Bayesian Networks

II. Probabilistic Independence and Separation in Graphs (part 3)

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1. **Basic Probability Calculus**

2. **Separation in undirected graphs**

3. **Separation in directed graphs**

4. **Markov networks**

Complete graphs, orderings

Definition 1. An undirected graph $G := (V, E)$ is called **complete**, if it contains all possible edges (i.e. if $E = \mathcal{P}^2(V)$).

Definition 2. Let $G := (V, E)$ be a directed graph.
A bijective map

$$\sigma : \{1, \dots, |V|\} \to V$$

is called an **ordering of (the vertices of)** G.

We can write an ordering as enumeration of V, i.e. as $v_1, v_2, \dots, v_n$ with $V = \{v_1, \dots, v_n\}$ and $v_i \neq v_j$ for $i \neq j$.

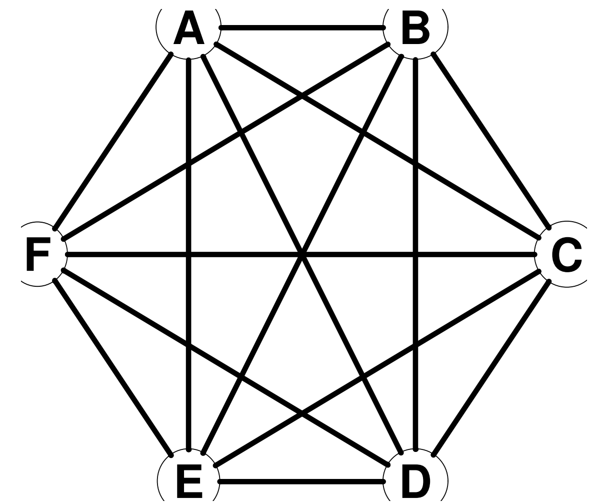


Figure 1: Undirected complete graph with 6 vertices.

Topological orderings (1/2)

Definition 3. An ordering $\sigma = (v_1, \ldots, v_n)$ is called **topological ordering** if

(i) all parents of a vertex have smaller numbers, i.e.

$$\text{fanin}(v_i) \subseteq \{v_1, \ldots, v_{i-1}\}, \quad \forall i = 1, \ldots, n$$

or equivalently

(ii) all edges point from smaller to larger numbers

$$(v, w) \in E \Rightarrow \sigma^{-1}(v) < \sigma^{-1}(w), \quad \forall v, w \in V$$

The reverse of a topological ordering – e.g. got by using the fanout instead of the fanin – is called **ancestral numbering**.

In general there are several topological orderings of a DAG.

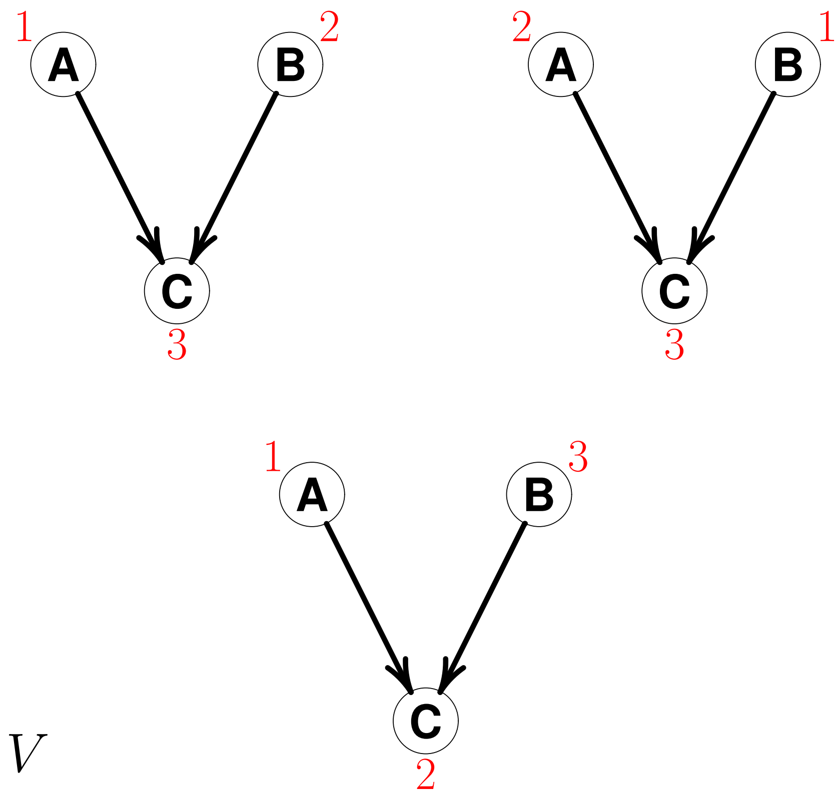


Figure 2: DAG with different topological orderings: $\sigma_1 = (A, B, C)$ and $\sigma_2 = (B, A, C)$. The ordering $\sigma_3 = (A, C, B)$ is not topological.

Topological orderings (2/2)

Lemma 1. *Let G be a directed graph. Then*

$$G \text{ is acyclic (a DAG)} \Leftrightarrow G \text{ has a topological ordering}$$

$\text{topological-ordering}(G = (V, E))$:
choose $v \in V$ with $\text{fanout}(v) = \emptyset$
$\sigma(|V|) := v$
$\sigma|_{\{1,\ldots,|V|-1\}} := \text{topological-ordering}(G \setminus \{v\})$
return σ

Figure 3: Algorithm to compute a topologcial ordering of a DAG.

Exercise: write an algorithm for checking if a given directed graph is a acyclic.

Complete DAGs

Definition 4. A DAG $G := (V, E)$ is called complete, if

(i) it has a topological ordering $\sigma = (v_1, \ldots, v_n)$ with

$$\text{fanin}(v_i) = \{v_1, \ldots, v_{i-1}\}, \quad \forall i = 1, \ldots, n$$

or equivalently

(ii) it has exactly one topological ordering

or equivalently

(iii) every additional edge introduces a cycle.

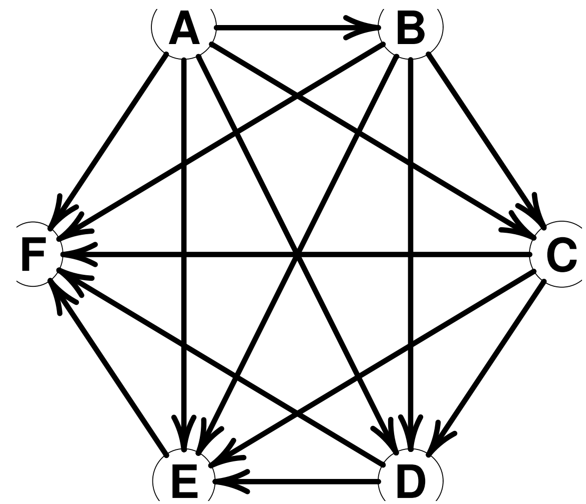


Figure 4: Complete DAG with 6 vertices. Its topological ordering is $\sigma = (A, B, C, D, E, F)$.

Graph representations of ternary relations on $\mathcal{P}(V)$

Definition 5. Let V be a set and I a ternary relation on $\mathcal{P}(V)$ (i.e. $I \subseteq \mathcal{P}(V)^3$). In our context I is often called an **independency model**.

Let G be a graph on V (undirected or DAG).
G is called a **representation of** I, if

$$I_G(X, Y|Z) \Rightarrow I(X, Y|Z) \quad \forall X, Y, Z \subseteq V$$

A representation G of I is called **faithful**, if

$$I_G(X, Y|Z) \Leftrightarrow I(X, Y|Z) \quad \forall X, Y, Z \subseteq V$$

Representations are also called **independency maps of** I or **markov w.r.t.** I, faithful representations are also called **perfect maps of** I.

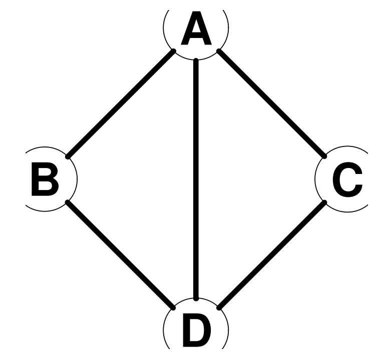


Figure 5: Non-faithful representation of

$$I := \{(A, B|\{C, D\}), (B, C|\{A, D\}), (B, A|\{C, D\}), (C, B|\{A, D\})\}$$

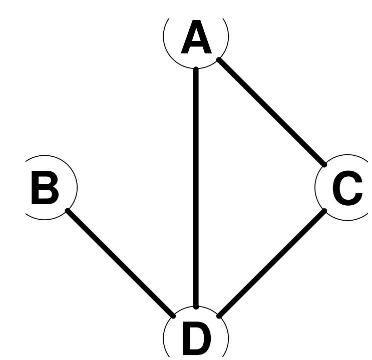


Figure 6: Faithful representation of I. Which I?

Faithful representations

In G also holds
$I_G(B, \{A, C\}|D), I_G(B, A|D), I_G(B, C|D), \ldots$
so G is not a representation of

$$I := \{(A, B|\{C, D\}), (B, C|\{A, D\}), (B, A|\{C, D\}), (C, B|\{A, D\})\}$$

at all. It is a representation of

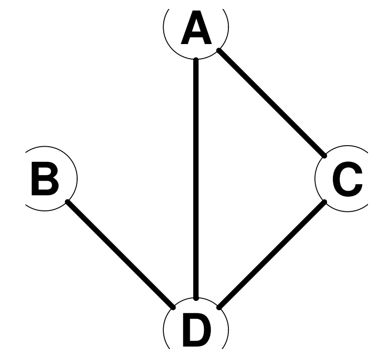


Figure 7: Faithful representation of J.

$$J := \{(A, B|\{C, D\}), (B, C|\{A, D\}), (B, \{A, C\}|D), (B, A|D), (B, C|D), (B, A|\{C, D\}), (C, B|\{A, D\}), (\{A, C\}, B|D), (A, B|D), (C, B|D)\}$$

and as all independency statements of J hold in G, it is faithful.

Trivial representations

For a complete undirected graph or a complete DAG $G := (V, E)$ there is

$$I_G \equiv \text{false},$$

i.e. there are no triples $X, Y, Z \subseteq V$ with $I_G(X, Y|Z)$. Therefore G represents any independency model I on V and is called **trivial representation**.

There are independency models without faithful representation.

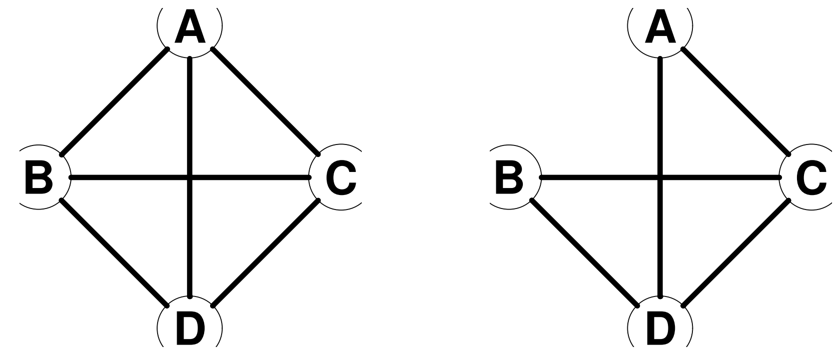


Figure 8: Independency model

$$I := \{(A, B|\{C, D\})\}$$

without faithful representation.

Minimal representations

Definition 6. A representation G of I is called **minimal**, if none of its subgraphs omitting an edge is a representation of I.

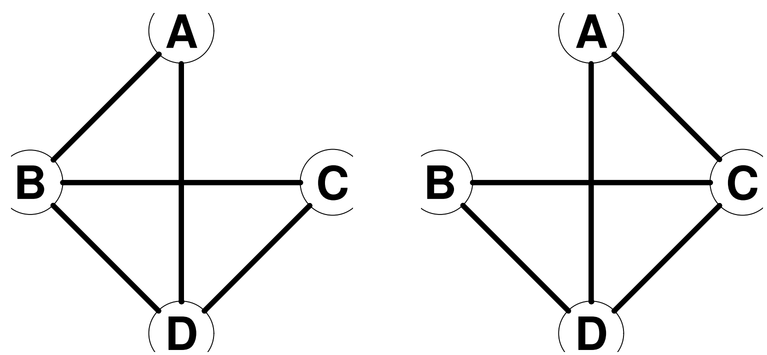


Figure 9: Different minimal undirected representations of the independency model

$$I := \{(A, B|\{C, D\}), (A, C|\{B, D\}), (B, A|\{C, D\}), (C, A|\{B, D\})\}$$

Minimal representations

Lemma 2 (uniqueness of minimal undirected representation)**.** *An independency model I has exactly one minimal undirected representation, if and only if it is*

(i) symmetric: $I(X,Y|Z) \Rightarrow I(Y,X|Z)$.

(ii) decomposable: $I(X,Y \cup W|Z) \Rightarrow I(X,Y|Z)$ *and* $I(X,W|Z)$

(iii) intersectable: $I(X,W|Z \cup Y)$ *and* $I(X,Y|Z \cup W) \Rightarrow I(X,Y \cup W|Z)$

Then this representation is $G = (V, E)$ *with*

$$E := \{\{x,y\} \in \mathcal{P}^2(V) \,|\, \textit{not } I(x,y|V \setminus \{x,y\}\}$$

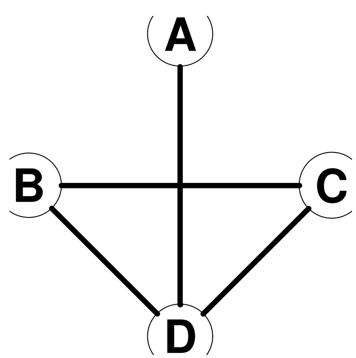
Minimal representations (2/2)

Example 1.

$$I := \{(A, B|\{C, D\}), (A, C|\{B, D\}), (A, \{B, C\}|D), (A, B|D), (A, C|D),\\ (B, A|\{C, D\}), (C, A|\{B, D\}), (\{B, C\}, A|D), (B, A|D), (C, A|D)\}$$

is symmetric, decomposable and intersectable.

Its unique minimal undirected representation is



If a faithful representation exists, obviously it is the unique minimal representation, and thus can be constructed by the rule in lemma 2.

Properties of conditional independency

relation	symmetry	decomposition	composition	strong union	weak union	contraction	intersection	strong transitivity	weak transitivity	chordality
u-separation	+	+	+	+	+	+	+	+	+	−
d-separation	+	+	+	−	+	+	+	−	+	+
cond. ind. in general JPD	+	+	−	−	+	+	−	−	−	−[1)]
cond. ind. in non-extreme JPD	+	+	−	−	+	+	+	−	−	−[1)]

[1)] + for decomposable JPDs.

Independency models that satisfy symmetry, decomposition, weak union, and contraction (as conditional independency of general JPDs) are called **semi-graphoids**. If they satisfy also intersection (as conditional independency of non-extreme JPDs), they are called **graphoids**.

Representation of conditional independency

Definition 7. We say, a graph **represents a JPD** p, if it represents the conditional independency relation I_p of p.

As for general JPDs the intersection property does not hold, they may have several minimal undirected representations.

For non-extreme JPDs all properties required for uniqueness of the minimal representation hold (symmetry, decomposition, intersection; see lemma 2), i.e. non-extreme JPDs have a unique minimal undirected representation.

To compute this representation we have to check $I_p(X, Y | V \setminus \{X, Y\})$ for all pairs of variables $X, Y \in V$, i.e.

$$p \cdot p^{\downarrow V \setminus \{X,Y\}} = p^{\downarrow V \setminus \{X\}} \cdot p^{\downarrow V \setminus \{Y\}}$$

Then the minimal representation is the complete graph on V omitting the edges $\{X, Y\}$ for that $I_p(X, Y | V \setminus \{X, Y\})$ holds.

Representation of conditional independency

Example 2. Let p be the JPD on $V := \{X, Y, Z\}$ given by:

Z	X	Y	$p(X, Y, Z)$
0	0	0	0.024
0	0	1	0.056
0	1	0	0.036
0	1	1	0.084
1	0	0	0.096
1	0	1	0.144
1	1	0	0.224
1	1	1	0.336

Checking $p \cdot p^{\downarrow V \setminus \{X,Y\}} = p^{\downarrow V \setminus \{X\}} \cdot p^{\downarrow V \setminus \{Y\}}$ one finds that the only independency relations of p are $I_p(X, Y|Z)$ and $I_p(Y, X|Z)$.

Its marginals are:

Z	X	$p(X, Z)$
0	0	0.08
0	1	0.12
1	0	0.24
1	1	0.56

Z	Y	$p(Y, Z)$
0	0	0.06
0	1	0.14
1	0	0.32
1	1	0.48

X	Y	$p(X, Y)$
0	0	0.12
0	1	0.2
1	0	0.26
1	1	0.42

X	$p(X)$
0	0.32
1	0.68

Y	$p(Y)$
0	0.38
1	0.62

Y	$p(Z)$
0	0.2
1	0.8

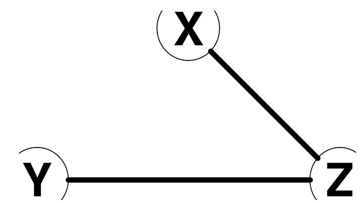
Representation of conditional independency

Example 2 (cont.).

Z	X	Y	$p(X,Y,Z)$
0	0	0	0.024
0	0	1	0.056
0	1	0	0.036
0	1	1	0.084
1	0	0	0.096
1	0	1	0.144
1	1	0	0.224
1	1	1	0.336

Checking $p \cdot p^{\downarrow V \setminus \{X,Y\}} = p^{\downarrow V \setminus \{X\}} \cdot p^{\downarrow V \setminus \{Y\}}$ one finds that the only independency relations of p are $I_p(X, Y|Z)$ and $I_p(Y, X|Z)$.

Thus, the graph



represents p, as its independency model is $I_G := \{(X, Y|Z), (Y, X|Z)\}$.

As for p only $I_p(X, Y|Z)$ and $I_p(Y, X|Z)$ hold, G is a faithful representation.

Factorization of a JPD according to a graph

Definition 8. Let p be a joint probability distribution of a set of variables V. Let $\mathcal{C}$ be a cover of V, i.e. $\mathcal{C} \subseteq \mathcal{P}(V)$ with $\bigcup_{\mathcal{X}\in\mathcal{C}} \mathcal{X} = V$.
p **factorizes according to** $\mathcal{C}$, if there are potentials

$$\psi_{\mathcal{X}} : \prod_{X\in\mathcal{X}} X \to \mathbb{R}_0^+, \quad \mathcal{X} \in \mathcal{C}$$

with

$$p = \prod_{\mathcal{X}\in\mathcal{C}} \psi_{\mathcal{X}}$$

In general, the potentials are not unique and do not have a natural interpretation.

Example 3.

Z	X	Y	$p(X,Y,Z)$
0	0	0	0.024
0	0	1	0.056
0	1	0	0.036
0	1	1	0.084
1	0	0	0.096
1	0	1	0.144
1	1	0	0.224
1	1	1	0.336

Z	X	$p(X,Z)$
0	0	0.08
0	1	0.12
1	0	0.24
1	1	0.56

Z	Y	$p(Y,Z)$	$p(Y\|Z)$
0	0	0.06	0.3
0	1	0.14	0.7
1	0	0.32	0.4
1	1	0.48	0.6

p factorizes according to $\mathcal{C} = \{\{X,Z\},\{Y,Z\}\}$ as

$$p = p(X,Z)\cdot p(Y|Z)$$

Factorization of a JPD according to a graph

Definition 9. Let G be an undirected graph. A maximal complete subgraph of G is called a **clique of** G. $\mathcal{C}_G$ denotes the set of all cliques of G.

p **factorizes according to** G, if it factorizes according to its clique cover $\mathcal{C}_G$.

The factorization induced by the complete graph is trivial.

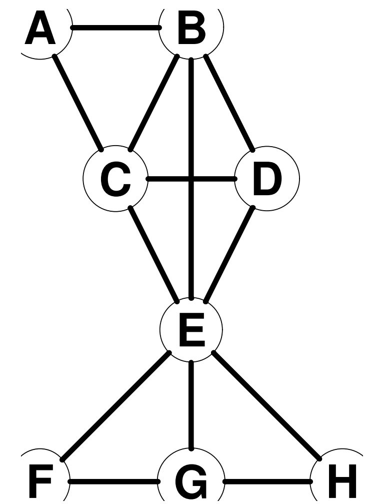
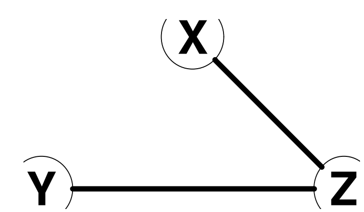


Figure 10: A graph with cliques $\{A, B, C\}$, $\{B, C, D, E\}$, $\{E, F, G\}$ and $\{E, G, H\}$.

Example 4. The JPD p from last example factorized according to the graph



as it has cliques $\mathcal{C} = \{\{X, Z\}, \{Y, Z\}\}$

Factorization and representation

Lemma 3. *Let p be a JPD of a set of variables V, G be an undirected graph on V. Then*

(i) p factorizes acc. to $G \Rightarrow G$ represents p.

(ii) If $p > 0$ then
p factorizes acc. to $G \Leftrightarrow G$ represents p.

(iii) If $p > 0$ then p factorizes acc. to its (unique) minimal representation.

(iv) If G is an undirected graph and $\psi_{\mathcal{X}}$ for $\mathcal{X} \in \mathcal{C}_G$ are any potentials on its cliques, then G represents the JPD

$$p := (\prod_{\mathcal{X} \in \mathcal{C}_G} \psi_{\mathcal{X}})^{|\emptyset}$$

Multiplication of potentials

Multiplication of potentials has the following properties:

(i) $dom(\psi_1\psi_2) = dom(\psi_1) \cup dom(\psi_2)$

(ii) The commutative law: $\psi_1\psi_2 = \psi_2\psi_1$

(iii) The associative law: $(\psi_1\psi_2)\psi_3 = \psi_1(\psi_2\psi_3)$

(iv) Existence of unit: 1 is a potential over the empty set where $1.\psi = \psi$ for all potentials ψ

Example 5.

B	A	$\psi(B,A)$
b_1	a_1	x_1
b_1	a_2	x_2
b_2	a_1	x_3
b_2	a_2	x_4

$\otimes$

B	C	$\psi(B,C)$
b_1	c_1	y_1
b_1	c_2	y_2
b_2	c_1	y_3
b_2	c_2	y_4

$=$

B	A	C	$\psi(B,A,C)$
b_1	a_1	c_1	x_1y_1
b_1	a_1	c_2	x_1y_2
b_1	a_2	c_1	x_2y_1
b_1	a_2	c_2	x_2y_2
b_2	a_1	c_1	x_3y_3
b_2	a_1	c_2	x_3y_4
b_2	a_2	c_1	x_4y_3
b_2	a_2	c_2	x_4y_4

with $x_i, y_i \in \mathbb{R}_0^+$

Markov networks

Definition 10. A pair $(G, (\psi_C)_{C\in\mathcal{C}_G})$ consisting of

(i) an undirected graph G on a set of variables V and

(ii) a set of potentials

$$\psi_C : \prod_{X\in C} \mathrm{dom}(X) \rightarrow \mathbb{R}_0^+, \quad C \in \mathcal{C}_G$$

on the cliques[1)] of G (called **clique potentials**)

is called a **markov network**.

[1)] on the product of the domains of the variables of each clique.

Thus, a markov network encodes

(i) a joint probability distribution factorized as

$$p = (\prod_{C\in\mathcal{C}_G} \psi_C)^{|\emptyset}$$

and

(ii) conditional independency statements

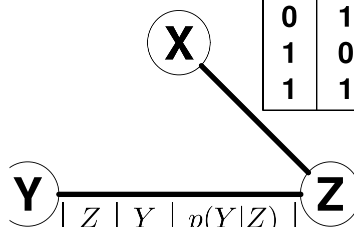
$$I_G(X, Y|Z) \Rightarrow I_p(X, Y|Z)$$

G represents p, but not necessarily faithfully.

If G is triangulated/chordal and $\mathcal{C} = C_1, \ldots, C_n$ a chain of cliques, then ψ_{C_i} can be replaced by the conditional probabilities $p^{\downarrow C_i|S_i}$ (without changing p).

Markov networks / examples

Z	X	$p(X,Z)$
0	0	0.08
0	1	0.12
1	0	0.24
1	1	0.56



Z	Y	$p(Y\|Z)$
0	0	0.3
0	1	0.7
1	0	0.4
1	1	0.6

Figure 11: Example for a markov network.

Chain of cliques

Definition 11. Let G be an undirected graph and $\mathcal{C}_G$ be its cliques. A sequence $C_1, \ldots, C_n$ of cliques of G is called **chain of cliques**, if

1. every clique occurs exactly once and
2. the **running intersection property** holds:

$$C_i \cap \bigcup_{j=1}^{i-1} C_j \subseteq C_k, \quad \forall i \exists k < i$$

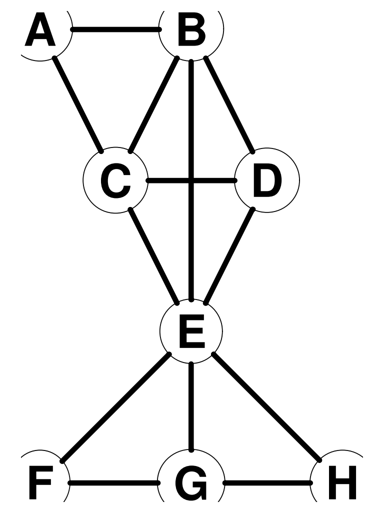


Figure 12: A graph with chain of cliques $\{A, B, C\}$, $\{B, C, D, E\}$, $\{E, F, G\}$ and $\{E, G, H\}$.

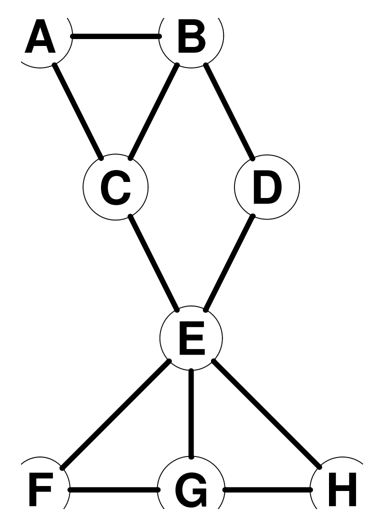


Figure 13: A graph with cliques $\{A, B, C\}$, $\{B, D\}$, $\{C, E\}$, $\{D, E\}$, $\{E, F, G\}$ and $\{E, G, H\}$, but without chain of cliques.

Triangulated/chordal graphs

Definition 12. Let G be an undirected graph.
G is called **triangulated** (or **chordal**), if every cycle of length ≥ 4 has a chord, i.e. it exists an additional edge in G between non-successive vertices of the cycle.

Lemma 4. *G is chordal $\Leftrightarrow$ I_G is chordal.*

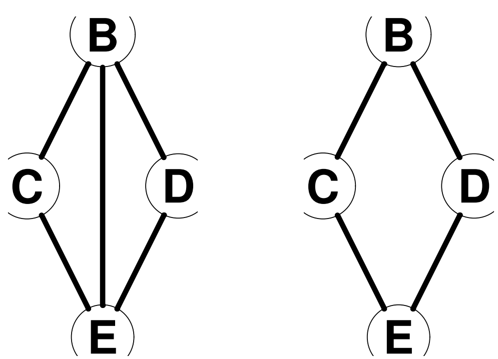


Figure 14: Cycle with chord and cycle without chord.

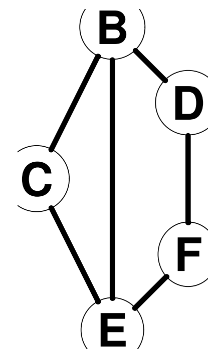


Figure 15: Chordal or non-chordal graph?

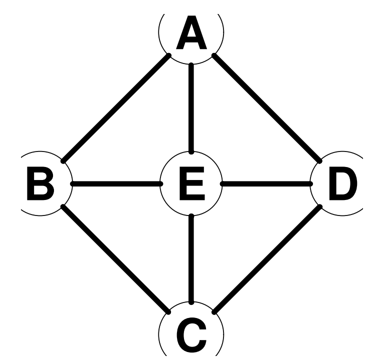


Figure 16: Chordal or non-chordal graph?

Perfect ordering

Definition 13. Let G be an undirected graph.
An ordering σ of (the vertices of) G is called **perfect**, if

(i) $\sigma(i)$ and its neighbors form a clique of the subgraph on $\sigma(\{1, \ldots, i\})$

or equivalently

(ii) the subgraph on

$$\text{fan}(\sigma(i)) \cap \sigma(\{1, \ldots, i-1\})$$

is complete for $i := 2, ..., n$.

A perfect ordering is also called a **perfect numbering**. The reverse of a perfect ordering is also called **elimination** or **deletion sequence**.

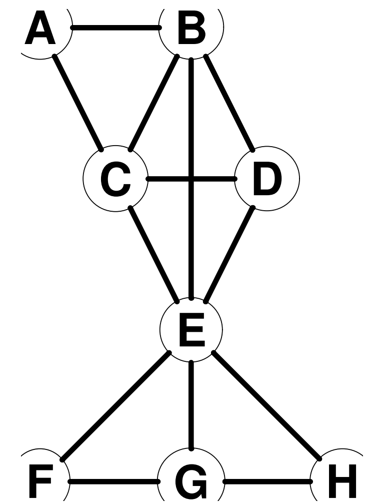


Figure 17: There are several perfect orderings of this graph, e.g., H, G, E, F, D, C, B, A and G, E, B, C, H, D, F, A.

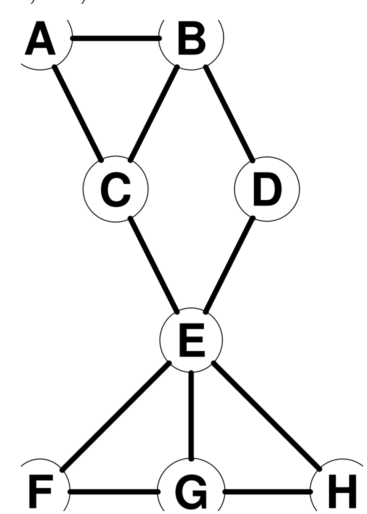


Figure 18: A graph without perfect ordering.

Triangulation, perfect ordering, and chain of cliques

Lemma 5. *Let G be an undirected graph. It is equivalent:*

(i) G is triangulated / chordal.

(ii) G admits a perfect ordering.

(iii) G admits a chain of cliques.

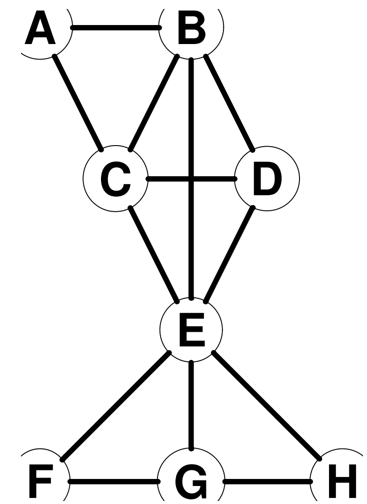


Figure 19: MCS finds the perfect ordering (A, B, C, D, E, F, G, H).

perfect-ordering-MCS$(G = (V, E))$:
for $i = 1, \ldots, |V|$ **do**
    $\sigma(i) := v \in V \setminus \sigma(\{1, \ldots, i-1\})$ with maximal $|\text{fan}_G(v) \cap \sigma(\{1, \ldots, i-1\})|$
        breaking ties arbitrarily
od
return σ

Figure 20: Algorithm to find a perfect ordering of a triangulated graph by maximum cardinality search.

Triangulation, perfect ordering, and chain of cliques

chain-of-cliques(G) :
$\mathcal{C}$:= *enumerate-cliques*(G)
σ := *perfect-ordering*(G)
Order $\mathcal{C}$ by ascending $\max(\sigma^{-1}(C))$ for $C \in \mathcal{C}$
    breaking ties arbitrarily
return $\mathcal{C}$

Figure 21: Algorithm to find a chain of cliques of a triangulated graph.

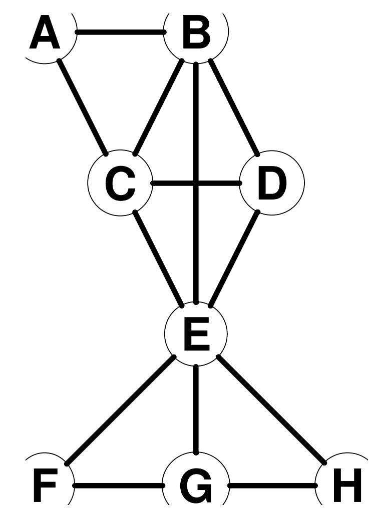


Figure 22: Based on the perfect ordering (A, B, C, D, E, F, G, H) the rank of the cliques is computed as $\{A, B, C\}$ (3) $\{B, C, D, E\}$ (5), $\{E, F, G\}$ (7) and $\{E, G, H\}$ (8). The algorithm outputs the chain of cliques $\{A, B, C\}$, $\{B, C, D, E\}$, $\{E, F, G\}$ and $\{E, G, H\}$.

Factorization and representation (2/2)

Definition 14. A joint probability distribution p is called **decomposable**, if its conditional independency relation I_p is chordal.

Warning. p being decomposable has nothing to do with I_p being decomposable!

Definition 15. Let G be a triangulated / chordal graph and $\mathcal{C} = C_1, \ldots, C_n$ a chain of cliques of G. Then

$$S_i := C_i \cap \bigcup_{j<i} C_j$$

is called the **i-th separator** and

$$R_i := C_i \setminus S_i$$

is called **i-th residual**

Lemma 6. *Let p be a JPD of a set of variables V, G be an undirected graph on V. If G represents p and p is decomposable (i.e. G triangulated/chordal), let $\mathcal{C} = C_1, \ldots, C_n$ be a chain of cliques, and then*

$$p = \prod_{i=1}^{n} p^{\downarrow R_i | S_i}$$

i.e. p factorizes in the conditional probability distributions of the residuals of the cliques given its separators.