On a hypergraph probabilistic graphical model

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Published online: 10 July 2020
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Abstract
We propose a directed acyclic hypergraph framework for a probabilistic graphical model that we call Bayesian hypergraphs. The space of directed acyclic hypergraphs is much larger than the space of chain graphs. Hence Bayesian hypergraphs can model much finer factorizations than Bayesian networks or LWF chain graphs and provide simpler and more computationally efficient procedures for factorizations and interventions. Bayesian hypergraphs also allow a modeler to represent causal patterns of interaction such as Noisy-OR graphically (without additional annotations). We introduce global, local and pairwise Markov properties of Bayesian hypergraphs and prove under which conditions they are equivalent. We also extend the causal interpretation of LWF chain graphs to Bayesian hypergraphs and provide corresponding formulas and a graphical criterion for intervention.

Keywords Graphical model · Hypergraph · Chain graph · Bayesian network · Intervention · Markov property · Factorization · Structural equation model

Mathematics Subject Classification (2010) 62-07 · 62-09 · 05C65 · 05C70 · 05C75

1 Introduction
Probabilistic graphical models are graphs in which nodes represent random variables and edges represent conditional independence assumptions. They provide a compact way to
represent the joint probability distributions of a set of random variables. In undirected graphical models, e.g., Markov networks (see [5, 27]), there is a simple rule for determining independence: two set of nodes \(A\) and \(B\) are conditionally independent given \(C\) if removing \(C\) separates \(A\) and \(B\). On the other hand, directed graphical models, e.g. Bayesian networks (see [14, 27, 43]), which consist of a directed acyclic graph (DAG) and a corresponding set of conditional probability tables, have a more complicated rule (d-separation) for determining independence. More complex graphical models include various types of graphs with edges of several types (e.g., [3, 11, 15, 31, 32, 34, 41, 42]), including chain graphs [19, 23], for which different interpretations have emerged [1, 7].

Probabilistic Graphical Models (PGMs) enjoy a well-deserved popularity because they allow explicit representation of structural constraints in the language of graphs and similar structures. From the perspective of efficient belief update, factorization of the joint probability distribution of random variables corresponding to variables in the graph is paramount, because it allows decomposition of the calculation of the evidence or of the posterior probability [21]. The proliferation of different PGMs that allow factorizations of different kinds leads us to consider a more general graphical structure in this paper, namely directed acyclic hypergraphs. Since there are many more hypergraphs than DAGs, undirected graphs, chain graphs, and, indeed, other graph-based networks, as discussed in Remark 8, Bayesian hypergraphs can model much finer factorizations and thus are more computationally efficient. When tied to probability distributions, directed acyclic hypergraphs specify independence (and possibly other) constraints through their Markov properties; we call the new PGM resulting from the directed acyclic hypergraphs and their Markov properties Bayesian hypergraphs. We provide such properties and show that they are consistent with the ones used in Bayesian networks, Markov networks, and LWF chain graphs, when the directed acyclic hypergraphs are suitably restricted. In particular, we define a projection operator, called shadow, that maps a Bayesian hypergraph to a chain graph, and show that the Markov properties of a Bayesian hypergraph are equivalent to those of its shadow (which is a chain graph). This also allows people to work with familiar separation criteria even in the case of Bayesian hypergraphs.

There are situations that may be of interest to a probabilistic or causal modeler that can be modeled more explicitly using Bayesian hypergraphs. In particular, some causal patterns, such as independence of causal influence (e.g., Noisy-OR), can be expressed graphically in Bayesian hypergraphs, while they require a numerical specification in DAGs or chain graphs. This is one of the important limitations to the Causal Representation Convention [38]. For example, suppose diseases \(A\) and \(B\) both increase symptoms \(C\), but the effect of \(B\) without \(A\) is quite trivial, while the effect of \(A\) alone is not (see Table 1b). The directed graph representation we have considered in Fig. 1, which is a DAG, offer no means to represent this interaction and to distinguish it from other circumstances in which \(A\) and \(B\) alone each have an effect on \(C\) (see Table 1a). Both interactions are only represented through the probability distribution associated with the graph. We describe this case in detail in Section 5.2, and we show that how using hypergraphs can help modelers to overcome this problem.

We provide a causal interpretation of Bayesian hypergraphs that extends the causal interpretation of LWF chain graphs [22], by giving corresponding formulas and a graphical criterion for intervention.

The paper is organized as follows: In Section 2, we introduce some common notations, terminology and concepts on graphs and hypergraphs. In Section 3 and Section 4, we review the Markov properties and factorizations in the case of undirected graphs and chain graphs.
Table 1 The conditional probability distribution $P(C|A, B)$ for a model with: (a) noisy functional dependence (Noisy-OR), and therefore $P(C = n|A = y, B = y) = P(C = n|A = y)P(C = n|B = y)$; (b) non-noisy functional dependence

|    | A=n       | A=y       |
|----|-----------|-----------|
|    | B=n       | B=y       | B=n       | B=y       |
| (a) |           |           |           |           |
| C  |           |           |           |           |
| n  | 1         | 0.2       | 0.02      |           |
| y  | 0.1       | 0.9       | 0.8       | 0.98      |
| (b) |           |           |           |           |
| C  |           |           |           |           |
| n  | 0.95      | 0.3       | 0.5       | 0.2       |
| y  | 0.05      | 0.7       | 0.5       | 0.8       |

In Section 5, we introduce the Bayesian hypergraphs model, discuss the factorizations, Markov properties and its relations to chain graphs. In Section 6, we discuss how interventions can be achieved in Bayesian hypergraphs. Section 7 concludes the paper and includes some directions for further work.

2 Terminology and concepts

In this paper, we use $[n]$ to denote the set $\{1, 2, \ldots, n\}$. For $a, b \in \mathbb{Z}$, We use $[a, b]$ to denote $\{k \in \mathbb{Z} : a \leq k \leq b\}$. Given a set $h$, we use $|h|$ to denote the number of elements in $h$.

2.1 Graphs

A graph $G = (V, E)$ is an ordered pair $(V, E)$ where $V$ is a finite set of vertices (or nodes) and $E \subseteq V \times V$ consists of a set of ordered pairs of vertices $(v, w) \in V \times V$. Given a graph $G$, we will use $V(G)$, $E(G)$ to denote the set of vertices and edges of $G$ respectively. An edge $(v, w) \in E$ is directed if $(w, v) \notin E$ and undirected if $(w, v) \in E$. We write $v \to w$ if $(v, w)$ is directed and $v \leftarrow w$ if $(v, w)$ is undirected. If $v \to w$ then we call $v$ a neighbor of $w$ and vice versa. If $v \to w$, then we call $v$ a parent of $w$ and $w$ a child of $v$. Let $pa_G(v)$ and $nb_G(v)$ denote the set of parents and neighbors of $v$, respectively. We say $v$ and $w$ are

Fig. 1 A simple DAG $G$
adjacent if either \((v, w) \in E\) or \((w, v) \in E\), i.e., either \(v \rightarrow w\), \(w \rightarrow v\) or \(v \leftarrow w\). We say an edge \(e\) is incident to a vertex \(v\) if \(v\) is contained in \(e\). We also define the boundary \(bd(v)\) of \(v\) by

\[
bd(v) = nb(v) \cup pa(v).
\]

Moreover, given \(\tau \subseteq V\), define

\[
\begin{align*}
\pa_G(\tau) &= \left(\bigcup_{v \in \tau} \pa_G(v)\right) \setminus \tau. \\
\nb_G(\tau) &= \left(\bigcup_{v \in \tau} \nb_G(v)\right) \setminus \tau. \\
\bd_G(\tau) &= \left(\bigcup_{v \in \tau} \bd_G(v)\right) \setminus \tau. \\
\cl_G(\tau) &= \bd_G(\tau) \cup \tau.
\end{align*}
\]

For every graph \(G = (V, E)\), we will denote the underlying undirected graph \(G^u = (V, E^u)\), i.e., \(E^u = \{(v, u) : (v, u) \in E \text{ or } (u, v) \in E\}\). A path in \(G\) is a sequence of distinct vertices \(v_0, \ldots, v_k\) such that \((v_i, v_{i+1}) \in E\) for all \(0 \leq i < k\). A path \(v_0, \ldots, v_k\) is directed if for all \(0 \leq i < k\), \((v_i, v_{i+1})\) is a directed edge, i.e., \((v_i, v_{i+1}) \in E\) but \((v_{i+1}, v_i) \notin E\). A cycle is a path with the modification that \(v_k = v_0\). A cycle is partially directed if at least one of the edges in the cycle is a directed edge. A graph \(G\) is acyclic if \(G\) contains no partially directed cycle. A vertex \(v\) is said to be an anterior of a vertex \(u\) if there is a path from \(v\) to \(u\). We remark that every vertex is also an anterior of itself. If there is a directed path from \(v\) to \(u\), we call \(v\) an ancestor of \(u\) and \(u\) a descendent of \(v\). Moreover, \(u\) is a non-descendent of \(v\) if \(u\) is not a descendent of \(v\). Let \(\text{ant}(u)\) and \(\text{an}(u)\) denote the set of anteriors and ancestors of \(u\) in \(G\) respectively. Let \(\text{de}(v)\) and \(\text{nd}(v)\) denote the set of descendents and non-descendents of \(v\) in \(G\) respectively. For a set of vertices \(\tau\), we also define \(\text{ant}(\tau) = \{\text{ant}(v) : v \in \tau\}\). Again, note that \(\tau \subseteq \text{ant}(\tau)\).

A subgraph of a graph \(G\) is a graph \(H\) such that \(V(H) \subseteq V(G)\) and each edge present in \(H\) is also present in \(G\) and has the same type. An induced subgraph of \(G\) by a subset \(A \subseteq V(G)\), denoted by \(G_A\) or \(G[A]\), is a subgraph of \(G\) that contains all and only vertices in \(A\) and all edges of \(G\) that contain only vertices in \(A\). A clique or complete graph with \(n\) vertices, denoted by \(K_n\), is a graph such that every pair of vertices is connected by an undirected edge.

Now we can define several basic graph representations used in probabilistic graphical models. An undirected graph is a graph such that every edge is undirected. A directed acyclic graph (DAG) is a graph such that every edge is directed and contains no directed cycles. A chain graph is a graph without partially directed cycles. Define two vertices \(v\) and \(u\) to be equivalent if there is an undirected path from \(v\) to \(u\). Then the equivalence classes under this equivalence relation are the chain components of \(G\). For a vertex set \(S\), define \(E^*(S)\) as the edge set of the complete undirected graph on \(S\). Given a graph \(G = (V, E)\) with chain components \(\{\tau : \tau \in \mathcal{D}\}\), the moral graph of \(G\), denoted by \(G^m = (V, E^m)\), is a graph such that \(V(G^m) = V(G)\) and \(E^m = E^u \cup \bigcup_{\tau \in \mathcal{D}} E^*(bd(\tau))\), i.e., the underlying undirected graph, where the boundary w.r.t. \(G\) of every chain component is made complete. The moral graphs are natural generalizations to chain graphs of the similar concept for DAGs given in [17] and [18].
2.2 Hypergraphs

Hypergraphs are generalizations of graphs such that each edge is allowed to contain more than two vertices. Formally, an (undirected) hypergraph is a pair $\mathcal{H} = (V, E)$, where $V = \{v_1, v_2, \ldots, v_n\}$ is the set of vertices (or nodes) and $E = \{h_1, h_2, \ldots, h_m\}$ is the set of hyperedges where $h_i \subseteq V$ for all $i \in [m]$. If $|h_i| = k$ for every $i \in [m]$, then we say $\mathcal{H}$ is a $k$-uniform (undirected) hypergraph. A directed hyperedge or hyperarc $h$ is an ordered pair, $h = (X, Y)$, of (possibly empty) subsets of $V$ where $X \cap Y = \emptyset$; $X$ is the called the tail of $h$ while $Y$ is the head of $h$. We write $X = T(h)$ and $Y = H(h)$. We say a directed hyperedge $h$ is fully directed if none of $H(h)$ and $T(h)$ are empty. A directed hypergraph is a hypergraph such that all of the hyperedges are directed. A $(s, t)$-uniform directed hypergraph is a directed hypergraph such that the tail and head of every directed edge have size $s$ and $t$ respectively. For example, any DAG is a $(1, 1)$-uniform hypergraph (but not vice versa). An undirected graph is a $(0, 2)$-uniform hypergraph. Given a hypergraph $\mathcal{H}$, we use $V(\mathcal{H})$ and $E(\mathcal{H})$ to denote the the vertex set and edge set of $\mathcal{H}$ respectively.

We say two vertices $u$ and $v$ are co-head (or co-tail) if there is a directed hyperedge $h$ such that $\{u, v\} \subseteq H(h)$ (or $\{u, v\} \subseteq T(h)$ respectively). Given another vertex $u \neq v$, we say $u$ is a parent of $v$, denoted by $u \rightarrow v$, if there is a directed hyperedge $h$ such that $u \in T(h)$ and $v \in H(h)$. If $u$ and $v$ are co-head, then $u$ is a neighbor of $v$. If $u, v$ are neighbors, we denote them by $u - v$. Given $v \in V$, we define parent ($pa(v)$), neighbor ($nb(v)$), boundary ($bd(v)$), ancestor ($an(v)$), anterior ($ant(v)$), descendent ($de(v)$), and non-descendent ($nd(v)$) for hypergraphs exactly the same as for graphs (and therefore use the same names). The same holds for the equivalent concepts for $\tau \subset V$. Note that it is possible that some vertex $u$ is both the parent and neighbor of $v$.

A partially directed cycle in $\mathcal{H}$ is a sequence $\{v_1, v_2, \ldots, v_k\}$ satisfying that $v_i$ is either a neighbor or a parent of $v_{i+1}$ for all $1 \leq i \leq k$ and $v_i \rightarrow v_{i+1}$ for some $1 \leq i \leq k$. Here $v_{k+1} \equiv v_1$. We say a directed hypergraph $\mathcal{H}$ is acyclic if $\mathcal{H}$ contains no partially directed cycle. For ease of reference, we call a directed acyclic hypergraph a DAH or a Bayesian hypergraph structure (as defined in Section 5). Note that for any two vertices $u, v$ in a directed acyclic hypergraph $\mathcal{H}$, $u$ can not be both the parent and neighbor of $v$ otherwise we would have a partially directed cycle.

Remark 1 DAHs are generalizations of undirected graphs, DAGs and chain graphs. In particular an undirected graph can be viewed as a DAH in which every hyperedge is of the form $(\emptyset, \{u, v\})$. A DAG is a DAH in which every hyperedge is of the form $(\{u\}, \{v\})$. A chain graph is a DAH in which every hyperedge is of the form $(\emptyset, \{u, v\})$ or $(\{u\}, \{v\})$.

We define the chain components of $\mathcal{H}$ as the equivalence classes under the equivalence relation where two vertices $v_i, v_t$ are equivalent if there exists a sequence of distinct vertices $v_1, v_2, \ldots, v_l$ such that $v_i$ and $v_{i+1}$ are co-head for all $i \in [l - 1]$. The chain components $\{\tau : \tau \in D\}$ yields an unique natural partition of the vertex set $V(\mathcal{H}) = \bigcup_{\tau \in D} \tau$ with the following properties:

**Proposition 1** Let $\mathcal{H}$ be a DAH and $\{\tau : \tau \in D\}$ be its chain components. Let $G$ be a graph obtained from $\mathcal{H}$ by contracting each element of $\{\tau : \tau \in D\}$ into a single vertex and creating a directed edge from $\tau_i \in V(G)$ to $\tau_j \in V(G)$ in $G$ if and only if there exists a hyperedge $h \in E(\mathcal{H})$ such that $T(h) \cap \tau_i \neq \emptyset$ and $H(h) \cap \tau_j \neq \emptyset$. Then $G$ is a DAG.
Suppose a hypergraph is a chain graph. We call a set \( A \) an anterior set if it can be generated by stepwise removal of terminal chain components. We denote the smallest ancestral set containing \( A \) such that \( \text{ant}(A) \) is indeed a DAG.

Proof First of all, clearly \( G \) is a directed graph. Now since \( \mathcal{H} \) is a DAH, there is no directed hyperedge such that both its head and tail intersect a common chain component. Hence \( G \) has no self-loop. It remains to show that there is no directed cycle in \( G \). Suppose for contradiction that there is a directed cycle \( \tau_1, \tau_2, \ldots, \tau_k \) in \( G \). Then by the construction of \( G \), there is a sequence of hyperedges \( \{h_1, h_2, \ldots, h_k\} \) such that \( T(h_i) \cap \tau_i \neq \emptyset \) and \( H(h_i) \cap \tau_{i+1} \neq \emptyset \) (with \( \tau_{k+1} \equiv \tau_1 \)). Since there is a path between any two vertices in the same component, it follows that there is a partially directed cycle in \( \mathcal{H} \), which contradicts that \( \mathcal{H} \) is acyclic. Hence we can conclude that \( G \) is indeed a DAG.

Note that the DAG obtained in Proposition 1 is unique and given a DAH \( \mathcal{H} \) we call such \( G \) the canonical DAG of \( \mathcal{H} \). The canonical DAG of a DAH is important in the factorization decomposition of a probability distribution according to the DAH. For details, see Section 5.2. A chain component \( \tau \) of \( \mathcal{H} \) is terminal if the out degree of \( \tau \) in \( G \) is 0, i.e., there is no \( \tau' \neq \tau \) such that \( \tau \rightarrow \tau' \) in \( G \). A chain component \( \tau \) is initial if the in degree of \( \tau \) in \( G \) is 0, i.e., there is no \( \tau' \neq \tau \) such that \( \tau' \rightarrow \tau \) in \( G \). We call a vertex set \( A \subseteq V(\mathcal{H}) \) an anterior set if it can be generated by stepwise removal of terminal chain components. We call \( A \) an ancestral set if both its head and tail intersect a common chain component. Hence, we remark that given a set \( A \), \( \text{ant}(A) \) is also the smallest ancestral set containing \( A \).

A sub-hypergraph of \( \mathcal{H} = (V, E) \) is a directed hypergraph \( \mathcal{H}' = (V', E') \) such that \( V' \subseteq V \) and \( E' \subseteq E \). Given \( S \subseteq V(\mathcal{H}) \), we say a directed hypergraph \( \mathcal{H}' \) is a sub-hypergraph of \( \mathcal{H} \) induced by \( S \), denoted by \( \mathcal{H}'_S \) or \( \mathcal{H}[S] \), if \( V(\mathcal{H}') = S \) and \( h \in E(\mathcal{H}') \) if and only if \( h \in E(\mathcal{H}) \) and \( H(h) \cup T(h) \subseteq S \).

To illustrate the relationship between a directed acyclic hypergraph and a chain graph, we will introduce the concept of a shadow of a directed acyclic hypergraph. Given a directed acyclic hypergraph \( \mathcal{H} \), let the (directed) shadow of \( \mathcal{H} \), denoted by \( \partial(\mathcal{H}) \), be a graph \( G \) such that \( V(G) = V(\mathcal{H}) \), and for every hyperedge \( h = (X, Y) \in E(\mathcal{H}) \), \( G[Y] \) is a clique (i.e. every two vertices in \( G[Y] \) are neighbors) and there is a directed edge from each vertex of \( X \) to each vertex of \( Y \) in \( G \).

Proposition 2 Suppose \( \mathcal{H} \) is a directed acyclic hypergraph and \( G \) is the shadow of \( \mathcal{H} \). Then

(i) \( G \) is a chain graph.
(ii) For every vertex \( v \in V(\mathcal{H}) = V(G) \), \( \text{nb}_G(v) = \text{nb}_\mathcal{H}(v) \) and \( \text{pa}_G(v) = \text{pa}_\mathcal{H}(v) \).

Proof For (i), note that since \( \mathcal{H} \) is acyclic, there is no partially directed cycle in \( \mathcal{H} \). It follows by definition that there is no partially directed cycle in \( G \). Hence, the shadow of a directed acyclic hypergraph is a chain graph. (ii) is also clear from the definition of the shadow.

2.3 Hypergraph drawing

In this subsection, we present how directed edges are drawn in this paper and illustrate the concepts with an example. For a fully directed hyperedge with two vertices (both head and tail contain exactly one vertex), we use the standard arrow notation. For a fully directed hyperedge with at least three vertices, we use a shaded polygon to represent that edge, with the darker side as the head and the lighter side as the tail. For hyperedges of the type \( (a, b, \ldots) \) we use an undirected line segment (i.e. \(-\)) to denote the hyperedge if \(|A| = 2\) and a shaded polygon with uniform gray color if \(|A| \geq 3\). For example, in Fig. 2, the directed hyperedges are \( (\{a, b\}, \{c\}), (\{a\}, \{c, d\}), (\{d\}, \{e, f\}) \), \( (\{c\}, \{e\}) \). Here \( a \) and \( b \) are co-tail, \( c \) and \( d \), \( e \) and \( f \) are co-head. Figure 2(2) shows the canonical DAG associated to \( \mathcal{H} \) with four chain components: \( \{a\}, \{b\}, \{c, d\}, \{e, f\} \). Figure 2(3) shows the shadow of \( \mathcal{H} \).
2.4 Construction of a directed acyclic hypergraph from chain graph

In this subsection, we show how to construct a directed acyclic hypergraph $H$ from a chain graph $G$ according to the LWF interpretation. We will then show later in Section 5.3 that the DAH model $H$ constructed from $G$ in this section admits the same Markov properties and factorization decomposition as the chain graph model $G$. This shows that the DAH model indeed generalizes the chain graph model (at least according to the LWF interpretation). Due to the expressiveness and generality of a directed hypergraph, other constructions may exist too. Let $G$ be a chain graph with $n$ vertices. We will explicitly construct a directed acyclic hypergraph $H$ on $n$ vertices that correspond to $G$. We remark that the construction essentially creates a hyperedge for each maximal clique in the moral graph of $G_{cl(\tau)}$ for every chain component $\tau$ of $G$.

Construction:

\[
V(H) = V(G).
\]

The edge set of $H$ is constructed in two phases:

Phase I:

- For each $v \in V(G)$, let $S_v$ be the set of children of $v$ in $G$. Consider the subgraph $G'$ of $G[S_v]$ induced by the undirected edges in $G[S_v]$. For each maximal clique (with vertex set $K$) in $G'$, add the directed hyperedge $(\{v\}, K)$ into $H$.
- Let $H'$ be the resulting hypergraph after performing the above procedure for every $v \in V(G)$. Now for every maximal clique $K$ (every edge in $K$ is undirected) in $G$, if $K \not\subseteq H(h)$ for every $h \in E(H')$, add the directed hyperedge $(\emptyset, K)$ into $H$.

Phase II: Let $H'$ be the resulting hypergraph constructed from Phase I and $\{\tau : \tau \in D\}$ be the chain components of $G$. Given $\tau$, let $H'_{\tau}$ be the hypergraph containing all the edges $h$ in $H'_{cl(\tau)}$ such that $H(h) \cap \tau \neq \emptyset$.

Define

\[
E(H) = \bigcup_{\tau \in D} \left\{ \left( \bigcup_{h \in E(H'_{\tau})} T(h), B \right) : B = \bigcap_{h \in F} H(h), F \subseteq E(H'_{\tau}) \right\}.
\]

Note that the resulting hypergraph $H$ is a directed acyclic hypergraph since a partially directed cycle $C$ in $H$ corresponds to a directed cycle in $G$. Moreover, the above construction gives us an injection from the family of chain graphs with $n$ vertices to the family of directed acyclic hypergraphs with $n$ vertices.

Figure 3 contains an example of a simple chain graph and its corresponding version in the hypergraph representation. Recall that every fully directed hyperedge is represented (in the drawing) by a colored convex region. The darker side is the head and the lighter side is the tail. We will detail the hyperedges existing in every phase of the construction:
Phase I: the hyperedges in $\mathcal{H}$ are $\{a, d, e\}$ and $\{b, e, f\}$ and $\{c, f\}$.

Phase II: For each chain component $\tau$, we obtain all subsets $B$ of $\tau$ which are the intersections of the heads of some set of hyperedges intersecting $\tau$. For each such $B$ obtained, create a hyperedge whose head is $B$ and whose tail is the union of the tails of the hyperedges containing $B$ in its head. In Fig. 3, for the chain component $\{d, e, f\}$, the set of such $B$’s is $\{\{d, e\}, \{e\}, \{e, f\}, \{f\}\}$. This is because $\{d, e\}$ is the head of the hyperedge $\{a, d, e\}$; $\{e\}$ is the intersection of the heads of the hyperedges $\{a, d, e\}$, $\{a, b, e\}$ and $\{b, e, f\}$, etc. Hence

$$E(\mathcal{H}) = \\{\{a, d, e\}, \{e, a, b\}, \{b, e, f\}, \{b, c, f\}\}.$$ 

In this particular example, the hyperedges $\{a, b, e\}$ and $\{b, c, f\}$ are created so that the resulting factorization according to the DAH is consistent with the LWF chain graph model: in particular, the factorization decomposition includes the cliques created due to the moralization operation in the chain graph model.

Hence the resulting hypergraph $\mathcal{H}$ is the one in Fig. 3(2).

For ease of reference, given a chain graph, we will call the hypergraph $\mathcal{H}$ constructed above the canonical LWF DAH of $G$. We say $\mathcal{H}$ is hypermoralized from $G$ if $\mathcal{H}$ is the canonical LWF DAH of $G$. Moreover, we call the family of all such hypergraphs (i.e. the canonical LWF DAH of some chain graph) LWF DAHs (Fig. 4).

Remark 2 In this section, we gave an injective mapping from the space of chain graphs to the space of directed acyclic hypergraphs. The LWF DAH constructed from a LWF chain graph $G$ has the same Markov properties as $G$. We show that later in Theorem 3. We believe

![Fig. 3](image1.png) a a simple chain graph $G$; b the corresponding DAH of $G$ in the LWF interpretation

![Fig. 4](image2.png) Relationship between chain graphs and directed acyclic hypergraphs

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some other types of chain graphs can be modeled by DAHs too (e.g. MVR DAHs) but we
do not explore them in this paper.

We will summarize the relations between a chain graph and its canonical LWF DAH in
the following lemma:

**Lemma 1** Let G be a chain graph and H be its canonical LWF DAH. Then we have

1. For each vertex \( v \in V(G) = V(H) \), \( nb_G(v) = nb_H(v) \) and \( pa_G(v) = pa_H(v) \).
2. G is the shadow of H.
3. H is a directed acyclic hypergraph.

**Proof** We will first show (i). Note that by our construction in Phase I, if two vertices are
neighbors in G, then they are co-head in H. Moreover, if u is the parent of v in G, then u
is still the parent of v in H. These relations remain true in Phase II. Hence we obtain
that \( nb_G(v) \subseteq nb_H(v) \) and \( pa_G(v) \subseteq pa_H(v) \) for all \( v \in V(H) \). It remains to show that
for each \( v \in V(H) \), no additional neighbor or parent of v (compared to the case in G) is
added in the construction. In Phase I, every hyperedge added is either of the form \((\emptyset, K)\)
or \((\{v\}, K)\) where \( K \subseteq V \) induces a complete undirected graph in G and w is the parent
of every element in K. Hence for every \( v \in V(H) \), no additional neighbor or parent of v
is added in Phase I. Now let us examine Phase II. Given an edge \( h = (A, B) \in E(H) \),
there exists some \( \tau \in D(G) \) such that \( B = \bigcap_{h \in \mathcal{F}} H(h) \) for some \( \mathcal{F} \subseteq E(H^*_\tau) \). Moreover,
\( A = \bigcup_{h \in \{E(H^*_\tau)\}} T(h) \). Note for every pair of elements \( u, v \in B \), \( u, v \) are already neighbors
in G since \( u, v \in H(h) \) for some \( h \in \mathcal{F} \) from Phase I. Moreover, for every \( v \in A, u \in B \),
v is already a parent of u in G since there exists some \( h \) constructed in Phase I such that
\( u \in H(h) \) and \( v \in T(h) \). Therefore, it follows that any edge defined in Phase II does not
create any new neighbor or parent for any \( v \in V(G) \). Thus, we can conclude that for all
\( v \in V(G) = V(H) \), \( nb_G(v) = nb_H(v) \) and \( pa_G(v) = pa_H(v) \).

(ii) is implied by (i) by the definition of a shadow. (iii) is implied by (ii) since G is acyclic
and G is the shadow of H. \( \square \)

### 3 Markov properties for undirected graphs

In this section, we will summarize some basic results on the Markov properties of undirected
digraphs. Let us first introduce some notations. In the rest of this week, let \( (X_\alpha)_{\alpha \in V} \)
be a collection of random variables taking values in some product space \( \mathcal{X} = \times_{\alpha \in V} X_\alpha \). Let P
be a probability measure on \( \mathcal{X} \). For a subset A of V, we use \( X_A \) to denote \( \times_{\alpha \in A} X_\alpha \) and
\( P_A \) is the marginal measure on \( X_A \). A typical element of \( X_A \) is denoted by \( x_A = (x_\alpha)_{\alpha \in A} \).

We will use the short notation \( A \perp B \mid C \) for \( X_A \perp X_B \mid X_C \).

Recall that an independence model \( \perp \) is a ternary relation over subsets of a finite set
V. The following properties have been defined for the conditional independencies of prob-
ability distributions. Let A, B, C, D be disjoint subsets of V where C may be the empty
set.

- **S1 (Symmetry)** \( A \perp B \mid C \implies B \perp A \mid C \);
- **S2 (Decomposition)** \( A \perp B \mid D \mid C \implies (A \perp B \mid C \text{ and } A \perp D \mid C) \);
- **S3 (Weak Union)** \( A \perp B \mid D \mid C \implies (A \perp B \mid DC \text{ and } A \perp D \mid BC) \);
- **S4 (Contraction)** \( (A \perp B \mid DC \text{ and } A \perp D \mid C) \iff A \perp BD \mid C \);
An independence model is a *semi-graphoid* if it satisfies the first four independence properties listed above. A discussion of conditional independence can be found in Dawid [6] where it is shown that any probability measure is a semi-graphoid. Also see Studeny [39] and Pearl [27] for a discussion of soundness and (lack of) completeness of these axioms. If a semi-graphoid further satisfies the intersection property, we say it is a *graphoid*. A compositional graphoid further satisfies the composition property. We follow the same naming convention as Frydenberg [8].

The following theorem by Pearl and Paz [26] gives a sufficient condition for the equivalence of (UG), (UL) and (UP).

**Theorem 1** [26] If $G$ is an undirected graph and $P$ satisfies (S5), then (UG), (UL) and (UP) are equivalent and $P$ is said to be $G$-Markovian if they hold.

Conditional independencies and thus Markov properties are closely related to factorizations. A probability measure $P$ on $\mathcal{X}$ is said to *factorize* according to $G$ if for each clique $h$ in $G$, there exist a non-negative function $\psi_h$ depending on $x_h$ only and there exists a product measure $\mu = \times_{\alpha \in V} \mu_\alpha$ on $\mathcal{X}$ such that $P$ has density $f$ with respect to $\mu$ where $f$ has the form

$$f(x) = \prod_{h \in C} \psi_h(x),$$

where $C$ is the set of maximal cliques in $G$. If $P$ factorizes according to $G$, we say $P$ has property (UF). It is known (see [19]) that

$$(UF) \implies (UG) \implies (UL) \implies (UP).$$

Moreover, in the case that $P$ has a positive and continuous density, it can be proven using Möbius inversion lemma that $(UP) \implies (UF)$. This result seems to have been discovered in various forms by a number of authors [36] and is usually attributed to Hammersley and Clifford [10] who proved the result in the discrete case.

### 4 Markov properties of chain graphs

We use the same notations as Section 3. Let $G$ be a chain graph and $P$ be a probability measure defined on some product space $\mathcal{X} = \times_{\alpha \in V(G)} \mathcal{X}_\alpha$. Then $P$ is said to be

**(CP) pairwise $G$-Markovian**, if for every pair $(v, u)$ of non-adjacent vertices with $u \in nd(v),$

$$v \perp u \mid nd(v) \setminus \{v, u\}.$$

**Reference**

1. [Dawid, 6]
2. [Studeny, 39]
3. [Pearl, 27]
(CL) local $G$-Markovian, relative to $G$, if for any vertex $v \in V(G)$,
\[ v \independent nd(v) \setminus cl(v) \mid bd(v). \]  
(3)

(CG) global $G$-Markovian, relative to $G$, if for all $A, B, C \subseteq V$ such that $C$ separates $A$ and $B$ in $(G_{ant}(A \cup B \cup C))^m$, the moral graph of the smallest ancestral set containing $A \cup B \cup C$, we have
\[ A \independent B \mid C. \]

The factorization in the case of a chain graph involves two parts. Suppose $\{\tau : \tau \in \mathcal{D}\}$ is the set of chain components of $G$. Then $P$ is said to factorize according to $G$ if it has density $f$ that satisfies:

(i) $f$ factorizes as in the directed acyclic case:
\[ f(x) = \prod_{\tau \in \mathcal{D}} f(x_{\tau} \mid x_{pa(\tau)}). \]

(ii) For each $\tau \in \mathcal{D}$, $f$ factorizes in the moral graph of $G_{\tau \cup pa(\tau)}$:
\[ f(x_{\tau} \mid x_{pa(\tau)}) = Z^{-1}(x_{pa(\tau)}) \prod_{h \in \mathcal{C}} \psi_h(x), \]
where $\mathcal{C}$ is the set of maximal cliques in $G_{m}^{\tau \cup pa(\tau)}$, $\psi_h(x)$ depends only on $x_h$ and
\[ Z^{-1}(x_{pa(\tau)}) = \int_{X_{\tau}} \prod_{h \in \mathcal{C}} \psi_h(x) \mu_\tau(dx_{\tau}). \]

If a probability measure $P$ factorizes according to $G$, then we say $P$ satisfies (CF). From arguments analogous to the directed and undirected cases, we have that in general
\[ (CF) \implies (CG) \implies (CL) \implies (CP). \]

If we assume (S5), then all Markov properties are equivalent.

Theorem 2 [8] Assume that a probability measure $P$ defined on a chain graph $G$ is such that (S5) holds for disjoint subsets of $V(G)$, then
\[ (CF) \iff (CG) \iff (CL) \iff (CP). \]

5 Bayesian Hypergraphs

A Bayesian hypergraph (BH) is a probabilistic graphical model that represents a set of variables and their conditional dependencies through an acyclic directed hypergraph $\mathcal{H}$. Hypergraphs contain many more edges than chain graphs. Thus a Bayesian hypergraph is a more general and powerful framework for studying conditional independence relations that arise in various statistical contexts.

5.1 Markov Properties of Bayesian hypergraphs

Analogously to the chain graph’s case, we can define the Markov properties of a Bayesian hypergraph in a variety of ways. Let $H$ be a directed acyclic hypergraph with chain components $\{\tau : \tau \in \mathcal{D}\}$. We say that a probability measure $P$ defined on $\mathcal{X} = \times_{\tau \in \mathcal{V}(\mathcal{H})} \mathcal{X}_{\tau}$ is:
pairwise $\mathcal{H}$-Markovian, relative to $\mathcal{H}$, if for every pair $(v, u)$ of non-adjacent vertices in $\mathcal{H}$ with $u \in nd(v)$,

$$v \perp u \mid nd(v) \setminus \{v, u\}. \quad (4)$$

local $\mathcal{H}$-Markovian, relative to $\mathcal{H}$, if for any vertex $v \in V(\mathcal{H})$,

$$v \perp nd(v) \setminus cl(v) \mid bd(v). \quad (5)$$

global $\mathcal{H}$-Markovian, relative to $\mathcal{H}$, if for all $A, B, C \subseteq V$ such that $C$ separates $A$ and $B$ in $(\partial(\mathcal{H}_{\text{ant}(A \cup B \cup C)}))^m$, the moral graph of the (directed) shadow of the smallest ancestral set containing $A \cup B \cup C$, we have

$$A \perp B \mid C.$$

**Definition 1** A Bayesian hypergraph is a triple $(V, \mathcal{H}, P)$ such that $V$ is a set of random variables, $\mathcal{H}$ is a DAH on the vertex set $V$ and $P$ is a multivariate probability distribution on $V$ such that the local Markov property, i.e., $(HL)$, holds with respect to the DAH $\mathcal{H}$.

Given a Bayesian hypergraph $(V, \mathcal{H}, P)$, we call $\mathcal{H}$ the Bayesian hypergraph structure or the underlying DAH of the Bayesian hypergraph. For ease of reference, we simply use $\mathcal{H}$ to denote the Bayesian hypergraph. Moreover, for a Bayesian hypergraph $\mathcal{H}$ whose underlying DAH is a LWF DAH, we call $\mathcal{H}$ a LWF Bayesian hypergraph.

**Remark 3** Observe that by Proposition 2 and the definitions of the hypergraph Markov properties, a Bayesian hypergraph has the same pairwise, local and global Markov properties as its shadow, which is a chain graph. Consequentially, any separation criteria (e.g., d-separation) for LWF chain graphs also apply to the shadow of the LWF Bayesian hypergraphs. This allows people to work with familiar separation criteria even in the case of Bayesian hypergraphs.

By Remark 3, we can derive the following corollaries from results on the Markov properties of chain graphs:

**Corollary 1**

$$(HG) \implies (HL) \implies (HP).$$

Furthermore, if we assume (S5), then the global, local and pairwise Markov properties are equivalent.

**Corollary 2** Assume that $P$ is such that (S5) holds for disjoint subsets of $V$. Then

$$(HG) \iff (HL) \iff (HP).$$

**Proof** This follows from Remark 3 and Theorem 2.

Given a chain graph $G$, a triple $(\alpha, B, \beta)$ is a complex in $G$ if $B$ is a connected subset of a chain component $\tau$, and $\alpha, \beta$ are two non-adjacent vertices in $bd(\tau) \cap bd(B)$. Moreover, $(\alpha, B, \beta)$ is a minimal complex if $B = B'$ whenever $B'$ is a subset of $B$ and $(\alpha, B', \beta)$ is a complex. Frydenberg [8] showed that two chain graphs have the same Markov properties

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1 or U-structure [4]
if they have the same underlying undirected graph and the same minimal complexes. In the case of a Bayesian hypergraph, by Remark 3 and the result on the Markov equivalence of chain graphs, we obtain the following conclusion on the Markov equivalence of Bayesian hypergraphs.

**Corollary 3** Two Bayesian hypergraphs have the same Markov properties if their shadows are Markov equivalent, i.e., their shadows have the same underlying undirected graph and the same minimal complexes.

### 5.2 Factorization according to Bayesian hypergraphs

The factorization of a probability measure $P$ according to a Bayesian hypergraph is similar to that of a chain graph. Before we present the factorization property, let us introduce some additional terminology.

Given a DAH $H$, we use $H^u$ to denote the undirected hypergraph obtained from $H$ by replacing each directed hyperedge $h = (A, B)$ of $H$ into an undirected hyperedge $A \cup B$. Given a family of sets $\mathcal{F}$, define a partial order $(\mathcal{F}, \leq)$ on $\mathcal{F}$ such that for two sets $A, B \in \mathcal{F}$, $A \leq B$ if and only if $A \subseteq B$. Let $\mathcal{M}(\mathcal{F})$ denote the set of maximal elements in $\mathcal{F}$, i.e., no element in $\mathcal{M}(\mathcal{F})$ contains another element as subset. When $\mathcal{F}$ is a set of directed hyperedges, we abuse the notation to denote $\mathcal{M}(\mathcal{F}) = \mathcal{M}(\mathcal{F}^u)$.

Let $H$ be a directed acyclic hypergraph, $D$ be the canonical DAG of the chain components of $H$. Assume that a probability distribution $P$ has a density $f$, with respect to some product measure $\mu = \times_{\alpha \in V} \mu_\alpha$ on $X = \times_{\alpha \in V} X_\alpha$. Now we say a probability measure $P$ factorizes according to $H$ if it has density $f$ such that

(i) $f$ factorizes as in the directed acyclic case:

$$f(x) = \prod_{\tau \in V(D)} f(x_\tau | x_{pa(\tau)}).$$

(ii) For each $\tau \in V(D)$, define $H^*_\tau$ to be the subhypergraph of $H_{\tau \cup pa(\tau)}$ containing all edges $h$ in $H_{\tau \cup pa(\tau)}$ such that $H(h) \subseteq \tau$.

$$f(x_\tau | x_{pa(\tau)}) = \prod_{h \in \mathcal{M}(H^*_\tau)} \psi_h(x).$$

where $\psi_h$ are non-negative functions depending only on $x_h$ and

$$\int_{X_{\tau}} \prod_{h \in \mathcal{M}(H^*_\tau)} \psi_h(x) \mu_\tau(dx_\tau) = 1.$$ Equivalently, we can also write $f(x_\tau | x_{pa(\tau)})$ as

$$f(x_\tau | x_{pa(\tau)}) = Z^{-1}(x_{pa(\tau)}) \prod_{h \in \mathcal{M}(H^*_\tau)} \psi_h(x),$$

where $Z^{-1}(x_{pa(\tau)}) = \int_{X_{\tau}} \prod_{h \in \mathcal{M}(H^*_\tau)} \psi_h(x) \mu_\tau(dx_\tau)$.

**Remark 4** Note that although (LWF) Bayesian hypergraphs are generalizations of Bayesian networks and LWF chain graph models, the underlying graph structures that represent the same factorizations may differ. The motivation behind this representational choice is that it is easier for a modeler to represent induced dependencies explicitly via directed hyperedges, rather than representing the absence of induced dependencies via directed...
hyperedges. As a consequence, the underlying graph structures of Bayesian networks and chain graph do not directly migrate to Bayesian hypergraphs.

We will illustrate with an example. Consider the graph in Fig. 5, which can be interpreted as a chain graph structure $G$ or a Bayesian hypergraph structure $\mathcal{H}$. Note that the factorizations, under the two interpretations, are different. In particular, the factorization, according to $G$, is

$$f_G(x) = f(x_a)f(x_b)\psi_{abc}(x)$$

for some non-negative functions $\psi_{abc}$. On the other hand, the factorization, according to $\mathcal{H}$, is

$$f_\mathcal{H}(x) = f(x_a)f(x_b)\psi_{ac}(x)\psi_{bc}(x)$$

for some non-negative functions $\psi_{ac}, \psi_{bc}$.

Remark 5 One of the key advantages of Bayesian hypergraphs is that they allow much finer factorizations of probability distributions compared to chain graph models. We will illustrate with a simple example in Fig. 6. Note that in Fig. 6(1), the factorization according to $G$ is

$$f(x) = f(x_a)f(x_b)f(x_{cd}|x_{ab}) = f(x_a)f(x_b)\psi_{abcd}(x)$$

In Figure 6 (2), the factorization according to $\mathcal{H}$ is

$$f(x) = f(x_a)f(x_b)f(x_{cd}|x_{ab}) = f(x_a)f(x_b)\psi_{abc}(x)\psi_{abd}(x)\psi_{cd}(x)$$

Note that although $G$ and $\mathcal{H}$ have the same global Markov properties, the factorization according to $\mathcal{H}$ is one step further compared to the factorization according to $G$. Suppose each of the variables of $\{a, b, c, d\}$ can take $k$ values. Then the factorization according to $G$ will require a conditional probability table of size $k^4$ while the factorization according to $\mathcal{H}$ only needs a table of size $\Theta(k^3)$ asymptotically. Hence, a Bayesian hypergraph model allows much finer factorizations and thus achieves higher memory efficiency.

Remark 6 We remark that the factorization formula defined in (7) is in fact the most general possible in the sense that it allows all possible factorizations of a probability distribution admitted by a DAH. In particular, given a Bayesian hypergraph $\mathcal{H}$ and one of its chain components $\tau$, the factorization scheme in (7) allows a distinct function for each maximal subset of $\tau \cup pa_D(\tau)$ that intersects $\tau$ ($pa_D$ is the parent of $\tau$ in the canonical DAG of $\mathcal{H}$). For each subset $S$ of $\tau \cup pa_D(\tau)$ that does not intersect $\tau$, recall that the factorization in (7)

Fig. 5 A simple Bayesian hypergraph $\mathcal{H}$
On a hypergraph probabilistic graphical model

Fig. 6  a a chain graph $G$; b a Bayesian hypergraph $\mathcal{H}$

can be rewritten as follows:

$$f(x_\tau \mid x_{pa(\tau)}) = \left( \prod_{h \in M^*(\mathcal{H}_\tau^\tau)} \psi_h(x) \right) \left/ \left( \int_{X_\tau} \prod_{h \in M^*(\mathcal{H}_\tau^\tau)} \psi_h(x) \mu_\tau(dx_\tau) \right) \right..$$

Observe that $\psi_S(x)$ is a function that does not depend on values of variables in $\tau$. Hence $\psi_S(x)$ can be factored out from the integral above and cancels out with itself in $f(x_\tau \mid x_{pa(\tau)})$. Thus, the factorization formula in (7) or (8) in fact allows distinct functions for all possible maximal subsets of $\tau \cup pa_D(\tau)$.

Table 2 lists some factorizations of three random variables and the corresponding BH representation. Entry 1 (top left) corresponds to a three-node Bayesian network: an uncoupled converging connection (unshielded collider) at $c$. Entry 3 (below entry 1) corresponds to a three-node Bayesian network like the one in entry 1, with the constraint that the conditional probability table factorizes as, for example, in a Noisy-OR functional dependence and, more generally, in a situation for which compositionality holds, such as MIN, MAX, or probabilistic sum [12, 13, 27]. Graphical modeling languages should capture assumptions

| Factorization                  | BH representation | Factorization                  | BH representation |
|-------------------------------|-------------------|-------------------------------|-------------------|
| $f(x) = f(x_a)f(x_b)\psi_{abc}(x)$ | ![Diagram](a) ![Diagram](b) ![Diagram](c) | $f(x) = f(x_{ab})\psi_{abc}(x)$ | ![Diagram](a) ![Diagram](b) ![Diagram](c) |
| $f(x) = f(x_a)f(x_b)\psi_{ac}(x)\psi_{bc}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) | $f(x) = f(x_{ab})\psi_{ac}(x)\psi_{bc}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) |
| $f(x) = f(x_a)f(x_b)\psi_{ac}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) | $f(x) = f(x_{ab})\psi_{ac}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) |
| $f(x) = f(x_a)f(x_b)f(x_c)$ | ![Diagram](a) ![Diagram](b) ![Diagram](c) | $f(x) = f(x_{ab})f(x_c)$ | ![Diagram](a) ![Diagram](b) ![Diagram](c) |
| $f(x) = \psi_{ac}(x)\psi_{bc}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) | $f(x) = f(x_c)\psi_{ac}(x)\psi_{ab}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) |
| $f(x) = f(x_c)\psi_{ac}(x)\psi_{bc}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) | $f(x) = f(x_c)\psi_{ac}(x)\psi_{bc}(x)$ | ![Diagram](a) ![Diagram](c) ![Diagram](b) |
graphically in a transparent and explicit way, as opposed to hiding them in tables or functions. By this criterion, the Bayesian hypergraph of entry 3 shows the increased power of our new PGM with respect to Bayesian networks and chain graphs.

For a detailed example of Noisy-OR functional dependence, consider the (much simplified) heart disease model of [9], shown in Fig. 7, and the family of nodes Obesity (O, with values Yes, No), Diet (D, with values Bad, Good), and Moderate Exercise (M, with values Yes, No). The Noisy-OR model is used to compute the conditional probability of O given M and D. Good diet prevents obesity, except when an inhibiting mechanism prevents that with probability \( q_{D \rightarrow O} \); moderate exercise prevents obesity except when an inhibiting mechanism prevents that with probability \( q_{M \rightarrow O} \). The inhibiting mechanisms are independent, and therefore the probability of being obese given both a good diet and moderate exercise is \( 1 - q_{D \rightarrow O} q_{M \rightarrow O} \). Equivalently, the probability of not being obese given both a good diet and moderate exercise is \( q_{D \rightarrow O} q_{M \rightarrow O} \). If we consider a situation with only the variables just described, the joint probability of Diet, Moderate Exercise, and Obesity factorizes exactly as in the Bayesian hypergraph of entry 3 (Fig. 8), with the caution that only half of the entries in the joint probability table are computed directly; the others are computed by the complement to one.

Similarly, entry 2 (top right) corresponds to a three node chain graph, while entry 4 (below entry 2) may be used to model a situation in which variables \( a \) and \( b \) are related by being effects of a common latent cause, while the mechanisms by which they, in turn, affect variable \( c \) are causally independent. While such a situation may be unusual, it is notable that it can be represented graphically in Bayesian hypergraphs. Therefore, the Bayesian hypergraph of entry 4 shows the increased power of our new PGM with respect to Bayesian networks and chain graphs.

For a detailed example, consider again the model shown in Fig. 7 and, this time, the structure in which Moderate Exercise, Serum LDL (S-LDL), Serum Triglycerides (S-T), and Cholesterol HDL (C-HDL) Ratio are parents (possible causes) of Atherosclerosis, and Diet is a parent of S-LDL, S-T, and C-HDL (Fig. 9a). As in the previous example, the Noisy-OR

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Fig. 7 A model of heart disease
assumption is made, and therefore, after marginalization of Diet (Fig. 9b), the computation of the joint probability of Moderate Exercise, S-LDL, S-T, C-HDL, and Atherosclerosis factorizes as in an entry 4, with a slight generalization due to the presence of four parents instead of two. As in entry 4, the parents (causes) are not marginally independent, due to their common dependence on Diet, but the conditional probability of the effect decomposes multiplicatively.

Moreover, as illustrated in Remark 5 and Table 2, a Bayesian hypergraph enables much finer factorization than a chain graph. In the factorization w.r.t. a chain graph $G$ with chain components $\{\tau : \tau \in V(D)\}$, $f(x_\tau | x_{pa(\tau)})$ is only allowed to be further factorized based on the maximal cliques in the moral graph of $G_{\tau \cup pa(\tau)}$, which is rather restrictive. In comparison, a Bayesian hypergraph $H$ allows factorization based on the maximal elements in all subsets of the power set of $\tau \cup pa_D(x)$. Finer factorizations have the advantage of memory saving in terms of the size of the probability table required. Moreover, factorizations according to Bayesian hypergraphs can be obtained directly from reading off the hyper-edges instead of having to search for all maximal cliques in the moral graph (in the chain graph’s case). Hence, Bayesian hypergraphs enjoy an advantage in heuristic adequacy as well as representational adequacy.

Next, we investigate the relationship between the factorization property and the Markov properties of Bayesian hypergraphs.

**Proposition 3** Let $P$ be a probability measure with density $f$ that factorizes according to a DAH $H$. Then

$$(HF) \implies (HG) \implies (HL) \implies (HP).$$

**Proof** It suffices to show $(HF) \implies (HG)$ since the other implications are proven in Corollary 1. Let $A, B, C \subseteq V(H)$ such that $C$ separates $A$ and $B$ in $G = (\partial(H_{ant(A \cup B \cup C)}))^m$.

Let $\tilde{A}$ be the connectivity components in $G \setminus C$ containing $A$ and let $\tilde{B} = V \setminus (\tilde{A} \cup C)$. Note that in $(\partial(H_{ant(A \cup B \cup C)}))^m$, every hyperedge $h = (T, H)$ becomes a complete graph on the vertex set $T \cup H$ because of moralization. Observe that since $C$ separates $A$ and $B$ in $G$, for every hyperedge $h = (T, H)$, $T \cup H$ is either a subset of $\tilde{A} \cup C$ or $\tilde{B} \cup C$. Let $H' = H_{ant(A \cup B \cup C)}$, $D'$ be the canonical DAG of the chain components of $H'$. For each $\tau \in V(D')$, define $H^*_\tau$ to be the subhypergraph of $H'_{\tau \cup pa(\tau)}$ containing all edges $h$ in $H'_{\tau \cup pa(\tau)}$ such that $H(h) \subseteq \tau$. We then obtain from the (HF) property that

$$f_{H'}(x) = \prod_{\tau \in V(D')} \prod_{h \in M(H^*_\tau)} \psi_h(x).$$

$$= \phi_1(x_{\tilde{A} \cup C})\phi_2(x_{\tilde{B} \cup C}).$$

**Fig. 8** An example of Noisy-OR: obesity
for some non-negative functions $\phi_1, \phi_2$. By integrating over the chain components not in $\text{ant}(A \cup B \cup C)$, it follows that

$$f(x) = \psi_1(x_{\bar{A} \cup C})\psi_2(x_{\bar{B} \cup C}).$$

for some non-negative functions $\psi_1, \psi_2$. Hence, we have that

$$\tilde{A} \perp \tilde{B} \mid C.$$

By (S2: Decomposition) property of conditional independencies, it follows that $A \perp B \mid C$.

Remark 7 Due to the generality of factorizations according to Bayesian hypergraphs, the reverse direction of the implication (HF) $\implies$ (HG) in Proposition 3 is generally not true. We will illustrate with the following example.

Consider the two Bayesian hypergraphs $\mathcal{H}_1$ and $\mathcal{H}_2$ in Fig. 10. Note that they have the same global Markov properties since the shadows of $\mathcal{H}_1$ and $\mathcal{H}_2$ are the same. However, the factorizations according to $\mathcal{H}_1$ and $\mathcal{H}_2$ are different. If we let $f_1, f_2$ denote the factorizations represented by $\mathcal{H}_1$ and $\mathcal{H}_2$, then

$$f_1(x) = f_1(x_a)f_1(x_b)f_1(x_{cd} \mid x_{ab})$$
$$= f_1(x_a)f_1(x_b)\psi_{abcd}(x)$$

while

$$f_2(x) = f_2(x_a)f_2(x_b)f_2(x_{cd} \mid x_{ab})$$
$$= f_2(x_a)f_2(x_b)\psi_{abc}(x)\psi_{abd}(x)\psi_{cd}(x)$$

This shows that (HG) does not generally imply (HF).
Remark 8 We remark that in our model, two Bayesian hypergraphs that are Markov equivalent may not be factorization-equivalent. This also implies that in general (HF) does not imply (HG). Below we present a combinatorial argument for why this cannot be resolved. We claim that the number of possible forms of factorizations admitted by Bayesian hypergraphs is much more than the number of conditional independence statements over the same set of variables. First, observe that the number of conditional independence statements on \( n \) variables is upper bounded by the number of ways to partition \( n \) elements into four disjoint sets \( A, B, C, D \). Each such partition induces a conditional statement \( A \perp \perp B | C \) and \( D \) is the set of unused variables. There are \( 4^n \) ways to partition \( n \) distinct elements into four ordered pairwise disjoint sets. Hence there are at most \( 4^n \) conditional independence statements on \( n \) variables.

On the other hand, we give a simple lower bound on the number of directed acyclic hypergraphs by simply counting the number of directed acyclic hypergraphs \( \mathcal{H} \) whose vertex sets can be partitioned into two sets \( A, B \) such that \( |A| = |B| = n/2 \) and every fully directed edge has its tail only from \( A \) and its head only from \( B \). Observe that there are \( 2^{n/2} \) subsets of \( A \) and \( B \) respectively. By Sperner’s theorem [37], the largest number of subsets of \( A \) none of which contain any other is upper bounded by \( \binom{n/2}{n/4} \). The same holds for \( B \). Hence there are at least \( \binom{n/2}{n/4}^2 \) possible directed hyperedges such that when viewed as undirected hyperedge, no edge contains any other as subset. Therefore, there are at least

\[
2^{\binom{n/2}{n/4}^2} = \Theta \left( 2^{2^{n+2}/3\pi n} \right)
\]

distinct factorizations admitted by DAHs whose directed edges have their tails only from \( A \) and their heads only from \( B \). Note that this number is much less than the total number of distinct factorizations admitted by DAHs, but is already much bigger than \( 4^n \), which is the upper bound on the number of conditional independence statements on \( n \) variables. Hence, there are many more factorizations allowed by Bayesian hypergraphs than the number of conditional independence statements on \( n \) variables, which suggests that (HG) does not imply (HF) in general.

5.3 Comparison between LWF chain graph and LWF Bayesian hypergraph

Let \( G \) be a LWF chain graph and \( \mathcal{H} \) be the canonical LWF DAH constructed from \( G \) described in Section 2.4. In this section, we show that \( \mathcal{H} \) and \( G \) admit the same Markov

\[a\] \[b\] \[c\] \[d\]
properties and factorization decomposition. Hence Bayesian hypergraphs generalize the LWF chain graphs.

**Theorem 3** Let $G$ be a chain graph and $\mathcal{H}$ be its canonical (LWF) DAH. We show that a probability measure $P$ satisfies the following:

(i) $P$ is pairwise $G$-Markovian if and only if $P$ is pairwise $\mathcal{H}$-Markovian.

(ii) $P$ is local $G$-Markovian if and only if $P$ is local $\mathcal{H}$-Markovian.

(iii) $P$ is global $G$-Markovian if and only if $P$ is global $\mathcal{H}$-Markovian.

**Proof** By Lemma 1, $nb_G(v) = nb_{\mathcal{H}}(v)$, $pa_G(v) = pa_{\mathcal{H}}(v)$. Hence the same equality holds for $nd_G(v)$, $bd_G(v)$, $cl_G(v)$, which gives us (i) and (ii) by definition of the Markov properties. (iii) results from the fact that for all $A, B, C \subseteq V(G) = V(\mathcal{H})$, $G_{ant(A \cup B \cup C)} = \partial(\mathcal{H}_{ant(A \cup B \cup C)})$.

**Theorem 4** Let $G$ be a chain graph and $\mathcal{H}$ be its canonical LWF DAH. Then a probability measure $P$ with density $f$ factorizes according to $G$ if and only if $f$ factorizes according to $\mathcal{H}$.

**Proof** Note that by Lemma 1, $G$ and $\mathcal{H}$ have the same set of chain components $\{\tau : \tau \in V(D)\}$. It suffices to show for every $\tau \in V(D)$, there exists a bijective map $\phi$ from the set of maximal edges in $(\mathcal{H}_\tau^*)^u$ to the set of maximal cliques in $(G_{\tau \cup pa(\tau)})^m$ such that for each maximal edge $h$ in $(\mathcal{H}_\tau^*)^u$, $\phi(h) = h$. For ease of reference, let $\mathcal{H}' = (\mathcal{H}_\tau^*)^u$ and let $G' = (G_{\tau \cup pa(\tau)})^m$. Define $\phi(h) = h$. We need to show two things: (1) for every maximal edge $h$ in $\mathcal{H}'$, $h$ induces a maximal clique in $G'$; (2) for every maximal clique $h$ in $G'$, $h$ is a maximal edge in $\mathcal{H}'$.

We first show (1). Suppose that $h$ is a maximal edge in $\mathcal{H}'$. Clearly, $h$ induces a clique in $G'$ because of the moralization. Suppose for the sake of contradiction that $h$ is not maximal in $G'$, i.e. there is a maximal clique $h'$ in $G'$ such that $h \subseteq h'$. Let $h'' = A \cup B$ where $A \subseteq pa(\tau)$ and $B \subseteq \tau$. There are two cases:

Case 1: $A = \emptyset$ or $B = \emptyset$.

Note that $B$ cannot be an empty set since $h$ is an edge in $\mathcal{H}'$ and every edge in $\mathcal{H}' = (\mathcal{H}_\tau^*)^u$ intersects $\tau$ by definition. If $A = \emptyset$, then $h'$ is a maximal clique in $\tau$. By Phase I of the construction, $h'$ either is a hyperedge in $\mathcal{H}'$ or is contained in the head of a hyperedge. In either case, since $h \subseteq h'$, it contradicts that $h$ is a maximal edge in $\mathcal{H}'$.

Case 2: $A \neq \emptyset$ and $B \neq \emptyset$.

Since $A \cup B$ induces a maximal clique in $G'$, it follows that for every $a \in A, b \in B$, $a \in pa(b)$. Hence $B$ the common children of some elements in $A$. Recall that in Phase I of our construction, for every $v$, $\{v\}, K_v$ is an hyperedge in $\mathcal{H}$ where $K_v$ is a maximal clique in the children of $v$ in $G$. Hence there exists $\mathcal{F} \subseteq E(\mathcal{H}_\tau^*)$ such that $B \subseteq \cap_{h \in \mathcal{F}} H(h)$. By maximality of $h'$, $B = \cap_{h \in \mathcal{F}} H(h)$. Now by our construction in Phase II, there exists a hyperedge

$$h'' = \left( \bigcup_{h \in E(\mathcal{H}_\tau^*))} T(h), B \right) \in E(\mathcal{H}_\tau^*).$$
Since every element in $A$ is a parent of every element in $B$, it follows that

$$A \subseteq \bigcup_{h \in E(H^\tau_1)} T(h).$$

By maximality of $A$, it follows that

$$h \subseteq h' = h'' \in E(H^\tau_1).$$

which contradicts the maximality of $h$ again.

Hence in both cases, we obtain by contradiction that $h$ induces a maximal clique in $G'$.

It remains to show (2). Suppose $h$ induces a maximal clique in $G'$. Observe that every hyperedge in $H'$ induces a clique in $G'$. Similar logic and case analysis above apply and it is not hard to see that $h$ is a maximal edge in $H'$. We will leave the details to the reader.

Example

In Fig. 11, both $G$ and its canonical LWF DAH $H$ have chain components $\{\{a\}, \{b\}, \{c\}, \{d, e, f\}\}$. Figure 11(2) shows the moral graph $G^m$ of $G$. The maximal cliques in $G^m$ are $\{ade, abce, cef\}$. Thus, by the factorization property of LWF chain graphs, we have that a probability measure $P$ with density $f$ that factorizes according to $G$ satisfies

$$f(x) = f(x_a)f(x_b)f(x_c)f(x_{d,e,f} | x_{a,b,c})$$

$$= f(x_a)f(x_b)f(x_c)\psi_{ade}(x)\psi_{abce}(x)\psi_{cef}(x).$$

Figure 11(3) gives the undirected hypergraph with edge set $\mathcal{M}(H)$. Observe that $\mathcal{M}(H)$ has the same members as the set of maximal cliques in $G^m$. Hence by the factorization property of Bayesian hypergraphs, they admit the same factorization.

Remark 9 One should notice that chain graphs also allow one to factorize the distribution as a product of potentials over (not necessarily maximal) complete sets [19]. This allows a finer model similar to DAHs. The approach presented in this paper is superior because the model is even more finely grained, more explicit, and graphically represented. We also note that the formalism of factor graphs provides an alternative graphical representation, one which emphasizes the factorization of the distribution [2, 16, 24] and is more commonly used as a secondary structure for message passing in inference algorithms. We do not use factor graphs in this paper.

Fig. 11 a a simple chain graph $G$; b The moral graph $G^m$ of $G$; c $\mathcal{M}(H)$ where $H$ is the canonical LWF DAH of $G$
6 Intervention in Bayesian hypergraphs

Formally, intervention in Bayesian hypergraphs can be defined analogously to intervention in LWF chain graphs [22]. In this section, we give graphical procedures that are consistent with the intervention formulas for chain graphs (9) and (10) and for Bayesian hypergraphs (11) and (12). Before we present the details, we need some additional definitions and tools to determine when factorizations according to two chain graphs or DAHs are equivalent in the sense that they could be written as products of the same type of functions (functions that depend on same set of variables). We say two chain graphs $G_1, G_2$ admit the same factorization decomposition if for every probability density $f$ that factorizes according to $G_1$, $f$ also factorizes according to $G_2$, and vice versa. Similarly, two DAHs $\mathcal{H}_1, \mathcal{H}_2$ admit the same factorization decomposition if for every probability density $f$ that factorizes according to $\mathcal{H}_1$, $f$ also factorizes according to $\mathcal{H}_2$, and vice versa.

6.1 Factorization equivalence and intervention in chain graphs

In this subsection, we will give graphical procedures to model intervention based on the formula introduced by Lauritzen and Richardson in [22]. Let us first give some background. In many statistical context, we would like to modify the distribution of a variable $Y$ by intervening externally and forcing the value of another variable $X$ to be $x$. This is commonly referred as conditioning by intervention or conditioning by action and denoted by $\text{Pr}(y \parallel x)$ or $\text{Pr}(y \mid X \leftarrow x)$. Other expressions such as $\text{Pr}(Y = y | set(X = x), X = \hat{x})$ or $\text{do}(X = x)$ have also been used to denote intervention conditioning (Neyman [25]; Rubin [35]; Spirtes et al. [38]; Pearl [28–30]).

Let $G$ be a chain graph and $\mathcal{D}$ be the corresponding DAG of the chain components of $G$. Moreover, assume further that a subset $A$ of variables in $V(G)$ are set such that for every $a \in A$, $x_a = a_0$. Lauritzen and Richardson, in [22], generalized the conditioning by intervention formula for DAGs and gave the following formula for intervention in chain graphs (where it is understood that the probability of any configuration of variables inconsistent with the intervention is zero). A probability density $f$ factorizes according to $G$ (with $A$ intervened) if

$$f(x \parallel x_A) = \prod_{\tau \in V(\mathcal{D})} f(x_{\tau \backslash A} \mid x_{pa(\tau)}, x_{\tau \cap A}).$$

(9)

Moreover, for each $\tau \in V(\mathcal{D})$,

$$f(x_{\tau \backslash A} \mid x_{pa(\tau)}, x_{\tau \cap A}) = Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) \prod_{h \in C} \psi_h(x)$$

(10)

where $C$ is the set of maximal cliques in $(G_{\tau \cup pa(\tau)})^m$ and $Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) = \int_{X_{\tau \backslash A}} \prod_{h \in C} \psi_h(x) \mu_{\tau \backslash A}(dx_{\tau \backslash A})$.

Let $G_1$ and $G_2$ be two chain graphs. Given a subset $A_1 \subseteq V(G_1)$ and $A_2 \subseteq V(G_2)$, we say $(G_1, A_1)$ and $(G_2, A_2)$ are factorization-equivalent if they become the same chain graph after removing from $G_i$ all vertices in $A_i$ together with the edges incident to vertices in $A_i$ for $i \in \{1, 2\}$. Typically, $A_i$ is a set of constant variables in $V(G_i)$ created by

\[2\]This term was defined for a different purpose in [40].
Thus it follows that every probability density $f$ that factorizes according to $G_1$ with $A_1$ intervened also factorizes according to $G_2$ with $A_2$ intervened, and vice versa.

**Theorem 5** Let $G_1$ and $G_2$ be two chain graphs defined on the same set of variables $V$. Moreover a common set of variables $A$ in $V$ are set by intervention such that for every $a \in A$, $x_a = a_0$. If $(G_1, A)$ and $(G_2, A)$ are factorization-equivalent, then $(G_1, A)$ and $(G_2, A)$ admit the same factorization decomposition.

**Proof** Let $G_0$ be the chain graph obtained from $G_1$ by removing all vertices in $A$ and the edges incident to $A$. It suffices to show that $G_1$ and $G_2$ both admit the same factorization decomposition as $G_0$. Let $D_1, D_0$ be the corresponding DAG of the chain components of $G_1$ and $G_0$ respectively. Let $\tau \in V(D_1)$ be an arbitrary chain component of $G_1$. By the factorization formula in (10), it follows that

$$f(x_{\tau \setminus A} \mid x_{pa(\tau)}, x_{\tau \cap A}) = Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) \prod_{h \in C} \psi_h(x)$$

where $C$ is the set of maximal cliques in $(G_{\tau \cup pa(\tau)})^m$ and $Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) = \int_{x_{\tau \setminus A}} \prod_{h \in C} \psi_h(x) \mu_{\tau \setminus A}(dx_{\tau \setminus A})$. Notice that for any maximal clique $h_1 \in C$ such that $h_1 \cap A = \emptyset$, $h_1$ is also a clique in $(G_0[\tau \setminus A])^m$. For $h_1 \in C$ with $h_1 \cap A \neq \emptyset$, there are two cases:

Case 1: $(h_1 \cap \tau) \setminus A \neq \emptyset$. In this case, observe that $h_1 \setminus A$ is also a clique in $(G_0[\tau \setminus A])^m$, thus is contained in some maximal clique $h'$ in $(G_0[\tau \setminus A])^m$. Since all variables in $A$ are pre-set as constants, it follows that $\psi_{h_1}(x)$ also appears in a factor in the factorization of $f$ according to $G_0$.

Case 2: $h_1 \cap \tau \subseteq A$. In this case, note that $h_1 \cap \tau$ is disjoint with $\tau \setminus A$. Hence $\psi_{h_1}(x)$ appears as a factor independently of $x_{\tau \setminus A}$ in both $Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A})$ and $\prod_{h \in C} \psi_h(x)$, which cancels out with itself.

Thus it follows that every probability density $f$ that factorizes according to $G_1$ also factorizes according to $G_0$. On the other hand, it is easy to see that for every $\tau' \in V(D_0)$ and every maximal clique $h'$ in $(G_0[\tau'])^m$, $h'$ is contained in some maximal clique $h$ in $(G_1[\tau])^m$ for some $\tau \in V(D_1)$. Hence we can conclude that $(G_1, A)$ and $(G_0, A)$ admit the same factorization decomposition. The above argument also works for $G_2$ and $G_0$. Thus, $(G_1, A)$ and $(G_2, A)$ admit the same factorization decomposition.

We now define a graphical procedure (call it redirection procedure) that is consistent with the intervention formula in (9) and (10). Let $G$ be a chain graph. Given an intervened set of variables $A \subseteq V(G)$, let $\hat{G}$ be the chain graph obtained from $G$ by performing the following operation: for every $u \in A$ and every undirected edge $e = \{u, w\}$ containing $u$, replace $e$ by a directed edge from $u$ to $w$; finally remove all the directed edges that point to some vertex in $A$. By replacing the undirected edge with a directed edge, we replace any feedback mechanisms that include a variable in $A$ with a causal mechanism. The intuition behind the procedure is the following. Since a variable that is set by intervention cannot be modified, the symmetric feedback relation is turned into an asymmetric causal one. Similarly, we can justify this graphical procedure as equivalent to removing the variables in $A$ from some equations in the Gibbs process on top of p. 338 of [22], as Lauritzen and Richardson [33] did for Equation (18) in [22].
Theorem 6 Let $G$ be a chain graph with a subset of variables $A \subseteq V(G)$ set by intervention such that for every $a \in A$, $x_a = a_0$. Let $\hat{G}$ be obtained from $G$ by the redirection procedure. Then $(G, A)$ and $(\hat{G}, A)$ admit the same factorization decomposition.

Proof It is not hard to see that removing from $\hat{G}$ and $G$ all vertices in $A$ and all edges incident to $A$ results in the same chain graph. Hence by Theorem (5), $(G, A)$ and $(\hat{G}, A)$ admit the same factorization decomposition.

Example 1 Consider the chain graph $G$ shown in Fig. 12. Let $\hat{G}$ be the graph obtained from $G$ through the redirection procedure described in this subsection. Let $G_0$ be the chain graph obtained from $G$ by deleting the vertex $c_0$ and the edges incident to $c_0$. We will compare the factorization decomposition according to formulas (9) and (10) as well as the graph structure $\hat{G}$ and $G_0$.

By formulas (9) and (10) proposed in [22], when $x_c$ is set as $c_0$ by intervention,
\[
\begin{align*}
f(x_{\parallel} x_c) &= f(x_a)f(x_b)f(x_{de} | x_{abc_0}) \\
&= f(x_a)f(x_b) \frac{\psi_{ac_0d}(x)\psi_{abde}(x)}{\sum_{d,e} \psi_{ac_0d}(x)\psi_{abde}(x)}.
\end{align*}
\]

Now consider the factorization according to $\hat{G}$. The chain components of $\hat{G}$ are \{\{a\}, \{b\}, \{c\}, \{d, e\}\} with $x_c$ set to be $c_0$. The factorization according to $\hat{G}$ as follows:
\[
\begin{align*}
f_{\hat{G}}(x_{\parallel} x_c) &= f_{\hat{G}}(x_a)f_{\hat{G}}(x_b)f_{\hat{G}}(x_c)f_{\hat{G}}(x_{de} | x_{abc_0}) \\
&= f_{\hat{G}}(x_a)f_{\hat{G}}(x_b)f_{\hat{G}}(x_c) \frac{\psi_{ac_0d}(x)\psi_{abde}(x)}{\sum_{d,e} \psi_{ac_0d}(x)\psi_{abde}(x)},
\end{align*}
\]
where $f(x_c) = 1$ when $x_c = c_0$ and otherwise 0. Hence $G$ and $\hat{G}$ admit the same factorization.

Now consider the factorization according to $G_0$. The chain components of $G_0$ are \{\{a\}, \{b\}, \{d, e\}\}. The factorization according to $G_0$ is as follows:
\[
\begin{align*}
f_{0}(x) &= f_{0}(x_a)f_{0}(x_b)f_{0}(x_{de} | x_{ab}) \\
&= f_{0}(x_a)f_{0}(x_b) \frac{\psi_{ad}(x)\psi_{abde}(x)}{\sum_{d,e} \psi_{ad}(x)\psi_{abde}(x)},
\end{align*}
\]
Observe that $f_0(x)$ has the same form of decomposition as $f(x_{\parallel} x_c)$ since $x_c$ is set to be $c_0$ in $\psi_{ac_0d}(x)$ (with the understanding that the probability of any configuration of variables

![Fig. 12](image-url)
with \( x_c \neq c_0 \) is zero). Hence we can conclude that \( G, \hat{G} \) (with \( x_c \) intervened) and \( G_0 \) admit the same factorization decomposition.

### 6.2 Factorization equivalence and intervention in Bayesian hypergraphs

Before we introduce the intervention formula for Bayesian hypergraphs, we first define a data-generating process for Bayesian hypergraphs, analogous to the data-generating process for chain graphs defined by Lauritzen and Richardson [22]. We also refer the readers to [22] for detailed expositions of the data-generating process for undirected graph and DAGs.

Let \( H \) be a DAH, \( D \) be its canonical DAG of the chain components of \( H \). Recall from Section 5.2 that a probability density \( f \) factorizes according to \( H \) as follows:

\[
f(x) = \prod_{\tau \in V(D)} f(x_\tau | x_{pa(\tau)})
\]

For each \( \tau \in V(D) \),

\[
f(x_\tau | x_{pa(\tau)}) = \prod_{h \in M(H_\tau)} \psi_h(x)
\]

where \( \psi_h \) are non-negative functions depending only on \( x_h \) and

\[
\int_{X_\tau} \prod_{h \in M(H_\tau)} \psi_h(x) \mu_\tau(dx_\tau) = 1.
\]

Similarly to the chain graph model, the data-generating process for a DAH has two loops. The outer loop deals with the assignment to the canonical DAG of chain components of \( H \):

\[
X_\tau \leftarrow H_\tau(X_{pa(\tau)}), \quad \tau \in V(D),
\]

with the restriction that when the variables in some component are to be updated, the variables in its parent components are already assigned values. Here \( H_\tau \) is the inner loop that updates the variables in the chain component \( \tau \), resulting in a system of structural equations via a Gibbs sampler. Following Lauritzen and Richardson’s notation [22], we describe the inner loop in the following form: let \( \epsilon_\tau = (\epsilon^1, \epsilon^2, \ldots) \) be a sequence of independent and identically uniformly distributed variables on the unit interval. The random variant of the Gibbs sampler yields:

function \( H_\tau \);

\[
\text{input} (x_{pa(\tau)}, \epsilon_\tau);
\]

\[
x_\tau \leftarrow x_\tau^0;
\]

\[
n \leftarrow 0;
\]

repeat until equilibrium:

\[
v \leftarrow \text{rand}(\tau);
\]

\[
n \leftarrow n + 1;
\]

\[
x_v \leftarrow h_v^\tau(x_{\tau\{v\}}, x_{pa(\tau)}, \epsilon^n);
\]

return \( x_\tau \)

and where \( h_v^\tau \) is chosen so that if \( U \) is uniformly distributed on the unit interval, then \( y_v = h_v^\tau(x_{\tau\{v\}}, x_{pa(\tau)}, U) \) has density \( f(y_v | x_{\tau\{v\}}, x_{pa(\tau)}) \), i.e., \( h_v^\tau \) is a direct Monte Carlo simulator for this conditional distribution. Given a set of variables \( A \subseteq V(H) \) and a set of fixed values \( \{x_a^* : a \in A\} \), if we replace the line updating the value \( x_a \) in the data-generating process by \( x_a \leftarrow x_a^* \), then we refer to this type of intervention as intervention by replacement.
We now propose the intervention formula for Bayesian hypergraphs. Given a DAH $\mathcal{H}$ and its canonical DAG $\mathcal{D}$, we say that a probability distribution $P$ is causally Markov with respect to $\mathcal{H}$ if for any $A \subseteq V(\mathcal{H})$, the density function $f$ of $P$ factorizes as follows:

$$f(x \| x_A) = \prod_{\tau \in V(\mathcal{D})} f(x_{\tau \setminus A} \mid x_{pa(\tau)}, x_{\tau \cap A})$$  \hspace{1cm} (11)

where

$$f(x_{\tau \setminus A} \mid x_{pa(\tau)}, x_{\tau \cap A}) = Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) \prod_{h \in \mathcal{M}(\mathcal{H}^*_\tau)} \psi_h(x).$$ \hspace{1cm} (12)

with $\mathcal{M}(\mathcal{H}^*_\tau)$ being defined the same way as in (7). $Z^{-1}(x_{pa(\tau)}, x_{\tau \cap A}) = \int_{X_{\tau \setminus A}} \prod_{h \in \mathcal{M}(\mathcal{H}^*_\tau)} \psi_h(x) \mu_{\tau \setminus A}(dx_{\tau \setminus A})$, and $\psi_h$ are non-negative functions that depend only on $x_h$. We show in the following theorem that intervention by replacement is consistent with the intervention formula in (11) and (12).

**Theorem 7** Let $X = \{X_v : v \in V(\mathcal{H})\}$ be determined by the system of structural equations corresponding to a DAH $\mathcal{H}$ in the data-generating process above. Let $P$ be the distribution of $X$. If intervention is carried out by replacement, then $P$ is causally Markov with respect to $\mathcal{H}$.

*Proof of Theorem 7* Let $\mathcal{D}$ be the canonical DAG of the chain components of $\mathcal{H}$ and $A \subseteq V(\mathcal{H})$ be the set of variables intervened by replacement. First, observe that $\{X_\tau, \tau \in V(\mathcal{D})\}$ satisfies the Markov property of the canonical DAG $\mathcal{D}$ (formed by the chain components of $\mathcal{H}$). The proof follows verbatim the same logic as in the case of DAGs (see, for example, [20], Theorem 2.20).

Now, for each $\tau \in V(\mathcal{D})$ and fixed $x_{pa(\tau)}$ consistent with $x_A$, the conditional distribution of the function $H_\tau(x_{pa(\tau)}, x_A)$ has density exactly $f(x_{\tau \setminus A} \mid x_{pa(\tau)}, x_{\tau \cap A})$ as the Gibbs sampler was designed to sample the variables in $\tau$ from this conditional distribution. Hence, the joint density of $X$ must follow the formula in (11) and (12).

**Definition 2** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Bayesian hypergraphs. Given a subset of variables $A_1 \subseteq V(\mathcal{H}_1)$ and $A_2 \subseteq V(\mathcal{H}_2)$, we say $(\mathcal{H}_1, A_1)$ and $(\mathcal{H}_2, A_2)$ are factorization-equivalent if performing the following operations to $\mathcal{H}_1$ and $\mathcal{H}_2$ results in the same directed acyclic hypergraph:

(i) Deleting all hyperedges with empty head, i.e., hyperedges of the form $(S, \emptyset)$.

(ii) Deleting every hyperedge that is contained in some other hyperedge, i.e., deleting $h$ if there is another $h'$ such that $T(h) \subseteq T(h')$ and $H(h) \subseteq H(h')$.

(iii) Shrinking all hyperedges of $\mathcal{H}_i$ containing vertices in $A_i$, i.e. replacing every hyperedge $h$ of $\mathcal{H}_i$ by $h' = (T(h) \setminus A_i, H(h) \setminus A_i)$ for $i \in \{1, 2\}$.

Typically, $A$ is a set of constant variables in $V$ created by intervention.

Moreover, we say $(\mathcal{H}_1, A_1)$, $(\mathcal{H}_2, A_2)$ admit the same factorization decomposition if every probability density $f$ that factorizes according to $\mathcal{H}_1$ with $A_1$ intervened also factorizes according to $\mathcal{H}_2$ with $A_2$ intervened, and vice versa.

**Theorem 8** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two DAHs defined on the same set of variables $V$. Moreover, a common set of variables $A$ in $V$ are set by intervention such that for every $a \in A$, $X_a = a_0$. If $(\mathcal{H}_1, A)$ and $(\mathcal{H}_2, A)$ are factorization-equivalent, then $(\mathcal{H}_1, A)$ and $(\mathcal{H}_2, A)$ admit the same factorization decomposition.
Proof Similar to the proof in Theorem 5, let $\mathcal{H}_0$ be the DAH obtained from $\mathcal{H}_1$ (or $\mathcal{H}_2$) by performing the operations above repeatedly. Let $D_1$ and $D_0$ be canonical DAG of the chain components of $\mathcal{H}_1$ and $\mathcal{H}_0$ respectively. First, note that performing the operation (i) does not affect the factorization since hyperedges of the form $h = (S, \emptyset)$ never appear in the factorization decomposition due to the fact that $H(h) \cap \tau = \emptyset$ for every $\tau \in V(D_1)$. Secondly, (ii) does not change the factorization decomposition too since if one hyperedge $h$ is contained in another hyperedge $h'$ as defined, then $\psi_h(x)$ can be simply absorbed into $\psi_{h'}(x)$ by replacing $\psi_{h'}(x)$ with $\psi_h(x) \cdot \psi_h(x)$.

Now let $\tau \in V(D_1)$ be an arbitrary chain component of $\mathcal{H}_1$ and $h_1 \in \mathcal{H}_1[\tau]^*$, i.e., the set of hyperedges in $\mathcal{H}_1$ whose head intersects $\tau$. Suppose that $\tau$ is separated into several chain components $\tau_1', \tau_2', \ldots, \tau_t'$ in $\mathcal{H}_0$ because of the shrinking operation. If $h_1 \cap A = \emptyset$, then $h_1$ is also a hyperedge in $\mathcal{H}_0[\tau \setminus A]^*$. If $h_1 \cap A \neq \emptyset$, there are two cases:

Case 1: $H(h_1) \subseteq A$. Then since variables in $A$ are constants, it follows that in (12), $\psi_{h_1}(x)$ does not depend on variables in $\tau \setminus A$. Hence $\psi_{h_1}(x)$ appears as a factor independent of variables in $\tau \setminus A$ in both $Z^{-1}(x_\text{pa}(\tau), x_{\tau \setminus A})$ and $\prod_{h \in \mathcal{M}(H'\tau)} \psi_h(x)$, thus cancels out with itself. Note that, $h_1$ does not exist in $\mathcal{H}_0$ too since $h_1$ becomes a hyperedge with empty head after being shrunk and thus is deleted in Operation (i).

Case 2: $H(h_1) \setminus A \neq \emptyset$. In this case, $H(h_1) \setminus A$ must be entirely contained in one of $\{\tau_1', \ldots, \tau_t'\}$. Without loss of generality, say $H(h_1) \setminus A \subseteq \tau_1'$ in $\mathcal{H}_0$. Then note that $h_1 \setminus A$ must be contained in some maximal hyperedge $h'$ in $E(\mathcal{H}_0)$ such that $H(h') \cap \tau_1' \neq \emptyset$.

Moreover, recall that variables in $A$ are constants. Hence $\psi_{h_1}$ must appear in some factor in the factorization of $f$ according to $\mathcal{H}_0$. Thus it follows that every probability density $f$ that factorizes according to $\mathcal{H}_1$ also factorizes according to $\mathcal{H}_0$. On the other hand, it is not hard to see that for every $\tau' \in V(D_0)$ and every hyperedge $h'$ in $(\mathcal{H}_0[\tau')]^*$, $h'$ is contained in some maximal hyperedge $h$ in $(\mathcal{H}_1[\tau])^*$ for some $\tau \in V(D_1)$. Hence we can conclude that $(\mathcal{H}_1, A)$ and $(\mathcal{H}_0, A)$ admit the same factorization decomposition. The above argument also works for $\mathcal{H}_2$ and $\mathcal{H}_0$. Thus, $(\mathcal{H}_1, A)$ and $(\mathcal{H}_2, A)$ admit the same factorization decomposition.

We now present a graphical procedure (call it redirection procedure) for modeling intervention in Bayesian hypergraph. Let $\mathcal{H}$ be a DAH and $D$ be the canonical DAG of the chain components of $\mathcal{H}$. Suppose a set of variables $x_A$ is set by intervention. We then modify $\mathcal{H}$ as follows: for each hyperedge $h \in E(\mathcal{H})$ such as $S = H(h) \cap A \neq \emptyset$, replace the hyperedge $h$ by $h' = (T(h) \cup S, H(h) \setminus S)$. If a hyperedge has empty set as its head, delete that hyperedge. Call the resulting hypergraph $\hat{\mathcal{H}}_A$. We will show that the factorization according to $\hat{\mathcal{H}}_A$ is consistent with (12).

Theorem 9 Let $\mathcal{H}$ be a Bayesian hypergraph and $\{\tau : \tau \in D\}$ be its chain components. Given an intervened set of variables $x_A$, let $\hat{\mathcal{H}}_A$ be the DAH obtained from $\mathcal{H}$ by replacing each hyperedge $h \in E(\mathcal{H})$ satisfying $S = H(h) \cap A \neq \emptyset$ by the hyperedge $h' = (T(h) \cup S, H(h) \setminus S)$ and removing hyperedges with empty head. Then $(\mathcal{H}, A)$ and $(\hat{\mathcal{H}}, A)$ admit the same factorization decomposition.

Proof This is a corollary of Theorem 8 since performing the operations (i)(ii)(iii) in the definition of factorization-equivalence of DAH to $\mathcal{H}$ and $\hat{\mathcal{H}}$ results in the same DAH. □
Example 2 Let $G$ be a chain graph as shown in Fig. 13a and $\mathcal{H}$ be the canonical LWF Bayesian hypergraph of $G$ as shown in Fig. 13b, constructed based on the procedure in Section 2.4. $\mathcal{H}$ has two directed hyperedges $\{(a, \{c, d\})\}$ and $\{(a, b), \{d, e\}\}$. Applying the redirection procedure for intervention in Bayesian hypergraphs leads to the Bayesian hypergraph $\hat{\mathcal{H}}$ in Fig. 13c. We show that using (9) and (10) for Fig. 13a leads to the same result as if one uses the factorization formula for the Bayesian hypergraph in Fig. 13c.

First, we compute $f(x||x_c)$ for chain graph in Fig. 13a. Based on (9) we have:

$$f(x||x_c) = f(x_a)f(x_b)f(x_{de} | x_{abc0}),$$

as the effect of the atomic intervention $do(X_c = c_0)$. Then, using (10) gives:

$$f(x||x_c) = f(x_a)f(x_b)\frac{\psi_{ac0d}(x)\psi_{abde}(x)}{\sum_{d,e} \psi_{ac0d}(x)\psi_{abde}(x)}.$$  \hspace{1cm} (13)
Now, we compute $f(x)$ for Bayesian hypergraph in Fig. 13c. Using (6) gives:

$$f(x || x_c) = f(x_a)f(x_b)f(x_d | x_{abc0}).$$

Applying formula (7) gives:

$$f(x || x_c) = f(x_a)f(x_b)f(x_c)\frac{\psi_{acod}(x)\psi_{abde}(x)}{\sum_{d,e} \psi_{acod}(x)\psi_{abde}(x)} \quad (14)$$

Note that $f(x_c) = 1$, when $x_c = c_0$, otherwise $f(x_c) = 0$. As a result, the right side of (13) and (14) are the same.

Remark 10 Figure 14 summarizes all the results in Section 6. Given a chain graph $G$ and its canonical LWF DAH $\mathcal{H}$, Theorem 4 shows that $G$ and $\mathcal{H}$ admit the same factorization decomposition. Suppose a set of variables $A$ is set by intervention. Theorem 5 and 6 show that the the DAH obtained from $G$ by the redirection procedure or deleting the variables in $A$ admit the same factorization decomposition, which is also consistent with the intervention formula introduced in [22]. Similarly, Theorem 8 and 9 show that the DAH obtained from $\mathcal{H}$ by the redirection procedure or shrinking the variables in $A$ admit the same factorization decomposition, which is consistent with a hypergraph analogue of the formula in [22].

7 Conclusion and future work

This paper presents Bayesian hypergraph, a new probabilistic graphical model. We showed that the model generalizes Bayesian networks, Markov networks, and LWF chain graphs, in the following sense: when the shadow of a Bayesian hypergraph is a chain graph, its Markov properties are the same as that of its shadow. We extended the causal interpretation of LWF chain graphs to Bayesian hypergraphs and provided corresponding formulas and two graphical procedures for intervention (as defined in [22]).

Directed acyclic hypergraphs can admit much finer factorizations than chain graphs, thus are more computationally efficient. The Bayesian hypergraph model also allows simpler and more general procedures for factorization as well as intervention. Furthermore, it allows a modeler to express independence of causal influence and other useful patterns, such as Noisy-OR, directly (i.e., graphically), rather than through annotations or the structure of a conditional probability table or function. We conjecture that the greater expressive power of Bayesian hypergraphs can be used to represent other PGMs and plan to explore the conjecture in future work.

Although the Bayesian hypergraph model admits much finer factorizations than the chain graph model, we note that our model does not yet expand the set of independence lists that can be represented by chain graphs. This is due to the fact that the Markov properties of the Bayesian hypergraphs are defined based on the shadow of the Bayesian hypergraph (which is a chain graph). One direction for future work is to design a hypergraph graphical model that admits a much larger set of independence lists than those allowed by chain graphs. Learning the structure and the parameters of Bayesian hypergraphs is another direction for future work. For this purpose, we will need to provide a criterion for Markov equivalence of Bayesian hypergraphs. The success of constraint-based structure learning algorithms for chain graphs leads us to hope that similar techniques would work for learning Bayesian hypergraphs. Of course, one should also explore whether a closed-form decomposable likelihood function can be derived in the discrete finite case.
Acknowledgments This work is primarily supported by Office on Naval Research grant ONR N00014-17-1-2842. The causal interpretation of Bayesian hypergraphs described in Section 6 was presented at the AAAI Spring Symposium “Beyond Curve Fitting: Causation, Counterfactuals, and Imagination-based AI (AAAI-WHY 2019),” Palo Alto, CA, March 25-27, 2019. Comments by reviewers and symposium participants are gratefully acknowledged.

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