Data Mining 2020
Bayesian Networks (1)

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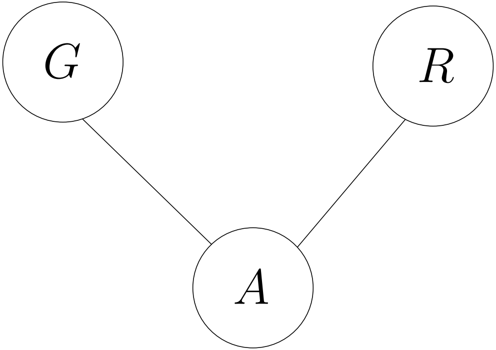
Do you like noodles?

		Do you like noodles?	
Race	Gender	Yes	No
Black	Male	10	40
	Female	30	20
White	Male	100	100
	Female	120	80

Do you like noodles? Undirected



$$G \perp\!\!\!\perp R \mid A$$

Strange: Gender and Race are prior to Answer, but this model says they are independent *given* Answer!

Do you like noodles?

Marginal table for Gender and Race:

	Race	
Gender	Black	White
Male	50	200
Female	50	200

From this table we conclude that Race and Gender are independent in the data.

cpr(G,R)$=1$

Do you like noodles?

Table for Gender and Race given Answer=yes:

	Race	
Gender	Black	White
Male	10	100
Female	30	120

cpr(G,R) = 0.4

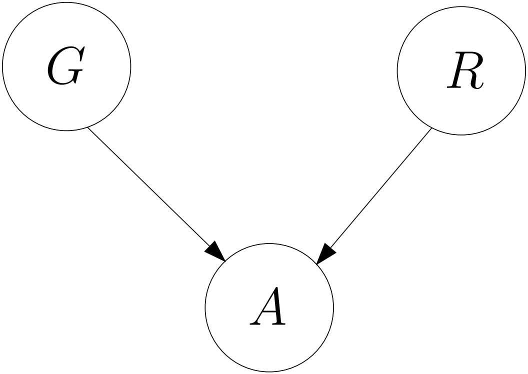
Table for Gender and Race given Answer=no:

	Race	
Gender	Black	White
Male	40	100
Female	20	80

cpr(G,R)=1.6

From these tables we conclude that Race and Gender are dependent given Answer.

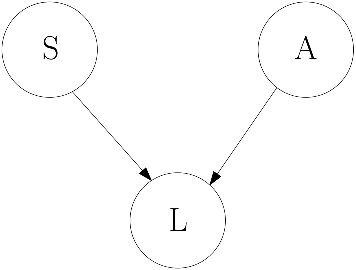
Do you like noodles? Directed



$$G \perp\!\!\!\perp R, \quad G \not\!\perp\!\!\!\perp R \mid A$$

Gender and Race are marginally independent
(but *dependent* given Answer).

Explaining away



- Smoking (S) and asbestos exposure (A) are independent, but become dependent if we observe that someone has lung cancer (L).
- If we observe L, this raises the probability of both S and A.
- If we subsequently observe S, then the probability of A drops (explaining away effect).

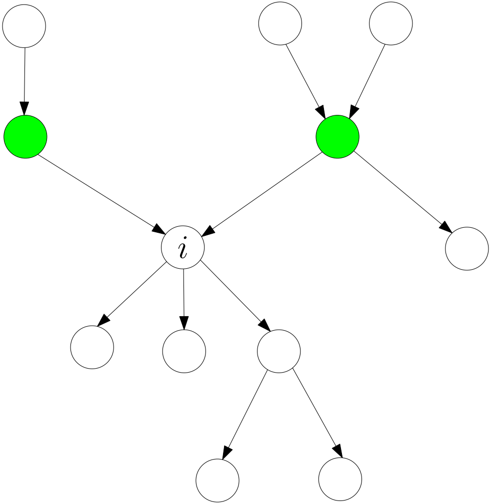
Directed Independence Graphs

$G = (K, E)$, K is a set of vertices and E is a set of edges with *ordered* pairs of vertices.

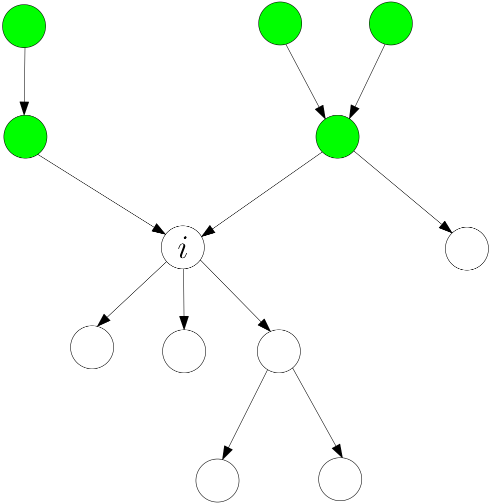
- No directed cycles (DAG)
- parent/child
- ancestor/descendant
- ancestral set

Because G is a DAG, there exists a *complete ordering* of the vertices that is respected in the graph (edges point from lower ordered to higher ordered nodes).

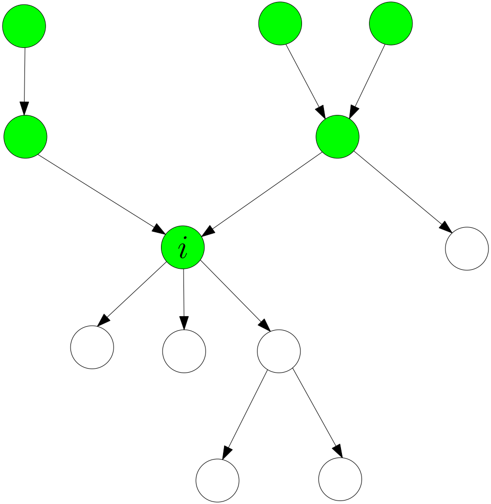
Parents Of Node i: pa(i)



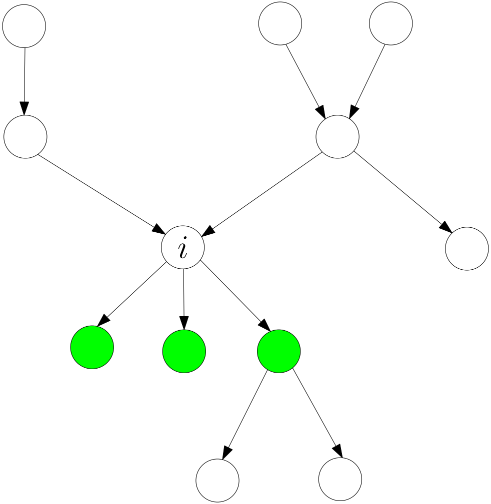
Ancestors Of Node i: an(i)



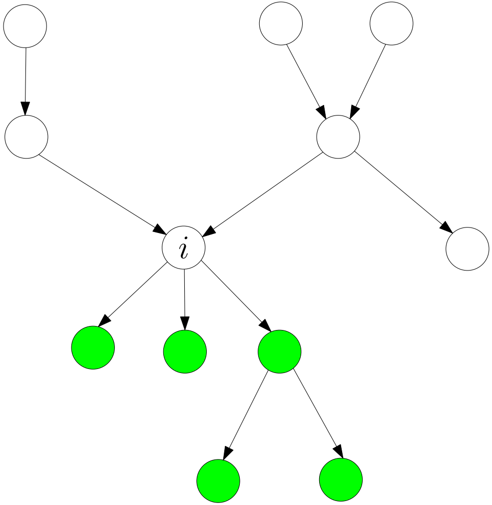
Ancestral Set Of Node i: $\text{an}^+(i)$



Children Of Node i: ch(i)



Descendants Of Node i: de(i)



Construction of DAG

Suppose that *prior knowledge* tells us the variables can be labeled $X_1, X_2, \ldots, X_k$ such that X_i is prior to X_{i+1}.
(for example: causal or temporal ordering)

Corresponding to this ordering we can use the product rule to factorize the joint distribution of $X_1, X_2, \ldots, X_k$ as

$$P(X) = P(X_1)P(X_2 \mid X_1) \cdots P(X_k \mid X_{k-1}, X_{k-2}, \ldots, X_1)$$

Note that:

1. This is an identity of probability theory, no independence assumptions have been made yet!
2. The joint probability of any initial segment $X_1, X_2, \ldots, X_j$ $(1 \leq j \leq k)$ is given by the corresponding initial segment of the factorization.

Constructing a DAG from pairwise independencies

Starting from the complete graph (containing arrows $i \rightarrow j$ for all $i < j$) an arrow from i to j is removed if $P(X_j \mid X_{j-1}, \ldots, X_1)$ does not depend on X_i, in other words, if

$$j \perp\!\!\!\perp i \mid \{1, \ldots, j\} \setminus \{i, j\}$$

More loosely

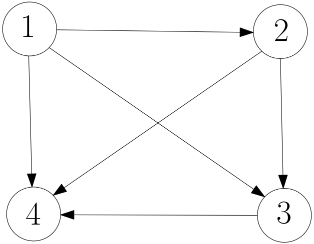
$$\boxed{j \perp\!\!\!\perp i \mid \text{prior variables}}$$

Compare this to pairwise independence

$$\boxed{j \perp\!\!\!\perp i \mid \text{rest}}$$

in undirected independence graphs.

Construction Of DAG

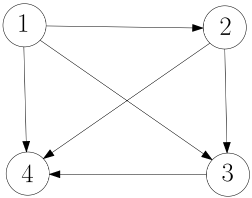


$$P(X) = P(X_1)P(X_2|X_1)P(X_3|X_1,X_2)P(X_4|X_1,X_2,X_3)$$

Suppose the following independencies are given:

1. $X_1 \perp\!\!\!\perp X_2$
2. $X_4 \perp\!\!\!\perp X_3|(X_1,X_2)$
3. $X_1 \perp\!\!\!\perp X_3|X_2$

Construction Of DAG

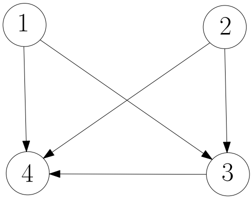


$$P(X) = P(X_1)\underbrace{P(X_2|X_1)}_{P(X_2)}P(X_3|X_1,X_2)P(X_4|X_1,X_2,X_3)$$

1. If $X_1 \perp\!\!\!\perp X_2$, then $P(X_2|X_1) = P(X_2)$.

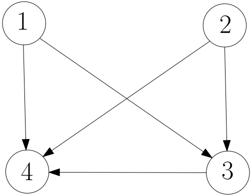
The edge $1 \rightarrow 2$ is removed.

Construction Of DAG



$$P(X) = P(X_1)P(X_2)P(X_3|X_1, X_2)P(X_4|X_1, X_2, X_3)$$

Construction Of DAG

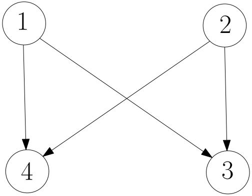


$$P(X) = P(X_1)P(X_2)P(X_3|X_1,X_2)\underbrace{P(X_4|X_1,X_2,X_3)}_{P(X_4|X_1,X_2)}$$

2. If $X_4 \perp\!\!\!\perp X_3 | (X_1, X_2)$, then $P(X_4|X_1,X_2,X_3) = P(X_4|X_1,X_2)$.

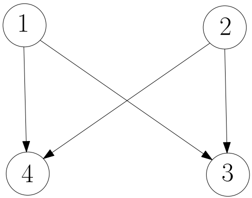
The edge $3 \rightarrow 4$ is removed.

Construction Of DAG



$$P(X) = P(X_1)P(X_2)P(X_3|X_1, X_2)P(X_4|X_1, X_2)$$

Construction Of DAG



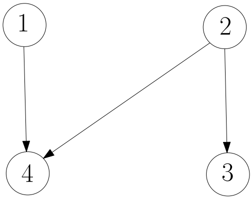
$$P(X) = P(X_1)P(X_2)\underbrace{P(X_3|X_1,X_2)}_{P(X_3|X_2)}P(X_4|X_1,X_2)$$

3. If $X_1 \perp\!\!\!\perp X_3|X_2$, then $P(X_3|X_1,X_2) = P(X_3|X_2)$

The edge $1 \to 3$ is removed.

Construction Of DAG

We end up with this independence graph and corresponding factorization:



$$P(X) = P(X_1)P(X_2)P(X_3|X_2)P(X_4|X_1, X_2)$$

Joint probability distribution of Bayesian Network

We can write the joint probability distribution more elegantly as

$$\boxed{P(X_1, \ldots, X_k) = \prod_{i=1}^{k} P(X_i \mid X_{pa(i)})}$$

Independence Properties of DAGs: d-separation and Moral Graphs

Can we infer other/stronger independence statements from the directed graph like we did using separation in the undirected graphical models?

Yes, the relevant concept is called d-separation.

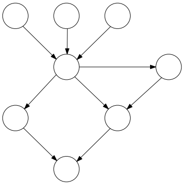
- establishing d-separation directly (Pearl)
- establishing d-separation via the moral graph and "normal" separation

We discuss the second approach.

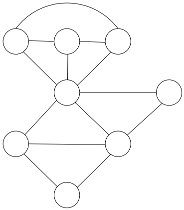
Independence Properties of DAGs: Moral Graph

Given a DAG $G = (K, E)$ we construct the moral graph G^m by marrying parents, and deleting directions, that is,

1. For each $i \in K$, we connect all vertices in $\text{pa}(i)$ with undirected edges.
2. We replace all directed edges in E with undirected ones.



DAG



Moral Graph

Independence Properties of DAGs: Moral Graph

The directed independence graph G possesses the conditional independence properties of its associated moral graph G^m. Why?

We have the factorisation:

$$
\begin{aligned}
P(X) &= \prod_{i=1}^{k} P(X_i \mid X_{pa(i)}) \\
&= \prod_{i=1}^{k} g_i(X_i, X_{pa(i)})
\end{aligned}
$$

by setting $g_i(X_i, X_{pa(i)}) = P(X_i \mid X_{pa(i)})$.

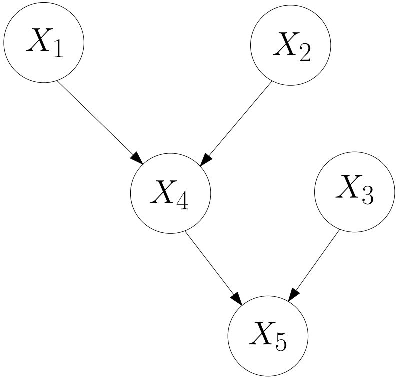
Independence Properties of DAGs: Moral Graph

We have the factorisation:

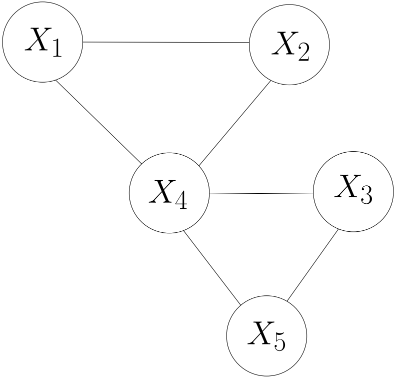
$$P(X) = \prod_{i=1}^{k} g_i(X_i, X_{pa(i)})$$

- We thus have a factorisation of the joint probability distribution in terms of functions $g_i(X_{a_i})$ where $a_i = \{i\} \cup pa(i)$.
- By application of the factorisation criterion the sets a_i become cliques in the undirected independence graph.
- These cliques are formed by moralization.

Moralisation: Example



Moralisation: Example



$\{i\} \cup pa(i)$ becomes a complete subgraph in the moral graph (by marrying all unmarried parents).

Moralisation Continued

Warning: the complete moral graph can obscure independencies!

To verify

$$i \perp\!\!\!\perp j \mid S$$

construct the moral graph of the induced subgraph on:

$$A = \mathrm{an}^+(\{i, j\} \cup S),$$

that is, A contains i, j, S and all their ancestors.

Let $G = (K, E)$ and $A \subseteq K$. The induced subgraph G_A contains nodes A and edges E', where

$$i \rightarrow j \in E' \Leftrightarrow i \rightarrow j \in E \text{ and } i \in A \text{ and } j \in A.$$

Moralisation Continued

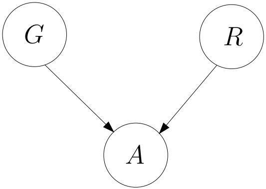
Since for $\ell \in A$, $pa(\ell) \in A$, we know that the joint distribution of X_A is given by

$$P(X_A) = \prod_{\ell \in A} P(X_\ell \mid X_{pa(\ell)})$$

which corresponds to the subgraph G_A of G.

1. This is a product of factors $P(X_\ell | X_{pa(\ell)})$, involving the variables $X_{\{\ell\} \cup pa(\ell)}$ only.
2. So it factorizes according to G_A^m, and thus the independence properties for undirected graphs apply.
3. Hence, if S separates i from j in G_A^m, then $i \perp\!\!\!\perp j \mid S$.

Full moral graph may obscure independencies: example

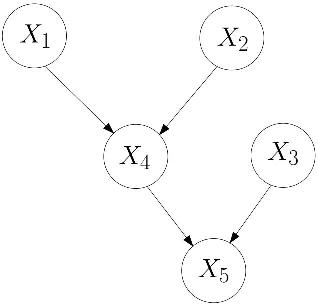


$$P(G,R,A) = P(G)P(R)P(A \mid G,R)$$

Does $G \perp\!\!\!\perp R$ hold? Summing out A we obtain:

$$\begin{aligned}
P(G,R) &= \sum_a P(G,R,A=a) && \text{(sum rule)}\\
&= \sum_a P(G)P(R)P(A=a \mid G,R) && \text{(BN factorisation)}\\
&= P(G)P(R)\sum_a P(A=a \mid G,R) && \text{(rule of summation)}\\
&= P(G)P(R) && (\textstyle\sum_a P(A=a \mid G,R) = 1)
\end{aligned}$$

Poll

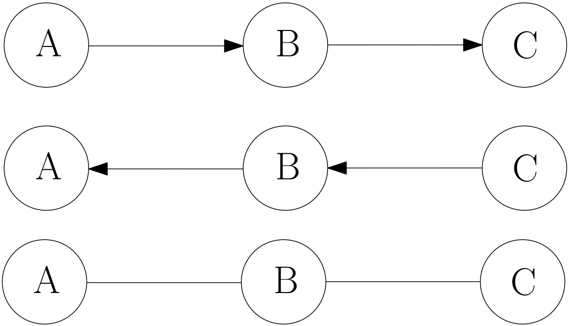


1. Are X_3 and X_4 independent?
2. Are X_1 and X_3 independent?
3. Are X_3 and X_4 independent given X_5?
4. Are X_1 and X_3 independent given X_5?

Equivalence

When no marrying of parents is required (there are no “immoralities” or “v-structures”), then the independence properties of the directed graph are identical to those of its undirected version.

These three graphs express the same independence properties:



Learning Bayesian Networks

1. Parameter learning: structure known/given; we only need to estimate the conditional probabilities from the data.
2. Structure learning: structure unknown; we need to learn the networks structure as well as the corresponding conditional probabilities from the data.

Maximum Likelihood Estimation

Find value of unknown parameter(s) that maximize the probability of the observed data.

n independent observations on binary variable $X \in \{1, 2\}$. We observe $n(1)$ outcomes $X = 1$ and $n(2) = n - n(1)$ outcomes $X = 2$.
What is the maximum likelihood estimate of $p(1)$?
The likelihood function (probability of the data) is given by:

$$L = p(1)^{n(1)}(1 - p(1))^{n-n(1)}$$

Taking the log we get

$$\mathcal{L} = n(1) \log p(1) + (n - n(1)) \log(1 - p(1))$$

Maximum Likelihood Estimation

Take derivative with respect to $p(1)$, equate to zero, and solve for $p(1)$.

$$\frac{d\mathcal{L}}{dp(1)} = \frac{n(1)}{p(1)} - \frac{n - n(1)}{1 - p(1)} = 0,$$

since $\frac{d \log x}{dx} = \frac{1}{x}$ (where log is the natural logarithm).

Solving for $p(1)$, we get

$$p(1) = \frac{n(1)}{n}.$$

This is just the fraction of one's in the sample!

ML Estimation of Multinomial Distribution

Let $X \in \{1, 2, \ldots, J\}$.

Estimate the probabilities $p(1), p(2), \ldots, p(J)$ of getting outcomes $1, 2, \ldots, J$. If in n trials, we observe $n(1)$ outcomes of 1, $n(2)$ of 2, ..., $n(J)$ of J, then the obvious guess is to estimate

$$p(j) = \frac{n(j)}{n}, \qquad j = 1, 2, \ldots, J.$$

This is indeed the maximum likelihood estimate.

BN-Factorisation

For a given BN-DAG, the joint distribution factorises according to

$$P(X) = \prod_{i=1}^{k} p(X_i \mid X_{pa(i)})$$

So to specify the distribution we have to estimate the probabilities

$$p(X_i \mid X_{pa(i)}) \qquad\qquad i = 1, 2, \ldots, k$$

for the conditional distribution of each variable given its parents.

ML Estimation of BN

The joint probability for n independent observations is

$$P(X^{(1)}, \ldots, X^{(n)}) = \prod_{j=1}^{n} P(X^{(j)})$$
$$= \prod_{j=1}^{n} \prod_{i=1}^{k} p(X_i^{(j)} \mid X_{pa(i)}^{(j)}),$$

where $X^{(j)}$ denotes the j-th row in the data table.

The likelihood function is therefore given by

$$L = \prod_{i=1}^{k} \prod_{x_i, x_{pa(i)}} p(x_i \mid x_{pa(i)})^{n(x_i, x_{pa(i)})}$$

where $n(x_i, x_{pa(i)})$ is a count of the number of records with $X_i = x_i$, and $X_{pa(i)} = x_{pa(i)}$.

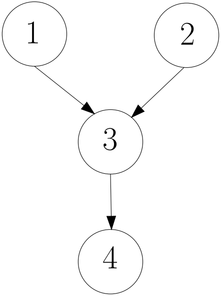
ML Estimation of BN

Taking the log of the likelihood function, we get

$$\boxed{\mathcal{L} = \sum_{i=1}^{k} \sum_{x_i, x_{pa(i)}} n(x_i, x_{pa(i)}) \log p(x_i \mid x_{pa(i)})}$$

- Maximize the log-likelihood function with respect to the unknown parameters $p(x_i \mid x_{pa(i)})$.
- This decomposes into a collection of independent multinomial estimation problems.
- Separate estimation problem for each X_i and configuration of $X_{pa(i)}$.

Example BN and Factorisation



$$P(X_1, X_2, X_3, X_4) = p_1(X_1)p_2(X_2)p_{3|12}(X_3|X_1, X_2)p_{4|3}(X_4|X_3)$$

Example BN: Parameters

$$P(X_1, X_2, X_3, X_4) = p_1(X_1)p_2(X_2)p_{3|12}(X_3|X_1, X_2)p_{4|3}(X_4|X_3)$$

Now we have to estimate the following parameters (X_4 ternary, rest binary):

$$p_1(1) \qquad p_1(2) = 1 - p_1(1)$$

$$p_2(1) \qquad p_2(2) = 1 - p_2(1)$$

$$\begin{array}{ll}
p_{3|1,2}(1|1,1) & p_{3|1,2}(2|1,1) = 1 - p_{3|1,2}(1|1,1) \\
p_{3|1,2}(1|1,2) & p_{3|1,2}(2|1,2) = 1 - p_{3|1,2}(1|1,2) \\
p_{3|1,2}(1|2,1) & p_{3|1,2}(2|2,1) = 1 - p_{3|1,2}(1|2,1) \\
p_{3|1,2}(1|2,2) & p_{3|1,2}(2|2,2) = 1 - p_{3|1,2}(1|2,2)
\end{array}$$

$$\begin{array}{lll}
p_{4|3}(1|1) & p_{4|3}(2|1) & p_{4|3}(3|1) = 1 - p_{4|3}(1|1) - p_{4|3}(2|1) \\
p_{4|3}(1|2) & p_{4|3}(2|2) & p_{4|3}(3|2) = 1 - p_{4|3}(1|2) - p_{4|3}(2|2)
\end{array}$$

Example Data Set

obs	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	1	1	1
3	1	1	2	1
4	1	2	2	1
5	1	2	2	2
6	2	1	1	2
7	2	1	2	3
8	2	1	2	3
9	2	2	2	3
10	2	2	1	3

Maximum Likelihood Estimation

obs	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	1	1	1
3	1	1	2	1
4	1	2	2	1
5	1	2	2	2
6	2	1	1	2
7	2	1	2	3
8	2	1	2	3
9	2	2	2	3
10	2	2	1	3

$$\hat{p}_1(1) = \frac{n(x_1 = 1)}{n} = \frac{5}{10} = \frac{1}{2}$$

Maximum Likelihood Estimation

obs	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	1	1	1
3	1	1	2	1
4	1	2	2	1
5	1	2	2	2
6	2	1	1	2
7	2	1	2	3
8	2	1	2	3
9	2	2	2	3
10	2	2	1	3

$$\hat{p}_2(1) = \frac{n(x_2 = 1)}{n} = \frac{6}{10}$$

Maximum Likelihood Estimation

obs	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	1	1	1
3	1	1	2	1
4	1	2	2	1
5	1	2	2	2
6	2	1	1	2
7	2	1	2	3
8	2	1	2	3
9	2	2	2	3
10	2	2	1	3

$$\hat{p}_{3|1,2}(1|1,1) = \frac{n(x_1 = 1, x_2 = 1, x_3 = 1)}{n(x_1 = 1, x_2 = 1)} = \frac{2}{3}$$

Maximum Likelihood Estimation

obs	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	1	1	1
3	1	1	2	1
4	1	2	2	1
5	1	2	2	2
6	2	1	1	2
7	2	1	2	3
8	2	1	2	3
9	2	2	2	3
10	2	2	1	3

$$\hat{p}_{3|1,2}(1|1,1) = \frac{n(x_1 = 1, x_2 = 1, x_3 = 1)}{n(x_1 = 1, x_2 = 1)} = \frac{2}{3}$$

ML Estimation of BN

The maximum likelihood estimate of $p(x_i \mid x_{pa(i)})$ is given by:

$$\boxed{\hat{p}(x_i \mid x_{pa(i)}) = \frac{n(x_i, x_{pa(i)})}{n(x_{pa(i)})},}$$

where

- $n(x_i, x_{pa(i)})$ is the number of records in the data with $X_i = x_i$ and $X_{pa(i)} = x_{pa(i)}$, and
- $n(x_{pa(i)})$ is the number of records in the data with $X_{pa(i)} = x_{pa(i)}$.