (triad pool)}, \quad e_1 = \{\text{ATP}, \text{ADP}\},$$

$$e_2 = \{\text{ATP}, \text{Pi}\}, \quad e_3 = \{\text{ADP}, \text{Pi}\},$$

$$\mathcal{E} = \{e_0, e_1, e_2, e_3\}.$$

**First iteration (star specialization).** We take the *star* specialization of the multi-valued line hypergraph (cf. Remark 1.14(ii)), namely $\mathsf{L}_H(\mathcal{H}) := L_{D^{\mathrm{max}}}(\mathcal{H})$, where $D^{\mathrm{max}}$ is given by $d_x = \deg_{\mathcal{H}}(x)$. Thus $\mathsf{L}_H(\mathcal{H}) = (\mathcal{E}, \mathcal{F})$ has vertex set $\mathcal{E}$ and hyperedge family $\mathcal{F} = \{\mathcal{E}_{\mathcal{H}}(x) : x \in V\}$, where

$$\mathcal{E}_{\mathcal{H}}(x) := \{\, e \in \mathcal{E} : x \in e \,\}.$$

Explicitly,

$$\mathcal{E}_{\mathcal{H}}(\text{ATP}) = \{e_0, e_1, e_2\},$$

$$\mathcal{E}_{\mathcal{H}}(\text{ADP}) = \{e_0, e_1, e_3\},$$

$$\mathcal{E}_{\mathcal{H}}(\text{Pi}) = \{e_0, e_2, e_3\}.$$

Hence

$$\mathcal{F} = \big\{\{e_0, e_1, e_2\},\ \{e_0, e_1, e_3\},\ \{e_0, e_2, e_3\}\big\}.$$

**Second iteration.** Define the second iterated line hypergraph (still under the same star specialization) by

$$\mathsf{L}_H^{(2)}(\mathcal{H}) \ := \ \mathsf{L}_H\big(\mathsf{L}_H(\mathcal{H})\big) = \mathsf{L}_H(\mathcal{E}, \mathcal{F}).$$

Its vertex set is $\mathcal{F}$. For each old vertex $e \in \mathcal{E}$, form the star in $\mathsf{L}_H(\mathcal{H})$:

$$\mathcal{F}_{\mathsf{L}_H(\mathcal{H})}(e) \ := \ \{\, F \in \mathcal{F} : e \in F \,\}.$$

Concretely, writing

$$F_{\mathrm{ATP}} := \{e_0, e_1, e_2\}, \quad F_{\mathrm{ADP}} := \{e_0, e_1, e_3\}, \quad F_{\mathrm{Pi}} := \{e_0, e_2, e_3\},$$

we obtain

$$\mathcal{F}_{\mathsf{L}_H(\mathcal{H})}(e_0) = \{F_{\mathrm{ATP}}, F_{\mathrm{ADP}}, F_{\mathrm{Pi}}\},$$
$$\mathcal{F}_{\mathsf{L}_H(\mathcal{H})}(e_1) = \{F_{\mathrm{ATP}}, F_{\mathrm{ADP}}\},$$
$$\mathcal{F}_{\mathsf{L}_H(\mathcal{H})}(e_2) = \{F_{\mathrm{ATP}}, F_{\mathrm{Pi}}\},$$
$$\mathcal{F}_{\mathsf{L}_H(\mathcal{H})}(e_3) = \{F_{\mathrm{ADP}}, F_{\mathrm{Pi}}\}.$$

Thus $\mathsf{L}_H^{(2)}(\mathcal{H})$ has three vertices $F_{\mathrm{ATP}}, F_{\mathrm{ADP}}, F_{\mathrm{Pi}}$ and four hyperedges given by the above stars.

**Interpretation.** This construction moves from *metabolite–process incidence* (the original $\mathcal{H}$) to *process–process co-participation* (the first line hypergraph $\mathsf{L}_H(\mathcal{H})$), and then to *co-participation-of-co-participations* (the second iterate $\mathsf{L}_H^{(2)}(\mathcal{H})$).

An iterated line superhypergraph repeatedly applies the line superhypergraph transformation to a superhypergraph, modeling evolving hierarchical incidence patterns across multiple levels.

**Definition 1.22** (Iterated line superhypergraphs). [30] For an initial level-$n$ superhypergraph $\mathcal{H}^{(n)}$, define

$$\mathbf{L}^0(\mathcal{H}^{(n)}) \ := \ \mathcal{H}^{(n)}, \qquad \mathbf{L}^{t+1}(\mathcal{H}^{(n)}) \ := \ \mathbf{L}\big(\mathbf{L}^t(\mathcal{H}^{(n)})\big) \quad (t \geq 0).$$

$\mathbf{L}^t(\mathcal{H}^{(n)})$ is level $n+t$.

**Example 1.23** (Iterated Line SuperHyperGraph: pathway modules $\rightarrow$ coupling channels $\rightarrow$ couplings of channels). Let the base set $V_0$ list reaction identifiers along a short signaling/glycolytic segment:

$$V_0 = \{r_1, \ r_2, \ r_3, \ r_4\}.$$

Form three level-1 supervertices (modules) as subsets of $V_0$:

$$M_1 = \{r_1, r_2\}, \qquad M_2 = \{r_2, r_3\}, \qquad M_3 = \{r_3, r_4\},$$

and set $V_1 = \{M_1, M_2, M_3\}$. Define level-1 superedges (module couplings)

$$E_1 = \{M_1, M_2\}, \qquad E_2 = \{M_2, M_3\},$$

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so $\mathcal{H}^{(1)} = (V_1, \mathcal{E}^{(1)})$ with $\mathcal{E}^{(1)} = \{E_1, E_2\}$. Apply the line SuperHyperGraph operator to obtain

$$\mathbf{L}\big(\mathcal{H}^{(1)}\big) = (V_2', \mathcal{E}_2'), \qquad V_2' = \mathcal{E}^{(1)} = \{E_1, E_2\},$$

and (nonempty) stars in $\mathcal{H}^{(1)}$:

$$\mathrm{Star}_{\mathcal{H}^{(1)}}(M_1) = \{E_1\}, \quad \mathrm{Star}_{\mathcal{H}^{(1)}}(M_2) = \{E_1, E_2\}, \quad \mathrm{Star}_{\mathcal{H}^{(1)}}(M_3) = \{E_2\}.$$

Thus

$$\mathcal{E}_2' = \big\{\ \{E_1\},\ \{E_1, E_2\},\ \{E_2\}\ \big\}.$$

Iterate once more to get the *Iterated Line SuperHyperGraph*

$$\mathbf{L}^2\big(\mathcal{H}^{(1)}\big) = \mathbf{L}\Big(\mathbf{L}\big(\mathcal{H}^{(1)}\big)\Big) = (V_3', \mathcal{E}_3'),$$

with

$$V_3' = \mathcal{E}_2' = \big\{\ \{E_1\},\ \{E_1, E_2\},\ \{E_2\}\ \big\},$$

and stars in $\mathbf{L}(\mathcal{H}^{(1)})$:

$$\mathrm{Star}_{\mathbf{L}(\mathcal{H}^{(1)})}(E_1) = \big\{\ \{E_1\},\ \{E_1, E_2\}\ \big\},$$

$$\mathrm{Star}_{\mathbf{L}(\mathcal{H}^{(1)})}(E_2) = \big\{\ \{E_1, E_2\},\ \{E_2\}\ \big\}.$$

Hence

$$\mathcal{E}_3' = \big\{\ \{\{E_1\}, \{E_1, E_2\}\},\ \{\{E_1, E_2\}, \{E_2\}\}\ \big\}.$$

Chemically, level 1 groups reactions into modules, level 2 turns module couplings into "channel vertices" and records which channels meet at a module, and level 3 records how those channels themselves co-occur via shared channel–vertices.

### 1.4. *Molecular Line Graph and Iterated Line Graph*

Molecular Graph models a molecule with atoms as vertices and bonds as edges, representing its structural connectivity [38–43]. Related concepts to the molecular graph include the chemical graph [44–48]. Molecular graphs have been extensively studied in a wide variety of research works [49–52].

Molecular Line Graph represents each bond of a molecular graph as a vertex, connecting them if the bonds share an atom (cf. [53, 54]). Molecular Iterated Line Graph repeatedly applies the line-graph transformation to reveal successive higher-order bond adjacency relationships [55–57].

**Definition 1.24** (Molecular Graph). [38,39] A *molecular graph* is a finite, simple, undirected graph $G = (V, E)$ in which each vertex $v \in V$ represents an atom and each edge $e = \{u, v\} \in E$ represents a chemical bond between atoms $u$ and $v$. (Optionally, vertex/edge labels may encode atom types and bond types or orders.)

**Example 1.25** (Methane $CH_4$). (cf. [58]) Consider methane, which consists of one carbon atom bonded to four hydrogen atoms. The molecular graph is

$$G = (V, E), \qquad V = \{C, H_1, H_2, H_3, H_4\}, \quad E = \{\{C, H_1\}, \{C, H_2\}, \{C, H_3\}, \{C, H_4\}\}.$$

Here the single carbon vertex $C$ is connected to each hydrogen vertex, forming a star graph $K_{1,4}$. This representation captures the tetrahedral bonding pattern of methane in a simplified graph-theoretic form.

**Definition 1.26** (Molecular Line Graph). (cf. [53,54]). Let $G = (V, E)$ be a molecular graph. The *molecular line graph* $L(G) = (V', E')$ is the (simple, undirected) line graph of $G$ defined by:

- $V' := E$ (each vertex of $L(G)$ corresponds to a bond of $G$);
- for distinct $e, e' \in V' = E$, $\{e, e'\} \in E'$ iff the two bonds $e$ and $e'$ share a common atom in $G$ (i.e., are incident in $G$).

Equivalently, two vertices of $L(G)$ are adjacent precisely when their corresponding edges of $G$ are incident.

**Example 1.27** (Linear chain on four atoms: $G = P_4$). (cf. [59]) Let $V = \{1, 2, 3, 4\}$ and $E = \{e_{12}, e_{23}, e_{34}\}$ with $e_{ij} := \{i, j\}$. Then the molecular line graph $L(G) = (V', E')$ has

$$V' := E = \{e_{12}, e_{23}, e_{34}\}, \qquad E' := \{\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}\},$$

so $L(G)$ is the path $P_3$. With vertex order $(e_{12}, e_{23}, e_{34})$, its adjacency matrix is

$$A(L(G)) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Iterating once,

$$L^2(G) = L(P_3) = P_2 \quad \text{with} \quad V'' = \{\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}\}, \ E'' = \{\{\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}\}\}.$$

Iterating again, $L^3(G) = L(P_2) = P_1$ (a single vertex). In general, $L(P_n) = P_{n-1}$ for $n \geq 2$, so $L^k(P_n) = P_{n-k}$ while defined.

**Definition 1.28** (Molecular Iterated Line Graph). For a molecular graph $G$, define the sequence $\{L^k(G)\}_{k \geq 0}$ recursively by

$$L^0(G) := G, \qquad L^{k+1}(G) := L(L^k(G)) \ \text{ for } k \geq 0.$$

The graph $L^k(G)$ is called the *k-th molecular iterated line graph* of $G$.

**Example 1.29** (Linear alkane backbone: $G = P_5$ (e.g., a pentane fragment)). (cf. [60]) Model a five-carbon chain by the simple molecular graph

$$V = \{C_1, C_2, C_3, C_4, C_5\}, \qquad E = \{e_{12} = \{C_1, C_2\},\ e_{23} = \{C_2, C_3\},\ e_{34} = \{C_3, C_4\},\ e_{45} = \{C_4, C_5\}\}.$$

Thus $G$ is the path $P_5$. By definition of the line graph, the first iterate has

$$V(L(G)) = E = \{e_{12}, e_{23}, e_{34}, e_{45}\}, \quad E(L(G)) = \{\{e_{12}, e_{23}\},\ \{e_{23}, e_{34}\},\ \{e_{34}, e_{45}\}\},$$

so $L(G) \cong P_4$. With vertex order $(e_{12}, e_{23}, e_{34}, e_{45})$, the adjacency matrix is

$$A(L(G)) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Iterating again,

$$L^2(G) = L(P_4) = P_3, \qquad A(L^2(G)) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Continuing,

$$L^3(G) = L(P_3) = P_2, \qquad L^4(G) = L(P_2) = P_1 \text{ (single vertex)}, \qquad L^5(G) = L(P_1) = P_0 \text{ (empty)}.$$

In general, for a path $P_n$ (an unbranched alkane backbone with $n$ carbon atoms),

$$L(P_n) = P_{n-1} \ \ (n \geq 2), \qquad L^k(P_n) = P_{n-k} \ \text{ while } n - k \geq 1.$$

**Size evolution.** If $|V(G)| = n$ and $|E(G)| = n - 1$ (a path), then

$$|V(L^k(G))| = n - k - 1, \qquad |E(L^k(G))| = n - k - 2 \quad (k = 0, 1, \ldots, n-2).$$

This explicitly tracks how bond–bond adjacencies (and higher) shrink along iterations.

**Example 1.30** (Aromatic ring: $G = C_6$ (benzene)). (cf. [61]) Let $G$ be the 6-cycle with vertices $V = \{C_1, \ldots, C_6\}$ and edges $E = \{\{C_1, C_2\}, \{C_2, C_3\}, \ldots, \{C_6, C_1\}\}$. Every edge in $G$ meets exactly two others, and the edge–adjacency pattern is itself a 6-cycle. Hence

$$L(G) \cong C_6, \qquad L^k(G) \cong C_6 \ \text{ for all } k \geq 1.$$

Thus benzene is a fixed point of the line-graph operator, reflecting the uniform bond–bond adjacency around the ring.

**Example 1.31** (Linear alkane backbone: $n$-pentane fragment $C_1 - C_2 - C_3 - C_4 - C_5$). We model an unbranched five–carbon backbone (as appears in $n$-pentane) by the simple molecular graph

$$G = (V, E), \qquad V = \{C_1, C_2, C_3, C_4, C_5\}, \quad E = \{e_{12}, e_{23}, e_{34}, e_{45}\},$$

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where $e_{ij} = \{C_i, C_j\}$ represents the covalent C–C bond.

*Adjacency matrix of G.* In the vertex order $(C_1, C_2, C_3, C_4, C_5)$, $G$ is the path $P_5$ with

$$A(G) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

*First iterate L(G): bond–bond adjacency.* By definition of the line graph, the vertices of $L(G)$ are the bonds of $G$:

$$V\big(L(G)\big) = E = \{e_{12}, e_{23}, e_{34}, e_{45}\}.$$

Two vertices of $L(G)$ are adjacent iff the corresponding bonds share a carbon in $G$. Thus $L(G) \cong P_4$ with edges

$$\{\{e_{12}, e_{23}\},\ \{e_{23}, e_{34}\},\ \{e_{34}, e_{45}\}\}.$$

In the order $(e_{12}, e_{23}, e_{34}, e_{45})$,

$$A\big(L(G)\big) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

*Counts:* $|V(L(G))| = 4$, $|E(L(G))| = 3$.

*Second iterate $L^2(G) = L(L(G))$.* Applying the line-graph operator to $P_4$ yields $P_3$. Its vertices correspond to the three edges of $L(G)$:

$$V\big(L^2(G)\big) = \{\{e_{12}, e_{23}\},\ \{e_{23}, e_{34}\},\ \{e_{34}, e_{45}\}\},$$

and the edges of $L^2(G)$ reflect shared adjacency:

$$E\big(L^2(G)\big) = \{\{\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}\},\ \{\{e_{23}, e_{34}\}, \{e_{34}, e_{45}\}\}\}.$$

In the order $(\{e_{12}, e_{23}\}, \{e_{23}, e_{34}\}, \{e_{34}, e_{45}\})$,

$$A\big(L^2(G)\big) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

*Counts:* $|V(L^2(G))| = 3$, $|E(L^2(G))| = 2$.

*Higher iterates and general pattern.* Continuing,

$$L^3(G) = L(P_3) = P_2, \qquad L^4(G) = L(P_2) = P_1 \ \text{(single vertex)},$$

$$L^5(G) = L(P_1) = P_0 \ \text{(empty)}.$$

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In general for an unbranched $n$-carbon chain $G = P_n$,

$$L(P_n) = P_{n-1} \ (n \geq 2), \qquad L^k(P_n) = P_{n-k} \quad \text{while } n - k \geq 1.$$

$G$ encodes atom–atom connectivity (C–C bonds). $L(G)$ turns bonds into vertices and records which bonds are *adjacent* at a common carbon—useful, e.g., for constructing bond–bond coupling terms in vibrational or NMR coupling models along an alkane backbone. Iterating to $L^2(G)$ captures adjacency among *bond–adjacency relations* themselves, which can organize higher-order constraints (e.g., sequential coupling pathways or coarse-grained segment interactions) in linear hydrocarbons such as $n$-pentane.

## 2. Molecular Line HyperGraph and Iterated Line HyperGraph

Molecular Hypergraph represents atoms as vertices and chemical bonds as hyperedges, capturing multi-atom interactions in a molecular structure [62–64]. Molecular hypergraphs have been the subject of various studies in recent years [65,66]. Molecular Line HyperGraph transforms a molecular hypergraph by representing bonds as vertices and connecting them when sharing common atoms. Iterated Line HyperGraph repeatedly applies the line-hypergraph transformation, revealing higher-order adjacency relationships between bonds in successive levels.

**Definition 2.1** (Molecular Hypergraph)**.** [62,63] A *molecular hypergraph* is a finite, simple, undirected hypergraph $\mathcal{H} = (V, E)$, where $V$ is the set of atoms and $E \subseteq 2^V \setminus \{\emptyset\}$ is the family of *bonds/interaction groups*. We allow $|e| \geq 2$ to encode multi-center interactions; multiple identical hyperedges are not allowed and loops are excluded. For $v \in V$, the (hypergraph) degree is $\deg_{\mathcal{H}}(v) := |\{ e \in E : v \in e \}|$.

**Example 2.2** (Molecular HyperGraph: Diborane $B_2H_6$ with three-center bonds)**.** Consider diborane with atoms

$$V = \{ B_1, B_2, \ H_{b1}, H_{b2}, \ H_{t1}, H_{t2}, H_{t3}, H_{t4} \},$$

where $H_{b1}, H_{b2}$ are bridging hydrogens and $H_{t1}, \ldots, H_{t4}$ are terminal hydrogens. Model two-center B–H bonds as size-2 hyperedges and each three-center two-electron bridge $B-H-B$ as a size-3 hyperedge:

$$E = \underbrace{\left\{ \{B_1, H_{t1}\}, \{B_1, H_{t2}\}, \{B_2, H_{t3}\}, \{B_2, H_{t4}\} \right\}}_{\text{terminal two-center bonds}}$$
$$\cup \underbrace{\left\{ \{B_1, H_{b1}, B_2\}, \{B_1, H_{b2}, B_2\} \right\}}_{\text{bridging three-center bonds}}.$$

The molecular hypergraph is $\mathcal{H} = (V, E)$. This representation captures both ordinary two-center bonds and multi-center $B-H-B$ interactions within the same hypergraph formalism.

**Example 2.3** (Molecular Hypergraph)**.** We encode ordinary B–H *two-center* bonds and *three-center* B–H–B bridges in a single molecular hypergraph $\mathcal{H} = (V, E)$.

*Atom (vertex) set.*
$$V = \{\, B_1, B_2,\ H_{b1}, H_{b2},\ H_{t1}, H_{t2}, H_{t3}, H_{t4}\,\}.$$

*Bond/interaction family (hyperedges).* Two-center terminals and three-center bridges:

$$E = \{e_{t1} = \{B_1, H_{t1}\},\ e_{t2} = \{B_1, H_{t2}\},\ e_{t3} = \{B_2, H_{t3}\},\ e_{t4} = \{B_2, H_{t4}\},$$

$$e_{b1} = \{B_1, H_{b1}, B_2\},\ e_{b2} = \{B_1, H_{b2}, B_2\}\,\}.$$

*Incidence matrix (rows: $B_1, B_2, H_{b1}, H_{b2}, H_{t1}, H_{t2}, H_{t3}, H_{t4}$; columns: $e_{t1}, e_{t2}, e_{t3}, e_{t4}, e_{b1}, e_{b2}$).*

$$
\mathbf{H} =
\begin{array}{c}
\\
B_1 \\ B_2 \\ H_{b1} \\ H_{b2} \\ H_{t1} \\ H_{t2} \\ H_{t3} \\ H_{t4}
\end{array}
\begin{array}{cccccc}
e_{t1} & e_{t2} & e_{t3} & e_{t4} & e_{b1} & e_{b2} \\
\left[\begin{array}{cccccc}
1 & 1 & 0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0
\end{array}\right]
\end{array}
$$

*Degrees and sanity check.*

$$\deg(B_1) = 4,\ \deg(B_2) = 4,\ \deg(H_{b1}) = \deg(H_{b2}) = \deg(H_{t1}) = \cdots = \deg(H_{t4}) = 1.$$

The total incidence count equals both the sum of vertex degrees and the sum of hyperedge sizes:

$$\sum_{v \in V} \deg(v) = 4 + 4 + 1 + 1 + 1 + 1 + 1 + 1 = 14$$

$$\sum_{e \in E} |e| = 2 + 2 + 2 + 2 + 3 + 3 = 14,$$

verifying consistency. This hypergraph cleanly unifies two-center and three-center bonding motifs in a single combinatorial object.

**Definition 2.4** (2-section (primal) of a Hypergraph)**.** For a hypergraph $\mathcal{F} = (\mathsf{V}, \mathsf{E})$, its *2-section* $\mathrm{Sec}_2(\mathcal{F})$ is the simple graph on vertex set $\mathsf{V}$ with an edge $\{x, y\}$ for distinct $x, y \in \mathsf{V}$ iff there exists $f \in \mathsf{E}$ such that $\{x, y\} \subseteq f$.

**Definition 2.5** (Line Hypergraph Operator)**.** Let $\mathcal{H} = (V, E)$ be any finite hypergraph. The *line hypergraph* (also called incidence-dual expansion) of $\mathcal{H}$ is

$$\mathsf{L}_H(\mathcal{H}) := (E, \mathsf{E}) \quad \text{with} \quad \mathsf{E} := \{\, N_{\mathcal{H}}(v) \subseteq E :\ v \in V,\ N_{\mathcal{H}}(v) \neq \emptyset \,\},$$

where

$$N_{\mathcal{H}}(v) := \{ e \in E : v \in e \}$$

collects all hyperedges of $\mathcal{H}$ incident to $v$. Thus vertices of $\mathsf{L}_H(\mathcal{H})$ are the bonds $E$ of $\mathcal{H}$, and each atom $v$ induces a hyperedge consisting of all bonds meeting $v$.

**Definition 2.6** (Molecular Line HyperGraph). For a molecular hypergraph $\mathcal{H} = (V, E)$, its *Molecular Line HyperGraph* is $\mathrm{MLH}(\mathcal{H}) := \mathsf{L}_H(\mathcal{H})$.

**Example 2.7** (Molecular Line HyperGraph of $B_2H_6$). Let $\mathcal{H} = (V, E)$ be as above and name the hyperedges

$$e_{t1} = \{B_1, H_{t1}\}, \quad e_{t2} = \{B_1, H_{t2}\}, \quad e_{t3} = \{B_2, H_{t3}\}, \quad e_{t4} = \{B_2, H_{t4}\},$$

$$e_{b1} = \{B_1, H_{b1}, B_2\}, \quad e_{b2} = \{B_1, H_{b2}, B_2\}.$$

The Molecular Line HyperGraph $\mathrm{MLH}(\mathcal{H}) = \mathsf{L}_H(\mathcal{H})$ has

$$V' := E = \{e_{t1}, e_{t2}, e_{t3}, e_{t4}, e_{b1}, e_{b2}\},$$

and for each atom $v \in V$ we add the hyperedge $\mathrm{Star}_{\mathcal{H}}(v) = \{ e \in E : v \in e \}$. Concretely,

$$\mathrm{Star}(B_1) = \{e_{t1}, e_{t2}, e_{b1}, e_{b2}\}, \qquad \mathrm{Star}(B_2) = \{e_{t3}, e_{t4}, e_{b1}, e_{b2}\},$$

$$\mathrm{Star}(H_{t1}) = \{e_{t1}\}, \ \mathrm{Star}(H_{t2}) = \{e_{t2}\}, \ \mathrm{Star}(H_{t3}) = \{e_{t3}\}, \ \mathrm{Star}(H_{t4}) = \{e_{t4}\},$$

$$\mathrm{Star}(H_{b1}) = \{e_{b1}\}, \ \mathrm{Star}(H_{b2}) = \{e_{b2}\}.$$

Thus the hyperedge set of $\mathrm{MLH}(\mathcal{H})$ is

$$E' = \big\{ \mathrm{Star}(v) : v \in V, \ \mathrm{Star}(v) \neq \emptyset \big\}.$$

Intuitively, each vertex of $\mathrm{MLH}(\mathcal{H})$ represents an original bond or multi-center interaction, and hyperedges group all such interactions incident to a common atom.

**Example 2.8** (Molecular Line HyperGraph: Cyclopropane $C_3H_6$ (C–C skeleton)). Consider the carbon triangle $(C_1C_2C_3)$ as a molecular hypergraph with only C–C bonds (each a size-2 hyperedge). Let

$$V = \{C_1, C_2, C_3\}, \qquad E = \{e_{12} = \{C_1, C_2\}, \ e_{23} = \{C_2, C_3\}, \ e_{31} = \{C_3, C_1\}\}.$$

The Molecular Line HyperGraph is $\mathrm{MLH}(\mathcal{H}) = \mathsf{L}_H(\mathcal{H}) = (E, E')$, where each atom $C_i$ contributes the (nonempty) star $N_{\mathcal{H}}(C_i) \subseteq E$:

$$N_{\mathcal{H}}(C_1) = \{e_{12}, e_{31}\},$$

$$N_{\mathcal{H}}(C_2) = \{e_{12}, e_{23}\},$$

$$N_{\mathcal{H}}(C_3) = \{e_{23}, e_{31}\}.$$

Hence

$$V\big(\mathrm{MLH}(\mathcal{H})\big) = E = \{e_{12}, e_{23}, e_{31}\}, \qquad E' = \{\{e_{12}, e_{31}\}, \ \{e_{12}, e_{23}\}, \ \{e_{23}, e_{31}\}\}.$$

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*2-section and adjacency (numerical form).* The 2-section $\mathrm{Sec}_2\big(\mathrm{MLH}(\mathcal{H})\big)$ is a simple graph on vertices $(e_{12}, e_{23}, e_{31})$ with edge set

$$\{\{e_{12}, e_{23}\},\ \{e_{23}, e_{31}\},\ \{e_{31}, e_{12}\}\},$$

i.e. a 3-cycle. Its adjacency matrix (in the order $e_{12}, e_{23}, e_{31}$) is

$$A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

This matches the classical line graph $L(C_3) \cong C_3$, confirming $\mathrm{Sec}_2\big(\mathrm{MLH}(\mathcal{H})\big) = L(\mathcal{H})$ in this instance. Chemically, vertices of MLH are the C–C bonds, and each hyperedge groups the two bonds that meet at a carbon, capturing bond–bond adjacencies around the strained three-membered ring.

**Theorem 2.9** (Molecular Line HyperGraph is a Line HyperGraph). *For every molecular hypergraph $\mathcal{H}$, $\mathrm{MLH}(\mathcal{H})$ is, by construction, a line hypergraph of $\mathcal{H}$; i.e.*

$$\mathrm{MLH}(\mathcal{H}) \;=\; \mathsf{L}_H(\mathcal{H}).$$

*Proof.* By definition, $\mathrm{MLH}(\mathcal{H})$ has vertex set $E$ and hyperedge set $\{\, N_{\mathcal{H}}(v) : v \in V,\ N_{\mathcal{H}}(v) \neq \emptyset \,\}$. This equals the line-hypergraph construction $\mathsf{L}_H(\mathcal{H})$ word for word. □

**Theorem 2.10** (Generalizes the Molecular Line Graph). *Let $G = (V, E)$ be a molecular graph (every $e \in E$ has $|e| = 2$). Then the 2-section of the Molecular Line HyperGraph recovers the ordinary line graph:*

$$\mathrm{Sec}_2\big(\mathrm{MLH}(G)\big) \;=\; L(G).$$

*Proof.* Vertices on both sides are $E$ (bonds of $G$). For distinct $e, e' \in E$, adjacency in $\mathrm{Sec}_2(\mathrm{MLH}(G))$ holds iff there exists a hyperedge $N_G(v)$ of $\mathrm{MLH}(G)$ with $\{e, e'\} \subseteq N_G(v)$. By definition of $N_G(v)$, this is equivalent to $v \in e \cap e'$, i.e. the two bonds meet at atom $v$. Thus $\{e, e'\}$ is an edge of $\mathrm{Sec}_2(\mathrm{MLH}(G))$ iff $e \cap e' \neq \emptyset$ in $G$, which is precisely the adjacency condition in $L(G)$. Hence $\mathrm{Sec}_2(\mathrm{MLH}(G)) = L(G)$. □

**Definition 2.11** (Molecular Iterated Line HyperGraph). For a molecular hypergraph $\mathcal{H}$, its *Molecular Iterated Line HyperGraph of order $k$* is

$$\mathrm{MILH}^{(k)}(\mathcal{H}) \;:=\; \mathsf{L}_H^k(\mathcal{H}) \qquad (k \in \mathbb{N}_0).$$

**Example 2.12** (Molecular Iterated Line HyperGraph: a linear C–C–C–C fragment). Consider a four-carbon chain fragment (e.g., a butane skeleton segment) with atoms

$$V = \{C_1, C_2, C_3, C_4\}, \qquad E = \{e_{12} = \{C_1, C_2\}, \ e_{23} = \{C_2, C_3\}, \ e_{34} = \{C_3, C_4\}\}.$$

The molecular hypergraph $\mathcal{H} = (V, E)$ is an ordinary graph (all hyperedges have size 2). Its Molecular Line HyperGraph $\mathrm{MLH}(\mathcal{H}) = \mathsf{L}_H(\mathcal{H})$ has

$$V^{(1)} := E = \{e_{12}, e_{23}, e_{34}\},$$

and hyperedges given by the stars of the atoms:

$$\mathrm{Star}(C_1) = \{e_{12}\}, \quad \mathrm{Star}(C_2) = \{e_{12}, e_{23}\}, \quad \mathrm{Star}(C_3) = \{e_{23}, e_{34}\}, \quad \mathrm{Star}(C_4) = \{e_{34}\}.$$

Now iterate once more to form the Molecular *Iterated* Line HyperGraph $\mathrm{MILH}^{(1)}(\mathrm{MLH}(\mathcal{H})) = \mathsf{L}_H(\mathrm{MLH}(\mathcal{H}))$. The new vertex set is the hyperedge set from the previous step,

$$V^{(2)} := \{ \ \{e_{12}\}, \ \{e_{12}, e_{23}\}, \ \{e_{23}, e_{34}\}, \ \{e_{34}\} \ \},$$

and for each $x \in V^{(1)} = \{e_{12}, e_{23}, e_{34}\}$ we add the star in $\mathrm{MLH}(\mathcal{H})$:

$$\mathrm{Star}_{\mathrm{MLH}}(e_{12}) = \{ \ \{e_{12}\}, \ \{e_{12}, e_{23}\} \ \},$$
$$\mathrm{Star}_{\mathrm{MLH}}(e_{23}) = \{ \ \{e_{12}, e_{23}\}, \ \{e_{23}, e_{34}\} \ \},$$
$$\mathrm{Star}_{\mathrm{MLH}}(e_{34}) = \{ \ \{e_{23}, e_{34}\}, \ \{e_{34}\} \ \}.$$

Hence the hyperedges of $\mathrm{MILH}^{(1)}$ are precisely these three sets. This concretely exhibits the iteration: vertices become "groups of adjacent bonds," and new hyperedges record which of those groups share a bond-vertex in the previous layer.

**Example 2.13** (Diborane $B_2H_6$: two-center and three-center bonding). We build $\mathrm{MILH}^{(2)}(\mathcal{H})$ starting from a molecular hypergraph that encodes both ordinary two-center B–H bonds and three-center two-electron $\mathrm{B-H-B}$ bridges.

*Level 0 (molecular hypergraph).* Let the atom set be

$$V = \{B_1, B_2, \ H_{b1}, H_{b2}, \ H_{t1}, H_{t2}, H_{t3}, H_{t4}\}.$$

Define the hyperedge family (two-center terminal bonds and three-center bridges)

$$E = \{e_{t1} = \{B_1, H_{t1}\}, \ e_{t2} = \{B_1, H_{t2}\}, \ e_{t3} = \{B_2, H_{t3}\}, \ e_{t4} = \{B_2, H_{t4}\},$$
$$e_{b1} = \{B_1, H_{b1}, B_2\}, \ e_{b2} = \{B_1, H_{b2}, B_2\} \ \}.$$

Thus $\mathcal{H} = (V, E)$ has $|V| = 8$ and $|E| = 6$.

*First iteration $L(H)$ (line hypergraph).* By definition, $L(H) = (E, \mathsf{E})$, where for each $v \in V$, $\mathrm{Star}_H(v) := \{\, e \in E : v \in e \,\}$ contributes a (nonempty) hyperedge. Explicitly,

$$\mathrm{Star}(B_1) = \{e_{t1}, e_{t2}, e_{b1}, e_{b2}\}, \quad \mathrm{Star}(B_2) = \{e_{t3}, e_{t4}, e_{b1}, e_{b2}\},$$

$$\mathrm{Star}(H_{t1}) = \{e_{t1}\}, \ \mathrm{Star}(H_{t2}) = \{e_{t2}\}, \ \mathrm{Star}(H_{t3}) = \{e_{t3}\}, \ \mathrm{Star}(H_{t4}) = \{e_{t4}\},$$

$$\mathrm{Star}(H_{b1}) = \{e_{b1}\}, \ \mathrm{Star}(H_{b2}) = \{e_{b2}\}.$$

Hence $|V(L(H))| = |E| = 6$ and $|\mathsf{E}| = 8$.

*Second iteration $L^2(H)$.* Vertices of $L^2(H)$ are the hyperedges of $L(H)$:

$$V\big(L^2(H)\big) = \Big\{\, \mathrm{Star}(x) \ : \ x \in V \,\Big\}.$$

For each $e \in E$, the star in $L(H)$ is the set of *previous* stars that contain $e$:

$$\mathrm{Star}_{L(H)}(e) := \{\, F \in \mathsf{E} \ : \ e \in F \,\}.$$

Enumerating,

$$\mathrm{Star}_{L(H)}(e_{t1}) = \{\mathrm{Star}(B_1), \mathrm{Star}(H_{t1})\},$$

$$\mathrm{Star}_{L(H)}(e_{t2}) = \{\mathrm{Star}(B_1), \mathrm{Star}(H_{t2})\},$$

$$\mathrm{Star}_{L(H)}(e_{t3}) = \{\mathrm{Star}(B_2), \mathrm{Star}(H_{t3})\},$$

$$\mathrm{Star}_{L(H)}(e_{t4}) = \{\mathrm{Star}(B_2), \mathrm{Star}(H_{t4})\},$$

$$\mathrm{Star}_{L(H)}(e_{b1}) = \{\mathrm{Star}(B_1), \mathrm{Star}(B_2), \mathrm{Star}(H_{b1})\},$$

$$\mathrm{Star}_{L(H)}(e_{b2}) = \{\mathrm{Star}(B_1), \mathrm{Star}(B_2), \mathrm{Star}(H_{b2})\}.$$

Thus $|\mathsf{E}(L^2(H))| = 6$ with four size-2 hyperedges (from terminals) and two size-3 hyperedges (from bridges).

*Chemical interpretation.* $L(H)$ reorganizes "interaction terms" (bonds) by common atoms; $L^2(H)$ captures how those *groupings* co-occur via shared interaction terms. The larger size-3 hyperedges in $L^2(H)$ reflect the cooperativity introduced by three-center B–H–B bonding.

**Example 2.14** (Benzene $C_6H_6$: $\sigma$ bonds plus a delocalized $\pi$ sextet)**.** We include the six two-center $\sigma$ C–C bonds and a six-center $\pi$ hyperedge to reflect aromatic delocalization, then compute $\mathrm{MILH}^{(2)}$.

*Level 0 (molecular hypergraph).* Let the carbon ring be $V = \{C_1, \ldots, C_6\}$ (indices mod 6). Define the hyperedge family

$$E = \big\{\, e_{12}, e_{23}, e_{34}, e_{45}, e_{56}, e_{61}, \ p \,\big\},$$

where $e_{i\,i+1} := \{C_i, C_{i+1}\}$ are the six $\sigma$ bonds and $p := \{C_1, C_2, C_3, C_4, C_5, C_6\}$ encodes the delocalized $\pi$ sextet. Hence $|V| = 6$, $|E| = 7$.

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*First iteration* $L(H)$. Vertices are $E$. For each $C_i$,

$$\text{Star}_H(C_i) = \{\, e_{i-1\,i},\ e_{i\,i+1},\ p \,\}.$$

Therefore

$$V\big(L(H)\big) = E, \qquad \mathsf{E} = \Big\{\, \{e_{12}, e_{61}, p\},\ \{e_{12}, e_{23}, p\},\ \ldots,\ \{e_{56}, e_{45}, p\} \Big\},$$

six (size-3) hyperedges total, one per carbon.

*Second iteration* $L^2(H)$. Vertices are the six triples above. For any $\sigma$ edge $e_{i\,i+1}$,

$$\text{Star}_{L(H)}(e_{i\,i+1}) = \big\{\, \text{Star}(C_i),\ \text{Star}(C_{i+1}) \,\big\} \quad \text{(size 2)}.$$

For the $\pi$ sextet $p$,

$$\text{Star}_{L(H)}(p) = \big\{\, \text{Star}(C_1), \text{Star}(C_2), \ldots, \text{Star}(C_6) \,\big\} \quad \text{(size 6)}.$$

Hence $L^2(H)$ has 6 vertices and 7 hyperedges: six size-2 hyperedges (one per $\sigma$ bond) and one size-6 hyperedge (from $p$).

*Chemical interpretation.* $L(H)$ records, for each carbon, the pair of adjacent $\sigma$ bonds together with the global $\pi$ channel. $L^2(H)$ then captures how "bond groups at carbons" co-occur via a shared $\sigma$ bond (yielding size-2 hyperedges) and how all such groups co-occur via the delocalized $\pi$ system (yielding a size-6 hyperedge), reflecting ring-wide aromatic coupling.

**Theorem 2.15** (Molecular Iterated Line HyperGraph is an Iterated Line HyperGraph)**.** *For every $k \geq 0$ and molecular hypergraph $\mathcal{H}$,*

$$\text{MILH}^{(k)}(\mathcal{H}) \;=\; \mathsf{L}_H^k(\mathcal{H}).$$

*Proof.* By definition of $\text{MILH}^{(k)}$ as $\mathsf{L}_H^k$, the identity is immediate. $\square$

**Definition 2.16** (Molecular iterated line hypergraph with 2-section normalization)**.** Let $G$ be a molecular (simple) graph. Define recursively

$$\text{MILH}^{(0)}(G) \;:=\; G, \qquad \text{MILH}^{(k+1)}(G) \;:=\; \mathsf{L}_H\Big(\text{Sec}_2\big(\text{MILH}^{(k)}(G)\big)\Big) \quad (k \geq 0),$$

where $\mathsf{L}_H(\cdot)$ denotes the molecular line hypergraph operator.

**Theorem 2.17** (Generalizes the Molecular Iterated Line Graph)**.** *Let $G$ be a molecular* graph. *For all $k \geq 0$,*

$$\text{Sec}_2\big(\text{MILH}^{(k)}(G)\big) \;=\; L^k(G),$$

*where $L^0(G) := G$ and $L^{k+1}(G) := L\big(L^k(G)\big).$*

*Proof.* We argue by induction on $k$.

*Base $k = 0$:* $\mathrm{Sec}_2(\mathrm{MILH}^{(0)}(G)) = \mathrm{Sec}_2(G) = G = L^0(G)$, since $G$ is a simple graph.

*Inductive step:* Assume $\mathrm{Sec}_2(\mathrm{MILH}^{(k)}(G)) = L^k(G)$. Set

$$X := \mathrm{Sec}_2\big(\mathrm{MILH}^{(k)}(G)\big).$$

Then $X$ is a (molecular) simple graph, hence Theorem 2.10 applies to $X$. Using Definition 2.16, we obtain

$$\mathrm{Sec}_2\big(\mathrm{MILH}^{(k+1)}(G)\big) = \mathrm{Sec}_2\Big(\mathsf{L}_H(X)\Big) = L(X) = L\big(\mathrm{Sec}_2(\mathrm{MILH}^{(k)}(G))\big) = L\big(L^k(G)\big) = L^{k+1}(G).$$

This completes the induction. $\square$

## 3. Molecular Line SuperHypergraph and Iterated Line SuperHypergraph

A Molecular $n$-SuperHypergraph models hierarchical molecular structures using nested sets of atoms or interactions up to depth $n$ (cf. [67–69]). A molecular line superhypergraph maps molecular superedges to vertices, linking them via shared atoms, enabling higher-order chemical connectivity analysis. A molecular iterated line superhypergraph repeatedly transforms molecular superedges into vertices, uncovering multi-level hierarchical connectivity in complex chemical structures.

**Definition 3.1** (Level-$n$ Molecular SuperHyperGraph)**.** Fix a finite base set $V_0$ of bond identifiers and an integer $n \geq 0$. Let $\mathcal{P}^0(V_0) = V_0$ and $\mathcal{P}^{k+1}(V_0) = \mathcal{P}(\mathcal{P}^k(V_0))$. A *level-$n$ molecular SuperHyperGraph* is a pair

$$\mathcal{H}^{(n)} = (V_n, \mathcal{E}) \quad \text{with} \quad V_n \subseteq \mathcal{P}^n(V_0), \qquad \emptyset \neq \mathcal{E} \subseteq \mathcal{P}(V_n) \setminus \{\emptyset\}.$$

Elements of $V_n$ are *$n$-supernodes*; elements of $\mathcal{E}$ are *$n$-superedges*. Incidence is the usual membership $v \in E$ for $v \in V_n$, $E \in \mathcal{E}$.

**Notation 2** (Stars)**.** *For $\mathcal{H}^{(n)} = (V_n, \mathcal{E})$ and $v \in V_n$, define the (nonempty-or-empty) star*

$$\mathrm{Star}_{\mathcal{H}}(v) := \{E \in \mathcal{E} : v \in E\} \subseteq \mathcal{E}.$$

*When forming hyperedges below we will use only the nonempty stars $\mathrm{Star}_{\mathcal{H}}(v) \neq \emptyset$.*

**Example 3.2** (Molecular SuperHyperGraph for ethanol $C_2H_5OH$; level $n = 1$)**.** Let the base set $V_0$ collect bond identifiers

$$V_0 := \{b_{\mathrm{CC}}, \ b_{\mathrm{CO}}, \ b_{\mathrm{OH}}, \ b_{C_1H_1}, \ b_{C_1H_2}, \ b_{C_1H_3}, \ b_{C_2H_1}, \ b_{C_2H_2}\}.$$

We form three 1-supervertices (subsets of $V_0$) corresponding to chemically meaningful groups:

$$T_{\text{methyl}} := \{ b_{C_1H_1}, b_{C_1H_2}, b_{C_1H_3} \},$$

$$T_{\text{methylene}} := \{ b_{\text{CC}}, b_{C_2H_1}, b_{C_2H_2} \},$$

$$T_{\text{hydroxyl}} := \{ b_{\text{CO}}, b_{\text{OH}} \}.$$

Set the level-1 vertex set $V_1 := \{T_{\text{methyl}}, T_{\text{methylene}}, T_{\text{hydroxyl}}\} \subseteq \mathcal{P}(V_0)$. Define two 1-superedges (nonempty subsets of $V_1$) reflecting adjacency of functional parts:

$$E_1 := \{T_{\text{methyl}}, T_{\text{methylene}}\}, \qquad E_2 := \{T_{\text{methylene}}, T_{\text{hydroxyl}}\}.$$

Then the level-1 Molecular SuperHyperGraph is

$$\mathcal{H}^{(1)} := (V_1, \mathcal{E}^{(1)}), \qquad \mathcal{E}^{(1)} := \{ E_1, E_2 \} \subseteq \mathcal{P}(V_1) \setminus \{\emptyset\}.$$

Here each 1-supervertex is a collection of bonds (a functional group), and each 1-superedge bundles the groups that are directly connected in the molecular framework.

**Definition 3.3** (Line SuperHyperGraph operator). Given $\mathcal{H}^{(n)} = (V_n, \mathcal{E})$, its *line SuperHyperGraph* is

$$\mathbf{L}(\mathcal{H}^{(n)}) := (V'_{n+1}, \mathcal{E}'_{n+1})$$

with

$$V'_{n+1} := \mathcal{E} \qquad \text{and} \qquad \mathcal{E}'_{n+1} := \{ \text{Star}_{\mathcal{H}}(v) \subseteq \mathcal{E} : v \in V_n, \ \text{Star}_{\mathcal{H}}(v) \neq \emptyset \}.$$

Thus each original superedge becomes a vertex; for every supernode $v$, we add a (hyper)edge consisting of all superedges incident with $v$.

**Definition 3.4** (Molecular Line SuperHyperGraph). Let $\mathcal{H}^{(n)}$ be a level-$n$ molecular Super-HyperGraph. Its *Molecular Line SuperHyperGraph* is the line SuperHyperGraph

$$\text{MLSH}(\mathcal{H}^{(n)}) := \mathbf{L}(\mathcal{H}^{(n)}).$$

**Example 3.5** (Molecular Line SuperHyperGraph of the ethanol example). Apply the line SuperHyperGraph operator to $\mathcal{H}^{(1)} = (V_1, \mathcal{E}^{(1)})$. By definition, the vertex set of $\mathbf{L}(\mathcal{H}^{(1)})$ is the previous superedge set:

$$V'_2 := \mathcal{E}^{(1)} = \{E_1, E_2\}.$$

For each $v \in V_1$, form the (nonempty) star $\text{Star}_{\mathcal{H}^{(1)}}(v) := \{ E \in \mathcal{E}^{(1)} : v \in E \}$. Explicitly,

$$\text{Star}_{\mathcal{H}^{(1)}}(T_{\text{methyl}}) = \{E_1\},$$

$$\text{Star}_{\mathcal{H}^{(1)}}(T_{\text{methylene}}) = \{E_1, E_2\},$$

$$\text{Star}_{\mathcal{H}^{(1)}}(T_{\text{hydroxyl}}) = \{E_2\}.$$

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The hyperedge set of the Molecular Line SuperHyperGraph is the collection of these nonempty stars:

$$\mathcal{E}_2' := \big\{\, \{E_1\},\ \{E_1, E_2\},\ \{E_2\} \,\big\} \ \subseteq\ \mathcal{P}(V_2') \setminus \{\emptyset\}.$$

Therefore

$$\mathrm{MLSH}\big(\mathcal{H}^{(1)}\big) \ :=\ \mathbf{L}\big(\mathcal{H}^{(1)}\big) \ =\ \big(V_2',\ \mathcal{E}_2'\big),$$

where vertices represent the original superedges $(E_1, E_2)$, and hyperedges record which of them meet at a common 1-supervertex in $\mathcal{H}^{(1)}$.

**Definition 3.6** (Molecular Iterated Line SuperHyperGraph). For $k \in \mathbb{N}_0$, the *Molecular Iterated Line SuperHyperGraph of order $k$* is

$$\mathrm{MILSH}^{(k)}\big(\mathcal{H}^{(n)}\big) \ :=\ \mathbf{L}^k\big(\mathcal{H}^{(n)}\big).$$

**Example 3.7** (Molecular Iterated Line SuperHyperGraph (second layer on ethanol)). Iterate the line construction once more:

$$\mathrm{MILSH}^{(2)}\big(\mathcal{H}^{(1)}\big) \ :=\ \mathbf{L}\Big(\mathrm{MLSH}\big(\mathcal{H}^{(1)}\big)\Big) \ =\ \mathbf{L}\big(V_2', \mathcal{E}_2'\big).$$

Its vertex set is the previous hyperedge set,

$$V_3' \ :=\ \mathcal{E}_2' \ =\ \big\{\, \{E_1\},\ \{E_1, E_2\},\ \{E_2\} \,\big\}.$$

For each $x \in V_2' = \{E_1, E_2\}$, compute the star in $\mathrm{MLSH}(\mathcal{H}^{(1)})$:

$$\mathrm{Star}_{\mathrm{MLSH}}(E_1) = \big\{\, \{E_1\},\ \{E_1, E_2\} \,\big\},$$
$$\mathrm{Star}_{\mathrm{MLSH}}(E_2) = \big\{\, \{E_1, E_2\},\ \{E_2\} \,\big\}.$$

Thus the hyperedge set at the second iteration is

$$\mathcal{E}_3' \ :=\ \big\{\, \{\{E_1\}, \{E_1, E_2\}\},\ \{\{E_1, E_2\}, \{E_2\}\} \,\big\} \ \subseteq\ \mathcal{P}(V_3') \setminus \{\emptyset\}.$$

Hence

$$\mathrm{MILSH}^{(2)}\big(\mathcal{H}^{(1)}\big) \ =\ \big(V_3',\ \mathcal{E}_3'\big),$$

which concretely illustrates how vertices (interaction groups) at one iteration become the "units" that are grouped into hyperedges at the next, thereby encoding higher-order incidence among functional parts through repeated line–superhypergraph lifting.

**Example 3.8** (Conjugated aromatic fragment (para–disubstituted benzene)). We construct a level 1 molecular SuperHyperGraph from bond identifiers of a benzene ring and compute its Molecular *Iterated* Line SuperHyperGraph up to the second iteration.

*Level 0 (base set of bonds).* Let

$$V_0 = \{\, b_{12}, b_{23}, b_{34}, b_{45}, b_{56}, b_{61} \,\}$$

denote the six C–C bonds of the cycle $C_6$ labeled in order.

*Level 1 (supervertices = fragments).* Define three chemically meaningful fragments (supervertices)

$$T_{\text{left}} := \{\, b_{12}, b_{23}, b_{34} \,\},$$

$$T_{\text{bridge}} := \{\, b_{23}, b_{34}, b_{45} \,\},$$

$$T_{\text{right}} := \{\, b_{45}, b_{56}, b_{61} \,\},$$

and set $V_1 := \{T_{\text{left}}, T_{\text{bridge}}, T_{\text{right}}\} \subseteq \mathcal{P}(V_0)$.

*Level 1 superedges (adjacent fragments).* Let

$$E_1 := \{T_{\text{left}}, T_{\text{bridge}}\}, \qquad E_2 := \{T_{\text{bridge}}, T_{\text{right}}\},$$

and $\mathcal{E}^{(1)} := \{E_1, E_2\} \subseteq \mathcal{P}(V_1) \setminus \{\emptyset\}$. Thus $\mathcal{H}^{(1)} = (V_1, \mathcal{E}^{(1)})$ is a level 1 molecular SuperHyperGraph.

*First line lift (Molecular Line SuperHyperGraph).* By Definition 3.3,

$$\text{MLSH}\big(\mathcal{H}^{(1)}\big) = \mathbf{L}\big(\mathcal{H}^{(1)}\big) = (V_2', \mathcal{E}_2'), \quad V_2' = \mathcal{E}^{(1)} = \{E_1, E_2\}.$$

For each $T \in V_1$ the nonempty star is

$$\text{Star}(T_{\text{left}}) = \{E_1\}, \quad \text{Star}(T_{\text{bridge}}) = \{E_1, E_2\}, \quad \text{Star}(T_{\text{right}}) = \{E_2\}.$$

Hence

$$\mathcal{E}_2' = \big\{\, \{E_1\}, \ \{E_1, E_2\}, \ \{E_2\} \,\big\} \subseteq \mathcal{P}(V_2') \setminus \{\emptyset\}.$$

*Second line lift (Molecular <u>Iterated</u> Line SuperHyperGraph).* The order-2 MILSH is

$$\text{MILSH}^{(2)}\big(\mathcal{H}^{(1)}\big) = \mathbf{L}^2\big(\mathcal{H}^{(1)}\big) = (V_3', \mathcal{E}_3'), \quad V_3' = \mathcal{E}_2' = \{\{E_1\}, \{E_1, E_2\}, \{E_2\}\}.$$

Stars in $\mathbf{L}(\mathcal{H}^{(1)})$ (taken at the vertices $E_1, E_2$) are

$$\text{Star}_\mathbf{L}(E_1) = \{\{E_1\}, \{E_1, E_2\}\}, \qquad \text{Star}_\mathbf{L}(E_2) = \{\{E_1, E_2\}, \{E_2\}\},$$

thus

$$\mathcal{E}_3' = \big\{\, \{\{E_1\}, \{E_1, E_2\}\}, \ \{\{E_1, E_2\}, \{E_2\}\} \,\big\}.$$

*Verification and interpretation.* All inclusions are explicit: $V_1 \subseteq \mathcal{P}(V_0)$, $\mathcal{E}^{(1)} \subseteq \mathcal{P}(V_1) \setminus \{\emptyset\}$, $V_2' = \mathcal{E}^{(1)} \subseteq \mathcal{P}^2(V_0)$, $\mathcal{E}_2' \subseteq \mathcal{P}(V_2') \setminus \{\emptyset\}$, etc. Chemically, level 1 groups contiguous $\pi$-segments; the first line lift turns their pairwise couplings into vertices and records which couplings meet at a fragment; the second lift captures *co-occurrence of coupling channels*, useful for modeling conjugation pathways in para–disubstituted benzenes.

**Example 3.9** (Hydrogen-bonded water trimer $(\text{H}_2\text{O})_3$)**.** We model the cyclic H-bond network and compute the order-2 Molecular Iterated Line SuperHyperGraph.

*Level 0 (base set of H-bonds).* Let $V_0 = \{h_{12}, h_{23}, h_{31}\}$, where $h_{ij}$ denotes the hydrogen bond from monomer $i$ (donor) to monomer $j$ (acceptor) in the cyclic trimer.

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*Level 1 (motif supervertices).* Define three donor/acceptor motifs (each a subset of bonds)

$$D_1 := \{h_{12}, h_{31}\}, \qquad D_2 := \{h_{23}, h_{12}\}, \qquad D_3 := \{h_{31}, h_{23}\},$$

and set $V_1 := \{D_1, D_2, D_3\} \subseteq \mathcal{P}(V_0)$.

*Level 1 superedges (adjacent motifs along the ring).* Let

$$E_1 := \{D_1, D_2\}, \qquad E_2 := \{D_2, D_3\}, \qquad E_3 := \{D_3, D_1\},$$

and $\mathcal{E}^{(1)} := \{E_1, E_2, E_3\} \subseteq \mathcal{P}(V_1) \setminus \{\emptyset\}$. Then $\mathcal{H}^{(1)} = (V_1, \mathcal{E}^{(1)})$ is a level 1 molecular Super-HyperGraph.

*First line lift (Molecular Line SuperHyperGraph).*

$$\mathrm{MLSH}(\mathcal{H}^{(1)}) = \mathbf{L}(\mathcal{H}^{(1)}) = (V_2', \mathcal{E}_2'), \qquad V_2' = \{E_1, E_2, E_3\}.$$

Nonempty stars at level 1 are

$$\mathrm{Star}(D_1) = \{E_1, E_3\}, \quad \mathrm{Star}(D_2) = \{E_1, E_2\}, \quad \mathrm{Star}(D_3) = \{E_2, E_3\},$$

hence

$$\mathcal{E}_2' = \{ \{E_1, E_3\}, \{E_1, E_2\}, \{E_2, E_3\} \}.$$

*Second line lift (Molecular <u>Iterated</u> Line SuperHyperGraph).*

$$\mathrm{MILSH}^{(2)}(\mathcal{H}^{(1)}) = \mathbf{L}^2(\mathcal{H}^{(1)}) = (V_3', \mathcal{E}_3'), \quad V_3' = \mathcal{E}_2'.$$

Stars in $\mathbf{L}(\mathcal{H}^{(1)})$ (taken at the vertices $E_1, E_2, E_3$) are

$$\mathrm{Star}_{\mathbf{L}}(E_1) = \{\{E_1, E_3\}, \{E_1, E_2\}\},$$
$$\mathrm{Star}_{\mathbf{L}}(E_2) = \{\{E_1, E_2\}, \{E_2, E_3\}\},$$
$$\mathrm{Star}_{\mathbf{L}}(E_3) = \{\{E_1, E_3\}, \{E_2, E_3\}\},$$

so

$$\mathcal{E}_3' = \{ \{\{E_1, E_3\}, \{E_1, E_2\}\}, \{\{E_1, E_2\}, \{E_2, E_3\}\}, \{\{E_1, E_3\}, \{E_2, E_3\}\} \}.$$

*Verification and interpretation.* All sets are explicitly contained in the required powersets: $V_1 \subseteq \mathcal{P}(V_0), \mathcal{E}^{(1)} \subseteq \mathcal{P}(V_1) \setminus \{\emptyset\}, V_2' = \mathcal{E}^{(1)} \subseteq \mathcal{P}^2(V_0)$, and so on. Physically, level 1 motifs encode each monomer's donor/acceptor participation; the first line lift turns motif–motif couplings into vertices and records which couplings meet at a motif; the second lift captures *cooperativity of coupling channels*, relevant to collective effects in cyclic H-bond networks.

**Theorem 3.10** (Well-definedness and level shift). *If $\mathcal{H}^{(n)} = (V_n, \mathcal{E})$ is a level-n molecular SuperHyperGraph, then $\mathbf{L}(\mathcal{H}^{(n)})$ is a level-(n+1) molecular SuperHyperGraph. More generally, for every $k \geq 0$, $\mathbf{L}^k(\mathcal{H}^{(n)})$ is level $n+k$.*

*Proof.* Since each superedge $E \in \mathcal{E}$ is a nonempty subset of $V_n \subseteq \mathcal{P}^n(V_0)$, we have $E \in \mathcal{P}(V_n) \subseteq \mathcal{P}(\mathcal{P}^n(V_0)) = \mathcal{P}^{n+1}(V_0)$. Thus $V'_{n+1} = \mathcal{E} \subseteq \mathcal{P}^{n+1}(V_0)$. Every hyperedge $\mathrm{Star}_{\mathcal{H}}(v)$ is a nonempty subset of $V'_{n+1}$ by construction, hence $\mathcal{E}'_{n+1} \subseteq \mathcal{P}(V'_{n+1}) \setminus \{\emptyset\}$. Therefore $\mathbf{L}(\mathcal{H}^{(n)})$ satisfies the definition at level $n+1$. The iterated statement follows by induction on $k$. $\square$

**Theorem 3.11** (Molecular Line SuperHyperGraph is a Line SuperHyperGraph)**.** *For any level-n molecular SuperHyperGraph $\mathcal{H}^{(n)}$, $\mathrm{MLSH}(\mathcal{H}^{(n)})$ coincides with the line SuperHyperGraph $\mathbf{L}(\mathcal{H}^{(n)})$ of Definition.*

*Proof.* By definition we set $\mathrm{MLSH}(\mathcal{H}^{(n)}) := \mathbf{L}(\mathcal{H}^{(n)})$, so the two objects are identical in vertex set and hyperedge set. $\square$

**Theorem 3.12** (Generalizes Molecular Line HyperGraph)**.** *Let $n = 0$ and regard a molecular hypergraph $H = (V, E)$ as $\mathcal{H}^{(0)} = (V, \mathcal{E})$ with $\mathcal{E} = E$. Then $\mathrm{MLSH}(\mathcal{H}^{(0)})$ equals the usual Molecular Line HyperGraph: its vertex set is $E$ and each atom $v \in V$ contributes the hyperedge $\mathrm{Star}_{\mathcal{H}}(v) = \{\, e \in E : \ v \in e \,\}$.*

*Proof.* When $n = 0$, supernodes are atoms and superedges are ordinary hyperedges. Definition 3.3 produces vertices $E$ and, for each $v \in V$, the hyperedge consisting of all $e \in E$ incident to $v$. This is precisely the line-hypergraph construction in the molecular hypergraph setting. $\square$

**Theorem 3.13** (Generalizes Molecular SuperHyperGraph)**.** *For any $n \geq 0$, $\mathrm{MLSH}(\mathcal{H}^{(n)})$ is itself a (level-n+1) molecular SuperHyperGraph. Hence the Molecular Line SuperHyperGraph generalizes the Molecular SuperHyperGraph by producing a valid superhypergraph one level higher.*

*Proof.* Immediate from Theorem 3.10. $\square$

**Theorem 3.14** (Molecular Iterated Line SuperHyperGraph is an Iterated Line SuperHyperGraph)**.** *For any $k \geq 0$ and level-n molecular SuperHyperGraph $\mathcal{H}^{(n)}$,*

$$\mathrm{MILSH}^{(k)}(\mathcal{H}^{(n)}) \;=\; \mathbf{L}^k(\mathcal{H}^{(n)}),$$

*i.e. it is the k-fold iterated line SuperHyperGraph of $\mathcal{H}^{(n)}$. Moreover, it is level n+k.*

*Proof.* The equality is by definition of $\mathrm{MILSH}^{(k)}$. The level statement follows from Theorem 3.10 by induction on $k$. $\square$

**Theorem 3.15** (Generalizes Molecular Iterated Line HyperGraph). *Let $n = 0$ and let $H = (V, E)$ be a molecular hypergraph. For all $k \geq 0$,*

$$\mathrm{MILSH}^{(k)}\big(\mathcal{H}^{(0)}\big) \quad \textit{equals the k-fold iterated Molecular Line HyperGraph of } H,$$

*obtained by repeatedly applying the line-hypergraph construction.*

*Proof.* For $n = 0$, $\mathbf{L}$ reduces to the molecular line-hypergraph operator by Theorem 3.12. Iteration preserves this identification, so $\mathbf{L}^k(\mathcal{H}^{(0)})$ is exactly the $k$-fold line-hypergraph iteration on $H$. □

**Theorem 3.16** (Generalizes Molecular SuperHyperGraph under iteration). *For any $n \geq 0$ and $k \geq 0$, $\mathrm{MILSH}^{(k)}\big(\mathcal{H}^{(n)}\big)$ is a (level-n+k) molecular SuperHyperGraph.*

*Proof.* Combine Theorems 3.10 and 3.14. □

## 4. Conclusion

In this paper, we introduced the notions of *Molecular Line SuperHyperGraphs* and *Molecular Iterated Line SuperHyperGraphs*, providing formal definitions and examining their potential applications. Looking ahead, we expect future work to extend these concepts using frameworks such as Fuzzy Graphs [70], Intuitionistic Fuzzy Graphs [71], Neutrosophic Graphs [72–75], Neutrosophic HyperGraphs [76,77], Uncertain Graphs [78,79], and Plithogenic Graphs [80–82]. We also anticipate developments in programming tools and libraries, as well as quantitative analyses carried out through computer-based machine learning and experimental investigations.

## 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.

## Conflicts of Interest

The authors confirm that there are no conflicts of interest related to the research or its publication.

## Use of Generative AI and AI-Assisted Tools

We use generative AI and AI-assisted tools for tasks such as English grammar checking, and we do not employ them in any way that violates ethical standards.

## Supplementary Information

No supplementary materials accompany this paper.

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