Probabilistic Graphical Models **Fall 2015**

Lecture 4 — October 21st

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4.1 Three Facts About Conditional Independence

1. **Can repeat variables:** $X \perp\!\!\!\perp Y, Z|Z, W$ is the same as $X, Z \perp\!\!\!\perp Y|Z, W$. The repetition is redundant but may be convenient notation.

2. **Decomposition:** $X \perp\!\!\!\perp Y, Z|W$ can be decomposed as $X \perp\!\!\!\perp Y|W$ and $X \perp\!\!\!\perp Z|W$.

3. **Trick:** extra conditioning on both sides of the equation doesn't change anything. E.g. the following two statements are always true.

$$p(x, y) = p(x|y)p(y) \tag{4.1}$$

$$p(x, y|z) = p(x|y, z)p(y|z) \tag{4.2}$$

4.2 Notation and probability review

Let us recall a few notations before establishing some properties of directed graphical models. Let $X_1, X_2, \ldots, X_n$ be random variables with distribution:

$$\mathbb{P}(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) = p_X(x_1, \ldots, x_n) = p(x)$$

where x stands for $(x_1, \ldots, x_n)$. Given $A \subset \{1, \ldots, n\}$, we denote the marginal distribution of x_A by:

$$p(x_A) = \sum_{x_{A^c}} p(x_A, x_{A^c}).$$

With this notation we can write the conditional distribution as:

$$p(x_A|x_{A^c}) = \frac{p(x_A, x_{A^c})}{p(x_{A^c})}$$

We also recall the so-called 'chain rule' stating:

$$p(x_1, \ldots, x_n) = p(x_1)p(x_2|x_1)p(x_3|x_2, x_1) \ldots p(x_n|x_1, \ldots, x_{n-1})$$

To end with notations and recalls, we remind the conditional independence characterization:

$$X \perp\!\!\!\perp Y \mid Z \Leftrightarrow p\,(x, y|z) = p\,(x|z)\,p\,(y|z) \Leftrightarrow p\,(x|y, z) = p\,(x|z) = \frac{p\,(x, y|z)}{p\,(y|z)}$$

4.3 Directed Graphical Model

4.3.1 Non-descendents

Let $nd(i) \triangleq \{j : \text{no path from } i \text{ to } j\}$. j are non-descendents of i.

4.3.2 First definitions and properties

Let $X_1, \dots, X_n$ be n random variables with distribution $p(x) = p_X(x_1, \dots, x_n)$.

Definition 4.1 *Let $G = (V, E)$ be a DAG with $V = \{1, \dots, n\}$. We say that $p(x)$ factorizes in G, denoted $p(x) \in \mathcal{L}(G)$ iff $p(x)$ is of the form:*

$$\forall x, p(x) = \prod_{i=1}^{n} f_i(x_i, x_{\pi_i}) \text{ such that } f_i \geq 0, \sum_{x_i} f(x_i, x_{\pi_i}) = 1 \;\; \forall x_{\pi_i} \tag{4.3}$$

where we recall that π_i stands for the set of parents of the vertex i in G.

We now show that because we assumed that G was a DAG, it implies a particular and convenient form for the f_i above. We have:

Proposition 4.2 *If $p(x) \in \mathcal{L}(G)$ then, for all $i \in \{1, \dots, n\}$, $f_i(x_i, x_{\pi_i}) = p(x_i|x_{\pi_i})$.*

Proof We prove this by induction on $n = |V|$, the cardinality of the set V. Since G is a DAG, there exists a leaf, *i.e.* a node with no children. Without loss of generality, we can assume that the leaf is labeled by n. We first notice:

$$\begin{aligned}
\forall x, p(x_1, \dots, x_{n-1}) &= \sum_{x_n} p(x_1, \dots, x_n) \\
&= \sum_{x_n} \prod_{i=1}^{n} f_i(x_i, x_{\pi_i}) \\
&= \sum_{x_n} f_n(x_n, x_{\pi_n}) \prod_{i=1}^{n-1} f_i(x_i, x_{\pi_i}) \\
&= \prod_{i=1}^{n-1} f_i(x_i, x_{\pi_i}) \sum_{x_n} f_n(x_n, x_{\pi_n}) \;\; (*) \\
&= \prod_{i=1}^{n-1} f_i(x_i, x_{\pi_i}) \\
&= g(x_1, \dots, x_{n-1}) \;\; (**)
\end{aligned} \tag{4.4}$$

The step $(*)$ is justified by the fact that n is a leaf and thus it never appears in any of the π_i for $i \in \{1, \dots, n-1\}$. Step $(**)$ is also justified by the same kind of reasoning: since n is a leaf it cannot appear in any of the π_i explaining why it is only a function, say g, of $x_1, \dots, x_{n-1}$.

From this result, we can use an induction reasoning noticing that $G - \{n\}$ is still a DAG. To conclude this proof, we simply need to show that, indeed, $f_n(x_n, x_{\pi_n}) = p(x_n|x_{\pi_n})$—this property will automatically propagates by induction. We have:

$$p(x_n, x_{\pi_n}) = \sum_{x_i, i \notin \{n\} \cup \pi_n} p(x) = \left(\sum_{x_i, i \notin \{n\} \cup \pi_n} g(x_1, \ldots, g_{n-1}) \right) f_n(x_n, x_{\pi_n}). \tag{4.5}$$

Noticing that $\sum_{x_i, i \notin \{n\} \cup \pi_n} g(x_1, \ldots, x_{n-1})$ is a function of only x_{π_n}, say $h(x_{\pi_n})$, we can derive:

$$p(x_n|x_{\pi_n}) = \frac{p(x_n, x_{\pi_n})}{\sum_{x_n} p(x_n, x_{\pi_n}) \sum_{x'_n} p(x'_n, x_{\pi_n})} \tag{4.6}$$

But since $\sum_{x_n} p(x_n, x_{\pi_n}) = 1$

$$p(x_n|x_{\pi_n}) = \frac{p(x_n, x_{\pi_n})}{\sum_{x'_n} p(x'_n, x_{\pi_n})} = \frac{h(x_{\pi_n}) f_n(x_n, x_{\pi_n})}{h(x_{\pi_n})} = f_n(x_n, x_{\pi_n}). \tag{4.7}$$

■

Hence we can give an equivalent definition for a DAG to the notion of factorization:

Definition 4.3 *(Equivalent definition) $p(x)$ factorizes in G, denoted $p(x) \in \mathcal{L}(G)$ iff:*

$$\forall x, p(x) = \prod_{i=1}^{n} p(x_i|x_{\pi_i}) \tag{4.8}$$

Example 4.3.1
- *(Trivial Graphs) Assume $E = \emptyset$,* i.e. *there is no edges. Then we have $p(x) = \prod_{i=1}^{n} p(x_i)$, implying the random variables $X_1, \ldots, X_n$ are independent. Hence variables are independent if they factorize in the empty graph.*
- *(Complete Graphs) Assume now we have a complete graph (thus with $n(n-1)/2$ edges as we need acyclic for it to be a DAG), we have: $p(x) = \prod_{i=1}^{n} p(x_i|x_1, \ldots, x_{i-1})$, the so-called 'chain rule' which is always true. Every random process factorizes in the complete graph.*

4.3.3 Graphs with three nodes

We give an insight of the different possible behaviors of a graph by thoroughly enumerating the possibilities for a 3-node graph.

- The two first options are the empty graph, leading to independence, and the complete graph that gives no further information than the chain rule.

- (Markov chain) A Markov chain is a certain type of DAG showed in Fig.(4.1). In this configuration we show that we have:

$$p(x, y, z) \in \mathcal{L}(G) \Rightarrow X \perp\!\!\!\perp Z \mid Y \tag{4.9}$$

Indeed we have:

$$p(z|y, x) = \frac{p(x, y, z)}{p(x, y)} = \frac{p(x, y, z)}{\sum_{z'} p(z', x, y)} = \frac{p(x)p(y|x)p(z|y)}{\sum_{z'} p(x)p(y|x)p(z'|y)} = p(z|y)$$

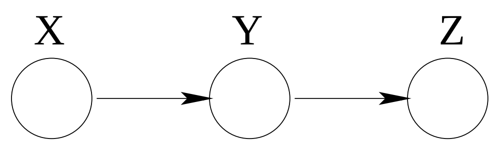


Figure 4.1. Markov Chain

- (Latent cause) It is the type of DAG given in Fig.(4.2). We show that:

$$p(x) \in \mathcal{L}(G) \Rightarrow X \perp\!\!\!\perp Y \mid Z \tag{4.10}$$

Indeed:

$$p(x, y|z)\frac{p(x, y, z)}{p(z)} = \frac{p(z)p(y|z)p(x|z)}{p(z)} = p(x|z)p(y|z)$$

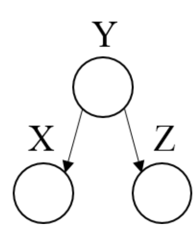


Figure 4.2. Latent cause

- (Explaining away) Represented in Fig.(4.3), we can show for this type of graph:

$$p(x) \in \mathcal{L}(G) \Rightarrow X \perp\!\!\!\perp Y \tag{4.11}$$

It basically stems from:

$$p(x, y) = \sum_z p(x, y, z) = p(x)p(y) \sum_z p(z) = p(x)p(y)$$

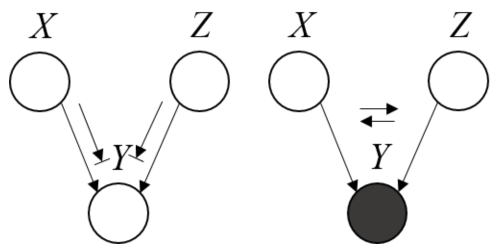


Figure 4.3. Explaining away, or V-structure

Remark 4.3.1 *The use of 'cause' is not advised since observational statistics provide with correlations and no causality notion. Note also that in the 'explaining away' graph, in general* $X \perp\!\!\!\perp Y | Z$ *is not true. Lastly, it is important to remember that not every relationship can be expressed in terms of graphical models. As a counter-example take the XOR function where* $Z = X \oplus Y$. *The three random variables are pairwise independent, but not mutually independent.*

4.3.4 Inclusion, reversal and marginalization properties

Inclusion property. Here is a quite intuitive proposition about included graphs and their factorization.

Proposition 4.4 *If* $G = (V, E)$ *and* $G' = (V, E')$ *then:*

$$E \subset E' \Leftrightarrow \mathcal{L}(G) \subset \mathcal{L}(G') \tag{4.12}$$

Proof We have $p(x) = \prod_{i=1}^{n} p(x_i, x_{\pi_i(G)})$. As $E \subset E'$ it is obvious that $\pi_i(G) \subset \pi_i(G')$. Therefore, going back to the definition of graphical models through potential $f_i(x_i, x_{\pi_i})$ we get the result. ■

Reversal property. We also have some reversal properties. Let us first define the notion of V-structure.

Definition 4.5 *We say there is a V-structure (figure 4.3) in* $i \in V$ *if* $|\pi_i| \geq 2$, *i.e.has two or more parents.*

Proposition 4.6 *(Markov equivalence) If* $G = (V, E)$ *is a DAG and if for* $(i, j) \in E, |\pi_i| = 0$ *and* $|\pi_j| \leq 1$, *then* (i, j) *may be reversed,* i.e. *if* $p(x)$ *factorizes in* G *then it factorizes in* $G' = (V, E')$ *with* $E' = (E - \{(i, j)\}) \cup \{(j, i)\}$.

In terms of 3-nodes graph, this property ensures us that the Markov chain and latent cause are equivalent. On the other hand the V-structure lead to a different class of graph compared to the two others.

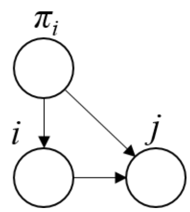


Figure 4.4. Edge (i,j) is covered

Definition 4.7 *An edge (i,j) is said to be covered if $\pi_j = \{i\} \cup \pi_i$.*

By reversing (i,j) we might not get a DAG as it might break the acyclic property. We have the following result:

Proposition 4.8 *Let $G = (V, E)$ be a graph and $(i,j) \in E$ a covered edge. Let $G' = (V, E')$ with $E' = (E - \{(i,j)\}) \cup \{(j,i)\}$, then if G' is a DAG, $\mathcal{L}(G) = \mathcal{L}(G')$.*

Marginalization. The underlying question is to know whether the marginalization of a distribution that factorizes in a graphical model also does. This is true for the marginalization with respect to leaf nodes but is not true generally.

Conditional independence. We finish this section by giving a result that explains that if $p(x)$ factorizes in G then every single random variable is independent from the set of its non-descendants given its parents. From now on, we denote by $\mathrm{nd}(i)$ the set of non-descendants of i.

Proposition 4.9 *If G is a DAG, then:*

$$p(x) \in \mathcal{L}(G) \Leftrightarrow X_i \perp\!\!\!\perp X_{nd(i) \setminus \pi_i} | X_{\pi_i} \tag{4.13}$$

Proof We will only prove the forward implication. Assume $(1, \ldots, n)$ is a topological order then:

$$\begin{cases} p(x) = \prod_{i=1}^{n} p(x_i | x_{\pi_i}) & : \text{ because } p(x) \in \mathcal{L}(G) \\ p(x) = \prod_{i=1}^{n} p(x_i | x_1, \ldots, x_{i-1}) & : \text{ chain rule, always true} \end{cases}$$

As we chose a topological order, we have $\pi_i \subset \{1, \ldots, i-1\}$, and we show by induction that:

$$p(x_i | x_{\pi_i}) = p(x_i | x_1, \ldots, x_{i-1}) = p(x_i | x_{\pi_i}, x_{\{1,\ldots,i-1\} - \pi_i}).$$

This directly implies that $X_i \perp\!\!\!\perp X_{\{1,\ldots,i-1\} \setminus \pi_i} | X_{\pi_i}$. The key idea now is to notice that for all i, there exist a topological order such that $\mathrm{nd}(i) = \{1, \ldots, i-1\}$. ■

4.3.5 Bayes ball algorithm

This is an intuitive "reacheability" algorithm to determine conditional independence in a DAG. Suppose we want to determine if X is conditionally independent from Z given Y. Place a ball on each of the nodes in X and let them bounce around according to some rules (described below) and see if any reaches Z. $X \perp\!\!\!\perp Z|Y$ is true if none reached Z, but not otherwise.

The rules are as follows for the three canonical graph structures. Note that the balls are allowed to travel in either direction along the edges of the graph.

1. **Markov chain:** Balls pass through when we do not observe Y, but are blocked otherwise.

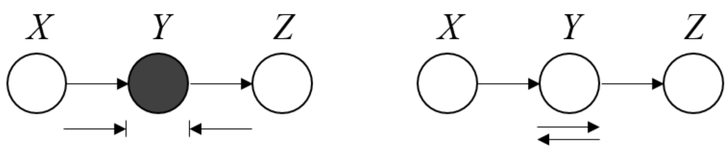


Figure 4.5. Markov chain rule: When Y is observed, balls are blocked (left). When Y is not observed, balls pass through (right)

2. **Two children:** Balls pass through when we do not observe Y, but are blocked otherwise.

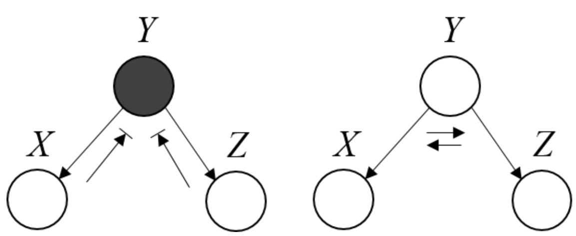


Figure 4.6. Rule when X and Z are Y's children: When Y is observed, balls are blocked (left). When Y is not observed, balls pass through (right)

3. **V-structure:** Balls pass through when we observe Y, but are blocked otherwise.

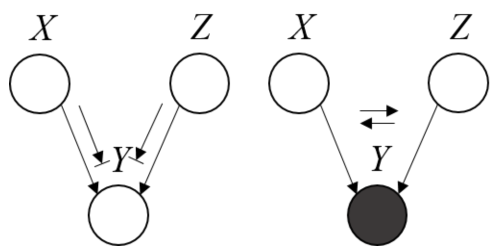


Figure 4.7. V-structure rule: When Y is not observed, balls are blocked (left). When Y is observed, balls pass through (right)

4.3.6 d-separation

We want to answer queries such as, given A, B and C three subsets, is $X_A \perp\!\!\!\perp X_B | X_c$ true? To answer those issues we need the d-separation notion, or directed separation. Indeed it is easy to see that the notion of separation is not enough in a directed graph and needs to be generalized.

Definition 4.10 *Let $a, b \in V$, a chain from a to b is a sequence of nodes, say $(v_1, \ldots, v_n)$ such that $v_1 = a$ and $v_n = b$ and $\forall j, (v_j, v_{j+1}) \in E$ or $(v_j, v_{j+1}) \in E$.*

We can notice that a chain is hence a path in the symmetrized graph, *i.e.* in the graph where if the relation $\rightarrow$ is true then $\leftrightarrow$ is true as well. Assume C is a set that is observed. We want to define a notion of being 'blocked' by this set C in order to answer the underlying question above.

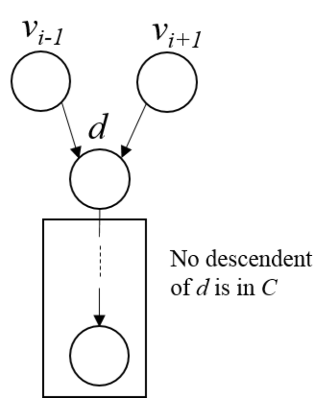


Figure 4.8. D-separation

Definition 4.11 *1. A chain from a et b is blocked at d if:*

- *either $d \in C$ and (v_{i-1}, d, v_{i+1}) is not a V-structure;*
- *or $d \notin C$ and (v_{i-1}, d, v_{i+1}) is a V-structure and no descendants of d is in C.*

2. *A chain from a to b is blocked if and only if it is blocked at any nodes.*

3. *A and B are said to be d-separated by C if and only if all chains that go from $a \in A$ to $b \in B$ are blocked.*

Example 4.3.2 • *(Markov chain) If you try to prove that any set of the future is independent to the past given the present with Markov theory, it might be difficult but the d-separation notion gives the results directly.*

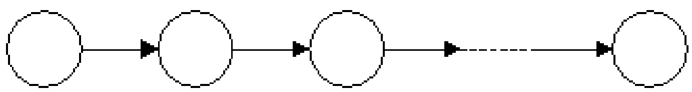


Figure 4.9. Markov chain

- *(Hidden Markov Model) Often used because we only observe a noisy observation of the random process.*

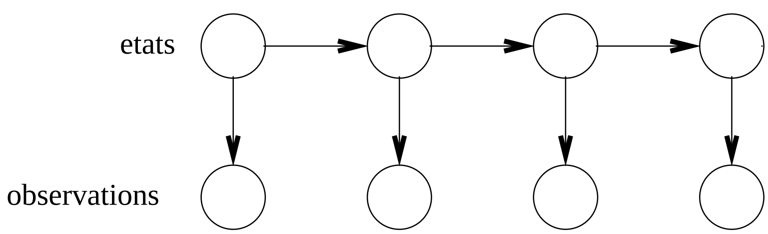


Figure 4.10. Hidden Markov Model

4.4 Undirected graphical models

4.4.1 Definition

Definition 4.12 *Let $G = (V, E)$ be a* **undirected graph***. We denote by $\mathcal{C}$ a set of cliques of G i.e.a set of sets of fully connected vertices. We say that a probability distribution p factorizes in G and denote $p \in \mathcal{L}(G)$ if $p(x)$ is of the form:*

$$p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C) \textit{ with } \psi_C \geq 0, Z = \sum_x \prod_{C \in \mathcal{C}} \psi_C(x_C).$$

The functions ψ_C are not probability distributions like in the directed graphical models. They are called potentials.

Remark 4.4.1 *With the normalization by Z of this expression, we see that the function ψ_C are defined up to a multiplicative constant.*

Remark 4.4.2 *We may restrict $\mathcal{C}$ to $\mathcal{C}_{max}$, the set of maximal cliques.*

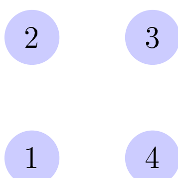
Remark 4.4.3 *This definition can be extended to any function: f is said to factorize in $G \iff f(x) = \prod_{C \in \mathcal{C}} \psi_C(x_C)$.*

4.4.2 Trivial graphs

Empty graphs We consider $G = (V, E)$ with $E = \emptyset$. For $p \in \mathcal{L}(G)$, we get:

$$p(x) = \prod_{i=1}^{n} \psi_i(x_i) \text{ as } \mathcal{C} = \{\{i\} \in V\}$$

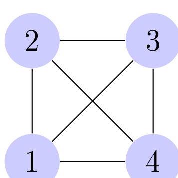
This gives us that $X_1, ..., X_n$ are mutually independent.



Complete graphs We consider $G = (V, E)$ with $\forall i, j \in V, (i, j) \in E$. For $p \in \mathcal{L}(G)$, we get:

$$p(x) = \frac{1}{Z}\psi_V(x_V) \text{ as } \mathcal{C} \text{ is reduced to a single set V}$$

This gives no further information upon the n-sample $X_1, ..., X_n$.



4.4.3 Separation and conditional dependence

Proposition 4.13 *Let $G = (V, E)$ and $G' = (V, E')$ be two undirected graphs.*

$$E \subseteq E' \Rightarrow \mathcal{L}(G) \subseteq \mathcal{L}(G')$$

Definition 4.14 *We say that p satisfies the* **Global Markov property** *w.r.t. G if and only if for all $A, B, S \subset V$ disjoint subsets: A and B are separated by $S \Rightarrow X_A \perp\!\!\!\perp X_B | X_S$.*

Proposition 4.15 *If $p \in \mathcal{L}(G)$ then, p satisfies the Global Markov property w.r.t. G.*

Proof We can consider that A, A', B, B', and S are disjoint sets and $A \cup B \cup S = V$. Without loss of generality as we could replace A and B by :

$$A' = A \cup \{a \in V/a \text{ and } A \text{ are not separated by } S\} \tag{4.14}$$

$$B' = V \setminus \{S \cup A'\} \tag{4.15}$$

A' and B' are separated by S. Note that

$$x_{A \oplus A'} \perp\!\!\!\perp x_{B \oplus B'} | x_S \Rightarrow x_A \perp\!\!\!\perp x_B | x_S \tag{4.16}$$

We consider $C \in \mathcal{C}$. It is not possible to have $C \cap A \neq \emptyset$ and $C \cap B \neq \emptyset$ as A and B are separated by S. Then $C \subset A \cup S$ or $C \subset B \cup S$. Let $\mathcal{D}$ be the set of cliques C such that $C \subset A \cup S$ and $\mathcal{D}'$ the set of all other cliques. We have:

$$p(x) = \frac{1}{Z} \prod_{\substack{C \in \mathcal{C} \\ C \subset A \cup S}} \psi_C(x_C) \prod_{C \in \mathcal{D}'} \psi_C(x_C) = f(x_{A \cup S}) g(x_{B \cup S})$$

$$\begin{aligned} p(x_A | x_S, x_B) &= \frac{p(x_A, x_B, x_S)}{p(x_S, x_B)} = \frac{f(x_A, x_S) g(x_S, x_B)}{\sum_{x'_A} f(x'_A, x_S) g(x_B, x_S)} \\ \text{(removed dependence on } x_B) &= \frac{f(x_A, x_S)}{\sum_{x'_A} f(x'_A, x_S)} \\ &= \frac{p(x_A, x_S)}{p(x_S)} \\ &= p(x_A | x_S) \end{aligned}$$

Thus, $X_A \perp\!\!\!\perp X_B | X_S$. ■

Théorème 4.16 *(Hammersley - Clifford) If $\forall x,\ p(x) > 0$ then $p \in \mathcal{L}(G) \iff p$ satisfies the global Markov property.*

4.4.4 Marginalization

As for directed graphical models, we also have a marginalization notion in undirected graphs. It is slightly different. If $p(x)$ factorizes in G, then $p(x_1, \ldots, x_{n-1})$ factorizes in the graph where the node n is removed and all neighbors are connected.

Proposition 4.17 *Let $G = (V, E)$ be an undirected graph, and $G' = (V', E')$ the graph obtained by marginalizing out n, ie. $V' = V \setminus \{n\}$. Let E' be the set of edge connecting all the neighbors of n. If $p \in \mathcal{L}(G)$ then $p(x_1, ..., x_{n-1}) \in \mathcal{L}(G')$ $\forall n$, so that undirected graphical models are closed under marginalization.*

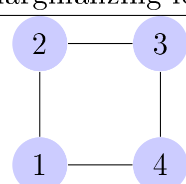
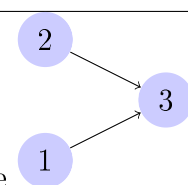
We now introduce the notion of Markov blanket

Definition 4.18 *For $i \in V$, the* **Markov blanket** *is the smallest set of nodes that makes X_i independent to the rest of the graph.*

Remark 4.4.4 *The Markov blanket in an undirected graph for $i \in V$ is the set of its neighbors. For a directed graph, it is the union of all parents, all children and parents of children.*

4.4.5 Relation between directed and undirected graphical models

Since now we have seen that many notions developed for directed graph naturally extended to undirected graphs. The raising question is thus to know whether we can find a theory including both directed and undirected graphs, in particular, is there a way—for instance by symmetrizing the directed graph as we have done repeatedly—to find a general equivalence between those two notions. The answer is no, as we will discuss—though it might work in some special cases described above.

	Directed graphical model	Undirected graphical model
Factorization	$p(x) = \prod_{i=1}^{n} p(x_i \vert x_{\pi_i})$	$p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C)$
Set independence	d-separation $[x_i \perp\!\!\!\perp x_{nd(i) \setminus \pi} \vert x_{\pi_i}]$	separation $[X_A \perp\!\!\!\perp X_B \vert X_S]$
Marginalization	not closed in general, only when marginalizing leaf nodes	closed
Difference	grid 	v-structure 

Let G be DAG. Can we find G' undirected such that $\mathcal{L}(G) = \mathcal{L}(G')$? $\mathcal{L}(G) \subset \mathcal{L}(G')$?

Definition 4.19 *Let $G = (V, E)$ be a* DAG*. The* **symmetrized graph** *of G is $\tilde{G} = (V, \tilde{E})$, with $\tilde{E} = \{(u, v), (v, u) / (u, v) \in E\}$, ie. an edge going the opposite direction is added for every edge in E.*

Definition 4.20 *Let $G = (V, E)$ be a* DAG*. The* **moralized graph** *$\bar{G}$ of G is the symmetrized graph $\tilde{G}$, where we add edge such that for all $v \in V$, π_v is a clique.*

We admit the following proposition:

Proposition 4.21 *Let G be a* DAG *without any V-structure, then $\bar{G} = \tilde{G}$ and $\mathcal{L}(G) = \mathcal{L}(\tilde{G}) = \mathcal{L}(\bar{G})$.*

In case there is a V-structure in the graph, we can only conclude:

Proposition 4.22 *Let G be a* DAG, *then* $\mathcal{L}(G) \subset \mathcal{L}(\bar{G})$.

$\bar{G}$ is minimal for the number of edges in the set H of undirected graphs such that $\mathcal{L}(G) \subset \mathcal{L}(H)$.

Not all conditional independence structure for random variables can be factorized in a graphical model (directed or undirected).