Bernoulli **21**(3), 2015, 1467–1493
DOI: 10.3150/14-BEJ611

Standard imsets for undirected and chain graphical models

TAKUYA KASHIMURA[1] and AKIMICHI TAKEMURA[1,2]

[1]*Department of Mathematical Informatics, Graduate School of Information Science and Technology, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan. E-mail: takemura@stat.t.u-tokyo.ac.jp*
[2]*JST, CREST, 5 Sanbancho, Chiyoda-ku, Tokyo, 102-0075, Japan*

We derive standard imsets for undirected graphical models and chain graphical models. Standard imsets for undirected graphical models are described in terms of minimal triangulations for maximal prime subgraphs of the undirected graphs. For describing standard imsets for chain graphical models, we first define a triangulation of a chain graph. We then use the triangulation to generalize our results for the undirected graphs to chain graphs.

Keywords: conditional independence; decomposable graph; maximal prime subgraph; triangulation

1. Introduction

The notion of imsets introduced by Studený [16] provides a very convenient algebraic method for encoding all conditional independence (CI) models which hold under a discrete probability distribution. However, a class of imsets does not satisfy the uniqueness property: a number of different imsets represent the same CI model.

Thus some questions related to the uniqueness property arise [16]. One of them is the task of characterizing equivalent imsets. For example, in the case of classical graphical models [9], their equivalence classes are characterized by Andersson *et al.* [1] and Frydenberg [3] in graphical terms. Studený [14] related a CI model induced by a imset to some face of a special polyhedral cone, and an algorithm for CI inference based on this cone is studied in [2].

Another question is to find a suitable representative for every equivalence class. This is motivated by a practical question about learning CI models (see Section 4.4 in [15] and Section 4 in [22]). As a subproblem of this, explicit expressions of imsets for important classes of graphical models, such as directed acyclic graphical (DAG) models and decomposable models, are given in [16]. Imsets for some chain graphical (CG) models are also known [18]. They are called standard imsets and have attractive simple forms. One of their advantages is that they give a simple method to test whether two graphs have the same CI model. Another advantage is that it provides a translation of graphical models into the framework of imsets. Thus standard imsets offer a new algebraic approach for learning graphical models [7,20].

In this paper, we derive standard imsets for undirected graphical (UG) models and general CG models. Our standard imsets generalize those for DAG models and decomposable models. For UG models, we consider all minimal triangulations of an undirected graph in accordance with maximal prime subgraphs and then use the standard imsets for minimal triangulations (which are

1350-7265

decomposable models) for defining our standard imset. For CG models, we first define a triangulation of a chain graph. We then use the triangulation to generalize our results for undirected graphs to chain graphs.

The organization of the paper is as follows. In Section 2, we summarize basic definitions and known facts on imsets and graphs, including standard imsets for DAG models and decomposable models. In Section 3, we derive standard imsets for UG models. In Section 4, we introduce a notion of triangulation of a chain graph and based on the triangulation we derive standard imsets for CG models. We conclude the paper with some remarks in Section 5.

2. Preliminaries

In this section, we summarize our notation, definitions and relevant preliminary results concerning conditional independence, imsets and graphical models.

2.1. Conditional independence and imsets

First, we set up notation for conditional independence and imsets following Studený [16].

Let N be a finite set of variables and let $\mathcal{P}(N) = \{A\colon\ A \subseteq N\}$ denote the power set of N. For convenience, we write the union $A \cup B$ of subsets of N as AB. A singleton set $\{i\}$ is simply written as i. As usual, $\mathbb{R}$, $\mathbb{Z}$, and $\mathbb{N}$ denote reals, integers and natural numbers, respectively. For pairwise disjoint subsets, $A, B, C \subseteq N$, we write this triplet by $\langle A, B \,|\, C\rangle$, and the set of all disjoint triplets $\langle A, B \,|\, C\rangle$ over N by $\mathcal{T}(N)$. As usual, for a probability distribution P over N, $A \perp\!\!\!\perp B \,|\, C\,[\mathrm{P}]$ denotes the conditional independence statement of variables in A and in B given the variables in C under P. The case $C = \varnothing$ corresponds to the marginal independence of A and B. In this paper, we regard a triplet $\langle A, B \,|\, C\rangle$ as an independence statement. Then the set of conditional independence statements under P is denoted as

$$\mathcal{M}_{\mathrm{P}} = \bigl\{\langle A, B \,|\, C\rangle \in \mathcal{T}(N)\colon\ A \perp\!\!\!\perp B \,|\, C\,[\mathrm{P}]\bigr\}.$$

We call $\mathcal{M}_{\mathrm{P}}$ the *conditional independence model* induced by P.

An *imset* over N is an integer-valued function $u : \mathcal{P}(N) \to \mathbb{Z}$, or alternatively, an element of $\mathbb{Z}^{|\mathcal{P}(N)|} = \mathbb{Z}^{2^{|N|}}$. The identifier δ_A of a set $A \subseteq N$ is defined as

$$\delta_A(B) = \begin{cases} 1, & B = A, \\ 0, & B \neq A,\ B \subseteq N. \end{cases}$$

For a triplet $\langle A, B \,|\, C\rangle \in \mathcal{T}(N)$, a *semi-elementary imset* $u_{\langle A,B \,|\, C\rangle}$ is defined as

$$u_{\langle A,B \,|\, C\rangle} = \delta_{ABC} + \delta_C - \delta_{AC} - \delta_{BC}.$$

If $A = a$ and $B = b$ are singletons, the imset $u_{\langle a,b \,|\, C\rangle}$ is called *elementary*. The set of all elementary imsets is denoted by $\mathcal{E}(N)$. Let $\mathrm{cone}(\mathcal{E}(N)) \subseteq \mathbb{R}^{2^{|N|}}$ be the polyhedral cone generated by all the elementary imsets. It can be shown that every elementary imset is a generator of an extreme ray of the cone($\mathcal{E}(N)$) [14]. A *combinatorial imset* is an imset which can be written as a non-negative integer combination of elementary imsets. The set of all combinatorial imsets is denoted by $\mathcal{C}(N)$. Let

$$\mathcal{S}(N) = \mathrm{cone}\big(\mathcal{E}(N)\big) \cap \mathbb{Z}^{|\mathcal{P}(N)|}.$$

An element of $\mathcal{S}(N)$ is called a *structural imset*. Note that $\mathcal{C}(N) \subseteq \mathcal{S}(N)$ by definition, however, it is known that this inclusion is strict for $|N| \geq 5$ [8].

A conditional independence statement induced by a structural imset is defined as follows:

Definition 2.1. *For $u \in \mathcal{S}(N)$ and a triplet $\langle A, B \,|\, C\rangle \in \mathcal{T}(N)$, we define a conditional independence statement with respect to u as*

$$A \perp\!\!\!\perp B \,|\, C\,[u] \quad\Longleftrightarrow\quad \exists k \in \mathbb{N}, \qquad k \cdot u - u_{\langle A,B\,|\,C\rangle} \in \mathcal{S}(N).$$

The independence model induced by u is denoted by

$$\mathcal{M}_u = \big\{\langle A, B \,|\, C\rangle \in \mathcal{T}(N)\colon\ A \perp\!\!\!\perp B \,|\, C\,[u]\big\}.$$

It can be shown that the structure of conditional independence models induced by structural imsets depends only on the face lattice of cone($\mathcal{E}(N)$), not on each imset [14]. Therefore implications of conditional independence models induced by imsets correspond to those of faces of cone($\mathcal{E}(N)$). The next lemma, which is very useful for our proofs in later sections, follows from this fact.

Lemma 2.2 (Studený [16]). *For $u, u' \in \mathcal{S}(N)$,*

$$\mathcal{M}_{u'} \subseteq \mathcal{M}_u \quad\Longleftrightarrow\quad \exists k \in \mathbb{N}, \qquad k \cdot u - u' \in \mathcal{S}(N).$$

The method of imsets is very powerful, because conditional independence models induced by discrete probability measures are always represented by structural imsets.

Theorem 2.3 (Studený [16]). *For every discrete probability measure* P *over N, there exists a structural imset $u \in \mathcal{S}(N)$ such that $\mathcal{M}_u = \mathcal{M}_{\mathrm{P}}$.*

2.2. Graphs and graphical models

Here we summarize relevant facts on graphs and graphical models following Lauritzen [9], Studený, Roverato and Štěpánová [18], Leimer [11], and Hara and Takemura [5].

Throughout this paper, we consider a simple graph $G = (V(G), E(G))$, $V(G) = N$, $E(G) \subseteq N \times N \setminus \{(a, a)\colon a \in N\}$. An edge $(a, b) \in E(G)$ is *undirected* if $(b, a) \in E(G)$. We denote an undirected edge by $a - b$. If $(b, a) \notin E(G)$, we call (a, b) *directed* and denote it by $a \to b$. An *undirected graph* (UG) contains only undirected edges, while a directed graph contains only directed ones. The *underlying graph* of a graph G is the undirected graph obtained from G by replacing every directed edge with an undirected one. For a subset $S \subseteq N$, G_S denotes the subgraph of G induced by S. In this paper when we refer to a subgraph of G, it is induced by some subset of N. A graph is *complete* if all vertices are joined by an edge. A subset $K \subseteq N$ is a *clique* if G_K is complete. In particular, an empty set $K = \varnothing$ is a clique. A clique K is maximal if no proper superset $K' \supset K$ is a clique in G. $\mathcal{K}_G$ denotes the set of maximal cliques of G.

Two vertices $a, b \in N$ are adjacent if $(a, b) \in E(G)$ or $(b, a) \in E(G)$. If $a \to b$, then a is a *parent* of b and b is a *child* of a. For a vertex $c \in N$, we denote the set of parents and the set of children of c in G by $\mathrm{pa}_G(c)$ and $\mathrm{ch}_G(c)$, respectively. For a subset $C \subseteq N$, let $\mathrm{pa}_G(C) = \bigcup_{c\in C} \mathrm{pa}_G(c) \setminus C$ and $\mathrm{ch}_G(C) = \bigcup_{c\in C} \mathrm{ch}_G(c) \setminus C$. We will omit the subscript G if it is obvious from the context.

A *path* of length $k \ge 0$ from a to b is a sequence $a = c_1, \dots, c_{k+1} = b$ of distinct vertices such that $(c_i, c_{i+1}) \in E(G)$ for $i = 1, \dots, k$. If a path contains only undirected edges, it is an undirected path and otherwise (i.e., it contains at least one directed edge) directed. Note that some authors use the term "semi-directed" instead of "directed". A vertex $a \in N$ is an *ancestor* of $b \in N$ if there exists a path from a to b. Let $\mathrm{an}_G(a)$ be the set of all ancestors of a. The ancestral set $\mathrm{an}_G(C)$ of a subset $C \subseteq N$ is defined as $\mathrm{an}_G(C) = \bigcup_{c\in C} \mathrm{an}_G(c)$. Note that $C \subseteq \mathrm{an}_G(C)$. Let $c_1, \dots, c_k$ be a path with $(c_k, c_1) \in E(G)$. Then we call the sequence $c_1, \dots, c_k, c_1$ a *cycle* of length k. Analogously to paths, a cycle is undirected if it contains only undirected edges, otherwise directed. A *directed acyclic graph* (DAG) is a directed graph containing no directed cycles.

A subset $C \subseteq N$ is said to be *connected* if there exists an undirected path from a to b for all $a, b \in C$ in the subgraph G_C. A *connectivity component of* G is a maximal connected subset in G with respect to set inclusion. The connectivity components in G form a partition of N. A *chain graph* (CG) G is a graph whose connectivity components $C_1, \dots, C_m$ can be ordered such that if $a \to b \in E(G)$ with $a \in C_i, b \in C_j$, then $i < j$. Equivalently, a chain graph is defined as a graph containing no directed cycles. The connectivity components of a chain graph are called *chain components*. The set of chain components of a chain graph G is denoted by $\mathcal{C}_G$. The chain components are most easily found by removing all directed edges from G before taking connectivity components. Both undirected graphs and directed acyclic graphs are chain graphs. In fact, a chain graph is undirected provided $m = 1$, and directed acyclic if each chain component contains only one vertex. Suppose two chain graphs G, H have the same underlying graph. Then we say H is *larger* than or equal to G if $a \to b$ in H implies $a \to b$ in G. In this case, we write $H \ge G$. From the definition, H has more undirected edges than G if H is larger than G.

We now discuss maximal prime subgraphs of an undirected graph G. A non-empty subset $\varnothing \neq S \subset N$ is a *separator* if the set $N \setminus S$ is not connected. $S = \varnothing$ is a separator if (and only if) G is not connected. A separator S is a *clique separator* if S is a clique. For two vertices $u, v \in N$ with $u - v \notin E(G)$, a set S is called a (u, v)*-separator* if u and v belong to different components of $G_{N\setminus S}$. A *minimal vertex separator* is a minimal (u, v)-separator for some $u, v \in N$ with respect to set inclusion relative to all (u, v)-separators. Note that a minimal vertex separator for some u, v maybe a strict subset of a minimal vertex separator for another pair. For $\langle A, B \mid C\rangle \in \mathcal{T}(N)$, we say that A and B are separated by C if C is (a, b)-separator for all $a \in A$ and $b \in B$.

A graph G is *prime* if G has no clique separators. Let G_V, $V \subseteq N$, be prime. Then G_V is a *maximal prime subgraph* (mp-subgraph) and V is a *maximal prime component* (mp-component) of G, if there is no proper superset $V' \supset V$ such that $G_{V'}$ is prime. From Lemma 2.1(iii) of [11], if V_1 and V_2 are distinct prime components then $G_{V_1\cap V_2}$ is complete. The set of mp-components of G is denoted by $\mathcal{V}_G$. There exists an order $V_1, \dots, V_m$, $m = |\mathcal{V}_G|$, of $\mathcal{V}_G$ such that

$$\forall i \in \{2, \dots, m\}, \exists k \in \{1, \dots, i-1\}, \qquad S_i \equiv V_i \cap \bigcup_{j<i} V_j \subseteq V_k.$$

This sequence is said to be *D-ordered*, or alternatively, to have a *running intersection property* (RIP) [9]. For each i, S_i is a clique minimal vertex separator. An important fact about RIP is that for each i, $\bigcup_{j<i} V_j \setminus S_i$ and $V_i \setminus S_i$ are separated by S_i in $H_{V_1 \cup \dots \cup V_i}$ by applying Corollary 2.7(i) of [11] recursively. Define $\mathcal{S}_G = \{S_2, \dots, S_m\}$. Then $\mathcal{S}_G$ is the set of all clique minimal vertex separators in G. Moreover, the number of $S \in \mathcal{S}_G$ which appears among $S_2, \dots, S_m$ may be more than one. This number is called the *multiplicity* of S in G, and written as $\nu_G(S)$. For any undirected graph G, $\mathcal{V}_G, \mathcal{S}_G$ and $\{\nu_G(S)\}_{S \in \mathcal{S}_G}$ are uniquely defined [11].

In graphical models, the class of models induced by *decomposable graphs* are well studied, because it has many good properties. There are several equivalent definitions of decomposable graphs. One of them is based on the decomposability of graphs. For an undirected graph G and a triplet $\langle A, B \mid C \rangle$ with $N = A \cup B \cup C$, we say that $\langle A, B \mid C \rangle$ *decomposes G into the subgraphs G_{AC} and G_{BC}* if C is a clique and separates A and B. The decomposition is proper if $A, B \neq \varnothing$. An undirected graph G is decomposable if it is complete or there exists $\langle A, B \mid C \rangle$ which properly decomposes G into decomposable subgraphs G_{AC} and G_{BC}. Decomposable graphs are characterized in terms of mp-subgraphs by Leimer [11]. An undirected graph G is decomposable if and only if all mp-components of G are cliques. Furthermore, for every undirected graph G with mp-components $V_1, \dots, V_m \in \mathcal{V}_G$, there exists a decomposable graph G' such that $V_1, \dots, V_m$ are maximal cliques of G'. The graph G' is obtained by adding edges in such a way that $V_1, \dots, V_m$ are cliques.

Another equivalent definition is a *chordal graph*, or alternatively *triangulated graph*. An undirected graph is chordal if every cycle of length more than or equal to four has a chord, that is, an edge between two non-consecutive vertices of the cycle. An undirected graph is chordal if and only of it is decomposable [9].

2.3. Conditional independence models induced by graphs

Here we summarize known facts on conditional independence models induced by graphs.

For directed acyclic graphs, there are two equivalent separation criteria *d-separation* [13,21] and *moralization* [10]. However we omit their details because we do not need them in this paper. For a triplet $\langle A, B \mid C \rangle \in \mathcal{T}(N)$, we write $A \perp\!\!\!\perp B \mid C\,[G]$ if A and B are separated given C by these criteria. Every directed acyclic graph G induces the formal independence model

$$\mathcal{M}_G = \{\langle A, B \mid C \rangle \in \mathcal{T}(N) \colon A \perp\!\!\!\perp B \mid C\,[G]\}, \tag{1}$$

which we call a *DAG model*. A probability measure P over N is *Markovian* with respect to a directed acyclic graph G if $\mathcal{M}_G \subseteq \mathcal{M}_{\mathrm{P}}$ and *perfectly Markovian* if the converse inclusion also holds.

For an undirected graph G and $\langle A, B \mid C \rangle \in \mathcal{T}(N)$, we have $A \perp\!\!\!\perp B \mid C\,[G]$ if A and B are separated by C in G [9,13]. An *UG model* $\mathcal{M}_G$ is again defined by (1). The definitions of a Markovian and a perfectly Markovian measure are analogous to the case of DAG models. It is known that a perfectly Markovian discrete measure exists for every undirected graph [4]. A decomposable model is defined as an independence model induced by a decomposable graph. A decomposable model is simultaneously an UG model and a DAG model.

Finally, we discuss chain graphs. A popular separation criterion for chain graphs is *moralization* [3]. For a chain graph G and a triplet $\langle A, B \mid C\rangle \in \mathcal{T}(N)$, let $H = G_{\mathrm{an}(ABC)}$. A *moral graph* H^{mor} of H is the undirected graph obtained by adding an undirected edge $a - b$ to the underlying graph of H whenever there is a chain component $C' \in \mathcal{C}_H$ such that $a, b \in \mathrm{pa}(C')$ and a and b are not adjacent in H. We define $A \perp\!\!\!\perp B \mid C\,[G]$ if $A \perp\!\!\!\perp B \mid C\,[H^{\mathrm{mor}}]$ holds. The definitions of a *CG model*, a Markovian measure and a perfectly Markovian measure are analogous to the other graphs. It is known that a perfectly Markovian discrete measure exists for every chain graph [17].

An important concept about chain graphs is the equivalence for graphs [16]. We say that G and H are *equivalent* if $\mathcal{M}_G = \mathcal{M}_H$. Equivalent chain graphs are characterized by Frydenberg [3]. A *complex* in G is a subgraph of G of the form $c_0 \to c_1 - \cdots - c_k \leftarrow c_{k+1}$, $k \geq 1$, and no other edges between $c_0, c_1, \ldots, c_{k+1}$ exist in G.

Theorem 2.4 (Frydenberg [3]). *Two chain graphs are equivalent if and only if their underlying graphs coincide and they have the same complexes.*

A more important fact is that every equivalence class has one distinguished representative.

Theorem 2.5 (Frydenberg [3]). *Every equivalence class $\mathcal{H}$ of chain graphs has the largest element $H_\infty \in \mathcal{H}$ such that $H \leq H_\infty$ for all $H \in \mathcal{H}$.*

2.4. Standard imsets for directed acyclic graphs and decomposable graphs

Let G be a directed acyclic graph. A *standard imset for G* is defined as follows [16]:

$$u_G = \delta_N - \delta_\varnothing + \sum_{i \in N} \{\delta_{\mathrm{pa}(i)} - \delta_{\{i\} \cup \mathrm{pa}(i)}\}. \tag{2}$$

This standard imset is a unique representative for equivalent graphs.

Lemma 2.6 (Studený [16]). *Let G be a directed acyclic graph. Then $u_G \in \mathcal{C}(N)$ and $\mathcal{M}_G = \mathcal{M}_{u_G}$ hold. Moreover, for a directed acyclic graph G', $\mathcal{M}_G = \mathcal{M}_{G'}$ if and only if $u_G = u_{G'}$.*

A standard imset for a decomposable graph H is defined by the sets of maximal cliques and clique minimal vertex separators in H [16]:

$$u_H = \delta_N - \sum_{K \in \mathcal{K}_H} \delta_K + \sum_{S \in \mathcal{S}_H} \nu_H(S) \cdot \delta_S. \tag{3}$$

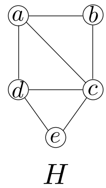

Figure 1. A decomposable graph H.

Example 2.7. Put $N = \{a, b, c, d, e\}$ and consider the decomposable graph H shown in Figure 1. The sets of maximal cliques and clique minimal vertex separators in H are $\mathcal{K}_H = \{abc, acd, cde\}$ and $\mathcal{S}_H = \{ac, cd\}$ (with multiplicities $\nu_H(ac) = \nu_H(cd) = 1$). Then the standard imset for H is

$$
\begin{aligned}
u_H &= \delta_{abcde} - \delta_{abc} - \delta_{acd} - \delta_{cde} + \delta_{ac} + \delta_{cd} \\
&= u_{\langle b,e \,|\, acd\rangle} + u_{\langle a,e \,|\, cd\rangle} + u_{\langle b,d \,|\, ac\rangle}.
\end{aligned}
$$

For a complete graph, its standard imset is the zero imset.

Since decomposable models can be viewed as DAG models, their imsets (2) and (3) lead to the same imset.

Lemma 2.8 (Studený [16]). *For every decomposable graph H, there exists a directed acyclic graph G such that $\mathcal{M}_G = \mathcal{M}_H$ and $u_G = u_H$.*

This implies that for a decomposable graph H, we have $u_H \in \mathcal{C}(N)$ and $\mathcal{M}_H = \mathcal{M}_{u_H}$ from Lemma 2.6.

As discussed in Section 1, these imsets for directed acyclic and decomposable graphs are not the only combinatorial ones representing their graphical models. However they are the simplest, "standard" representations [2]. A standard imset gives a simpler criterion of testing a conditional independence statement than other imsets.

Lemma 2.9 (Bouckaert *et al.* [2]). *For a directed acyclic (resp. decomposable) graph G, $\langle A, B \,|\, C\rangle \in \mathcal{M}_G$ if and only if $u_G - u_{\langle A,B \,|\, C\rangle} \in \mathcal{C}(N)$, which is also equivalent to $u_G - u_{\langle A,B \,|\, C\rangle} \in \mathcal{S}(N)$, where u_G is the standard imset in (2) or (3).*

3. Standard imsets for general undirected graphs

In this section, we derive imsets for general undirected graphs. Our construction is based on a concept of a triangulation.

3.1. General undirected graphical models

For generalizing the result of decomposable graphs to general undirected graphs, consider constructing a decomposable graph from a given undirected graph by adding edges. The resulting graph is called a *triangulation* of the input graph [6]. A triangulation G' of G is minimal if there is no triangulation G'' of G such that $E(G'') \subset E(G')$. From Lemma 2.21 of [9], it follows that G' is a minimal triangulation of G if and only if removing any edge in $E(G') \setminus E(G)$ from G' makes the resulting graph non-decomposable. In general, there are many minimal triangulations of a graph. In the following, we denote the set of all minimal triangulations of G by $\mathfrak{T}(G)$. As for separations of an input graph and a minimal triangulation, the following lemma holds.

Lemma 3.1. *For every undirected graph H and a triplet $\langle A, B \mid C\rangle \in \mathcal{M}_H$, there exists a minimal triangulation H' of H such that $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$.*

Proof. It suffices to show the existence of a triangulation H' such that $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$. In fact, if H' is not minimal, we can obtain a minimal triangulation by removing edges from H', because removing edges does not destroy the relation $A \perp\!\!\!\perp B \mid C$.

We construct a desired triangulation as follows (see Figure 2). Let $N = A' \cup B' \cup C'$ be a partition of the vertex set such that

$$A' = \{i \in N\colon\ i \text{ is connected with } A \text{ in } H_{N\setminus C}\},$$
$$C' = C \quad \text{and} \quad B' = N \setminus A'C'.$$

Construct the graph H' by adding edges so that $H'_{A'C'}$ and $H'_{B'C'}$ are complete. This H' is clearly decomposable, and hence, a triangulation of H. From the construction, A' and B' are not connected to each other in $H'_{N\setminus C'}$. Thus $A \subseteq A'$ and $B \subseteq B'$ are not connected to each other in $H'_{N\setminus C}$, which means $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$. □

For a general undirected graph H, we can obtain an imset representing this UG model by using all minimal triangulations. The following theorem is the first main result of this paper.

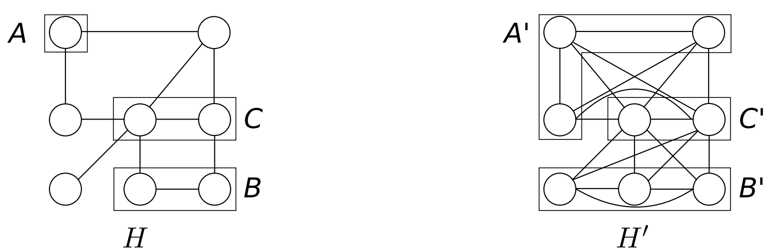

Figure 2. A construction of H' from an undirected graph H in Lemma 3.1.

Theorem 3.2. *Let H be an undirected graph. Put*

$$v_H = \sum_{H' \in \mathfrak{T}(H)} u_{H'}, \tag{4}$$

where $\mathfrak{T}(H)$ is the set of minimal triangulations of H and $u_{H'}$ for $H' \in \mathfrak{T}(H)$ are defined by (3). *Then $v_H \in \mathcal{C}(N)$ and $\mathcal{M}_H = \mathcal{M}_{v_H}$.*

Proof. Since the class of combinatorial imsets is closed under the addition, it is evident that the imset v_H is combinatorial.

For every undirected graph H, there exists a discrete probability measure P with $\mathcal{M}_{\mathrm{P}} = \mathcal{M}_H$ [4]. Moreover, Theorem 2.3 implies that there is a structural imset $w \in \mathcal{S}(N)$ such that $\mathcal{M}_{\mathrm{P}} = \mathcal{M}_w$. Then, for $H' \in \mathfrak{T}(H)$, we have

$$\mathcal{M}_{u_{H'}} = \mathcal{M}_{H'} \subseteq \mathcal{M}_H = \mathcal{M}_{\mathrm{P}} = \mathcal{M}_w,$$

which implies $k_{H'} \cdot w - u_{H'} \in \mathcal{S}(N)$ for some $k_{H'} \in \mathbb{N}$ from Lemma 2.2. Therefore, putting $k = \sum_{H' \in \mathfrak{T}(H)} k_{H'}$, it follows that $k \cdot w - v_H \in \mathcal{S}(N)$. That is, $\mathcal{M}_{v_H} \subseteq \mathcal{M}_w = \mathcal{M}_H$.

Conversely, for every $\langle A, B \mid C \rangle \in \mathcal{M}_H$, there exists $H' \in \mathfrak{T}(H)$ such that $\langle A, B \mid C \rangle \in \mathcal{M}_{H'}$ from Lemma 3.1. Thus, $u_{H'} - u_{\langle A,B \mid C \rangle} \in \mathcal{S}(N)$ from Lemma 2.9. Hence, we have

$$v_H - u_{\langle A,B \mid C \rangle} = \sum_{H'' \in \mathfrak{T}(H) \setminus H'} u_{H''} + (u_{H'} - u_{\langle A,B \mid C \rangle}) \in \mathcal{S}(N),$$

which implies $\langle A, B \mid C \rangle \in \mathcal{M}_{v_H}$. □

The imset v_H in (4) is a generalization of the case of decomposable graphs, because for a decomposable graph H, the set of minimal triangulations contains H only. An example of this imset is given in the next section.

3.2. Some consideration toward a definition of standard imsets for general undirected graphs

The imset defined in the last section through all minimal triangulations has 'extra' additional parts as shown in the following example.

Example 3.3. Put $N = \{a, b, c, d, e\}$. Consider the graph H in Figure 3 and its minimal triangulations H_1, H_2. Then the imset v_H in (4) is

$$\begin{aligned} v_H &= u_{H_1} + u_{H_2} \\ &= (\delta_N - \delta_{abd} - \delta_{bcd} - \delta_{cde} + \delta_{bd} + \delta_{cd}) \\ &\quad + (\delta_N - \delta_{abc} - \delta_{acd} - \delta_{cde} + \delta_{ac} + \delta_{cd}) \\ &= (u_{\langle ab,e \mid cd \rangle} + u_{\langle a,c \mid bd \rangle}) + (u_{\langle ab,e \mid cd \rangle} + u_{\langle b,d \mid ac \rangle}) \\ &= 2 \cdot u_{\langle ab,e \mid cd \rangle} + u_{\langle a,c \mid bd \rangle} + u_{\langle b,d \mid ac \rangle}. \end{aligned}$$

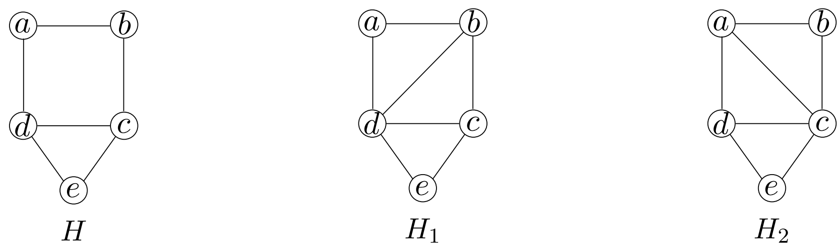

Figure 3. Non-decomposable graph H and its minimal triangulations H_1, H_2.

It can be seen that $ab \perp\!\!\!\perp e \mid cd$ holds in both H_1 and H_2. This is expressed as the coefficient 2 of $u_{\langle ab,e \mid cd\rangle}$. Now consider an imset u_H with this coefficient 1, that is,

$$u_H = u_{\langle ab,e \mid cd\rangle} + u_{\langle a,c \mid bd\rangle} + u_{\langle b,d \mid ac\rangle}. \tag{5}$$

From Lemma 3.1, $\langle A, B \mid C\rangle \in \mathcal{M}_H$ is equivalent to $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$ for some minimal triangulation H' of H. Hence, for example, letting $\langle A, B \mid C\rangle \in \mathcal{M}_{H_1}$, we have

$$\begin{aligned} & u_{H_1} - u_{\langle A,B \mid C\rangle} \in \mathcal{S}(N) \\ \implies \quad & u_{H_1} + u_{\langle b,d \mid ac\rangle} - u_{\langle A,B \mid C\rangle} \in \mathcal{S}(N) \\ \iff \quad & u_H - u_{\langle A,B \mid C\rangle} \in \mathcal{S}(N) \\ \implies \quad & \langle A, B \mid C\rangle \in \mathcal{M}_{u_H}. \end{aligned}$$

Since the same result holds for $\langle A, B \mid C\rangle \in \mathcal{M}_{H_2}$, we have $\mathcal{M}_{v_H} = \mathcal{M}_H \subseteq \mathcal{M}_{u_H}$. Also, since $v_H - u_H = u_{\langle ab,e \mid cd\rangle} \in \mathcal{S}(N)$, we have $\mathcal{M}_{v_H} \supseteq \mathcal{M}_{u_H}$ from Lemma 2.2. Thus $\mathcal{M}_{v_H} = \mathcal{M}_{u_H} = \mathcal{M}_H$.

Note that a graph such as the one in Figure 4 has an exponential number of minimal triangulations, which makes infeasible to calculate v_H in (4) actually.

The above examples suggest that it suffices to use only minimal triangulations of each mp-subgraph and not of the whole of the graph. In particular, the new imset (5) in Example 3.3 seems to be defined as follows: First, consider the graph obtained by adding edges to the input graph in such a way that all mp-subgraphs are complete (Figure 5(a)), and consider its standard

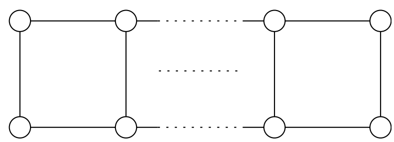

Figure 4. A graph with an exponential number of minimal triangulations.

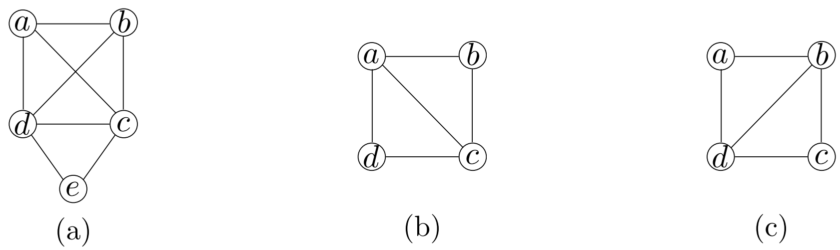

Figure 5. Mp-subgraphs in the new imset.

imset ($u_{\langle ab,e\,|\,cd\rangle}$). Next, for each mp-subgraph which is not complete, consider their minimal triangulations (Figure 5(b), (c)) and their standard imsets ($u_{\langle a,c\,|\,bd\rangle}, u_{\langle b,d\,|\,ac\rangle}$). We show in the following sections that this idea is correct.

3.3. Minimal triangulations and mp-subgraphs

We show in this section that all minimal triangulations for an undirected graph are obtained by computing minimal triangulations for each mp-subgraph.

The following facts give the way of adding edges to obtain a minimal triangulation:

Lemma 3.4 (Ohtsuki *et al.* [12]). *A triangulation H' of an undirected graph H is minimal if and only if for each $u - v$ added by this triangulation, no (u, v)-separators of H is a clique in H'.*

Lemma 3.5. *For an ordering $V_1, \dots, V_m$ of mp-components of an undirected graph H satisfying RIP, $\bigcup_{k<i} V_k \setminus S_i$ and $V_i \setminus S_i$ are separated by S_i in the whole graph H for each i.*

Proof. From Corollary 2.7(i) of [11], $\bigcup_{k<i} V_k \setminus S_i$ and $V_i \setminus S_i$ are separated by S_i in $H_{V_1\cup\cdots\cup V_i}$ for each i. For $i = m$, the desired conclusion already holds. Thus we show in the case of $i < m$. Suppose that there exists $p > i$ such that there exists a path from some vertex $a \in \bigcup_{k<i} V_k \setminus S_i$ to some vertex $b \in V_i \setminus S_i$ in $H_{V_1\cup\cdots\cup V_p\setminus S_i}$. Let $p > i$ be the minimum number with this property. Choose a vertex $x \in V_p \setminus S_p$ of the path. Since $\bigcup_{k<p} V_k \setminus S_p$ and $V_p \setminus S_p$ are separated by S_p in $H_{V_1\cup\cdots\cup V_p}$ and x leads to $a, b \in \bigcup_{k<p} V_k$, the path must contain vertices of S_p. Since S_p is a clique and is contained in V_q for some $1 \le q < p$ from the definition of RIP, there also exists a path from a to b in $H_{V_1\cup\cdots\cup V_{p-1}\setminus S_i}$. However this contradicts minimality of p, and hence the desired conclusion holds. $\square$

From these lemmas, we have the following result about the relation between mp-subgraphs and minimal triangulations of a graph.

Lemma 3.6. *For an undirected graph H, a graph H' obtained by a minimal triangulation of each mp-subgraph is a minimal triangulation of H. Conversely, all minimal triangulations of H are obtained in this way.*

Proof. Let w be a cycle $a_1, \dots, a_n, a_{n+1} = a_1, n \geq 4$, of length more than or equal to 4 in H'. First, consider the case that w is not contained in one mp-component. Let V_i be the last mp-component in an ordering $V_1, \dots, V_m$ satisfying RIP such that w intersects $V_i \setminus S_i$. Choose a vertex x of w such that $x \in V_i \setminus S_i$. Since no edge in H' outside mp-components is added, two (distinct) branches of w out of x lead to distinct elements $y, z \in S_i$. Since S_i is a clique, y and z are adjacent in H, which means that the cycle w has a chord. We next consider the case $\{a_1, \dots, a_n\} \subseteq V$ for some mp-component $V \in \mathcal{V}_H$ in H. Since H'_V is decomposable, the cycle w also has a chord in H'. Therefore H' is decomposable. Moreover, from an equivalent characterization of a minimal triangulation, it follows that H' is minimal since removing one edge from H' makes it non-decomposable. Thus the first statement is proved.

To prove the converse, consider an edge $u - v$ added by a triangulation H' of H. Let $u \in V_i \setminus S_j, v \in V_j \setminus S_j$ and $i < j$. Then by Lemma 3.5 $u \in \bigcup_{k<j} V_k \setminus S_j$ and $v \in V_j \setminus S_j$ are separated by S_j in H. Since S_j is also a clique in H', H' is not a minimal triangulation from Lemma 3.4. □

3.4. Definition and properties of standard imsets for undirected graphs

We define a standard imset for an undirected graph using Lemma 3.6.

Definition 3.7. *For an undirected graph H, a standard imset u_H for H is defined as*

$$u_H = \delta_N - \sum_{V \in \mathcal{V}_H} \delta_V + \sum_{S \in \mathcal{S}_H} \nu_H(S) \cdot \delta_S + \sum_{V \in \mathcal{V}_H} \sum_{G \in \mathfrak{T}(H_V)} u_G, \tag{6}$$

where for each $G \in \mathfrak{T}(H_V)$, $V \in \mathcal{V}_H$, u_G is the standard imset given by (3):

$$u_G = \delta_V - \sum_{K \in \mathcal{K}_G} \delta_K + \sum_{S \in \mathcal{S}_G} \nu_G(S) \cdot \delta_S.$$

Note that, if H is decomposable, the last term of u_H vanishes because all mp-components are cliques [11]. Thus this imset coincides with (3).

We show that this imset represents an UG model.

Theorem 3.8. *For an undirected graph H, define u_H as* (6). *Then $u_H \in \mathcal{C}(N)$ and $\mathcal{M}_H = \mathcal{M}_{u_H}$.*

Proof. The first three terms of (6) correspond to the standard imset for the decomposable graph such that all $V \in \mathcal{V}_H$ are cliques. Thus, this imset is combinatorial, and hence, $u_H \in \mathcal{C}(N)$.

Let H' be a minimal triangulation of H. Since a minimal triangulation is done in each mp-subgraph from Lemma 3.6, the following relations hold:

$$\begin{gathered}\mathcal{K}_{H'} = \bigcup_{V\in\mathcal{V}_H} \mathcal{K}_{H'_V}, \qquad \mathcal{S}_{H'} = \mathcal{S}_H \cup \Bigl(\bigcup_{V\in\mathcal{V}_H} \mathcal{S}_{H'_V}\Bigr), \\ \mathcal{K}_{H'_{V_1}} \cap \mathcal{K}_{H'_{V_2}} = \varnothing, \qquad \mathcal{S}_{H'_{V_1}} \cap \mathcal{S}_{H'_{V_2}} = \varnothing, \qquad \forall V_1, V_2 \in \mathcal{V}_H, V_1 \neq V_2, \\ \mathcal{S}_H \cap \mathcal{S}_{H'_V} = \varnothing, \qquad \forall V \in \mathcal{V}_H, \qquad \nu_H(S) = \nu_{H'}(S), \qquad \forall S \in \mathcal{S}_H.\end{gathered}$$

To verify the disjointness $\mathcal{S}_H \cap \mathcal{S}_{H'_V} = \varnothing$, we note the fact that for every mp-component V, the elements of $\mathcal{S}_{H'_V}$ are not cliques in H_V, because otherwise $S \in \mathcal{S}_{H'_V}$, being a separator in H'_V, is a clique separator in H_V, which contradicts the primeness of H_V. Now consider RIP ordering $V_1, \dots, V_m$ of mp-components of H. For the last mp-component V_m, the elements of $\mathcal{S}_{H'_{V_m}}$ are not cliques in H and intersect $V_m \setminus S_m$. Since elements of $\mathcal{S}_H$ are cliques in H and since the elements of $\mathcal{S}_{H'_{V_i}}$ for $i < m$ do not intersect $V_m \setminus S_m$, the class $\mathcal{S}_{H'_{V_m}}$ is disjoint with those other ones. By decreasing induction on m, the disjointness $\mathcal{S}_H \cap \mathcal{S}_{H'_V} = \varnothing$ holds.

Hence a standard imset for the decomposable graph H' given by (3) is

$$\begin{aligned} u_{H'} &= \delta_N - \sum_{K\in\mathcal{K}_{H'}} \delta_K + \sum_{S\in\mathcal{S}_{H'}} \nu_{H'}(S)\cdot\delta_S \\ &= \delta_N - \sum_{V\in\mathcal{V}_H}\sum_{K\in\mathcal{K}_{H'_V}} \delta_K + \sum_{S\in\mathcal{S}_H} \nu_H(S)\cdot\delta_S + \sum_{V\in\mathcal{V}_H}\sum_{S\in\mathcal{S}_{H'_V}} \nu_{H'}(S)\cdot\delta_S \\ &= \delta_N - \sum_{V\in\mathcal{V}_H} \delta_V + \sum_{S\in\mathcal{S}_H} \nu_H(S)\cdot\delta_S \\ &\quad + \sum_{V\in\mathcal{V}_H}\Bigl\{\delta_V - \sum_{K\in\mathcal{K}_{H'_V}} \delta_K + \sum_{S\in\mathcal{S}_{H'_V}} \nu_{H'_V}(S)\cdot\delta_S\Bigr\} \\ &= \delta_N - \sum_{V\in\mathcal{V}_H} \delta_V + \sum_{S\in\mathcal{S}_H} \nu_H(S)\cdot\delta_S + \sum_{V\in\mathcal{V}_H} u_{H'_V}. \end{aligned} \tag{7}$$

In particular, the comparison with (6) gives $u_H - u_{H'} \in \mathcal{C}(N)$. Let $v_H = \sum_{H'\in\mathfrak{T}(H)} u_{H'}$ given in (4). Then v_H is written as

$$\begin{aligned} v_H &= \sum_{H'\in\mathfrak{T}(H)}\Bigl\{\delta_N - \sum_{V\in\mathcal{V}_H} \delta_V + \sum_{S\in\mathcal{S}_H} \nu_H(S)\cdot\delta_S + \sum_{V\in\mathcal{V}_H} u_{H'_V}\Bigr\} \\ &= \bigl|\mathfrak{T}(H)\bigr|\cdot\Bigl\{\delta_N - \sum_{V\in\mathcal{V}_H} \delta_V + \sum_{S\in\mathcal{S}_H} \nu_H(S)\cdot\delta_S\Bigr\} + \sum_{H'\in\mathfrak{T}(H)}\sum_{V\in\mathcal{V}_H} u_{H'_V} \end{aligned}$$

$$= \left|\mathfrak{T}(H)\right| \cdot \left\{\delta_N - \sum_{V \in \mathcal{V}_H} \delta_V + \sum_{S \in \mathcal{S}_H} \nu_H(S) \cdot \delta_S\right\}$$
$$+ \sum_{V \in \mathcal{V}_H} \sum_{G \in \mathfrak{T}(H_V)} n_H(V, G) \cdot u_G,$$

where $n_H(V, G) = |\{H' \in \mathfrak{T}(H)\colon\ H'_V = G\}|$ for $V \in \mathcal{V}_H$ and $G \in \mathfrak{T}(H_V)$, is the number of minimal triangulations $H' \in \mathfrak{T}(H)$ such that $H'_V = G$. Note that u_H in (6) is obtained by replacing the coefficients of the right-hand side by one. Thus, u_H and v_H belong to the relative interior of the same face of cone$(\mathcal{E}(N))$. Hence, we have $\mathcal{M}_{u_H} = \mathcal{M}_{v_H}$, which means $\mathcal{M}_{u_H} = \mathcal{M}_H$ from Theorem 3.2. □

Example 3.9. Consider the graph H in Figure 3 again. The sets of mp-components and clique minimal vertex separators are $\mathcal{V}_H = \{abcd, cde\}$ and $\mathcal{S}_H = \{cd\}$. Since $V_2 = cde$ is a clique, the minimal triangulation of its subgraph H_{V_2} is itself. As for $V_1 = abcd$, the minimal triangulations of H_{V_1} are given in Figure 5(b), (c). Then the standard imset for H in (6) is

$$u_H = \delta_{abcde} - \delta_{abcd} - \delta_{cde} + \delta_{cd}$$
$$+ (\delta_{abcd} - \delta_{abd} - \delta_{bcd} + \delta_{bd}) + (\delta_{abcd} - \delta_{abc} - \delta_{acd} + \delta_{ac})$$
$$= u_{\langle ab,e\,|\,cd\rangle} + u_{\langle a,c\,|\,bd\rangle} + u_{\langle b,d\,|\,ac\rangle},$$

which coincides with (5).

As in the case of directed acyclic graphs and decomposable graphs, our standard imset for an undirected graph provides a simpler criterion.

Corollary 3.10. *For an undirected graph H and every triplet $\langle A, B\,|\,C\rangle \in \mathcal{T}(N)$, the followings are equivalent*:

(i) $\langle A, B\,|\,C\rangle \in \mathcal{M}_H$,
(ii) $u_H - u_{\langle A,B\,|\,C\rangle} \in \mathcal{C}(N)$,
(iii) $u_H - u_{\langle A,B\,|\,C\rangle} \in \mathcal{S}(N)$.

Proof. The implication (ii) ⇒ (iii) ⇒ (i) is obvious from the definition and Theorem 3.8. Thus, we only need to consider the implication (i) ⇒ (ii). For $\langle A, B\,|\,C\rangle \in \mathcal{M}_H$, Lemma 3.1 implies that $\langle A, B\,|\,C\rangle \in \mathcal{M}_{H'}$ for some minimal triangulation H' of H. Hence, $u_{H'} - u_{\langle A,B\,|\,C\rangle} \in \mathcal{C}(N)$ from Lemma 2.9. For every $V \in \mathcal{V}_H$, some minimal triangulation G of H_V coincides with H'_V from Lemma 3.6. Thus, $u_H - u_{H'} \in \mathcal{C}(N)$ from (7), which implies that

$$u_H - u_{\langle A,B\,|\,C\rangle} = (u_H - u_{H'}) + (u_{H'} - u_{\langle A,B\,|\,C\rangle}) \in \mathcal{C}(N).$$ □

Remark 3.11. In the case of directed acyclic graphs and chain graphs, some graphs may induce the same conditional independence model, and we have to consider the uniqueness of standard imsets for these graphs (cf. Lemma 2.6). However, in the case of undirected graphs, two different graphs cannot have the same conditional independence model. Thus, it is not necessary to consider the uniqueness question.

4. Standard imsets for general chain graphs

In this section, we define a standard imset for a chain graph, which is a generalization of an undirected graph and a directed acyclic graph. Studený and Vomlel [19], and Studený, Roverato and Štěpánová [18] give standard imsets for chain graphs which are equivalent to some directed acyclic graph. Using this result, we can derive imsets for general chain graphs. Moreover, we show that these imsets fully represent CG models by similar arguments as in the case of undirected graphs. In the later part of this section, we show the uniqueness of these imsets for equivalent chain graphs using the concept of a feasible merging.

4.1. Generalization of a triangulation to chain graphs

First, we introduce a concept which generalizes a triangulation of an undirected graph. In the case of an undirected graph, a triangulation of a graph is defined as a decomposable graph obtained by adding edges to the input graph. Since decomposable models can be interpreted as an undirected graph which is equivalent to some directed acyclic graph, we can define a triangulation of a chain graph in the same way.

Definition 4.1. *A chain graph $H' = (V(H'), E(H'))$, $V(H') = V(H)$ is said to be a triangulation of a chain graph H if H' satisfies that*

(i) *$a - b \in E(H')$ whenever $a - b \in E(H)$,*
(ii) *$a \to b \in E(H')$ whenever $a \to b \in E(H)$, and*
(iii) *H' is equivalent to some directed acyclic graph G, that is, $\mathcal{M}_{H'} = \mathcal{M}_G$.*

A triangulation H' of H is said to be minimal if there is no triangulation H'' of H such that $E(H'') \subset E(H')$ and $a \to b \in E(H')$ whenever $a \to b \in E(H'')$.

Note that the notion of a minimal triangulation of Definition 4.1 is consistent with the notion of a minimal triangulation of an undirected graph. See also Remark 4.5 below. Hence for a chain graph H, we also denote the set of its minimal triangulations by $\mathfrak{T}(H)$.

The condition (iii) has been characterized by Andersson *et al.* [1] in graphical terms. For a chain graph H and a chain component $C \in \mathcal{C}_H$, a closure graph for C is defined as the moral graph $\overline{H}(C) = (H_{C \cup \mathrm{pa}(C)})^{\mathrm{mor}}$.

Proposition 4.2 (Andersson *et al.* [1]). *A chain graph is equivalent to some directed acyclic graph if and only if $\overline{H}(C)$ is decomposable for every chain component $C \in \mathcal{C}_H$.*

Lemma 4.3 (cf. Remark 4.2 in [1]). *For $a \in N$ and $A \subseteq N$, let $\mathrm{ch}_A(a) = \mathrm{ch}(a) \cap A$ be the set of all children in H that occur in A. For any chain component $C \in \mathcal{C}_H$, the closure graph $\overline{H}(C) = (H_{C \cup \mathrm{pa}(C)})^{\mathrm{mor}}$ is decomposable if and only if:*

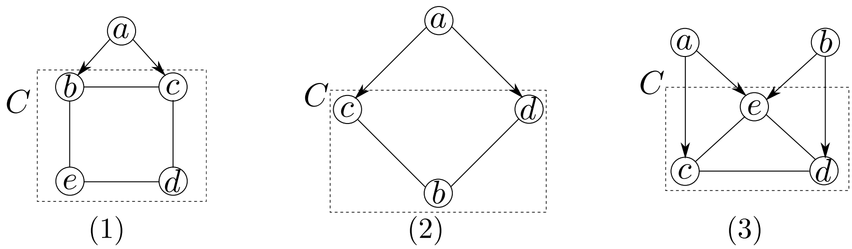

Figure 6. Examples of chain graphs violating the conditions of Lemma 4.3.

(i) *H_C is decomposable,*
(ii) *for every $a \in \mathrm{pa}(C)$, and every non-adjacent pair $c, d \in \mathrm{ch}_C(a)$, we have $c \perp\!\!\!\perp d \mid (\mathrm{ch}_C(a) \setminus cd)\,[H_C]$ (in particular $\mathrm{ch}_C(a) \setminus cd \neq \varnothing$), and*
(iii) *for every distinct pair $a, b \in \mathrm{pa}(C)$, and every $c \in \mathrm{ch}_C(a) \setminus \mathrm{ch}_C(b)$, $d \in \mathrm{ch}_C(b) \setminus \mathrm{ch}_C(a)$, we have $c \perp\!\!\!\perp d \mid (\mathrm{ch}_C(a)\,\mathrm{ch}_C(b) \setminus cd)\,[H_C]$ (in particular, $\mathrm{ch}_C(a)\,\mathrm{ch}_C(b) \setminus cd \neq \varnothing$, and c, d are non-adjacent).*

Example 4.4. We show in Figure 6 the examples of chain graphs which violate the conditions of Lemma 4.3. These graphs have only one chain component C and its parent set. In Figure 6(1), the subgraph H_C is not decomposable. In Figure 6(2), c and d are not separated by $\mathrm{ch}_C(a) \setminus cd = \varnothing$ because of a path $c - b - d$. In Figure 6(3), $c \in \mathrm{ch}_C(a) \setminus \mathrm{ch}_C(b)$ and $d \in \mathrm{ch}_C(b) \setminus \mathrm{ch}_C(a)$ are adjacent. Thus, c and d are not separated by $\mathrm{ch}_C(a)\,\mathrm{ch}_C(b) \setminus cd = e$. Their closure graphs are shown in Figure 7. These figures show that they are not decomposable, which implies that the graphs in Figure 6 are not equivalent to any directed acyclic graph from Proposition 4.2.

As these facts suggest, it is enough to consider a minimal triangulation of $H_{C \cup \mathrm{pa}(C)}$ for each chain component $C \in \mathcal{C}_H$ instead of the whole H. In fact, if a CG model induced by H coincides with none of DAG models, then at least one of the conditions (i), (ii) or (iii) in Lemma 4.3 is violated. When these conditions are violated, by adding edges between vertices in some C or between a vertex in C and a vertex in $\mathrm{pa}(C)$, we can satisfy these conditions without adding any

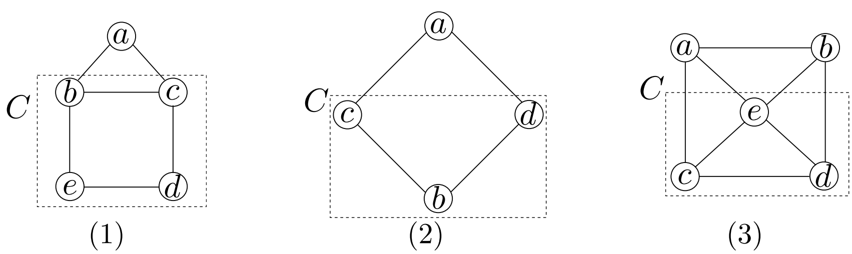

Figure 7. The closure graphs of Figure 6.

other edges. Conversely, all minimal triangulations of H are obtained by a minimal triangulation of $H_{C \cup \mathrm{pa}_H(C)}$ for each chain component $C \in \mathcal{C}_H$. Suppose that, for a triangulation H' of H, there exists $C \in \mathcal{C}_H$ such that the vertex set $V(\overline{H}(C))$ is a proper subset of $V(\overline{H'}(C'))$ for some $C' \in \mathcal{C}_{H'}$. This is the case when by the triangulation we add undirected edges among two distinct components of H or directed edges between the component C and some vertices which are not parents of C in H. Since $\overline{H'}(C')$ is decomposable by Proposition 4.2, the same is true for its induced subgraph over the vertex set $V(\overline{H}(C))$. Thus, we only need to add edges among $C \cup \mathrm{pa}_H(C)$. Moreover, the set of chain components of a triangulation is identical with that of the input graph.

Remark 4.5. The above argument shows how to obtain a minimal triangulation of chain graphs. Let H be a chain graph. For each $C \in \mathcal{C}_H$ and the parent set $\mathrm{pa}(C)$ in H, a minimal triangulation $H'_{C\cup \mathrm{pa}(C)}$ of $H_{C\cup \mathrm{pa}(C)}$ is obtained as follows. Let $G = \overline{H}(C)$ be a closure graph of a chain component C and G' be a minimal triangulation of G. Then for $F = \overline{E}(G') \setminus \overline{E}(G)$ one constructs a minimal triangulation $H'_{C\cup \mathrm{pa}(C)}$ by adding

- an undirected edge $a — b$ provided $(a, b) \in F$ and $a, b \in C$,
- a directed edge $a \to b$ provided $(a, b) \in F$, $a \in \mathrm{pa}(C)$ and $b \in C$.

Indeed, one gets a chain graph consistent with the chain components order for H, because every vertex in $\mathrm{pa}(C)$ has at least one arrow towards C.

Note also that in case of an undirected graph the obtained minimal triangulation is an undirected graph.

Example 4.6. Consider minimal triangulations of the graphs in Figure 6. Examples of minimal triangulations of closure graphs (Figure 7) for these graphs are shown in Figure 8. In Figure 8(1), a minimal triangulation of the closure graph is obtained by adding the edge $c — e$. Since c and e belong to the same chain component, adding the edge $c — e$ gives a minimal triangulation (Figure 9(1)) of the chain graph in Figure 6(1). In Figure 8(2), the edge $a — b$ is added. Since a and b belong to different chain components and there are directed edges from the chain component of a to that of b, a minimal triangulation (Figure 9(2)) of the graph in Figure 6(2) is obtained by adding the edge $a \to b$. As for the conditions of Lemma 4.3, $c \perp\!\!\!\perp d \mid (\mathrm{ch}_{H,C}(a) \setminus cd)\, [H_C]$ holds

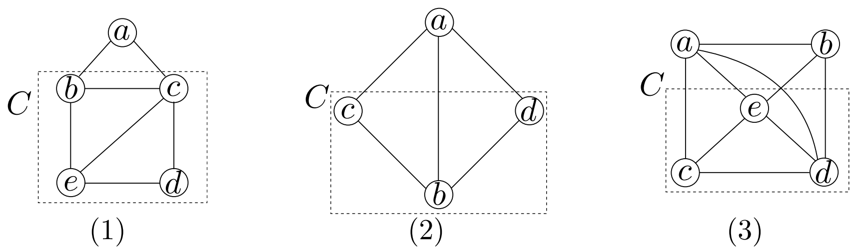

Figure 8. Examples of minimal triangulations of Figure 7.

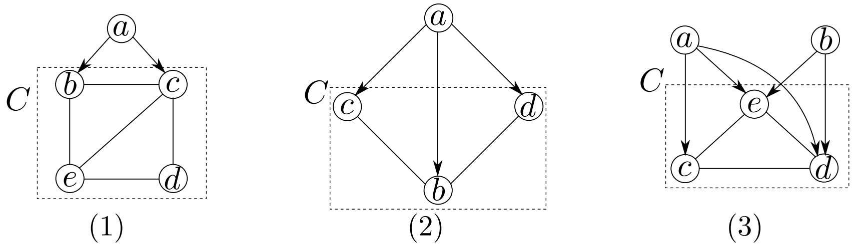

Figure 9. Examples of minimal triangulations of Figure 6.

because $\mathrm{ch}_{H,C}(a) \setminus cd = b$. In Figure 8(3), we add the edge $a - d$, hence, obtain the graph in Figure 9(3) in the same way as (2). Since $\mathrm{ch}_{H,C}(b) \setminus \mathrm{ch}_{H,C}(a) = \varnothing$ in this graph, the condition (iii) is satisfied automatically.

The following lemma immediately holds from the above discussion.

Lemma 4.7. *For a chain graph H and a chain component $C \in \mathcal{C}_H$, assume that $\overline{H}(C)$ is decomposable. Then for every minimal triangulation H' of H, we have $H_{C\cup \mathrm{pa}_H(C)} = H'_{C\cup \mathrm{pa}_{H'}(C)}$.*

Corollary 4.8. *For a chain graph H and a subset $K \subseteq N$ of the vertex set, assume that $H_{\mathrm{an}(K)}$ is equivalent to some directed acyclic graph. Then for every minimal triangulation H' of H, $H_{\mathrm{an}_H(K)} = H'_{\mathrm{an}_{H'}(K)}$ holds.*

Proof. Evidently, $\mathrm{an}_H(K) = \mathrm{an}_{H'}(K)$ holds. Also, for every chain component $C \in \mathcal{C}_{H_{\mathrm{an}(K)}}$, the closure graph $\overline{H}(C)$ is decomposable from Proposition 4.2. Hence, from Lemma 4.7, for every minimal triangulation H', we have $H_{C\cup \mathrm{pa}_H(C)} = H'_{C\cup \mathrm{pa}_{H'}(C)}$, which implies the corollary. □

As for separations of a chain graph and its minimal triangulation, we have a similar result to Lemma 3.1 for undirected graphs. See Figure 10.

Lemma 4.9. *For every chain graph H and triplet $\langle A, B \mid C\rangle \in \mathcal{M}_H$, there exists a minimal triangulation H' of H such that $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$.*

Proof. As in the case of undirected graphs, it suffices to find a triangulation H' which satisfies $\langle A, B \mid C\rangle \in \mathcal{M}_{H'}$. First, we construct a triangulation of a subgraph $H_{\mathrm{an}(ABC)}$, and then consider the whole graph H.

From the definition of the separation criterion of a chain graph, we have $\langle A, B \mid C\rangle \in \mathcal{M}_G$ for $G = (H_{\mathrm{an}(ABC)})^{\mathrm{mor}}$. We define a partition of $N' = \mathrm{an}_H(ABC)$ as in the same way of the proof of Lemma 3.1, that is,

$$A' = \{i \in N' \colon i \text{ is connected with } A \text{ in } G_{N'\setminus C}\},$$
$$C' = C \quad \text{and} \quad B' = N' \setminus A'C'.$$

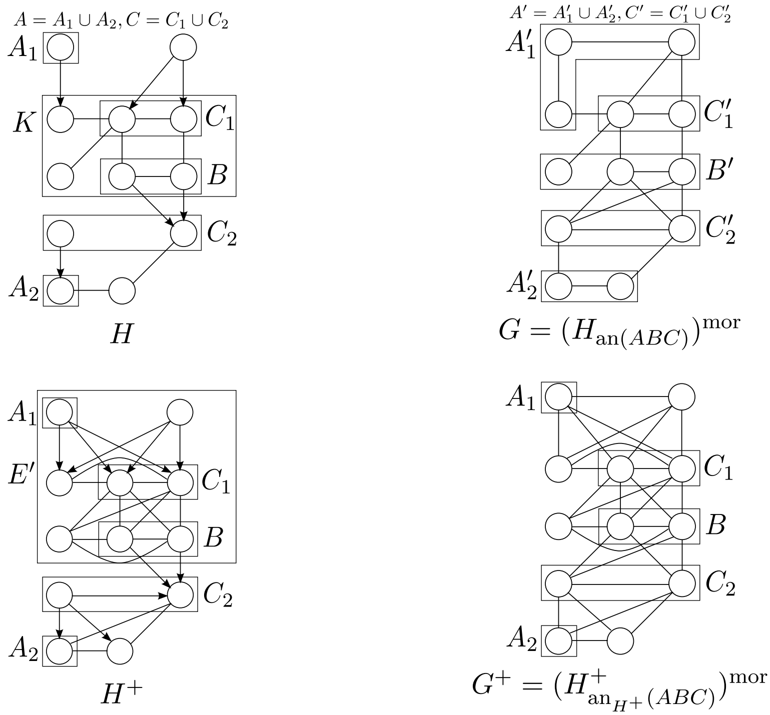

Figure 10. A construction of H^+ from a chain graph H in Lemma 4.9.

Then for each $K \in \mathcal{C}_H$, $K \subseteq N'$, we define a local graph $H^+(K)$ over $E' = K \cup \mathrm{pa}_H(K)$ as a graph obtained by removing edges between $A' \cap E'$ and $B' \cap E'$ from the graph which has an undirected graph over K and has all directed edges $a \to b$ from $a \in \mathrm{pa}(K)$ to $b \in K$. The graph H^+ is defined as the union of these local graphs over N' and outside $H^+_{N'}$ as the same as H. Since H^+ is also a chain graph, H and H^+ have the same components and their parent sets. Therefore, we have $\mathrm{an}_{H^+}(ABC) = \mathrm{an}_H(ABC)$. Moreover, closure graphs $\overline{H^+}(K)$ for components K are cliques over E' with removed edges between $A' \cap E'$ and $B' \cap E'$, and therefore $\overline{H^+}(K)$ is decomposable. This means that $H^+_{\mathrm{an}_{H^+}(ABC)}$ is equivalent to some acyclic directed graph from Proposition 4.2. Let $G^+ = (H^+_{\mathrm{an}_{H^+}(ABC)})^{\mathrm{mor}}$. From the construction of H^+, there is no edge between A' and B' in G^+. Thus, we also have $\langle A, B \mid C \rangle \in \mathcal{M}_{G^+}$.

Next, we consider the whole graph. Let H' be a minimal triangulation of H^+ (which may be H^+ itself). Since $(H^+_{\mathrm{an}_{H^+}(ABC)})^{\mathrm{mor}}$ is decomposable, $H^+_{\mathrm{an}_{H^+}(ABC)} = H'_{\mathrm{an}_{H'}(ABC)}$ from Corollary 4.8. Therefore, we have $G' = (H^+_{\mathrm{an}_{H^+}(ABC)})^{\mathrm{mor}} = (H'_{\mathrm{an}_{H'}(ABC)})^{\mathrm{mor}}$, which implies that $\langle A, B \mid C \rangle \in \mathcal{M}_{H'}$. □

4.2. Definition and properties of standard imsets for chain graphs

In this section, we define a standard imset for a chain graph and show that it fully represents the CG model induced by this graph.

When a chain graph H is equivalent to some directed acyclic graph, its standard imset is defined as follows [18,19]:

$$u_H = \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \left\{ \delta_{\mathrm{pa}_H(C)} - \sum_{K \in \mathcal{K}_{\overline{H}(C)}} \delta_K + \sum_{S \in \mathcal{S}_{\overline{H}(C)}} \nu_{\overline{H}(C)}(S) \cdot \delta_S \right\}. \tag{8}$$

This definition is a generalization of that of a directed acyclic graph (2) and a decomposable graph (3). Moreover, we have the following lemma about this imset.

Proposition 4.10 (Studený *et al.* [18]). *Assume that two chain graphs H_1, H_2 are equivalent to some directed acyclic graph. Then $\mathcal{M}_{H_1} = \mathcal{M}_{H_2}$ if and only if $u_{H_1} = u_{H_2}$.*

Therefore, for a chain graph H which is equivalent to some directed acyclic graph, we have $u_H \in \mathcal{C}(N)$ and $\mathcal{M}_H = \mathcal{M}_{u_H}$ from Lemma 2.6. Furthermore, we have the following corollary from Lemma 2.9:

Corollary 4.11. *Suppose that a chain graph H is equivalent to some directed acyclic graph and let u_H be given in (8). For a triplet $\langle A, B \mid C \rangle \in \mathcal{T}(N)$, the followings are equivalent*:

(i) $\langle A, B \mid C \rangle \in \mathcal{M}_H$,
(ii) $u_H - u_{\langle A, B \mid C \rangle} \in \mathcal{C}(N)$,
(iii) $u_H - u_{\langle A, B \mid C \rangle} \in \mathcal{S}(N)$.

Note that every closure graph $\overline{H}(C)$, $C \in \mathcal{C}_H$, is decomposable from Proposition 4.2. Thus (8) is also written as

$$u_H = \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{ \delta_{\mathrm{pa}(C)} - \delta_{C\,\mathrm{pa}(C)} + u_{\overline{H}(C)} \},$$

where $u_{\overline{H}(C)}$ is the standard imset (3) for the decomposable graph $\overline{H}(C)$. This equation suggests that a generalization of (8) is given by replacing $u_{\overline{H}(C)}$ as in (6). For $C \in \mathcal{C}_H$ and $V \subseteq C \cup \mathrm{pa}(C)$, let $\overline{H}(C)_V$ be the subgraph of the closure graph $\overline{H}(C)$ induced by V.

Definition 4.12. *A standard imset u_H for a chain graph H is defined by*

$$u_H = \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{ \delta_{\mathrm{pa}_H(C)} - \delta_{C\,\mathrm{pa}_H(C)} + u_{\overline{H}(C)} \}, \tag{9}$$

where $u_{\overline{H}(C)}$, $C \in \mathcal{C}_H$, *is the standard imset for the undirected graph* $\overline{H}(C)$ *given by* (6):

$$u_{\overline{H}(C)} = \delta_{C\,\mathrm{pa}_H(C)} - \sum_{V \in \mathcal{V}_{\overline{H}(C)}} \delta_V + \sum_{S \in \mathcal{S}_{\overline{H}(C)}} \nu_{\overline{H}(C)}(S) \cdot \delta_S$$

$$+ \sum_{V \in \mathcal{V}_{\overline{H}(C)}} \sum_{G \in \mathfrak{T}(\overline{H}(C)_V)} u_G.$$

Note that when H is a connected undirected graph this imset coincides with (6), because the sum in (9) has only one term and $\delta_{\mathrm{pa}_H(C)} = \delta_\varnothing$, $\delta_N = \delta_{C\,\mathrm{pa}_H(C)}$. We can easily prove that the same conclusion holds for any undirected graph by considering each connected component. This imset gives a representation of CG models. The proof is similar to the case of undirected graphs.

Theorem 4.13. *For a chain graph* H, *let a standard imset* u_H *for* H *be defined by* (9). *Then* $u_H \in \mathcal{C}(N)$ *and* $\mathcal{M}_H = \mathcal{M}_{u_H}$.

Proof. The argument in Section 4.1 implies that $\mathcal{C}_H = \mathcal{C}_{H'}$ and $\mathrm{pa}_H(C) = \mathrm{pa}_{H'}(C), \forall C \in \mathcal{C}_H$, for a minimal triangulation H' of H. Thus a standard imset $u_{H'}$ for H' given by (8) is

$$u_{H'} = \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_{H'}} \{\delta_{\mathrm{pa}_{H'}(C)} - \delta_{C\,\mathrm{pa}_{H'}(C)} + u_{\overline{H'}(C)}\}$$

$$= \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{\delta_{\mathrm{pa}_H(C)} - \delta_{C\,\mathrm{pa}_H(C)} + u_{\overline{H'}(C)}\}.$$

As in the proof (of implication $\mathcal{M}_H \subseteq \mathcal{M}_{u_H}$) of Theorem 3.8, we have $u_{\overline{H}(C)} - u_{\overline{H'}(C)} \in \mathcal{S}(N)$ for $C \in \mathcal{C}_H$, which shows that $u_H - u_{H'} \in \mathcal{S}(N)$. Also, putting $v_H = \sum_{H' \in \mathfrak{T}(H)} u_{H'}$, we have

$$v_H = \sum_{H' \in \mathfrak{T}(H)} \left[\delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{\delta_{\mathrm{pa}(C)} - \delta_{C\,\mathrm{pa}(C)} + u_{\overline{H'}(C)}\}\right]$$

$$= \left|\mathfrak{T}(H)\right| \cdot \left[\delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{\delta_{\mathrm{pa}(C)} - \delta_{C\,\mathrm{pa}(C)}\}\right] + \sum_{H' \in \mathfrak{T}(H)} \sum_{C \in \mathcal{C}_H} u_{\overline{H'}(C)}$$

$$= \left|\mathfrak{T}(H)\right| \cdot \left[\delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \{\delta_{\mathrm{pa}(C)} - \delta_{C\,\mathrm{pa}(C)}\}\right]$$

$$+ \sum_{C \in \mathcal{C}_H} \sum_{G \in \mathfrak{T}(\overline{H}(C))} n_H(C, G) \cdot u_G,$$

where $n_H(C, G) = |\{H' \in \mathfrak{T}(H); \overline{H'}(C) = G\}|$ for $C \in \mathcal{C}_H$ and $G \in \mathfrak{T}(\overline{H}(C))$, is the number of minimal triangulations H' of H such that $\overline{H'}(C) = G$. Therefore, as in the proof of Theorem 3.8 for the case of an undirected graph, u_H and v_H belong to the relative interior of the same face of $\mathrm{cone}(\mathcal{E}(N))$. Thus, we have $\mathcal{M}_{u_H} = \mathcal{M}_{v_H}$.

For every chain graph, there exists a discrete measure P over N such that $\mathcal{M}_{\mathrm{P}} = \mathcal{M}_H$ [17]. Moreover, Theorem 2.3 implies that $\mathcal{M}_{\mathrm{P}} = \mathcal{M}_w$ for some $w \in \mathcal{S}(N)$. Hence for every $H' \in \mathfrak{T}(H)$, we have

$$\mathcal{M}_{u_{H'}} = \mathcal{M}_{H'} \subseteq \mathcal{M}_H = \mathcal{M}_{\mathrm{P}} = \mathcal{M}_w,$$

which implies that $k_{H'} \cdot w - u_{H'} \in \mathcal{S}(N)$ for some $k_{H'} \in \mathbb{N}$ from Lemma 2.2. Putting $k = \sum_{H' \in \mathfrak{T}(H)} k_{H'}$, we have $k \cdot w - v_H \in \mathcal{S}(N)$. Therefore $\mathcal{M}_{u_H} = \mathcal{M}_{v_H} \subseteq \mathcal{M}_w = \mathcal{M}_H$.

Conversely, for every $\langle A, B \,|\, C\rangle \in \mathcal{M}_H$, there exists $H' \in \mathfrak{T}(H)$ such that $\langle A, B \,|\, C\rangle \in \mathcal{M}_{H'}$ from Lemma 4.9. Thus $u_{H'} - u_{\langle A,B \,|\, C\rangle} \in \mathcal{S}(N)$ from Corollary 4.11. Hence, we have

$$u_H - u_{\langle A,B \,|\, C\rangle} = (u_H - u_{H'}) + (u_{H'} - u_{\langle A,B \,|\, C\rangle}) \in \mathcal{S}(N)$$

and $\langle A, B \,|\, C\rangle \in \mathcal{M}_{u_H}$. □

As in the case of undirected graphs, we have the following corollary.

Corollary 4.14. *For a chain graph H and every triplet $\langle A, B \,|\, C\rangle \in \mathcal{T}(N)$, the followings are equivalent*:

(i) $\langle A, B \,|\, C\rangle \in \mathcal{M}_H$,
(ii) $u_H - u_{\langle A,B \,|\, C\rangle} \in \mathcal{C}(N)$,
(iii) $u_H - u_{\langle A,B \,|\, C\rangle} \in \mathcal{S}(N)$.

4.3. Feasible merging

From now on, we will consider the uniqueness of the standard imsets for chain graphs in Definition 4.12.

In the case of chain graphs which are equivalent to some directed acyclic graphs, the uniqueness of their standard imsets defined by (8) is given in Proposition 4.10. Its proof is based on the concept called a feasible merging [18]. In this section, we review its definition and properties.

Let H be a chain graph. A pair of its chain components $U, L \in \mathcal{C}_H$ is said to form a meta-arrow $U \rightrightarrows L$ if there exists a directed edge $a \to b \in E(H)$ for some $a \in U, b \in L$. The *merging of a meta-arrow* $U \rightrightarrows L$ is the operation of replacing every directed edge $a \to b \in E(H)$, $a \in U, b \in L$, with $a - b$. The merging of $U \rightrightarrows L$ is called *feasible* if the following two conditions are satisfied:

(i) $K \equiv \mathrm{pa}(L) \cap U$ is a clique in H, and
(ii) $\mathrm{pa}(L) \setminus U \subseteq \mathrm{pa}(b)$ for any $b \in K$.

By this definition, the merging is feasible if and only if $\mathrm{pa}(L)$ is a clique in the closure graph $\overline{H}(U)$. Moreover, for the resulting graph H' and the chain component M obtained by the merging of $U \rightrightarrows L$, $\mathrm{pa}_H(L)$ is a clique in $\overline{H'}(M)$.

Example 4.15. We show some examples of feasible and infeasible mergings in Figure 11. The left-hand side graphs of these figures are input graphs containing $K = \{b, c\}, L = \{d, e\}$ and

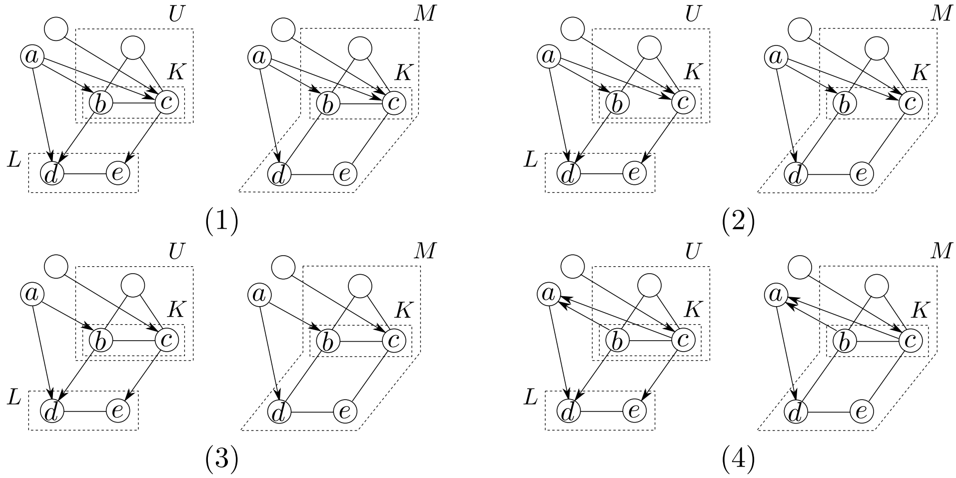

Figure 11. Examples of a feasible merging (1) and examples of infeasible merging (2), (3), (4).

$\mathrm{pa}(L) = \{a, b, c\}$, and the right-hand side graphs the resulting graphs obtained by the merging $U \rightrightarrows L$ in the input ones. In Figure 11(1), K is a clique, and $\mathrm{pa}(L) \setminus U = \{a\} = \mathrm{pa}(b) \subset \mathrm{pa}(c)$. Thus both conditions are satisfied, and the merging is feasible. Especially, the input graph and resulting graph have the same complexes. In Figure 11(2), since K is not a clique, the condition (i) is not satisfied. Also in Figure 11(3), the condition (ii) is violated because $\mathrm{pa}(L) \setminus U = \{a\} \not\subseteq \mathrm{pa}(c)$. Hence, the mergings of $U \rightrightarrows L$ in (2) and (3) are infeasible. Note that, in Figure 11(2), the merging of $U \rightrightarrows L$ destroys a complex $b \to d - e \leftarrow c$. Similarly, a complex $a \to d - e \leftarrow c$ vanishes in Figure 11(3). As in Figure 11(3), the condition (ii) is not satisfied in (4). In this case, the resulting graph has a directed cycle $a \to d - e - c \to a$, and hence, it is not a chain graph.

As shown in these examples, the resulting graph by a feasible merging is also a chain graph and has the same complexes as the input graph. Thus, we have the following important lemma from Theorem 2.4.

Lemma 4.16 (Studený *et al.* [18]). *Let H be a chain graph and H' be a graph obtained by the merging of $U \rightrightarrows L$ in H. Then $\mathcal{M}_H = \mathcal{M}_{H'}$ if and only if the merging is feasible.*

The operation of merging can be performed without leaving the equivalence class. Especially, every larger equivalent graph is obtained by a series of feasible merging operations.

Theorem 4.17 (Studený *et al.* [18]). *Let G and H be chain graphs such that $\mathcal{M}_G = \mathcal{M}_H$ and $H \geq G$. Then there exists a sequence of chain graphs $G = H_1, \ldots, H_r = H$, $r \geq 1$, such that H_{i+1} is obtained by the operation of feasible merging in H_i for all $i = 1, \ldots, r-1$.*

From Theorem 2.5, for proving that equivalent chain graphs have a common property, it suffices to prove that the property is shared by a pair of graphs of the class such that one is obtained by a feasible merging from the other.

4.4. Uniqueness of standard imsets for chain graphs

In this section, we show that equivalent chain graphs have the same standard imset.

Theorem 4.18. *Let H_1, H_2 be chain graphs. Then $\mathcal{M}_{H_1} = \mathcal{M}_{H_2}$ if and only if $u_{H_1} = u_{H_2}$.*

To prove this theorem, the following fact is useful.

Lemma 4.19 (cf. the proof of Theorem 20 in [18]). *For a chain graph H which is equivalent to some directed acyclic graph, let H' be a graph obtained from H by a feasible merging of a meta-arrow $U \rightrightarrows L$, and let M denote the merged chain component. Then $K \subseteq N$ is a maximal clique of $\overline{H'}(M)$ if and only if K is either a maximal clique of $\overline{H}(L)$ or a maximal clique of $\overline{H}(U)$ different from* $\mathrm{pa}_H(L)$.

In a chain graph H which is equivalent to some directed acyclic graph, every mp-subgraph of $\overline{H}(C), C \in \mathcal{C}_H$, is complete, because a closure graph $\overline{H}(C)$ is decomposable. As mentioned in Section 2.2, the graph obtained by adding edges to an undirected graph such that its all mp-components become maximal cliques is decomposable. The following lemma can be easily proved by Lemma 32 of [18] and Lemma 2.1(i), (ii) of [11].

Lemma 4.20. *For a chain graph H, define H' and M as in Lemma 4.19. Then $K \subseteq N$ is an mp-component of $\overline{H'}(M)$ if and only if K is either an mp-component of $\overline{H}(L)$ or an mp-component of $\overline{H}(U)$ different from* $\mathrm{pa}_H(L)$.

The chain graph in Lemma 4.20 need not be equivalent to an acyclic directed graph as in Lemma 4.19. Also note that $\mathrm{pa}_H(L)$ can never be an mp-component of $\overline{H}(L)$, and, therefore, never an mp-component of $\overline{H'}(M)$. This can be shown by contradiction: if $\mathrm{pa}(L)$ is an mp-component of $\overline{H}(L)$, then an ordering $V_1, \dots, V_m$ of its mp-components satisfying RIP and $V_1 = \mathrm{pa}(L)$ exists from Theorem 2.5 of [11]. Then $V_1 \setminus S_2$ and $V_2 \setminus S_2$ are separated by S_2 from Lemma 3.5. However, $x \in V_1 \setminus S_2$ must have a child in L, which leads to some vertex in $V_2 \setminus S_2$ since L is a connected component. This gives a contradiction with the above separation.

We now prove Theorem 4.18 using this result.

Proof of Theorem 4.18. Let $H = H_1$. Note that the standard imset for H given by (9) is

$$u_H = \delta_N - \delta_\varnothing + \sum_{C \in \mathcal{C}_H} \left\{ \delta_{\mathrm{pa}(C)} - \sum_{V \in \mathcal{V}_{\overline{H}(C)}} \delta_V + \sum_{S \in \mathcal{S}_{\overline{H}(C)}} \nu_{\overline{H}(C)}(S) \cdot \delta_S \right\}$$

$$+ \sum_{C \in \mathcal{C}_H} \sum_{V \in \mathcal{V}_{\overline{H}(C)}} \sum_{G \in \mathfrak{T}(\overline{H}(C)_V)} u_G.$$

We first show that $u_H = u_{H'}$ for a chain graph H' obtained from H by feasible merging of a meta-arrow $U \rightrightarrows L$. Let M denote the merged chain component. Since the closure graphs for every chain component C except for U, L, M are the same in H and in H', we have to show that the contribution in $u_{H'}$ corresponding to M is the sum of contributions in u_H corresponding to L and U. Since $\mathrm{pa}(L)$ is a clique (in all three considered graphs $\overline{H}(L)$, $\overline{H}(U)$ and $\overline{H'}(M)$), letting $V = \mathrm{pa}(L)$, we have

$$\sum_{G\in\mathfrak{T}(\overline{H}(U)_V)} u_G = \sum_{G\in\mathfrak{T}(\overline{H}(L)_V)} u_G = \sum_{G\in\mathfrak{T}(\overline{H'}(M)_V)} u_G = 0.$$

Also, from Lemma 4.20, mp-components in $\overline{H'}(M)$ except for $\mathrm{pa}_H(L)$ are identical with those of either $\overline{H}(L)$ or $\overline{H}(U)$. Therefore, we have

$$\sum_{V\in\mathcal{V}_{\overline{H}(L)}} \sum_{G\in\mathfrak{T}(\overline{H}(L)_V)} u_G + \sum_{V\in\mathcal{V}_{\overline{H}(U)}} \sum_{G\in\mathfrak{T}(\overline{H}(U)_V)} u_G = \sum_{V\in\mathcal{V}_{\overline{H'}(M)}} \sum_{G\in\mathfrak{T}(\overline{H'}(M)_V)} u_G, \tag{10}$$

whether $\mathrm{pa}(L)$ is an mp-component of $\overline{H}(U)$ or not.

From (10) and $\mathrm{pa}_H(U) = \mathrm{pa}_{H'}(M)$ (see Lemma 32 in [18]), $u_H = u_{H'}$ is reduced to

$$\begin{aligned} &- \sum_{V\in\mathcal{V}_{\overline{H}(L)}} \delta_V + \sum_{S\in\mathcal{S}_{\overline{H}(L)}} \nu_{\overline{H}(L)}(S)\cdot\delta_S + \delta_{\mathrm{pa}_H(L)} \\ &\quad - \sum_{V\in\mathcal{V}_{\overline{H}(U)}} \delta_V + \sum_{S\in\mathcal{S}_{\overline{H}(U)}} \nu_{\overline{H}(U)}(S)\cdot\delta_S \\ &= - \sum_{V\in\mathcal{V}_{\overline{H'}(M)}} \delta_V + \sum_{S\in\mathcal{S}_{\overline{H'}(M)}} \nu_{\overline{H'}(M)}(S)\cdot\delta_S, \end{aligned}$$

which is the same as the equation (7) in [18] if all mp-components V are maximal cliques. Indeed, one can construct a chain graph H^* over vertices $L \cup U \cup \mathrm{pa}(L)$ having U and L as components (and possibly some other singleton components in $\mathrm{pa}(L) \setminus U$) such that the mp-subgraphs of $\overline{H}(L)$ and $\overline{H}(U)$ are maximal cliques in $\overline{H^*}(L)$ and $\overline{H^*}(U)$. This graph is equivalent to an acyclic directed graph, which is the assumption for validity of the formula (7) in [19]. Then the similar argument for the proof of Proposition 20 in [18] holds by Lemma 4.20 and Theorem 2.5 in [11] for the above equation. Thus we have $u_H = u_{H'}$.

Let H_∞ be the largest chain graph (cf. Theorem 2.5) in the equivalence class containing H_1, H_2. Then we have $u_{H_1} = u_{H_\infty}$ from Theorem 4.17. Also we have $u_{H_2} = u_{H_\infty}$, which implies Theorem 4.18. □

5. Concluding remarks

In this paper, we defined standard imsets for undirected graphical models and chain graphical models. The crucial concept to derive them was a minimal triangulation. For an undirected graph, its imset was defined through all minimal triangulations of the graph. Moreover, we gave a more brief form of a standard imset using the structure of mp-subgraphs. For a chain graph, we generalized a triangulation of undirected graph. Then a standard imset for a chain graph was derived through an analogous argument as the undirected case. We also showed the uniqueness of standard imsets for equivalent chain graphs.

For directed acyclic graphs and decomposable graphs, the number of non-zero elements of their standard imsets is linear in $|N|$, while (6) and (9) may have exponential number of non-zero elements. Especially, for a prime undirected graph, imsets defined by (4) coincide with (6). Thus there is a question whether we can find an imset with smaller numbers of non-zero elements.

This is related to the degree of combinatorial imsets. The degree of a combinatorial imset is defined as the sum of positive coefficients when it is written as a non-negative integer combination of elementary imset [16]. An imset with the smallest degree is considered as a basic representative of an equivalence class in Section 7.3 in [16]. In fact, a standard imset for a directed acyclic graph has the smallest degree. Our definition of a standard imset has the smallest degree for some graphs. One of such examples is a 4-cycle graph. It is easy to see that the smallest degree in the equivalence class is 2, and (6) achieves this bound. Although, for other cycle graphs, (6) does not achieve the smallest degree, it may be possible to derive an imset with the smallest degree through our definition.

Acknowledgements

We are very grateful to a referee for very careful and constructive comments.

References

[1] Andersson, S.A., Madigan, D. and Perlman, M.D. (1997). On the Markov equivalence of chain graphs, undirected graphs, and acyclic digraphs. *Scand. J. Stat.* **24** 81–102. MR1436624

[2] Bouckaert, R., Hemmecke, R., Lindner, S. and Studený, M. (2010). Efficient algorithms for conditional independence inference. *J. Mach. Learn. Res.* **11** 3453–3479. MR2756190

[3] Frydenberg, M. (1990). The chain graph Markov property. *Scand. J. Stat.* **17** 333–353. MR1096723

[4] Geiger, D. and Pearl, J. (1993). Logical and algorithmic properties of conditional independence and graphical models. *Ann. Statist.* **21** 2001–2021. MR1245778

[5] Hara, H. and Takemura, A. (2010). A localization approach to improve iterative proportional scaling in Gaussian graphical models. *Comm. Statist. Theory Methods* **39** 1643–1654.

[6] Heggernes, P. (2006). Minimal triangulations of graphs: A survey. *Discrete Math.* **306** 297–317. MR2204109

[7] Hemmecke, R., Lindner, S. and Studený, M. (2010). Learning restricted Bayesian network structures. Preprint. Available at arXiv:1011.6664v1.

[8] Hemmecke, R., Morton, J., Shiu, A., Sturmfels, B. and Wienand, O. (2008). Three counter-examples on semi-graphoids. *Combin. Probab. Comput.* **17** 239–257. MR2396350

[9] Lauritzen, S.L. (1996). *Graphical Models*. *Oxford Statistical Science Series* **17**. New York: Oxford Univ. Press. MR1419991

[10] Lauritzen, S.L., Dawid, A.P., Larsen, B.N. and Leimer, H.-G. (1990). Independence properties of directed Markov fields. *Networks* **20** 491–505. Special issue on influence diagrams. MR1064735

[11] Leimer, H.-G. (1993). Optimal decomposition by clique separators. *Discrete Math*. **113** 99–123. MR1212872

[12] Ohtsuki, T., Cheung, L.K. and Fujisawa, T. (1976). Minimal triangulation of a graph and optimal pivoting order in a sparse matrix. *J. Math. Anal. Appl*. **54** 622–633. MR0485552

[13] Pearl, J. (1988). *Probabilistic Reasoning in Intelligent Systems*: *Networks of Plausible Inference*. *The Morgan Kaufmann Series in Representation and Reasoning*. San Mateo, CA: Morgan Kaufmann. MR0965765

[14] Studený, M. (1994/1995). Description of structures of stochastic conditional independence by means of faces and imsets (a series of three papers). *Int. J. Gen. Syst*. **23** 123–137, 201–219, 323–341.

[15] Studený, M. (2001). On non-graphical description of models of conditional independence structure. In *HSSS Workshop on Stochastic Systems for Individual Behaviours*, Louvain la Neuve, Belgium.

[16] Studený, M. (2005). *Probabilistic Conditional Independence Structures*. London: Springer.

[17] Studený, M. and Bouckaert, R.R. (1998). On chain graph models for description of conditional independence structures. *Ann. Statist*. **26** 1434–1495. MR1647685

[18] Studený, M., Roverato, A. and Štěpánová, Š. (2009). Two operations of merging and splitting components in a chain graph. *Kybernetika* (*Prague*) **45** 208–248. MR2518149

[19] Studený, M. and Vomlel, J. (2009). A reconstruction algorithm for the essential graph. *Internat. J. Approx. Reason*. **50** 385–413. MR2514506

[20] Studený, M., Vomlel, J. and Hemmecke, R. (2010). A geometric view on learning Bayesian network structures. *Internat. J. Approx. Reason*. **51** 573–586. MR2644598

[21] Verma, T. and Pearl, J. (1990). Causal networks: Semantics and expressiveness. In *Uncertainty in Artificial Intelligence*, 4. *Mach. Intelligence Pattern Recogn*. **9** 69–76. Amsterdam: North-Holland. MR1166827

[22] Vomlel, J. and Studený, M. (2007). Graphical and algebraic representatives of conditional independence models. In *Advances in Probabilistic Graphical Models* 55–80. Berlin: Springer.

Received February 2011 and revised January 2014