



Bayesian networks

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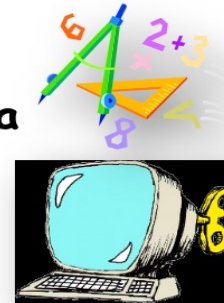
In a nutshell



Raw data



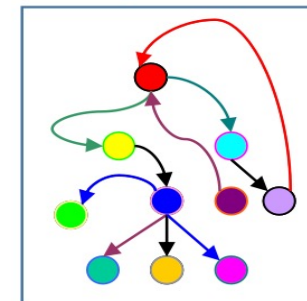
Cleaned data



Machine Learning



Statistical Methods



Network inference

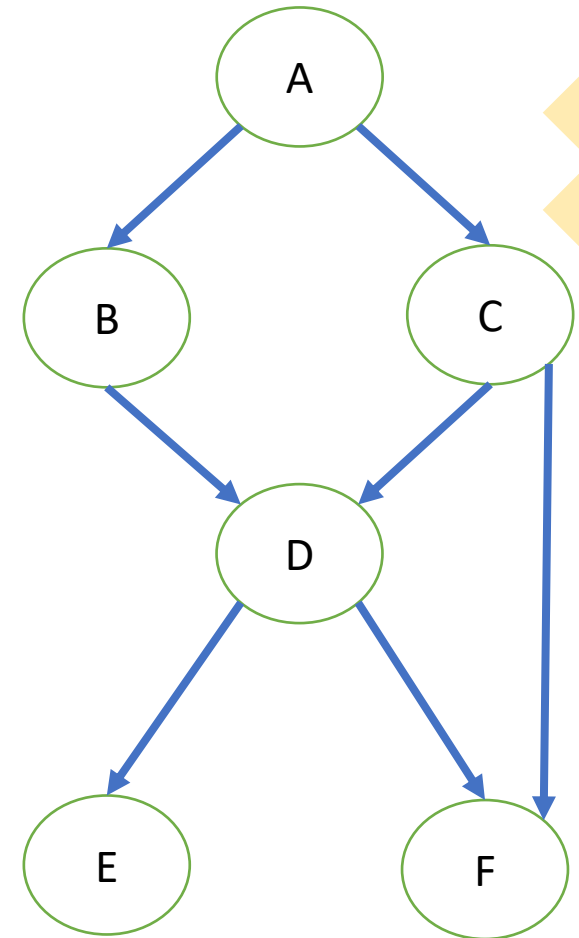
So, we aim to estimate the network structure, determining what depends on what and how, in the form of a network.

Discrete Data: Train Use Survey

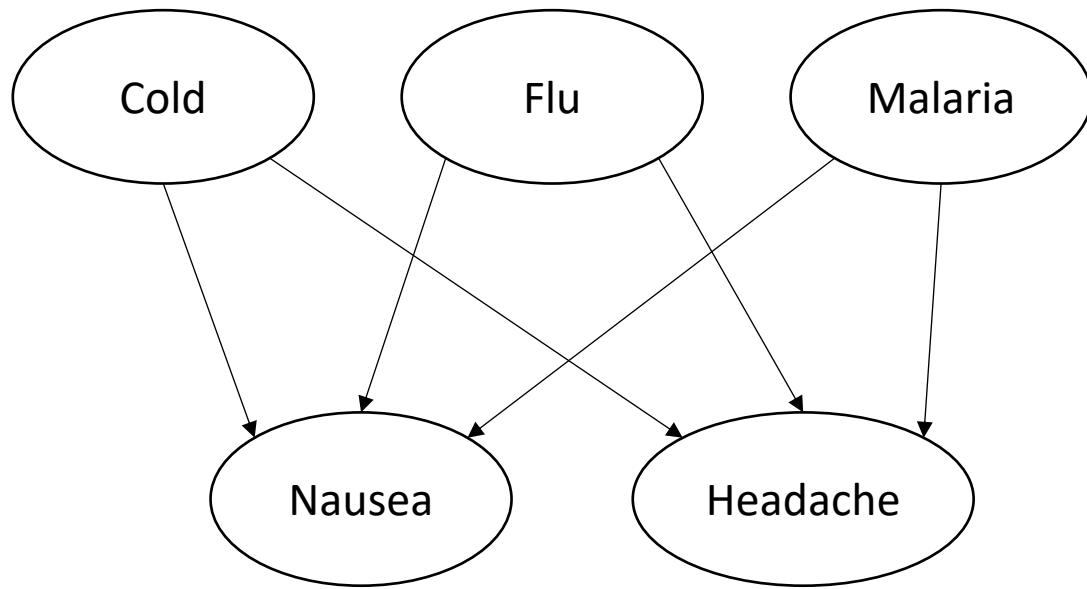
| • "Age" | "Residence" | "Education" | "Occupation" | "Sex" | "Travel" |
|-----------|-------------|-------------|--------------|-------|----------|
| • "adult" | "big" | "high" | "emp" | "F" | "car" |
| • "adult" | "small" | "uni" | "emp" | "M" | "car" |
| • "adult" | "big" | "uni" | "emp" | "F" | "train" |
| • "adult" | "big" | "high" | "emp" | "M" | "car" |
| • "adult" | "big" | "high" | "emp" | "M" | "car" |
| • "adult" | "small" | "high" | "emp" | "F" | "train" |
| • "adult" | "big" | "high" | "emp" | "F" | "car" |
| • "young" | "big" | "uni" | "emp" | "F" | "train" |

Bayesian networks (BNs)

- **Marriage between** graph theory and probability theory.
- **Nodes** represent **variables** and **edges** represent **(conditional) dependence** between variables.
- Bayesian Networks are **directed networks**.
- If the directions of the dependencies are important in your project, go for a Bayesian network.



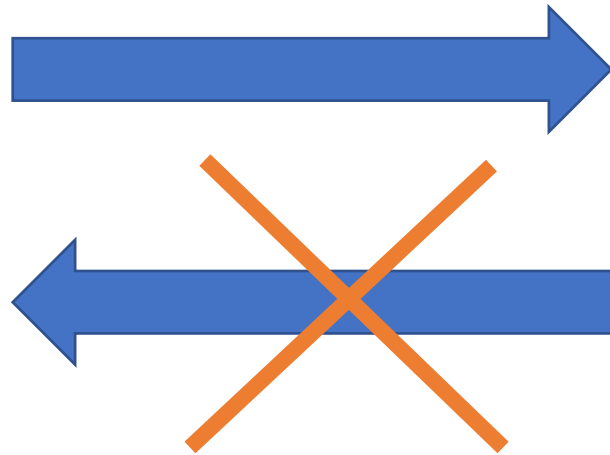
Example 1:



- A Bayesian network could represent the **probabilistic relationships** between **diseases** and **symptoms**.
- Bayesian network with causes (diseases) Cold, Flu, and Malaria and effects (symptoms) Nausea and Headache.

Note

Causal
Network



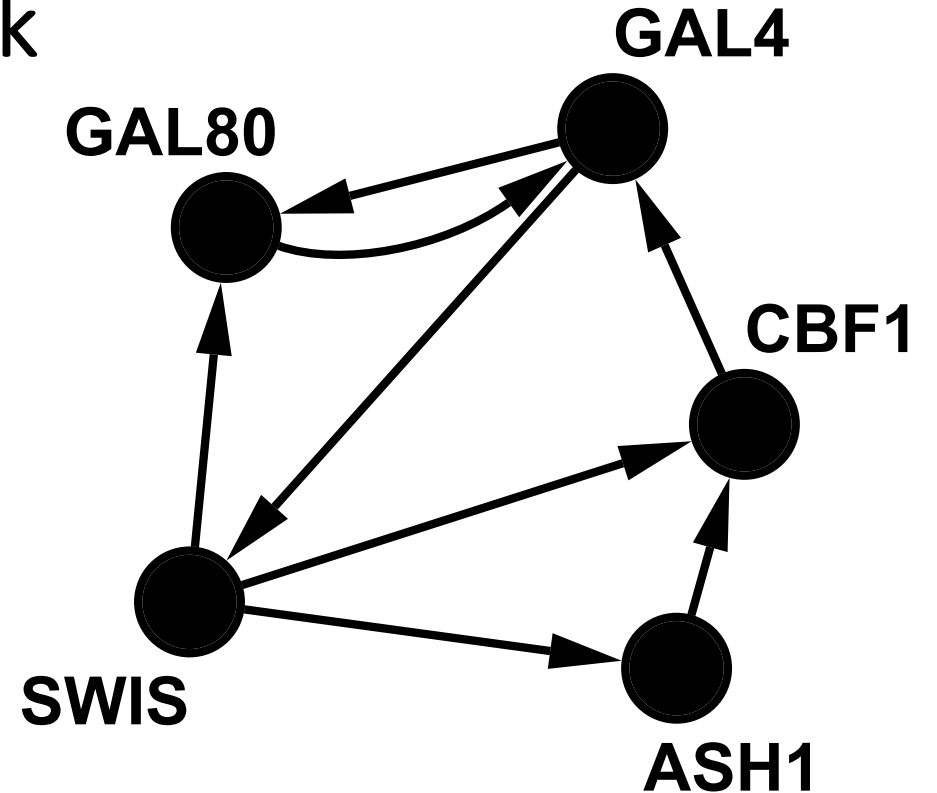
Not necessarily

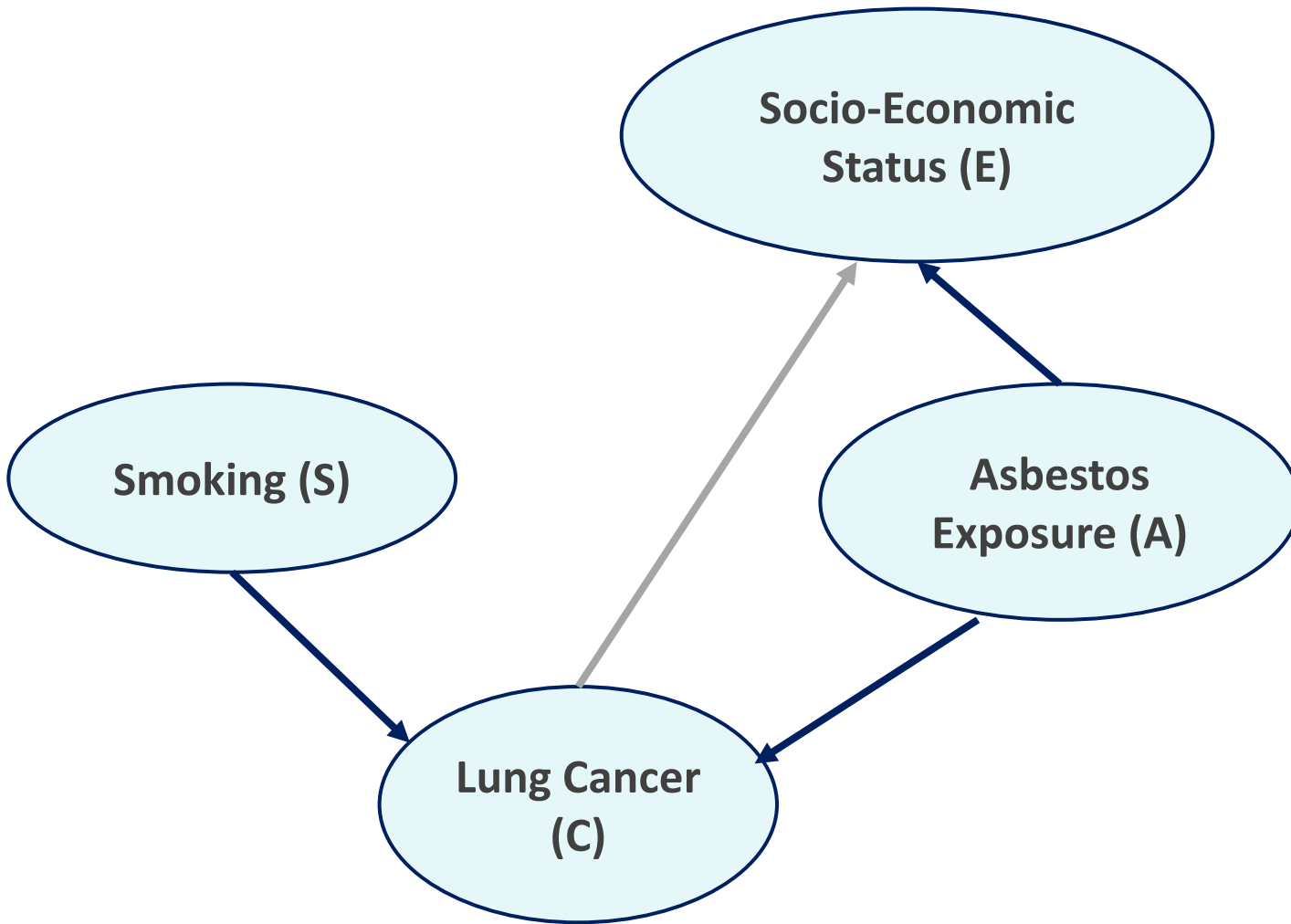
Bayesian
Network

Example 2: Gene regularity network

Network of $n = 5$ genes in *Saccharomyces cerevisiae* (yeast). The data obtained from synthetically designed yeast cells grown with different carbon sources: galactose (“switch on”) or glucose (“switch off”), Cantone et al. (2009).

- Dynamic Bayesian Network Models



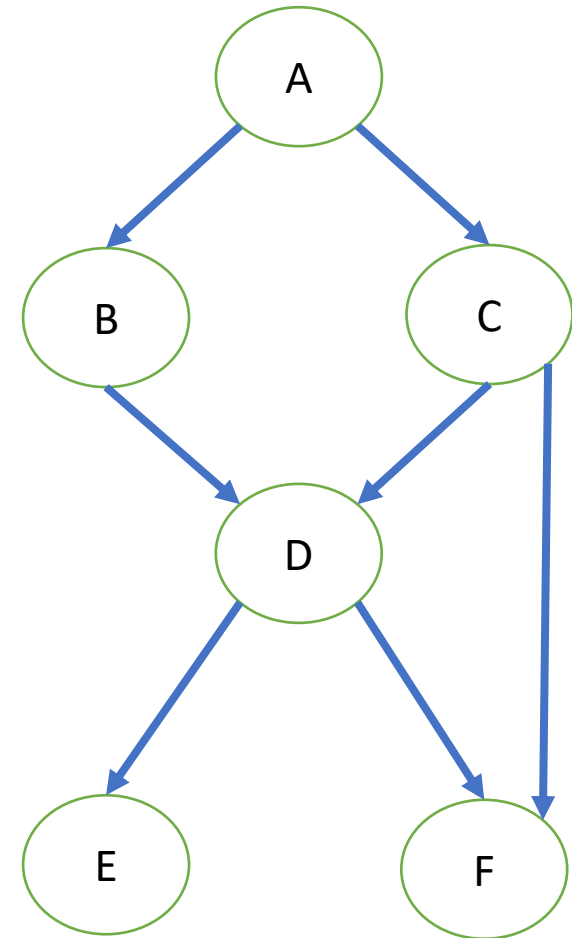


Some applications of BNs

- Biology (Gene Regulatory Network, ...)
- Medicine
- Document Classification. ...
- Image Processing. ...
- Spam Filter
-

See here:

<https://data-flair.training/blogs/bayesian-network-applications/>



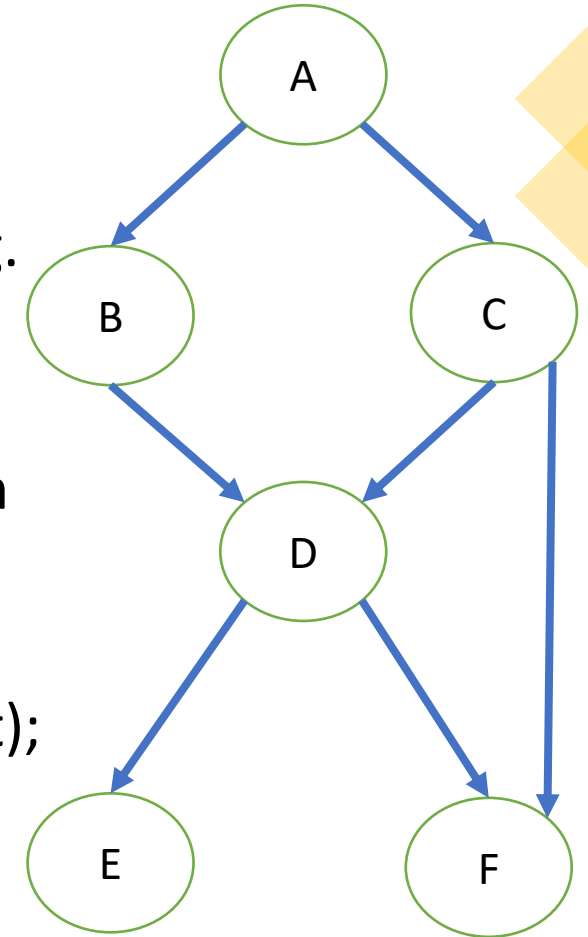
Bayesian networks

- **The first component** of a BN is a graph.

A graph G is a mathematical object with:

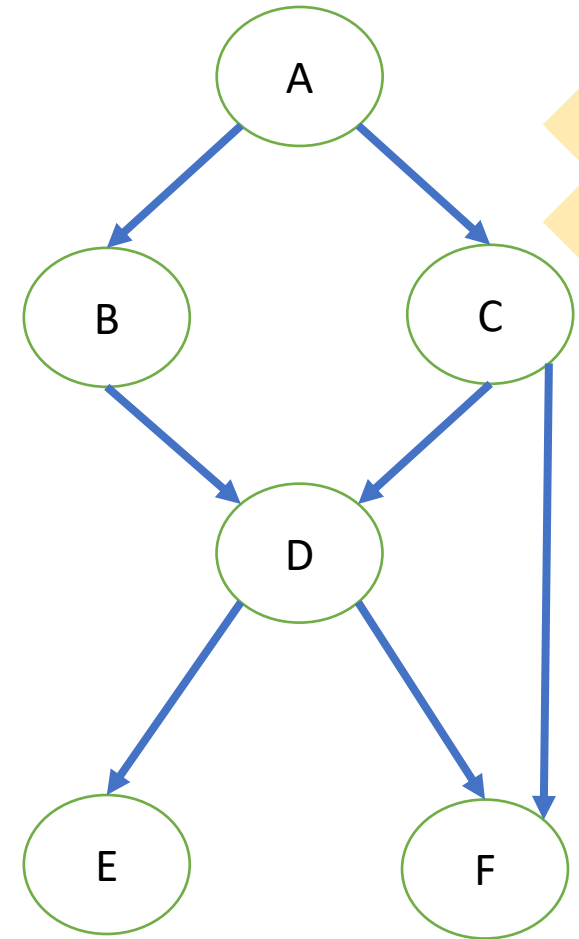
- a set of nodes $V = \{v_1, \dots, v_N\}$;
- a set of **arcs** A which are identified by pairs of nodes in V , e.g. $a_{ij} = (v_i, v_j)$.

- **The second component** of a BN is the probability distribution $P(X)$, should be such that the BN:
 - can be learned efficiently from data;
 - is flexible (distributional assumptions should not be too strict);
 - is easy to query to perform inference.



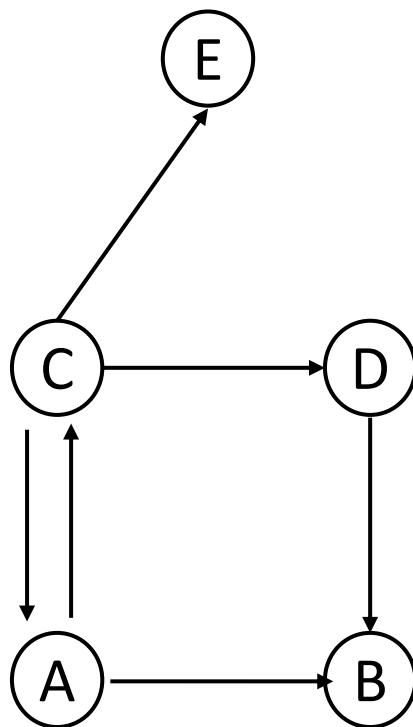
Static Bayesian network as Directed Acyclic Graph (DAG)

- contains only **directed** arcs and does not contain any loops/cycle.

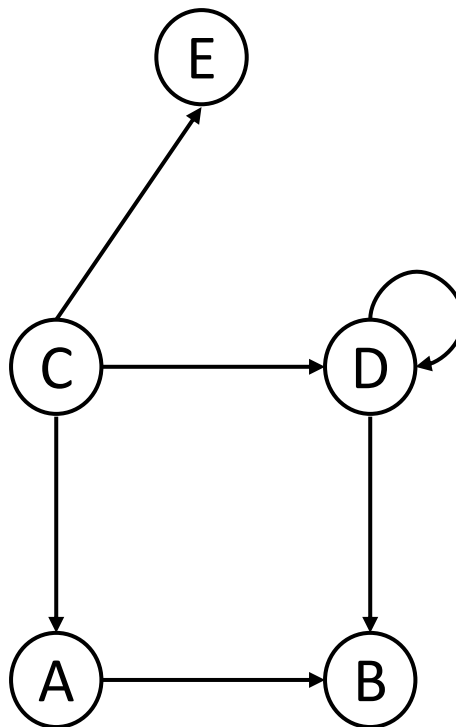


DAG: Which one is a Directed acyclic graph(No loops/no cycle)?

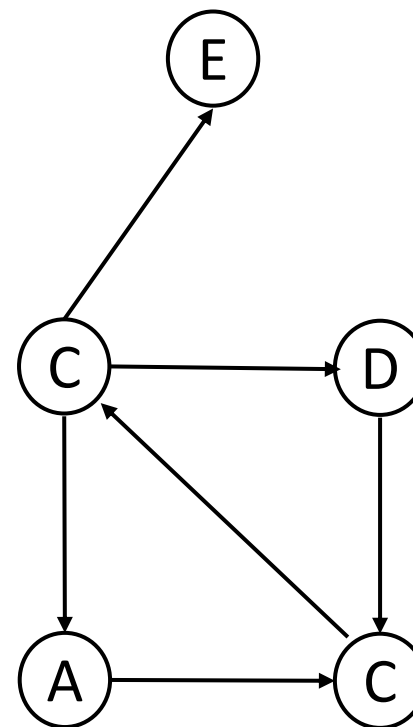
1



2

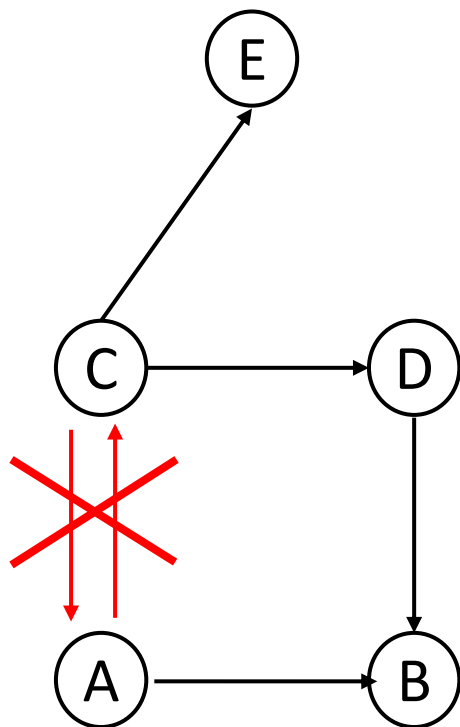


3

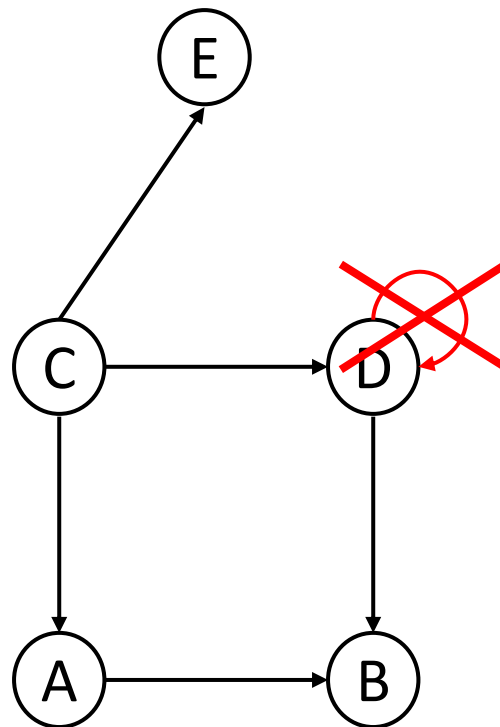


DAG: Directed acyclic graph: No loops/no cycle

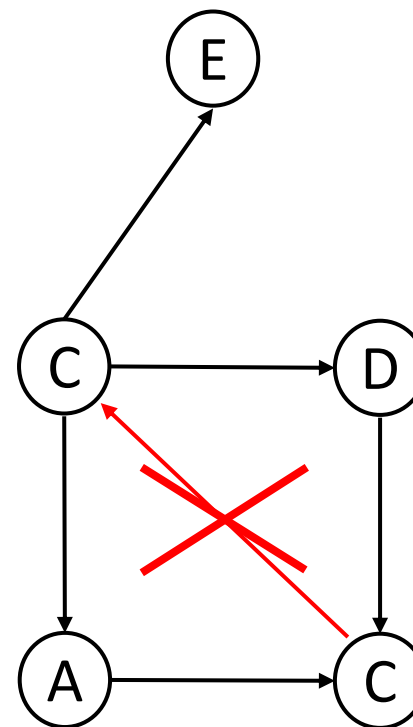
1



2

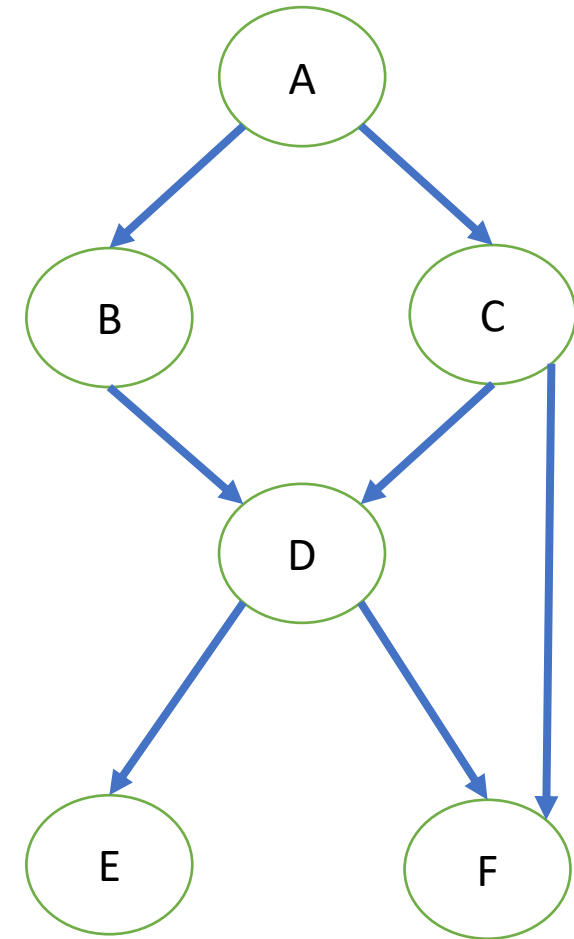


3



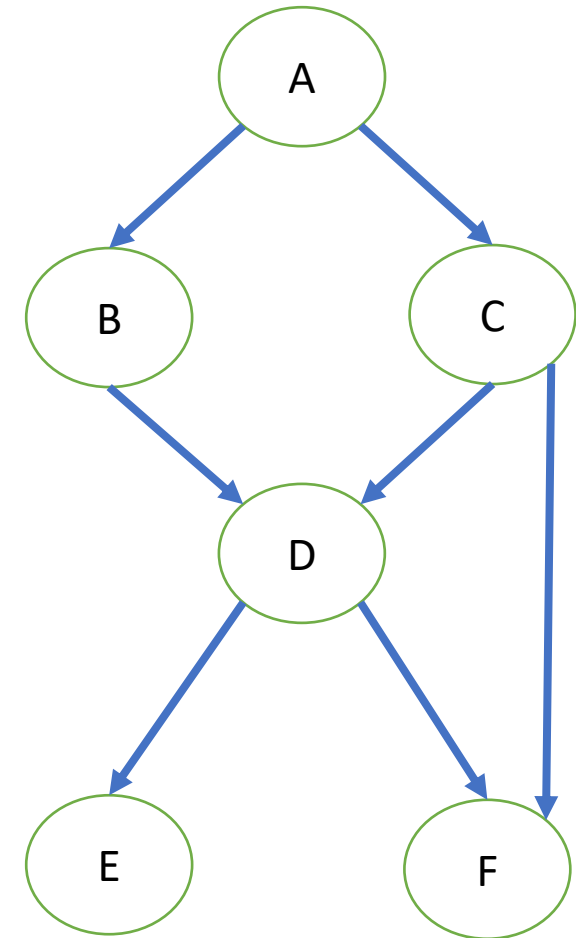
Interpretation of edges in BNs

- If there is an **edge** from one variable to another, **the later depends on the former**.
- Variables that **are not linked (lack of edges)** are **conditionally independent**.



Bayesian networks

- A is a **parent** node of B .
- B is a **child** node of A .
- The **parent node set** of D is the set $\{B, C\}$.
- D is a **common child** node of B and C .
- A has **no parents**. That is the parent set of A is an empty set.
- (B, C) is a **(co-)parent** node of D (another parent).

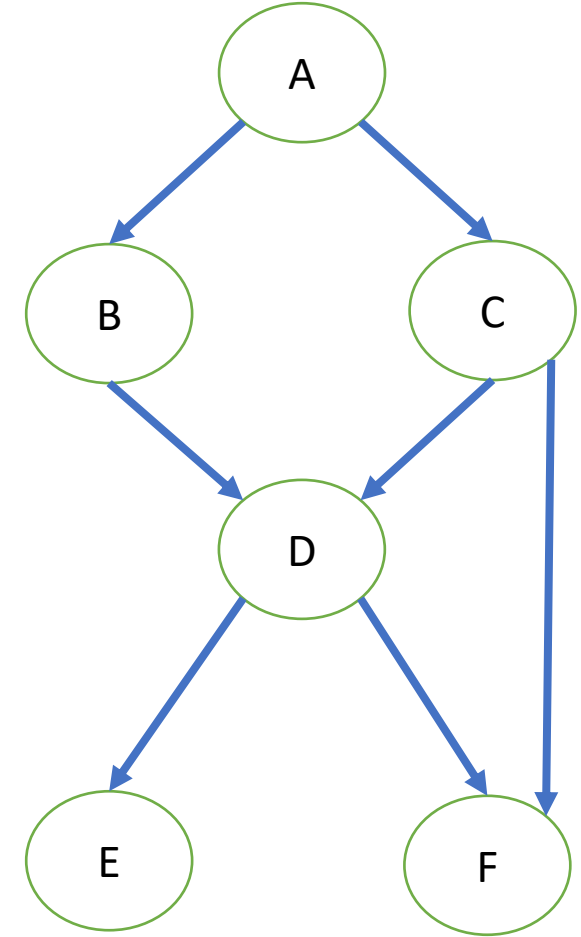


Bayesian networks

- Node X is an **ancestor** of node Y if there is a **path** of directed edges leading from X to Y :

$$X \rightarrow \dots \rightarrow Y$$

- Y is then called a **descendant** of X .



Bayesian networks and Markov assumption

- **Markov assumption** leads to a factorization of the joint probability distribution:

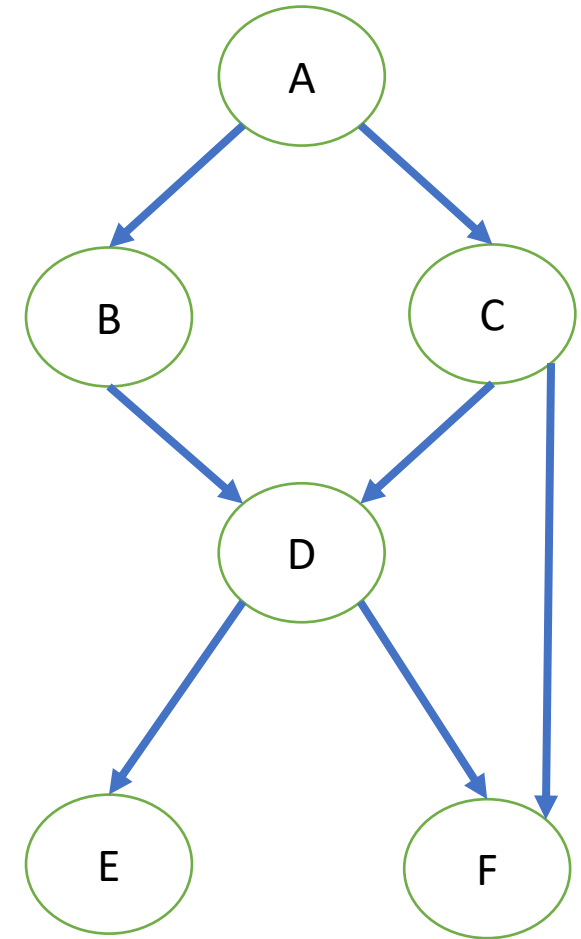
$$P(A, B, C, D, E, F) =$$

$$P(A) P(B|A) P(C|A) P(D|B, C) P(E|D) P(F|C, D)$$

→ $P(\text{child} | \text{parent(s)})$

- **Markov assumption:**

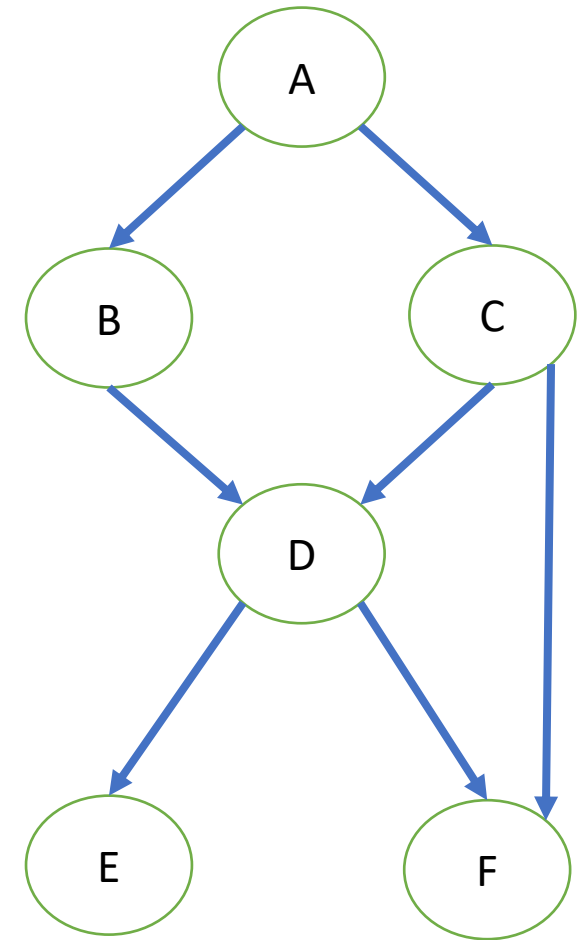
Every **node** in a Bayesian network is **conditionally independent** of its non-descendants, given its parents (only the parents).



Bayesian networks and Markov assumption

Which node is conditionally independent of node D given D's parent nodes?

- a. $A \perp\!\!\!\perp D \mid \{B, C\}$
- b. $E \perp\!\!\!\perp D \mid \{B, C\}$
- c. $F \perp\!\!\!\perp D \mid \{B, C\}$



Example: Train Use Survey

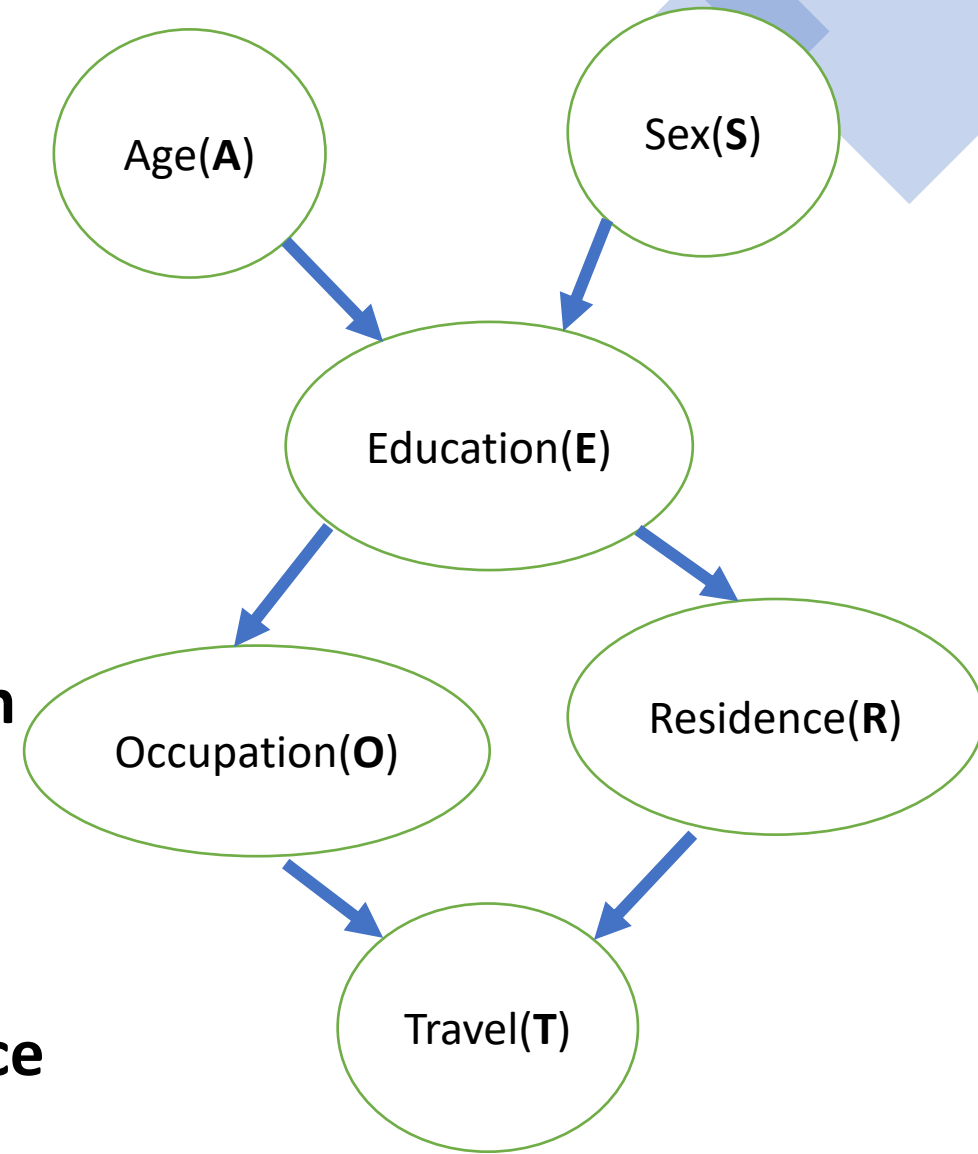
- Consider a survey whose aim is to **investigate the usage patterns** of different means of **transport**, with a **focus** on **cars** and **trains**.
- Such surveys are used to assess **customer satisfaction** across different social groups, to evaluate public policies or for urban planning.
- Some other real-world examples can also be found, in **Kenett et al. (2012)**.

Data: Train Use Survey

| Age | Residence | Education | Occupation | Sex | Travel |
|-----------|-----------|-----------|------------|-----|---------|
| • "adult" | "big" | "high" | "emp" | "F" | "car" |
| • "adult" | "small" | "uni" | "emp" | "M" | "car" |
| • "adult" | "big" | "uni" | "emp" | "F" | "train" |
| • "adult" | "big" | "high" | "emp" | "M" | "car" |
| • "adult" | "big" | "high" | "emp" | "M" | "car" |
| • "adult" | "small" | "high" | "emp" | "F" | "train" |
| • "adult" | "big" | "high" | "emp" | "F" | "car" |
| • "young" | "big" | "uni" | "emp" | "F" | "train" |

Example: Train Use Survey

- **Age** and **sex** are not influenced by any other variable.
- **Age** and **sex** have a direct influence on **Education**.
- **Education** strongly influences both **occupation** and **residence**
- **Transports** are directly influenced by both **occupation** and **residence**.
- This **DAG** represents the **dependence relationships** between: **Age** , **Sex**, **Education**, **Occupation**, **Residence** and **Travel**.



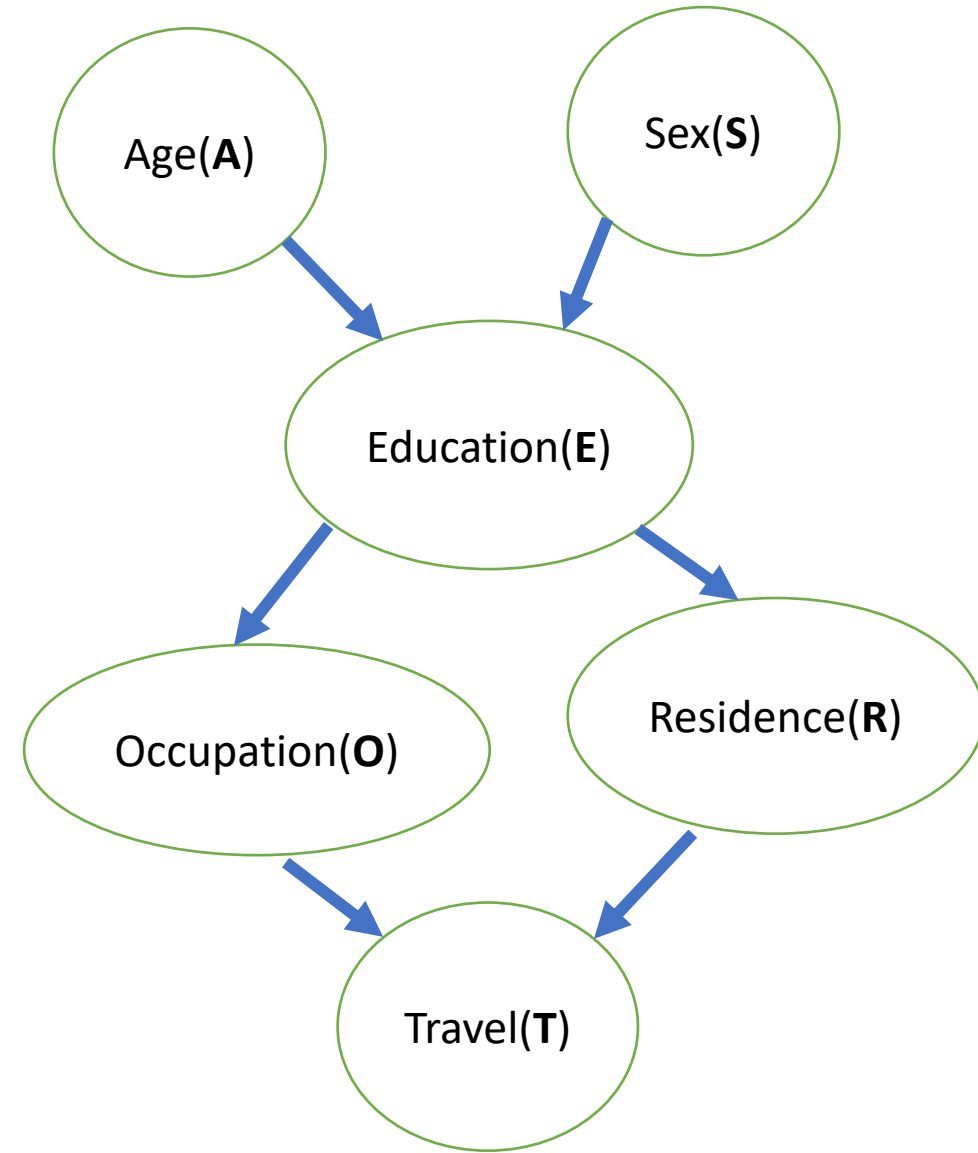
Example: Train Use Survey

The probabilistic relationship:

[A] [S] [E | A:S] [O | E] [R | E] [T | O:R]

[child | parents]

This type of representation
is what we will see when we use
bnlearn package in practical.

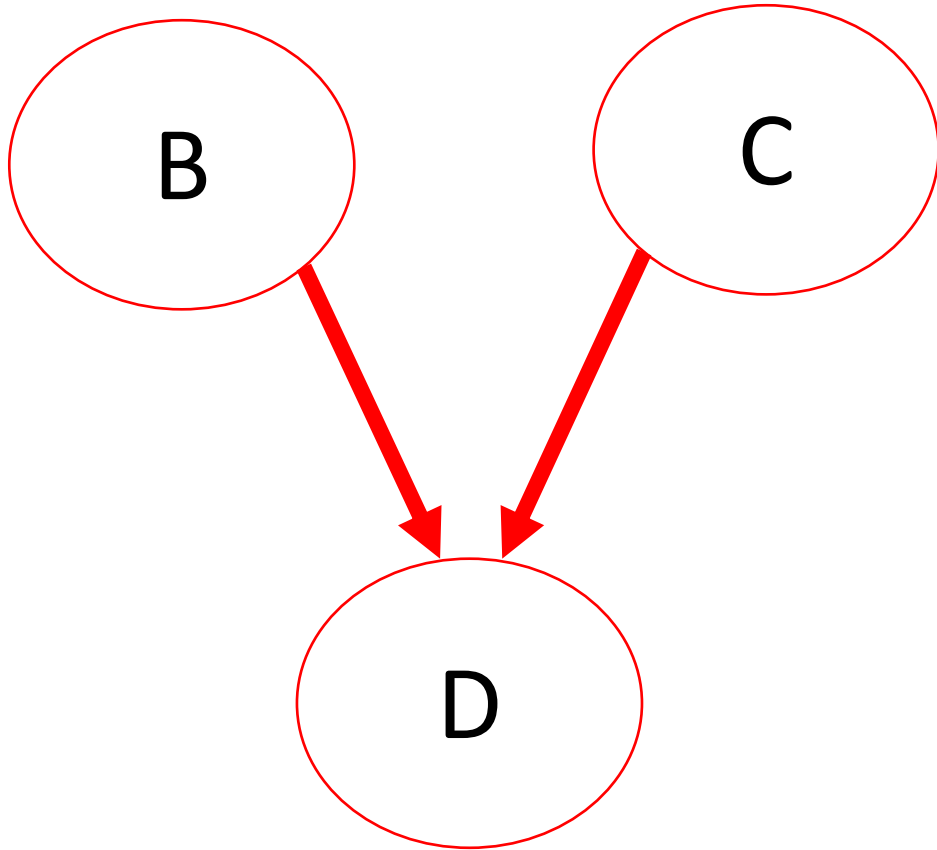


- Think about the application of this concept in your field for a few minutes and discuss that in pairs.
- Consider the following questions for reflection in your field:
 - ✓ What variables are present in your potential project?
 - ✓ Why are these variables important?
 - ✓ What motivates your interest in understanding their interdependencies?
 - ✓ How does this understanding contribute to your work or goals?

Some terminologies

v-structure

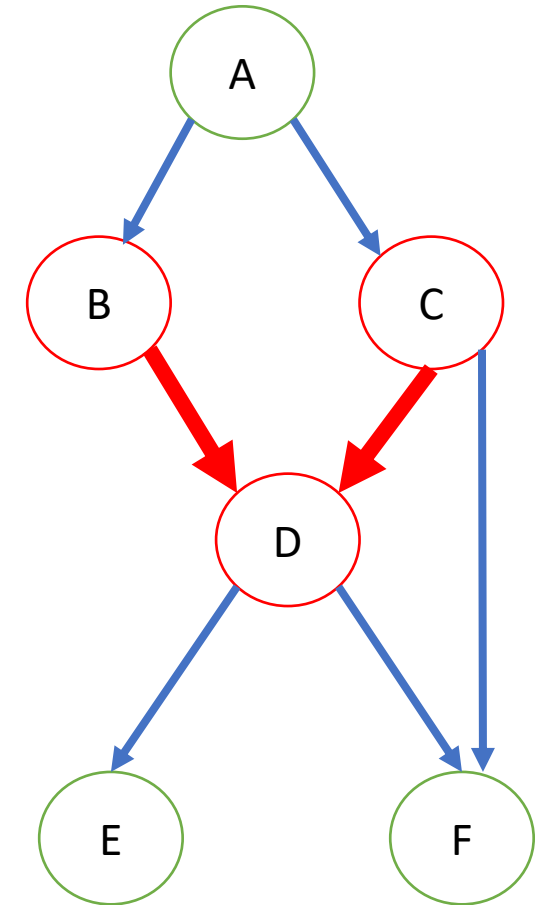
Important for interpretation



v-structure

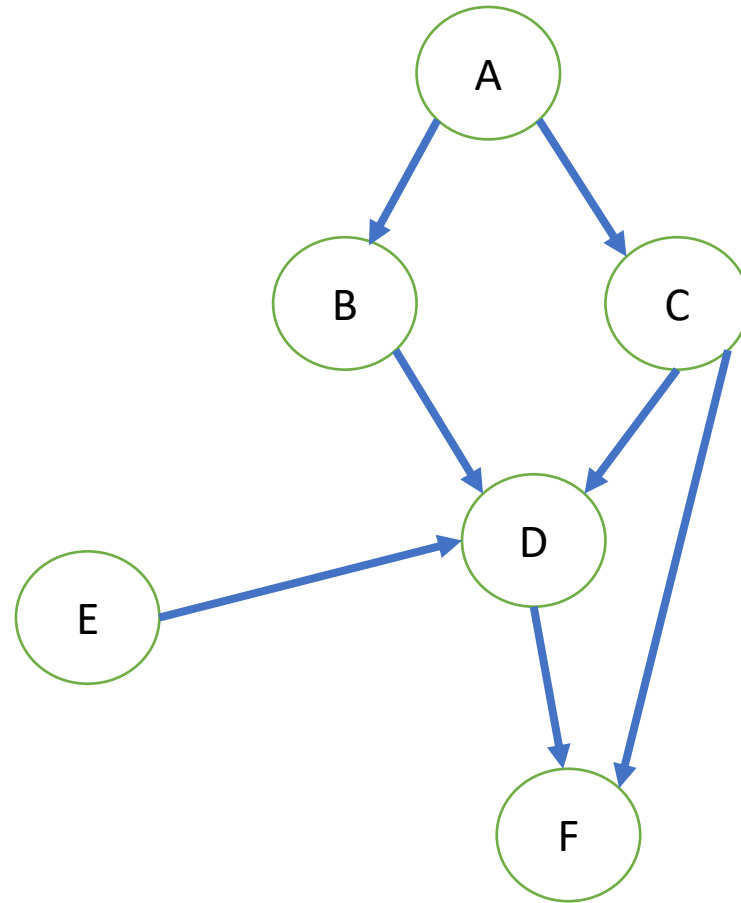
Important for interpretation

- D has the parent nodes B and C, and there is no connection between the nodes **B** and **C**.



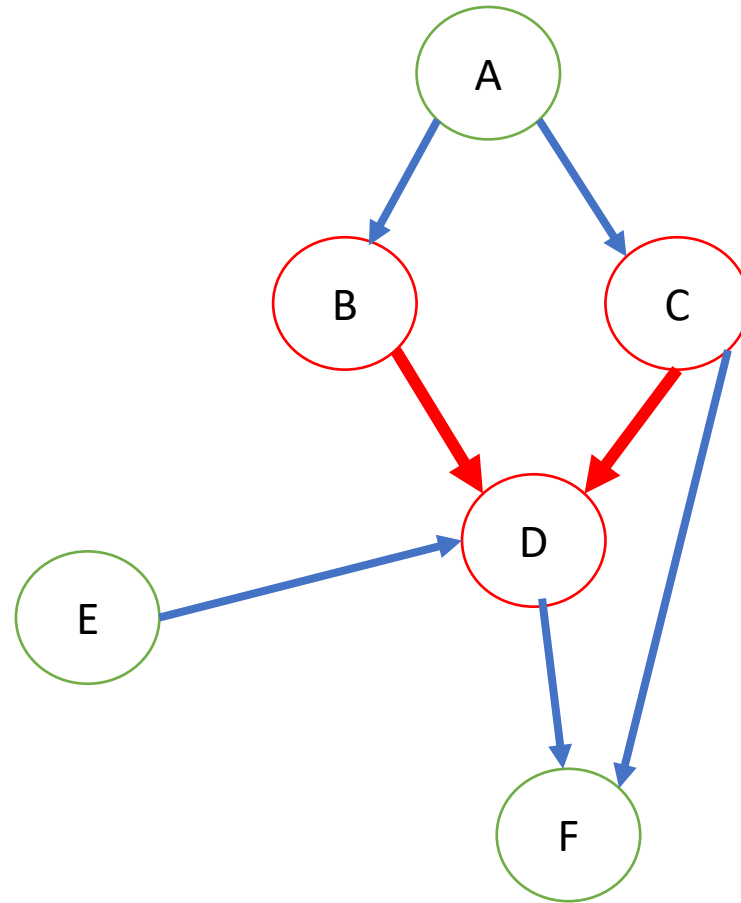
v-structure

How many v-structures do you see?



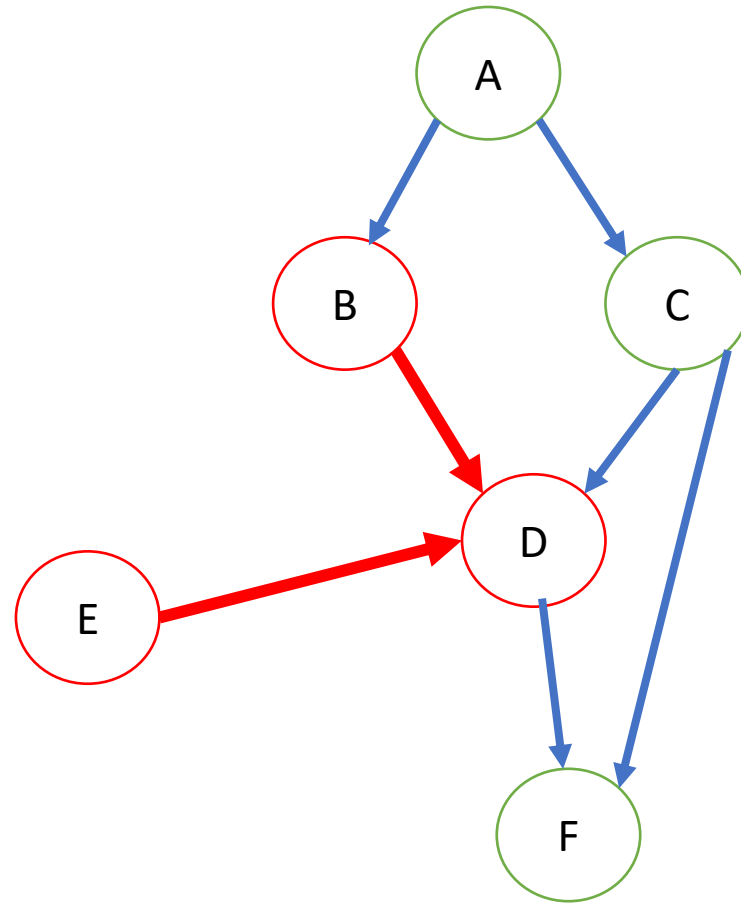
v-structure

1



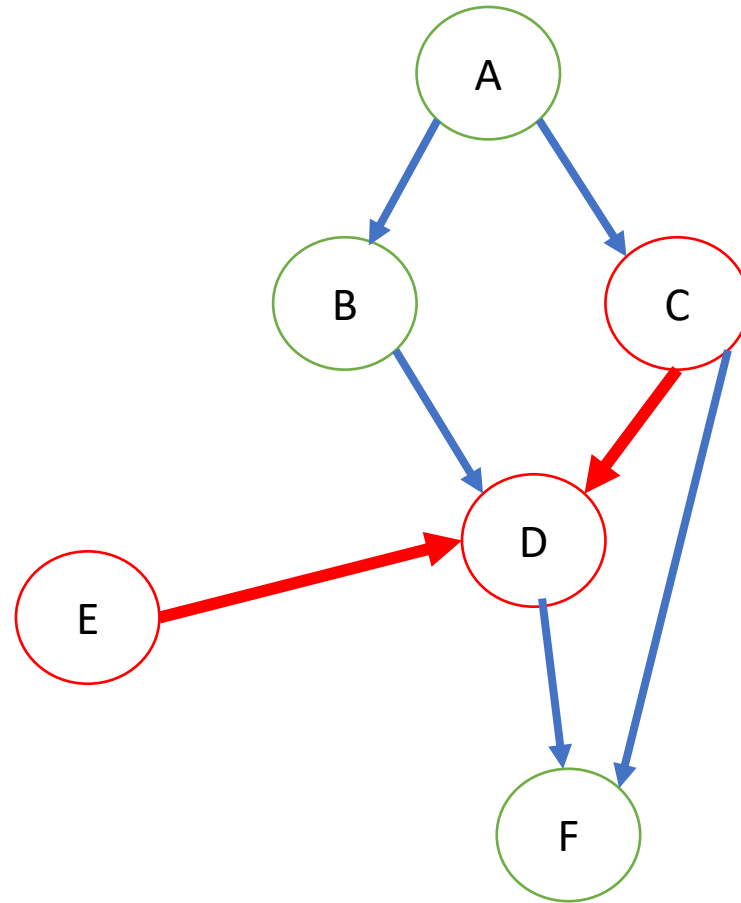
v-structure

2



v-structure

3



Markov Blanket

Graph \mathbf{G} has n nodes, $\mathbf{X}_1, \dots, \mathbf{X}_n$.

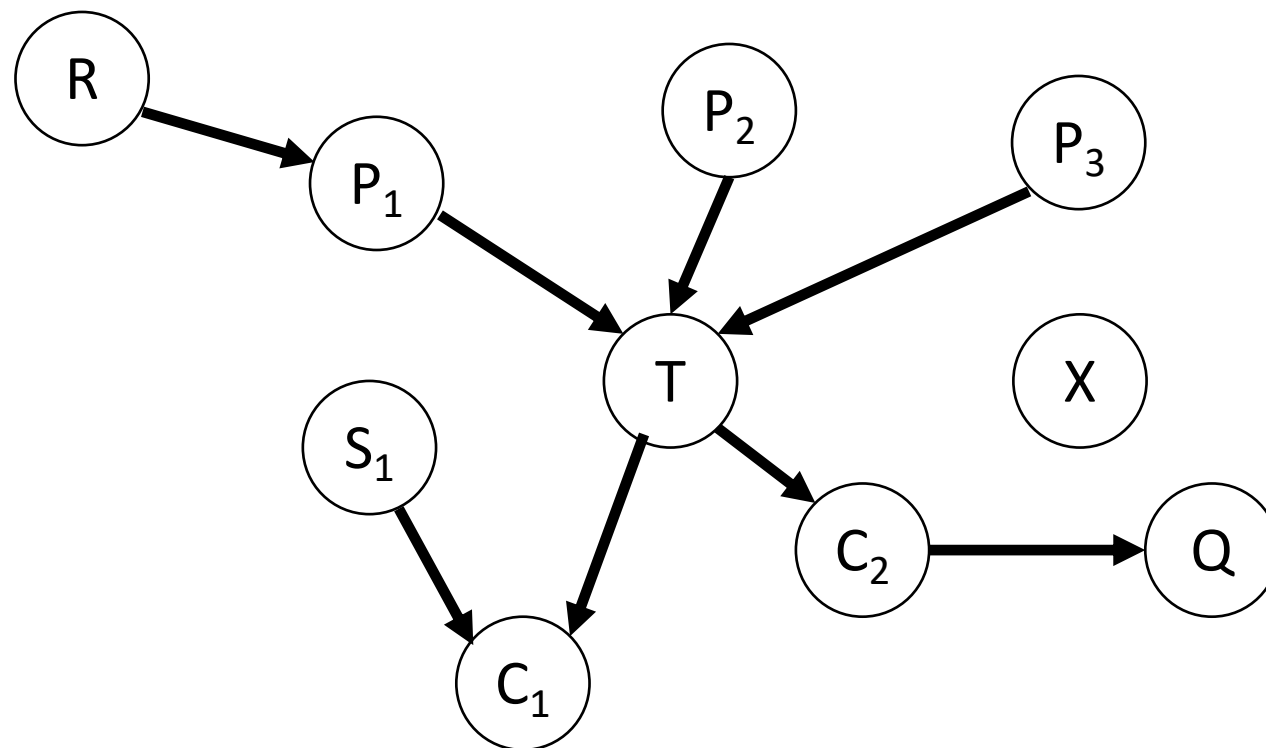
The Markov blanket of the node X_i ($i = 1, \dots, n$) includes:

- **all parent** nodes of X_i
- **all child** nodes of X_i
- **all "co-parent"** nodes of X_i

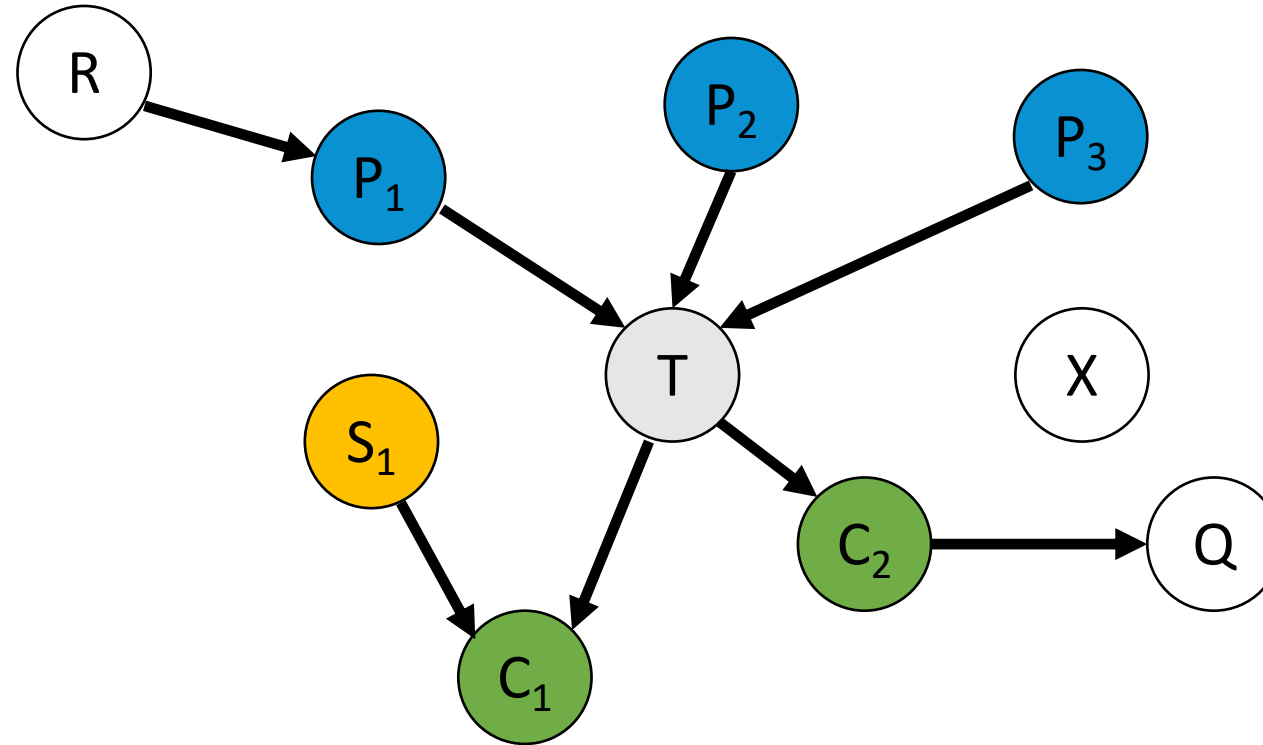
We denote the **Markov Blanket** of X_i symbolically as **MB**(X_i).

Using **bnlearn** package, **mb()** function can be used to show the Markov blankets.

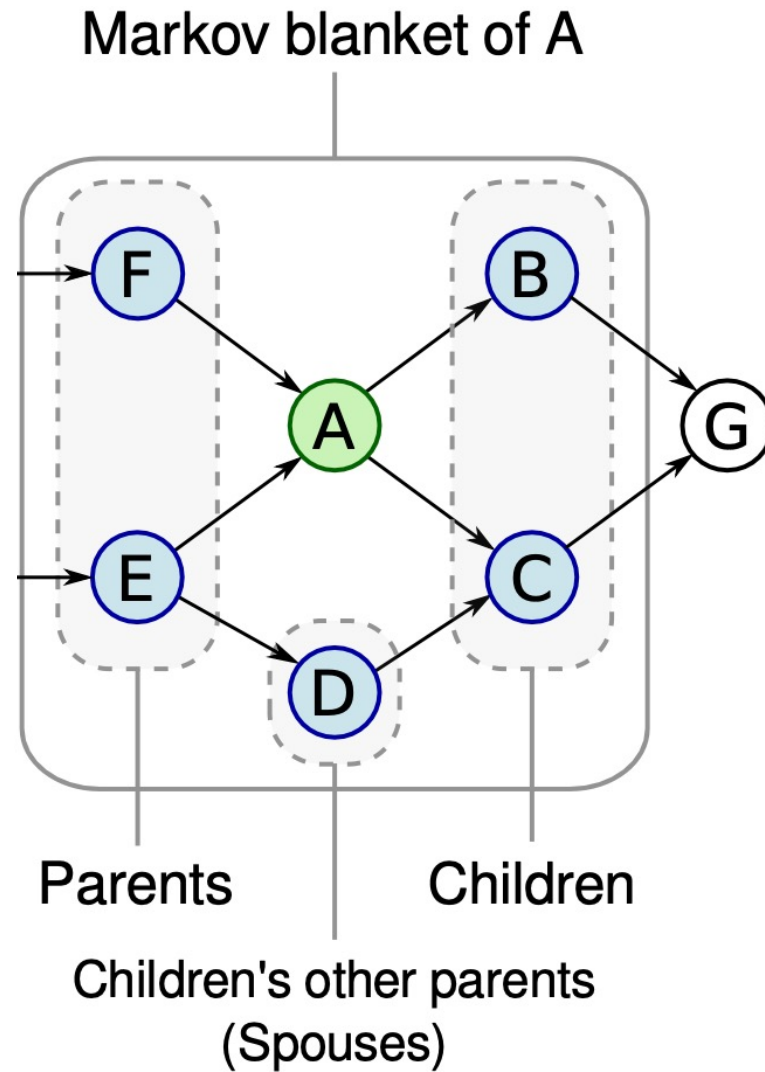
Markov Blanket of T?



Markov Blanket



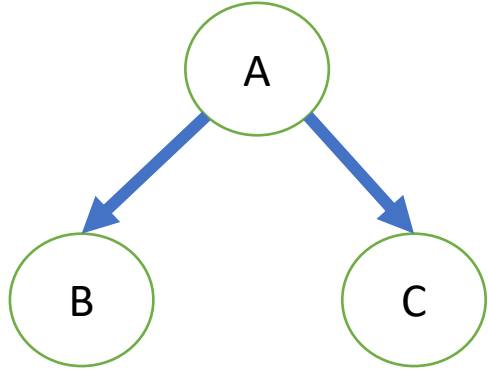
Example Markov blanket of a target T , consisting of **three parents (blue nodes)**, **two children (green)** and **one spouse (orange)**. All other nodes are conditionally independent of T given $MB(T)$.



We can easily use the DAG to solve the **feature selection** problem.

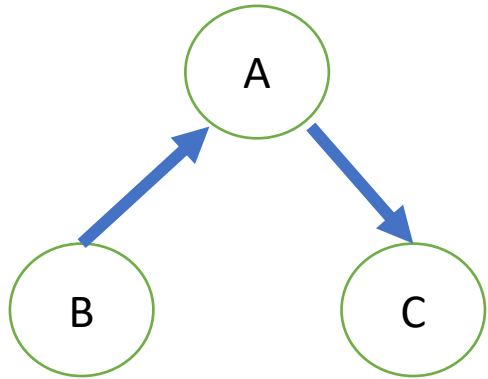
We can restrict ourselves to the **Markov blanket** to perform any kind of inference on the target node and disregard the rest.

Fundamental connections



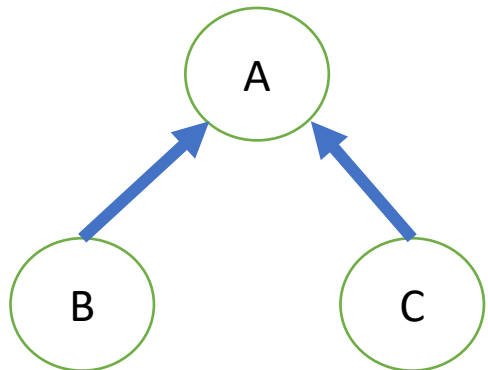
$$B \leftarrow A \rightarrow C$$

Divergent connection



$$B \rightarrow A \rightarrow C$$

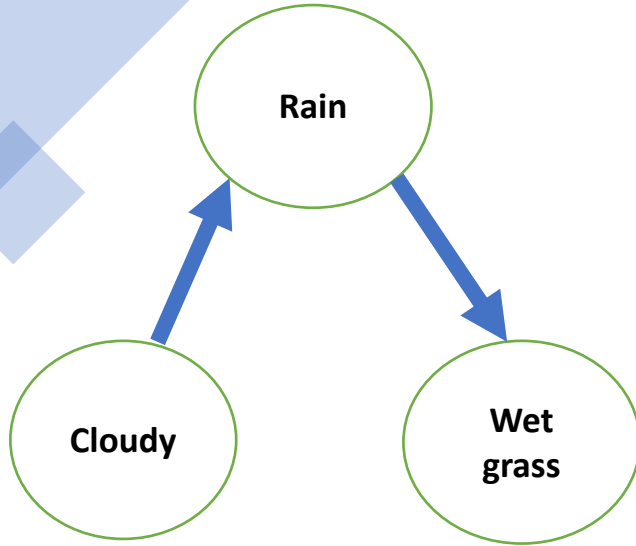
Serial connection



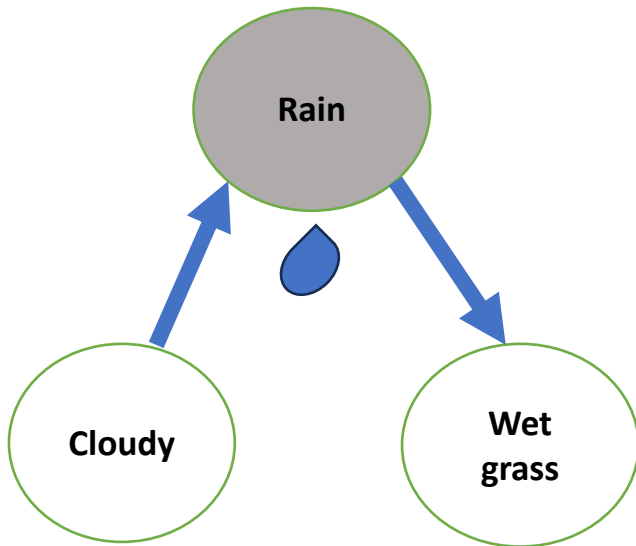
$$B \rightarrow A \leftarrow C$$

Convergent connection

Some examples:



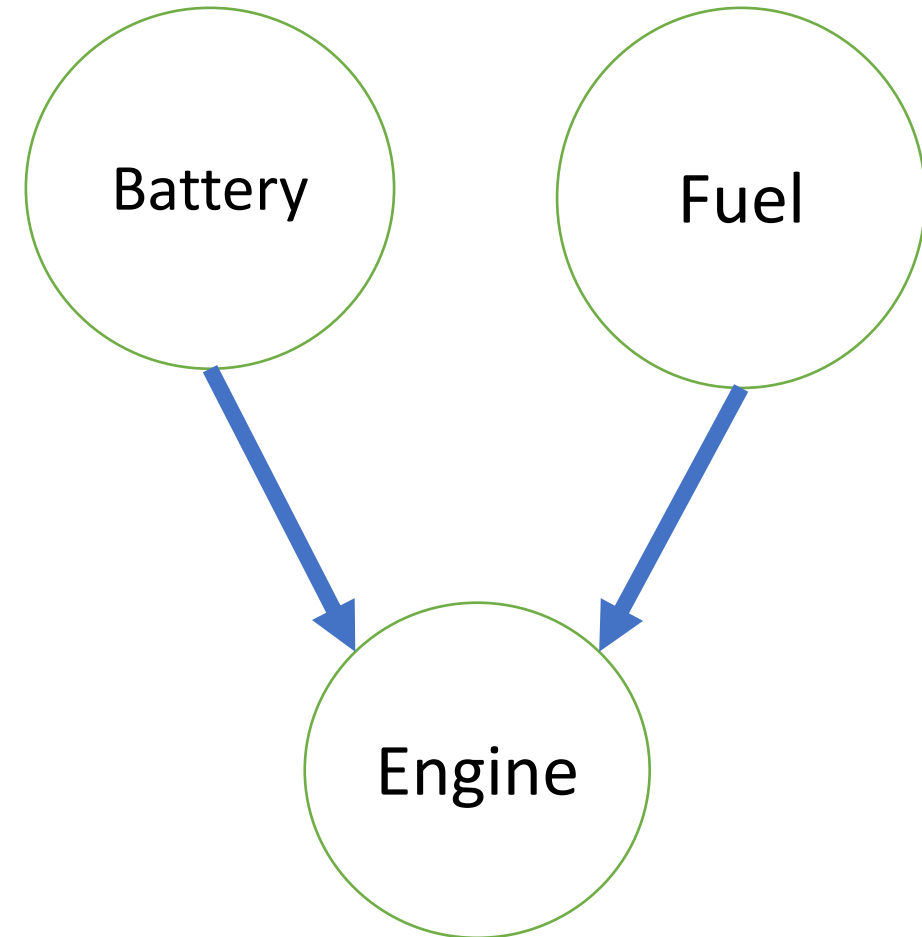
- Both variables **Cloudy** and **Wet grass** are **statistically dependent**.
- **Cloudiness** increases the probability of **rain** and thus indirectly the probability of a **wet grass**.
- **Conditional** on the variable **Rain**, the two variables **Cloudy** and **wet grass** are stochastically independent of each other.



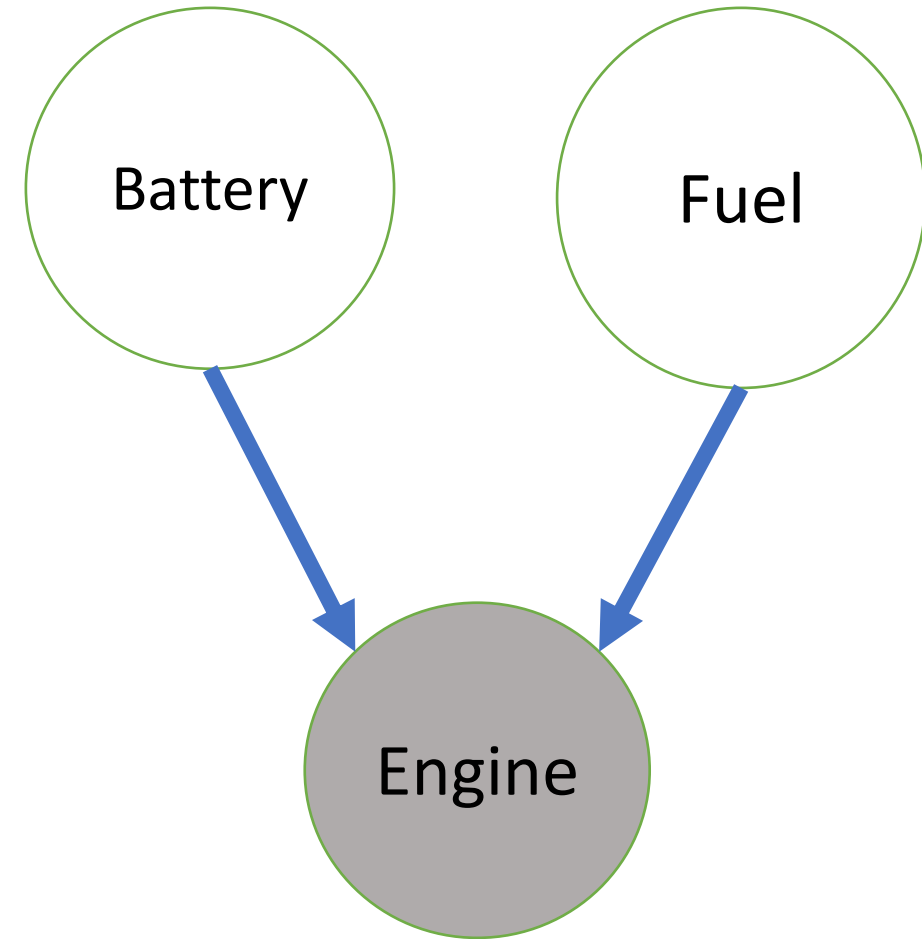
- 1) If it is known whether it rains or not, the state of cloudiness has no influence on the probability that the grass is wet.
- 2) If it is known whether it rains or not, the condition of the grass has no influence on the probability of the state of the clouds.

Some examples:

- The binary variable **Battery** indicates if the car battery is working or not.
- The binary variable **Fuel** indicates whether the tank of the car is empty or not.
- The binary variable **Engine** indicates whether the car can be started or not.
- **Battery** and **Fuel** are **stochastically independent**.



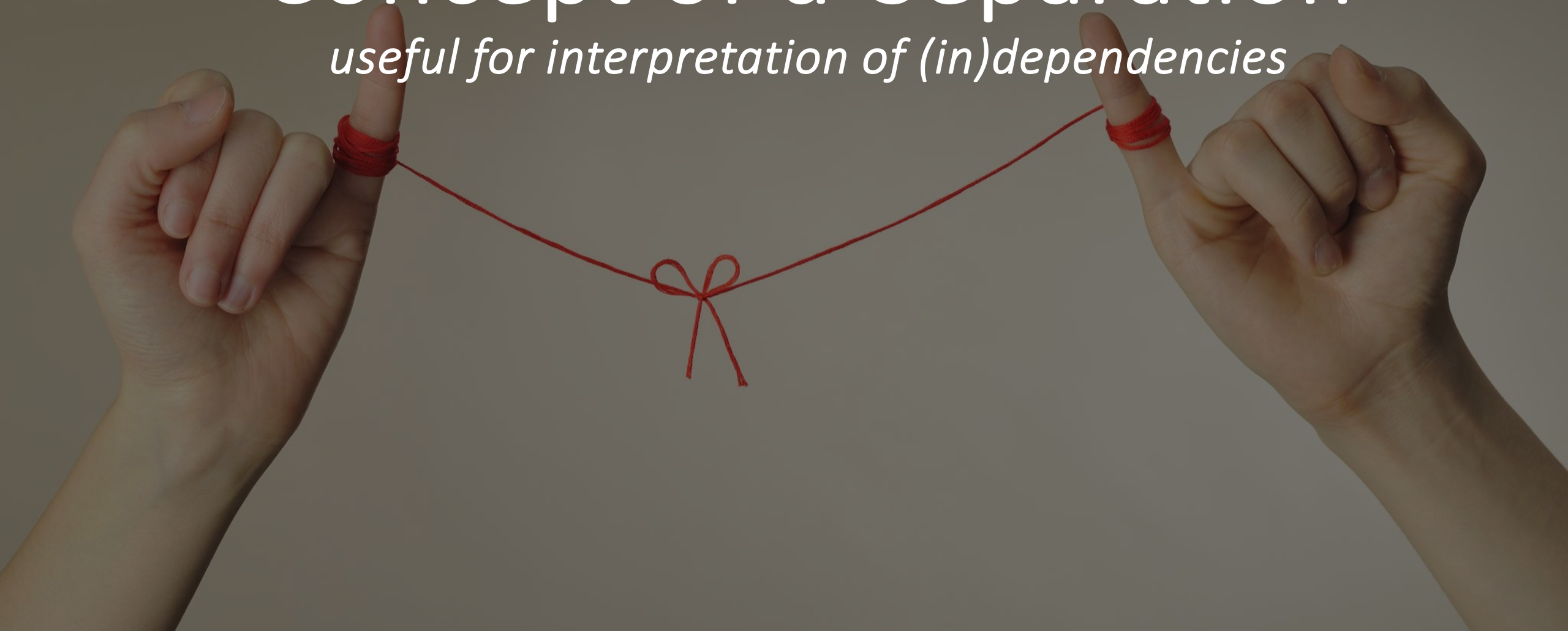
Some examples:



- However, **conditional** on the variable **Engine**, the two variables **Battery** and **Fuel** become **stochastically dependent**.
- When the car cannot be started, the probability that the fuel tank of the car is empty increases with the information that the battery is operating.

Concept of d-Separation

useful for interpretation of (in)dependencies



Concept of d-Separation

- In Bayesian networks, **the (in-)dependence relations** between the nodes (or variables) are easily obtained with the help of the **d-separation**.
- If two nodes/variables are d-separated, they are conditionally independent.
- It is very useful for interpretation.
- **dsep()** in **bnlearn** package.

Path

- **Definition of directed path**

There is a **directed path** from node X_i to node X_j in a graph G if one can move from X_i to X_j by **following directed edges** (according to their edge directions).

$$X_i \rightarrow \dots \rightarrow X_j$$

- **Definition of (any) path (path, trail)**

There is a **path (trail)** between the nodes X_i and X_j , if the two nodes are connected to each other through a **sequence of edges** (does not matter in which direction).

- In a **path or trail**, each node can appear **only once**.

$$X_i \rightarrow X_{i+1} \leftarrow \dots \rightarrow X_j$$

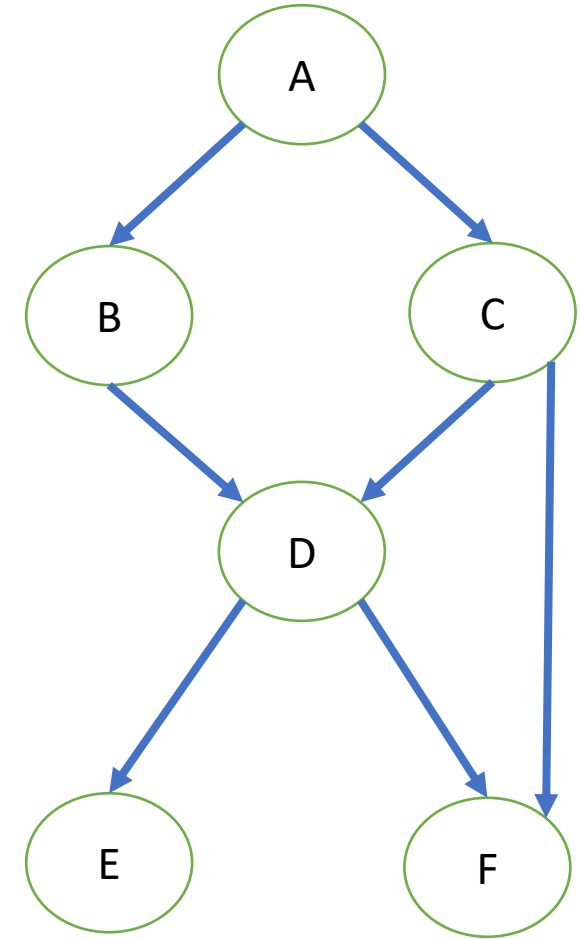
- Are these valid paths?

1. $A \rightarrow C \rightarrow F \leftarrow D \leftarrow B \leftarrow A \leftarrow C$

2. $A \rightarrow D \leftarrow B \leftarrow C$

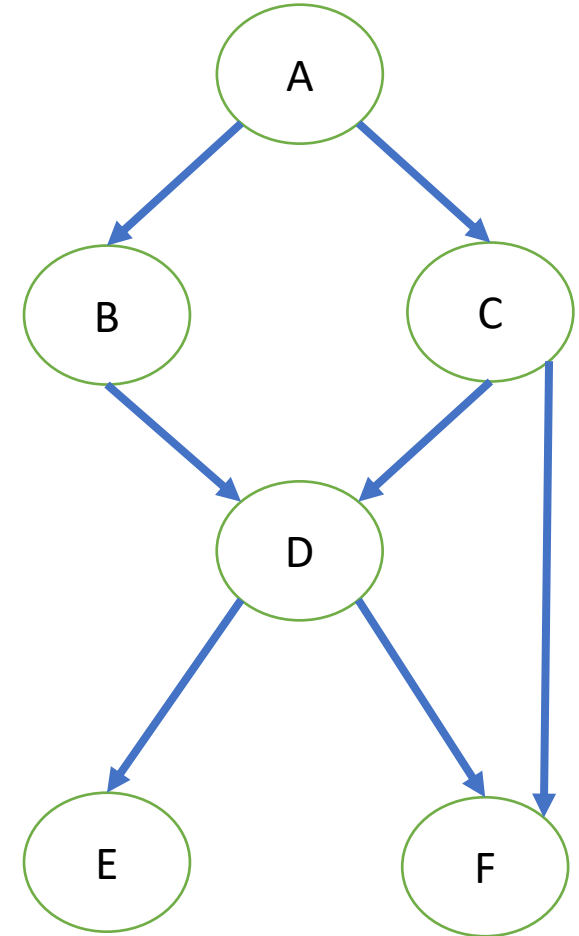
3. $C \rightarrow F \leftarrow D \leftarrow B \leftarrow A$

- One more paths?



Example of (directed) paths

- Examples of directed paths:
- $A \rightarrow B \rightarrow D \rightarrow F$
- $A \rightarrow C \rightarrow D$
- We have the paths (trails):
- $A \rightarrow B \rightarrow D \leftarrow C$
- $B \rightarrow D \leftarrow C$
- $A \rightarrow C \rightarrow F \leftarrow D \leftarrow B$



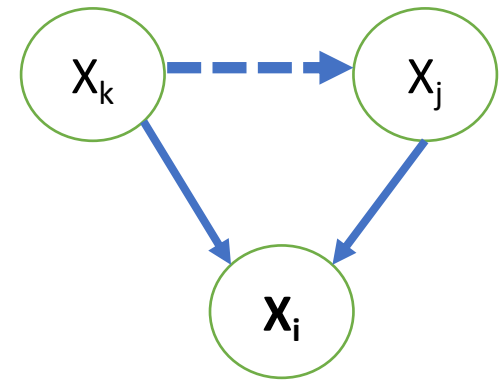
Collider

In a trail / path the node X_i ($i = 1, \dots, n$) is a collider if two edges converge on X_i .

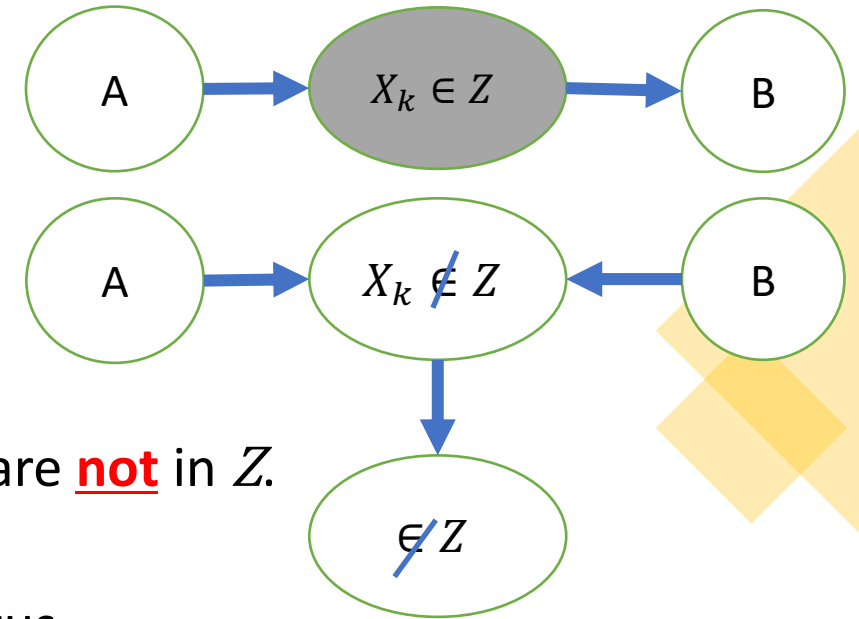
E.g.: $X_w \rightarrow X_k \rightarrow X_i \leftarrow X_j \rightarrow X_m$

- **Note:** This definition does not require that $X_k \rightarrow X_i \leftarrow X_j$ is a v-structure.

The nodes X_k and X_j can be in a parent-child relationship.

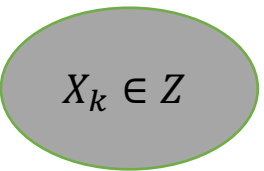
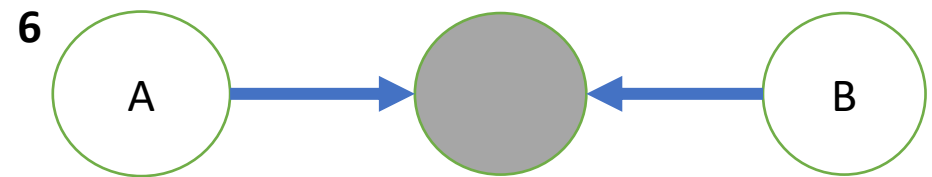
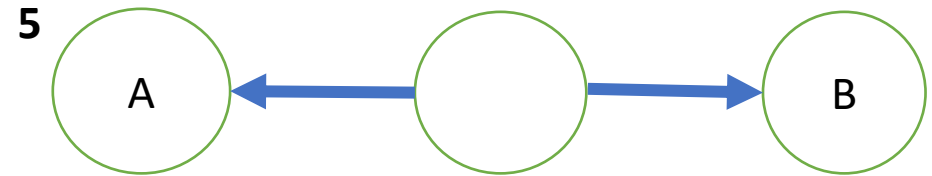
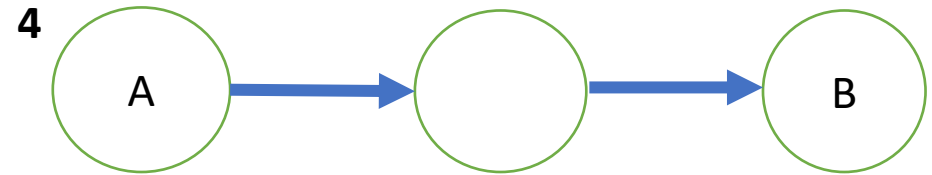
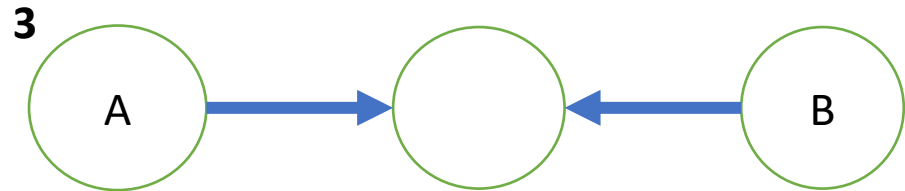
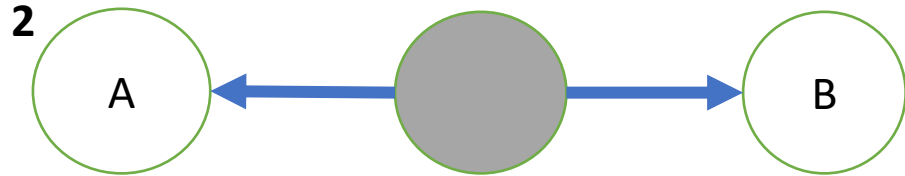
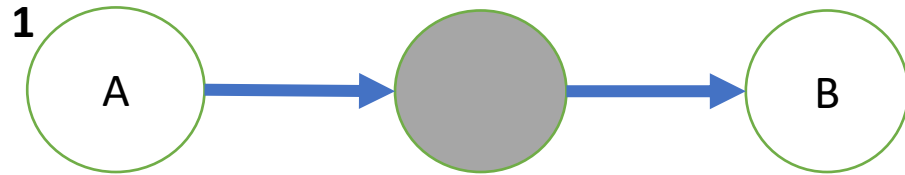


Blocked path

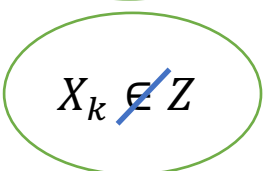


- We consider the nodes A and B and a subset Z , where A and B are **not** in Z .
- Being in Z means the node is observed. That is, we know its status.
- A path (trail) between A and B is **blocked** when the trail leads through any node X_k and:
 - (1) X_k **is not** a collider and X_k is an element of Z (X_k is observed).
 - (2) X_k is a collider and neither X_k nor a descendant of X_k is an element of Z (**not** observed).

Which ones are blocked?



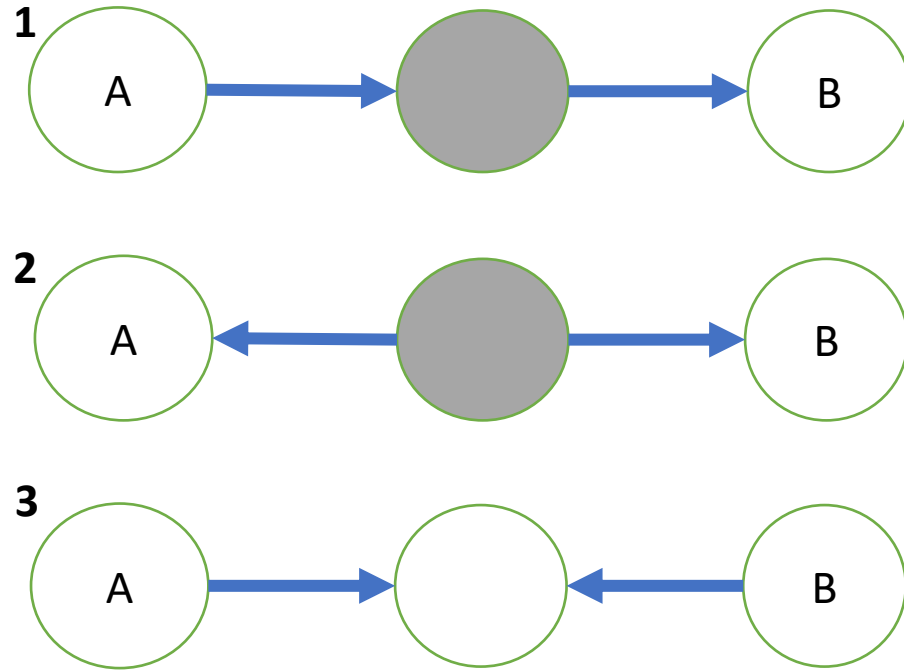
observed



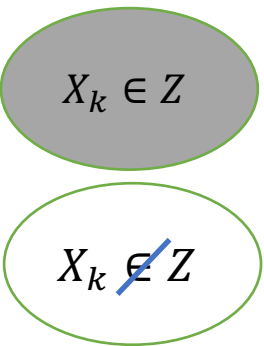
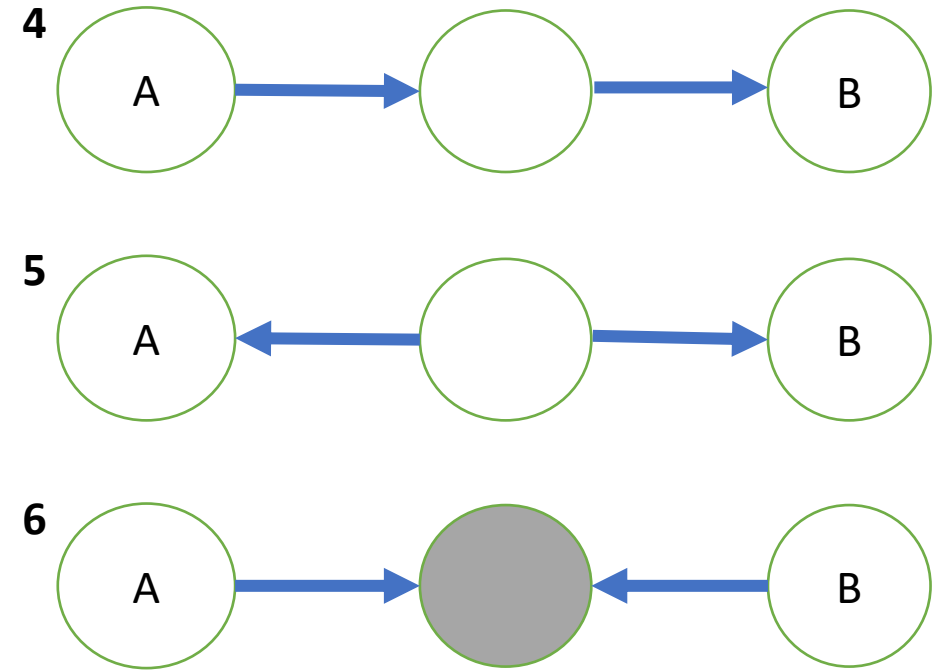
unobserved

The filled (grey) nodes are elements of the set Z (known). The empty (white) nodes are not elements of Z .

Blocked paths between A and B



Open paths between A and B



The filled (grey) nodes are elements of the set Z (known). The empty (white) nodes are not elements of Z.

Definition: d-Separation

d-Separation

- The nodes X_i and X_j are **d-separated** with respect to Z , when every path between X_i and X_j is **blocked** (conditional on Z).
- When X_i and X_j are d-separated given Z , then X_i and X_j are **stochastically independent** (conditional on Z).

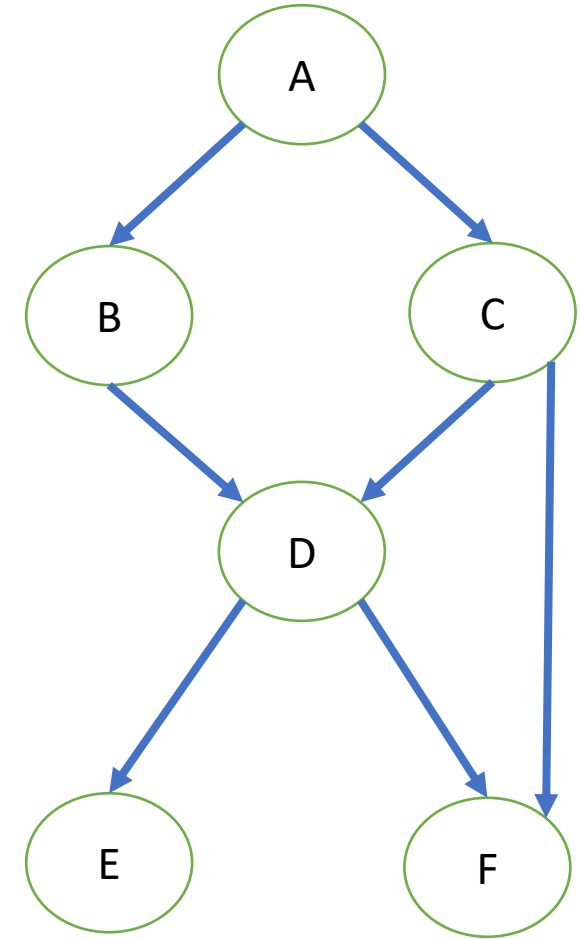
Example

A and D are d-separated conditional on $Z = \{B, C\}$?

A and F are d-separated conditional on $Z = \{D, C\}$?

B and C are d-separated conditional on $Z = \{A\}$?

B and C are d-separated conditional on $Z = \{A, D\}$?



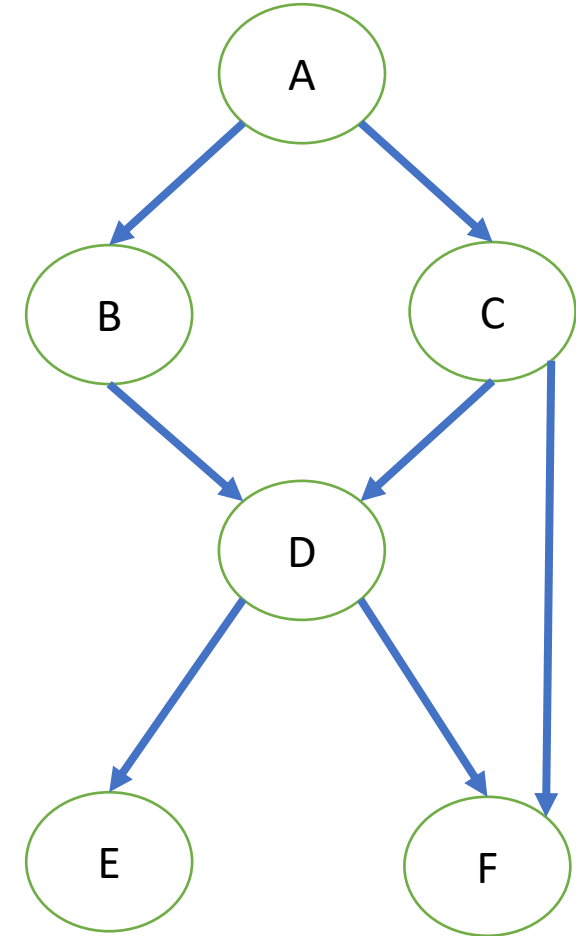
Example

A and D are d-separated conditional on $Z = \{B, C\}$.

A and F are d-separated conditional on $Z = \{D, C\}$.

B and C are d-separated conditional on $Z = \{A\}$.

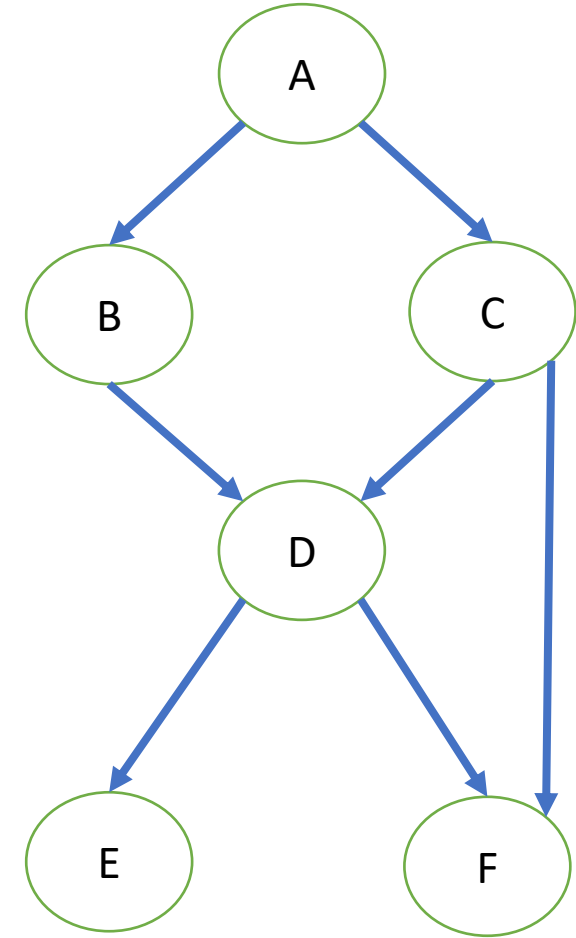
B and C are **not** d-separated conditional on $Z = \{A, D\}$ **why?**



- **The software does everything for you.**

Static Bayesian networks

- **The first component** of a BN is a graph. A graph G is a mathematical object with:
 - a set of nodes $V = \{v_1, \dots, v_N\}$;
 - a set of arcs A which are identified by pairs for nodes in V , e.g. $a_{ij} = (v_i, v_j)$.
- **The second component** of a BN is the probability distribution $P(X)$, should be such that the BN:
 - can be learned efficiently from data;
 - is flexible (distributional assumptions should not be too strict);
 - is easy to query to perform inference.



- Second component:

The probability distribution $P(X)$

Types of BN:

- The **three most common choices** in the literature (by far), are:
- **Discrete BNs:** X and the $(X_i \mid X_i's \text{ parents})$ are **multinomial**;
- **Gaussian BNs (GBNs):** X is **multivariate normal** and the $(X_i \mid X_i's \text{ parents})$ are univariate normal;
- **Conditional linear Gaussian BNs (CLGBNs):** CLGBNs contain both discrete and continuous nodes and combine **discrete BNs** and **GBNs** to obtain a mixture-of-Gaussians network.

Discrete BNs

- The joint probability distribution is a **multinomial distribution**, assigning a probability to each **combination of states of variables**.



Multinomial distribution

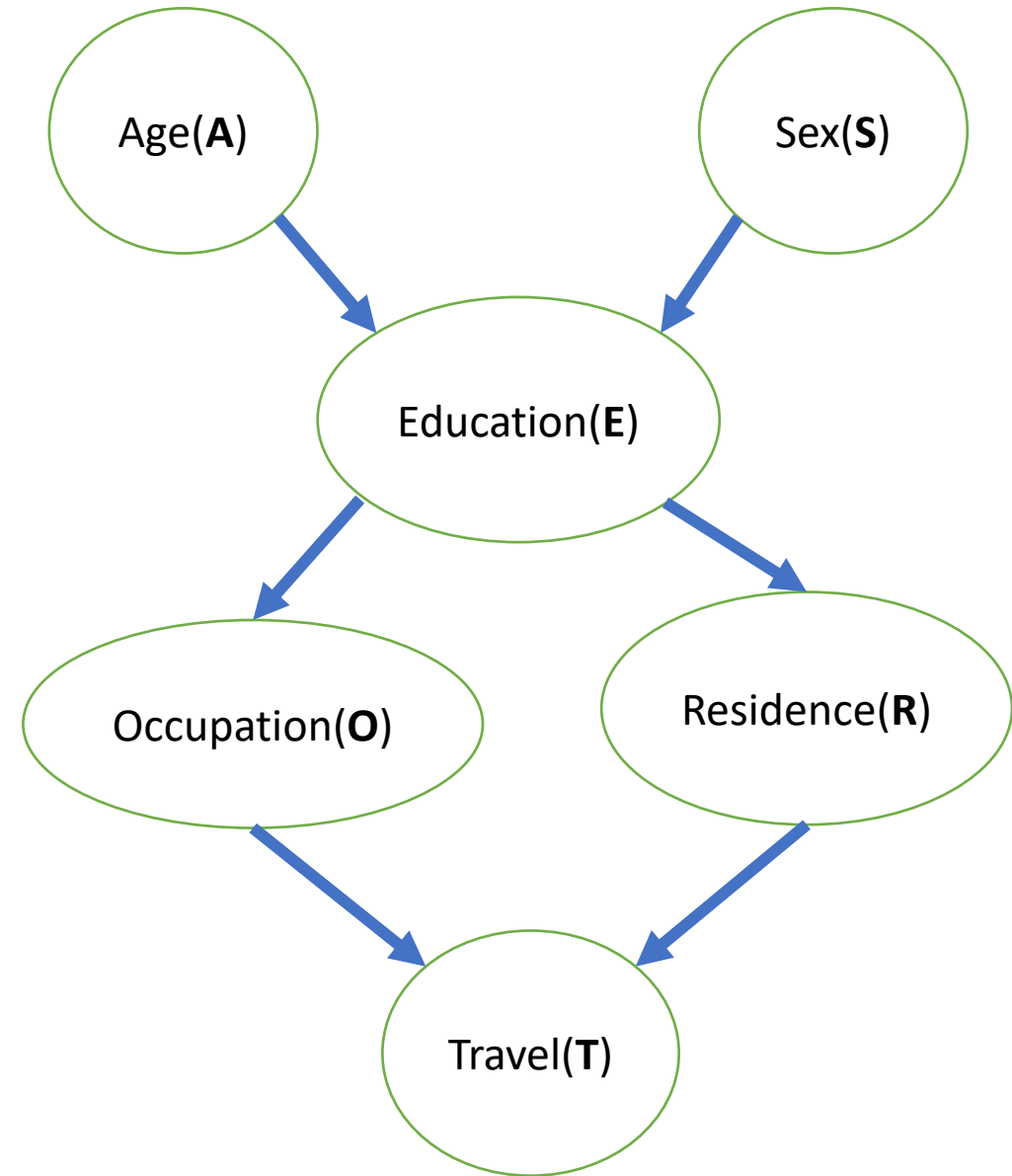
- A multinomial distribution involves a process that has a set of k possible results ($X_1, X_2, X_3, \dots, X_k$) with associated probabilities ($p_1, p_2, p_3, \dots, p_k$) such that $\sum p_i = 1$.
- Then for n repeated trials of the process, let x_i indicate the number of times that the result X_i occurs, subject to the restraints that $0 \leq x_i \leq n$ and $\sum x_i = n$.

$$P(X_1 = x_1, X_2 = x_2, \dots, X_k = x_k) = \frac{n!}{x_1! x_2! \dots x_k!} p_1^{x_1} p_2^{x_2} \dots p_k^{x_k}$$

Using BNs it can be decomposed.

Example of Discrete BNs

- **Age** and sex are not influenced by any other variable.
- **Age** and sex have a direct influence on **Education**.
- **Education** strongly influences both **occupation** and **residence**.
- **Transports** are directly influenced by both **occupation** and residence.
- $2^6 - 1 = 63$



| Young | Adult | Old |
|-------|-------|-----|
| 0.3 | 0.5 | 0.2 |

Age

| M | F |
|-----|-----|
| 0.6 | 0.4 |

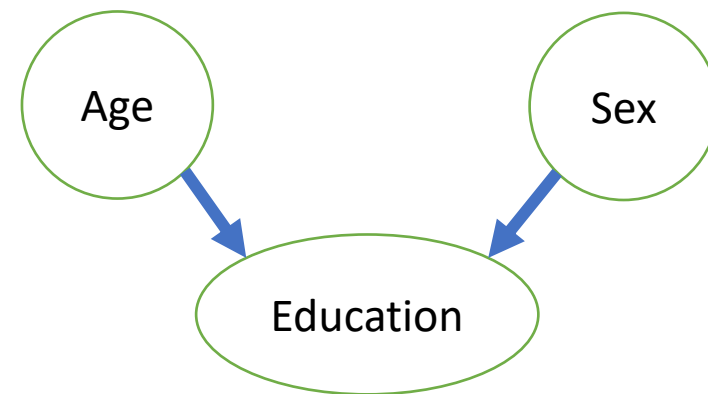
Sex

| | Emp | Self |
|------|------|------|
| High | 0.96 | 0.04 |
| Uni | 0.92 | 0.08 |

Education

Occupation

| | High | Uni |
|----------|------|------|
| Young& M | 0.75 | 0.25 |
| Adult& M | 0.72 | 0.28 |
| Old& M | 0.88 | 0.12 |
| Young& F | 0.64 | 0.36 |
| Adult& F | 0.70 | 0.30 |
| Old& F | 0.90 | 0.10 |

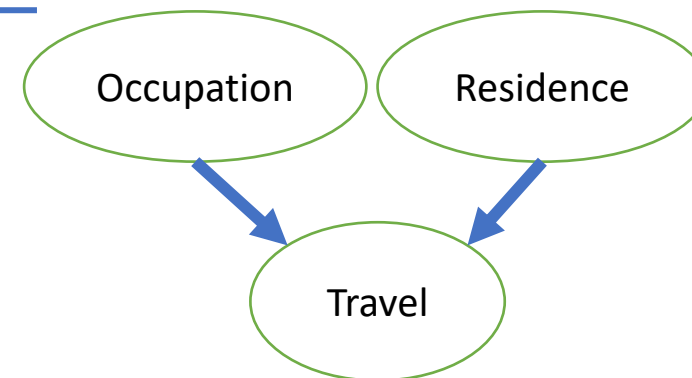


| | Small | Big |
|------|-------|------|
| High | 0.25 | 0.75 |
| Uni | 0.20 | 0.80 |

Education

Residence

| | Car | Train | Other |
|-------------|------|-------|-------|
| Small& Emp | 0.48 | 0.42 | 0.10 |
| Small& Self | 0.56 | 0.36 | 0.08 |
| Big& Emp | 0.58 | 0.24 | 0.18 |
| Big & Self | 0.70 | 0.21 | 0.09 |

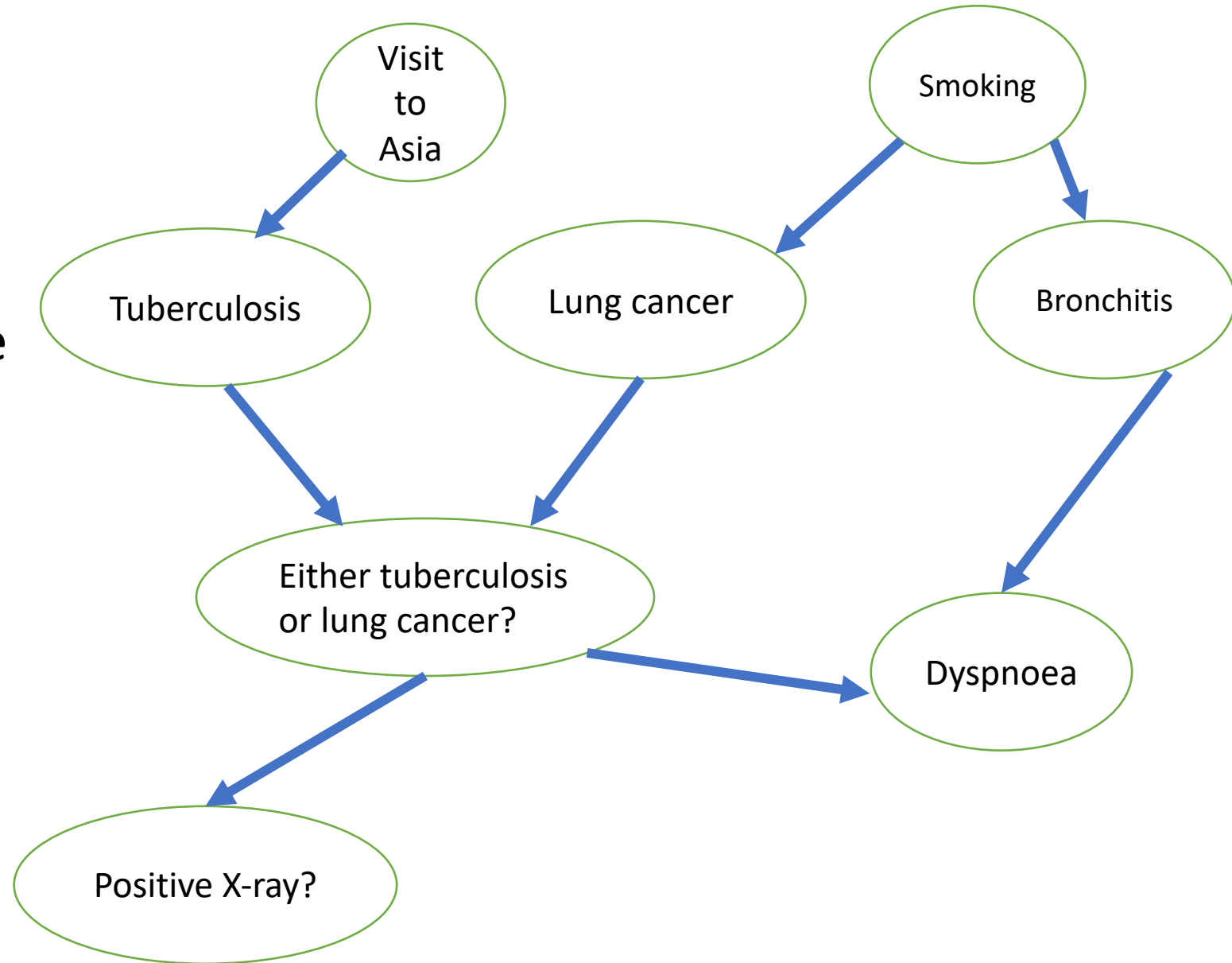


Overall, **fewer parameters:**

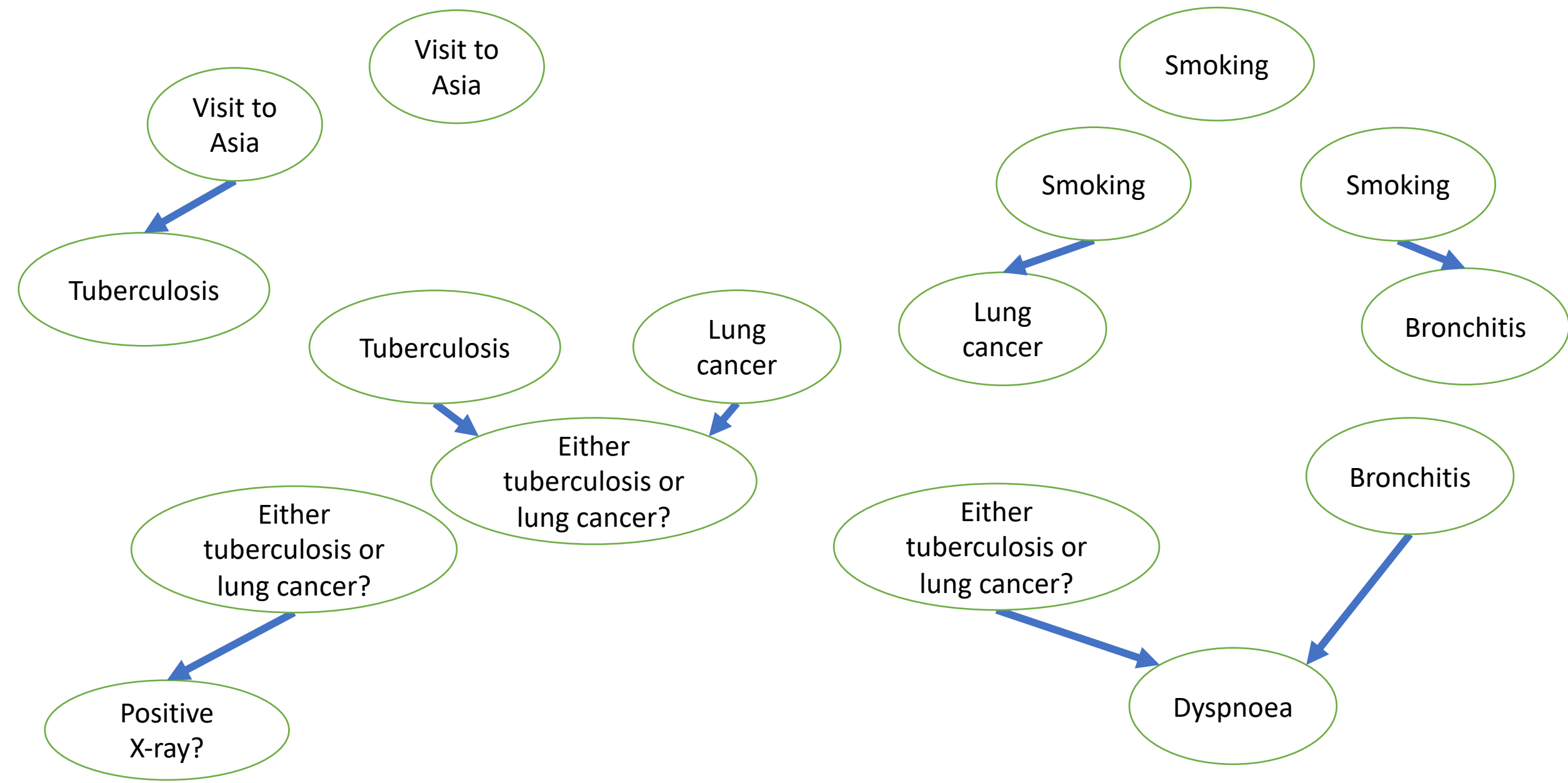
16 parameters only !

A classic example of BN is the **ASIA network** from Lauritzen & Spiegelhalter (1988), which includes a collection of binary variables. It describes a simple **diagnostic problem for tuberculosis and lung cancer**.

Total parameters of X :
 $2^8 - 1 = 255$



• Overall parameters of the $X_i | X_i$'s parents : 18



Learning the dag structure:

- It is not always possible or desired to rely on prior knowledge of the phenomenon we are modeling to decide which arcs are present in the graph and which are not.
- Therefore, the structure of the DAG itself maybe the object of our investigation.
- E.g., in genetics and systems biology reconstructing the molecular pathways and networks underlying complex disease and metabolic processes (Sachs et al., (2005)).

Learning the dag structure:

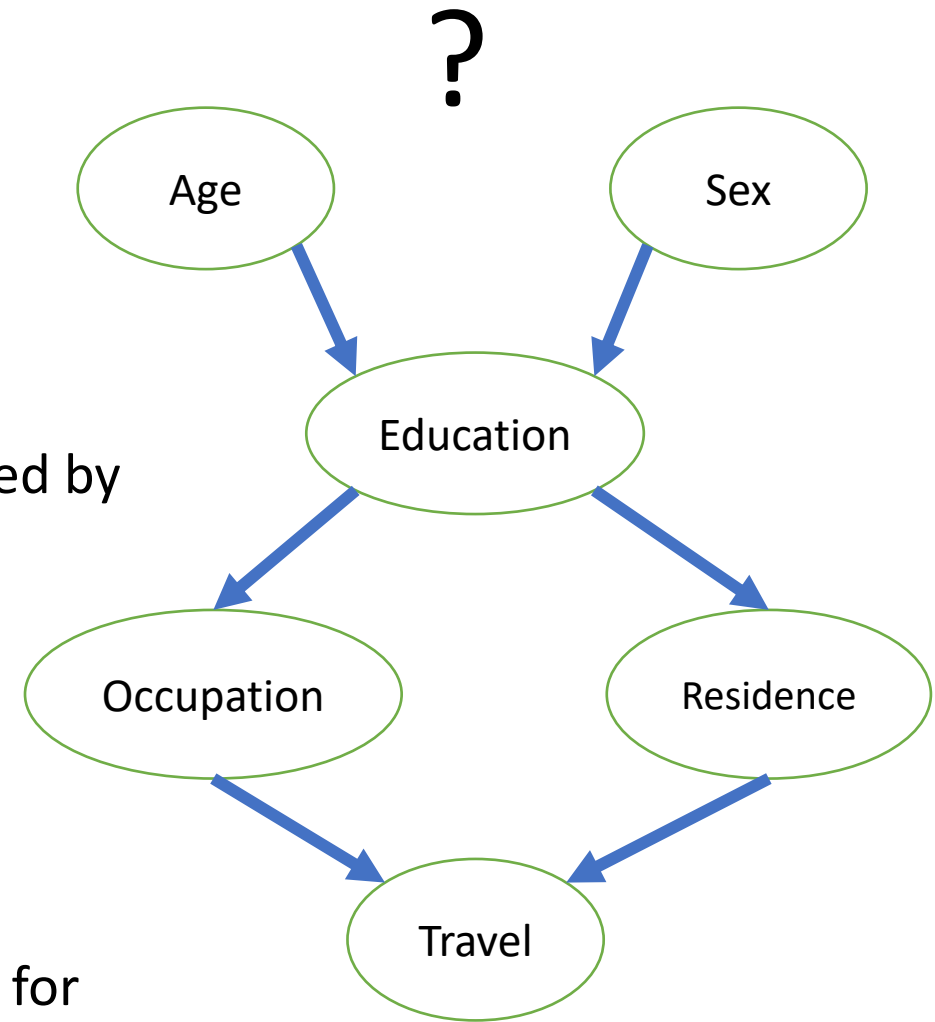
- Several algorithms have been presented in literature for this problem,
- Despite the variety of theoretical backgrounds and terminology they can all be traced to only three approaches:
 - *constraint-based*,
 - *score-based* and
 - *hybrid*.

Constraint-based :

Conditional independence test

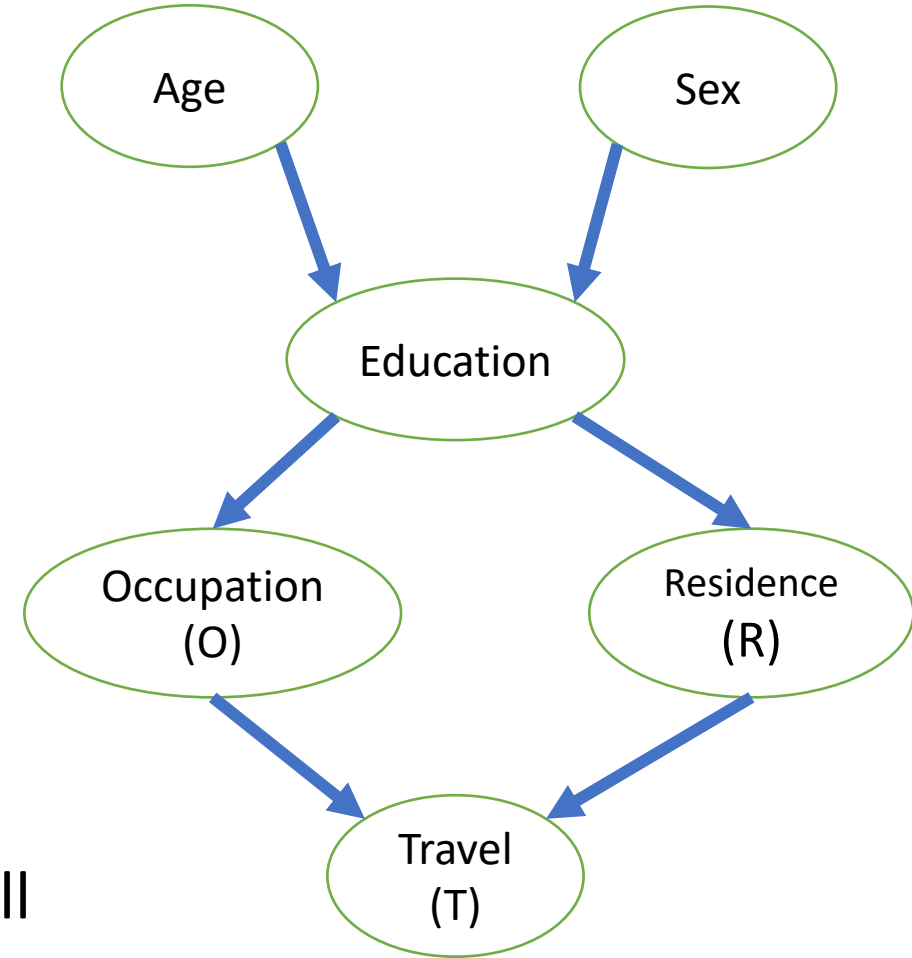
(Pearl 1990, Verma and Pearl, 1991)

- It focuses on presence of individual arcs.
- It can be used to assess whether the dependency is supported by the data.
- $H_0: T \perp\!\!\!\perp_P E \mid \{O, R\}$, they are independent, no edge
- $H_1: T \not\perp\!\!\!\perp_P E \mid \{O, R\}$, they are dependent, edge
- If the **null hypothesis** is **rejected**, the arcs can be considered for **inclusion** otherwise for **exclusion**.
- This approach operates edgewise.



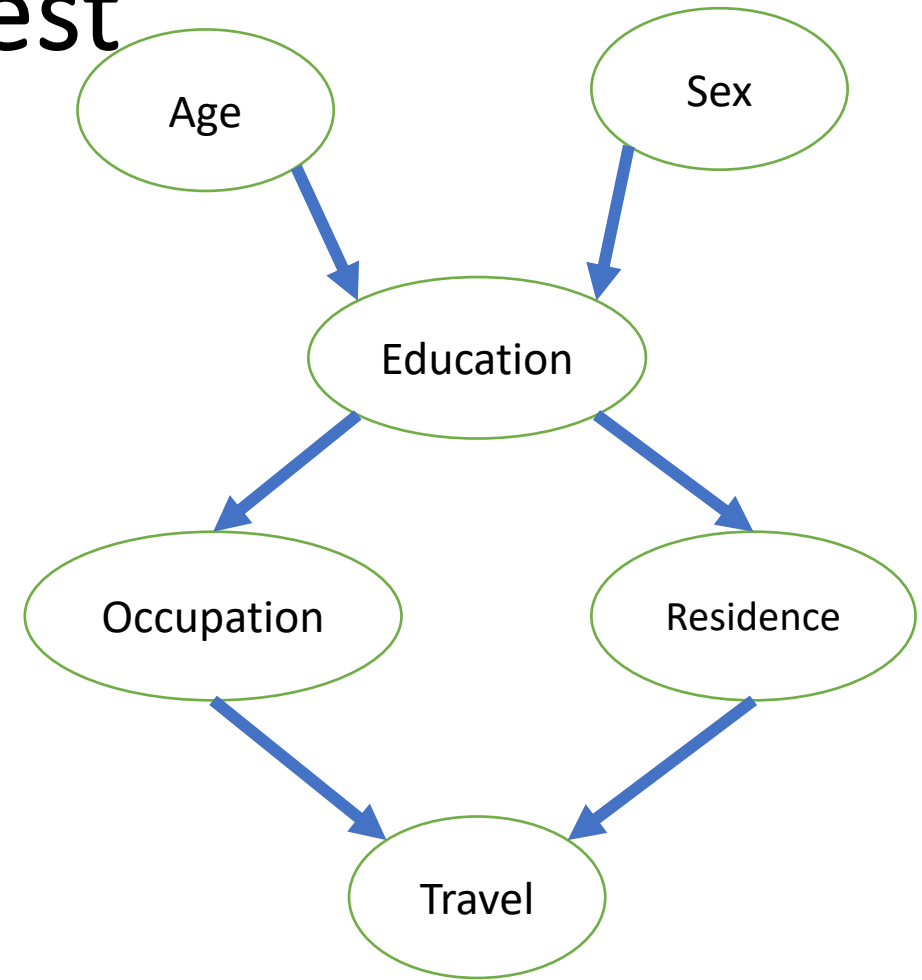
Conditional independence test

- $H_0: T \perp\!\!\!\perp E \mid \{O, R\}$,
- $H_1: T \not\perp\!\!\!\perp E \mid \{O, R\}$
- Performing this test H_0 by adapting the **log-likelihood ratio**, G^2 , or **Pearson's X^2** test.
- If the **null hypothesis** is **rejected**, the arcs can be considered for **inclusion** otherwise for **exclusion** (small p-value).



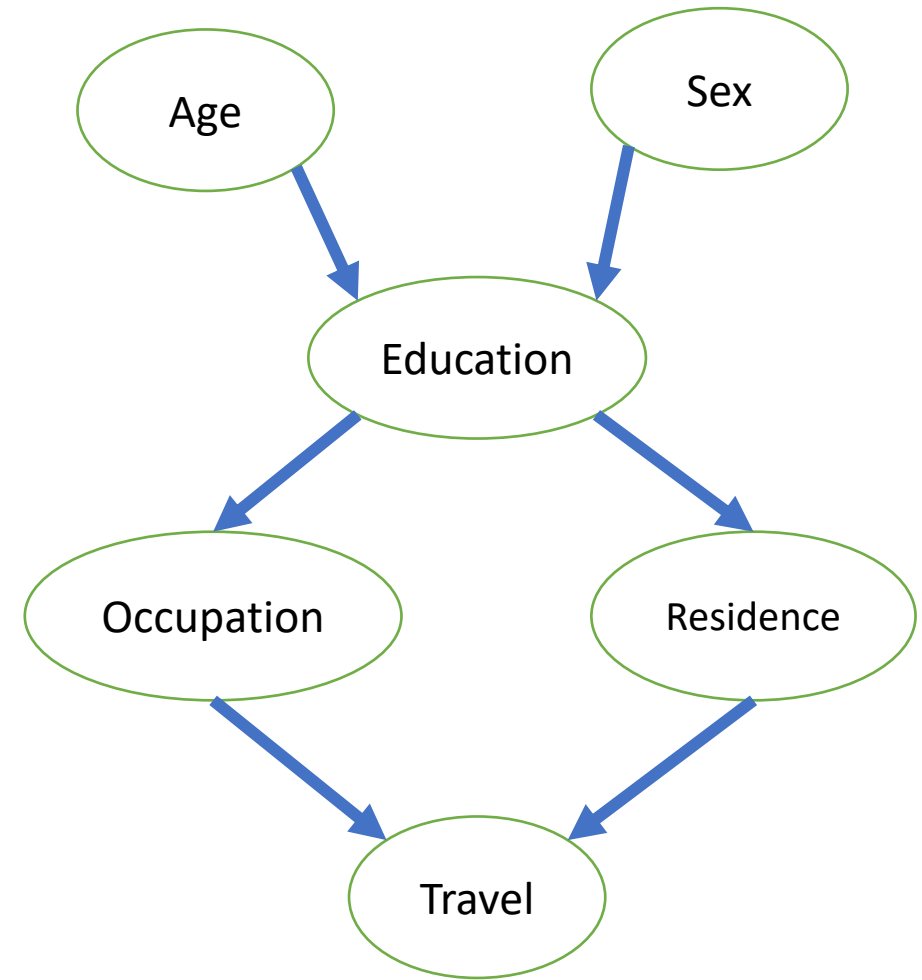
Conditional independence test

- the null hypothesis ***is not*** rejected,
p-value > α ---- there is no edge.
- The null hypothesis is rejected
p-value < α ----- there is an edge.
- α is usually 0.05 or 0.01.
- We will discuss this in practical.



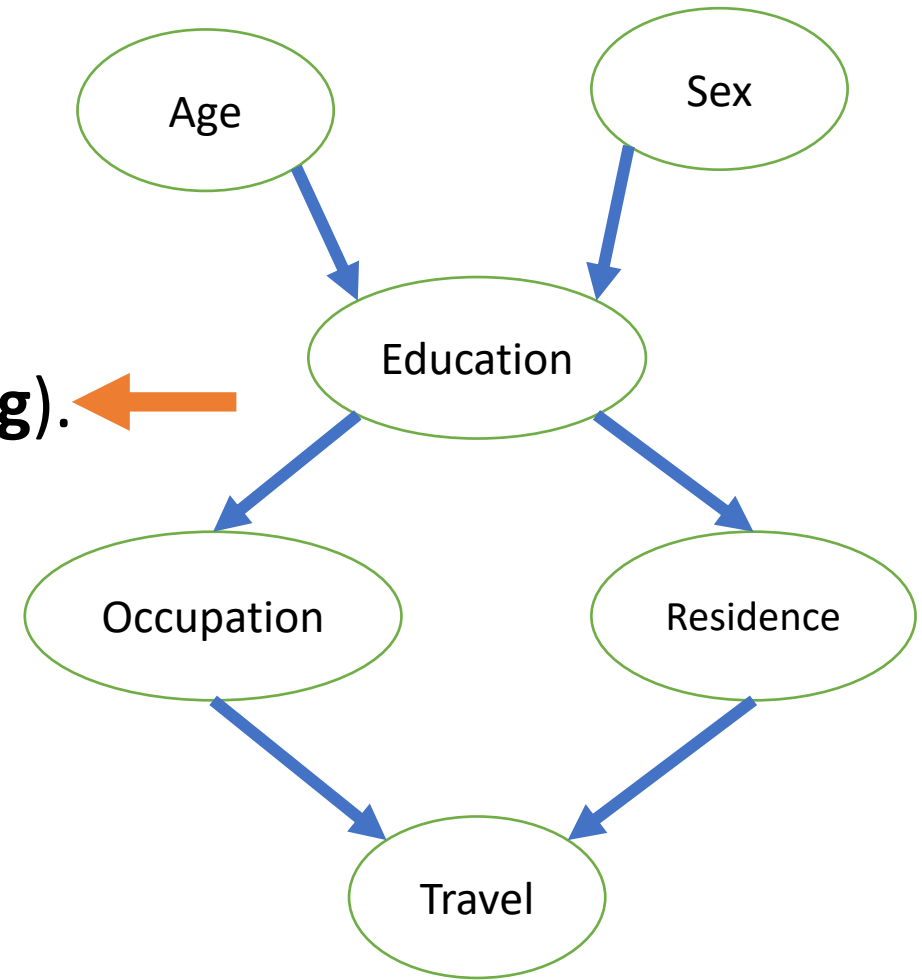
Network score

- Each candidate BN is assigned a network score reflecting its **goodness of fit**.
- Bayesian information criterion (**BIC**).
- Bayesian Dirichlet equivalent uniform (**BDeu**).



Algorithms that search for the DAG given the data
(maximize a given network score)

- **Greedy search algorithm (such as Hill-climbing).**
- **Genetic algorithm.**
- **Simulated annealing** (Bouckaert, 1995).



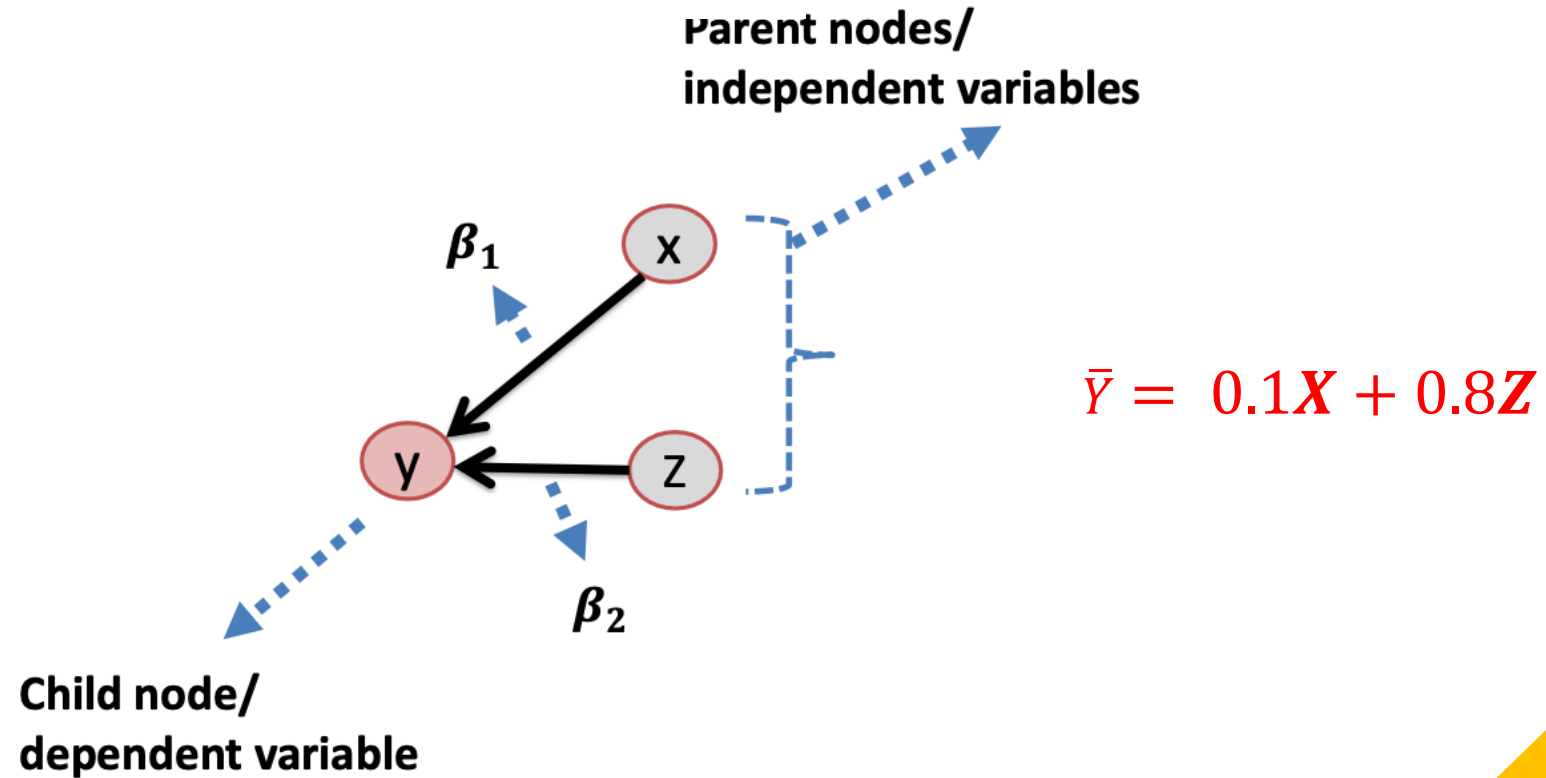


Continuous (Gaussian)
Bayesian Network

Continuous BNs

- Every node follows a **normal distribution**.
- Nodes without any parents (root nodes), are described by the univariate normal distribution.
- The local distribution of each node can be equivalently expressed as a **Gaussian linear model** which includes an intercept and the **node's parents as explanatory variables (predictors)**, **without any interaction term**.
- **Child** $\sim \beta_1 * \text{Parent1} + \beta_2 * \text{parent2} + \dots$

Edges: presence or absence of a coefficient

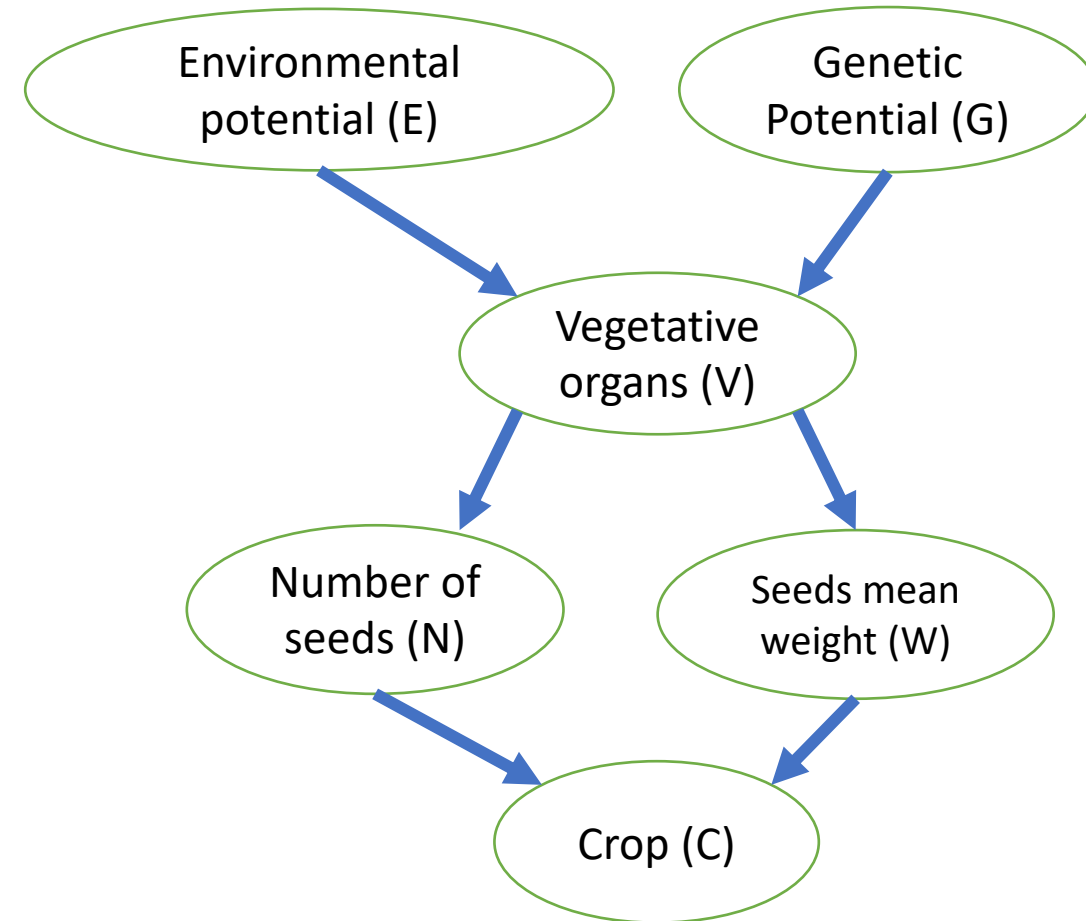


$$\overline{Child} \sim \beta_1 * \text{Parent1} + \beta_2 * \text{parent2} + \dots$$

Example of continuous BNs

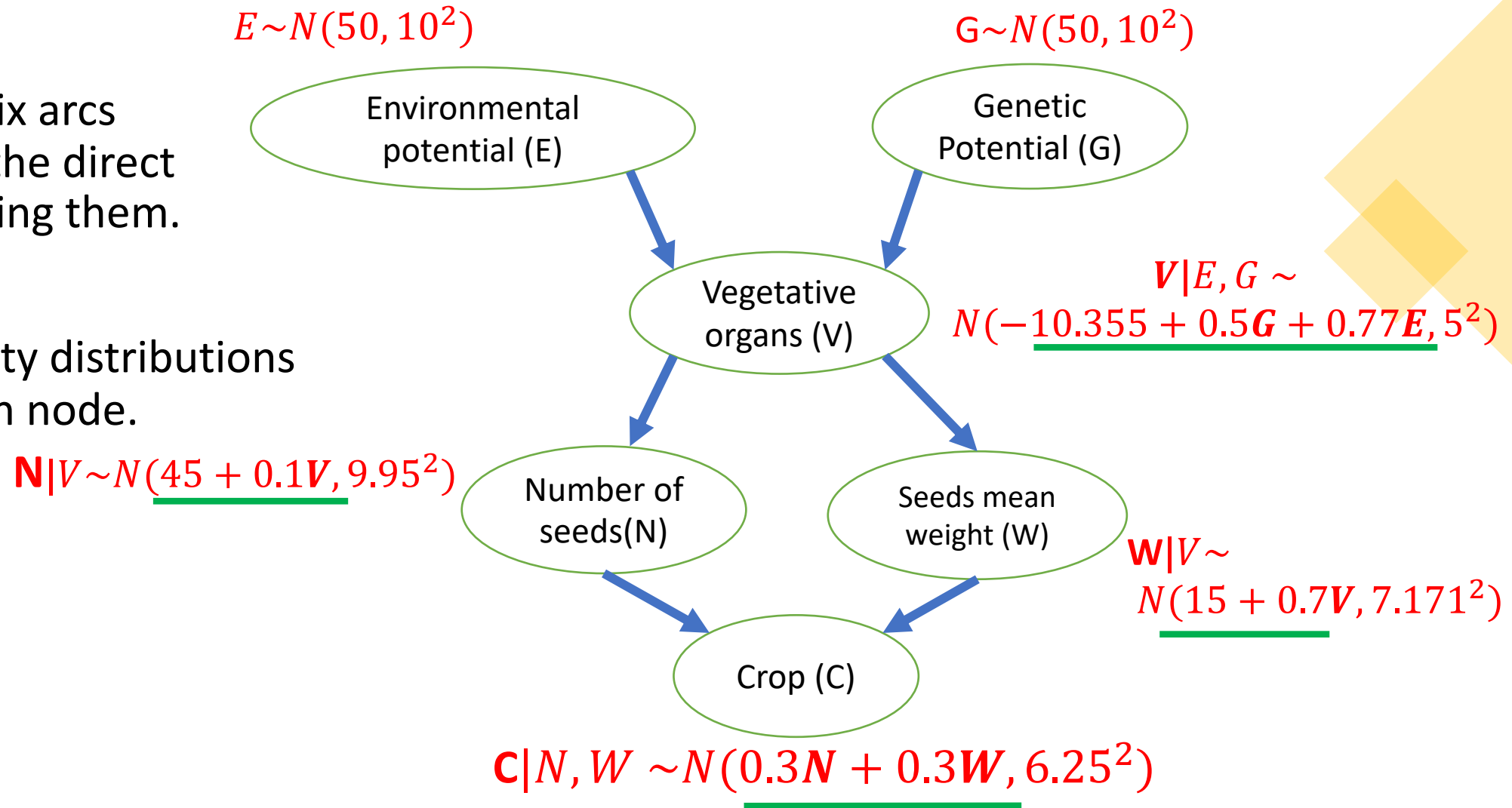
For the analysis of a particular plant:

- **Genetic Potential (G):** Genotype effect (a single score).
- **Environmental potential (E):** Environmental (location and season) effect (a single score).
- **Vegetative organs (V):** Roots, stems, etc., grow and accumulate reserves exploited for reproduction and summarises all the information available on constituted reserves.
- **Number of seeds (N)** is determined at the flowering time.
- **Seeds mean weight (W)** is assessed in the plant's life.
- **Crop (C):** The harvested grain mass.



Example

- Six variables and six arcs corresponding to the direct dependencies linking them.
- The local probability distributions are shown for each node.



N means normal/ Gaussian distribution.

$\overline{Child} \sim \beta_1 * \text{Parent1} + \beta_2 * \text{parent2} + \dots$

Some remarks

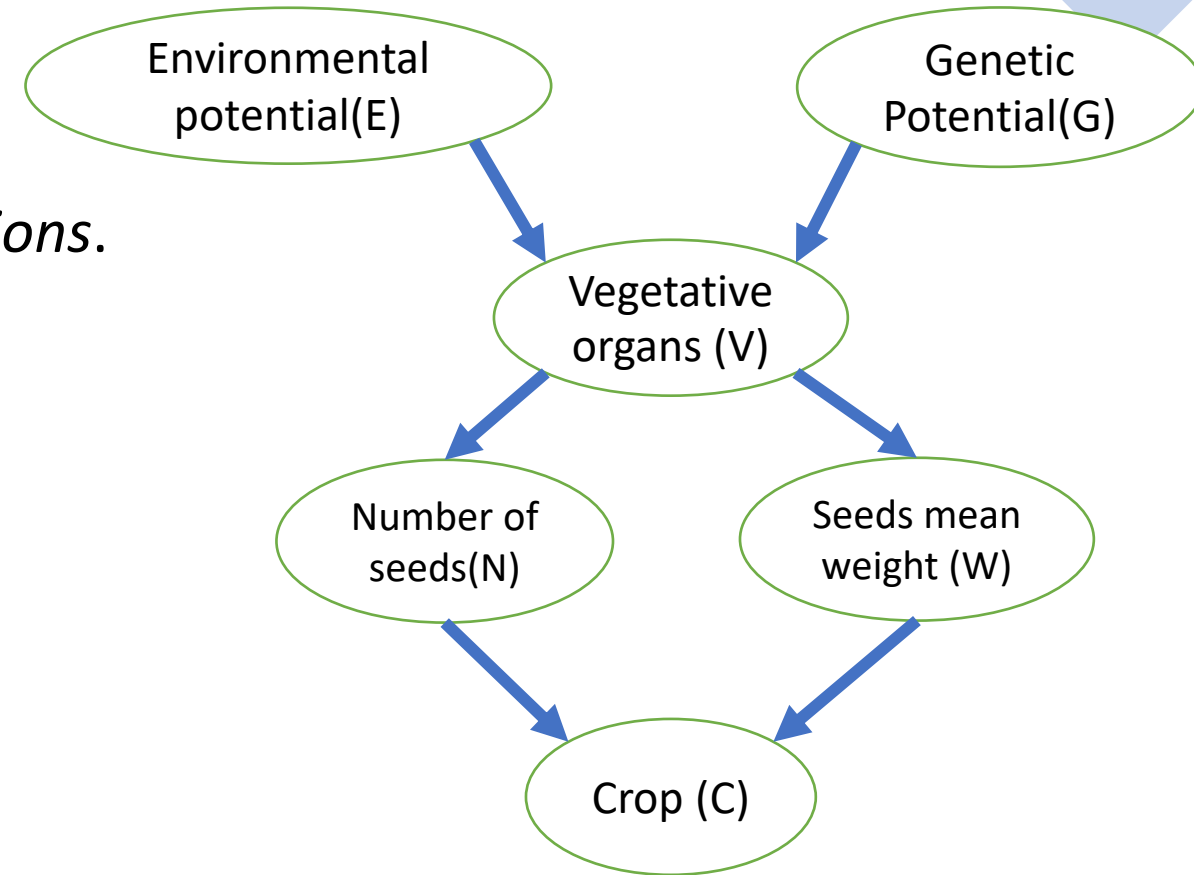
- WHY **linear dependencies**?
- **Closed-form results** for many inference procedures.
- Relatively **simple models** often perform better than very **sophisticated ones**.
- $\overline{Child} \sim \beta_1 * \text{Parent1} + \beta_2 * \text{parent2} + \dots$

Learning the DAG Structure: Tests and Scores

- Often expert knowledge on the data is not detailed enough to completely specify the structure of the DAG. In such cases, if sufficient data are available, we can infer a sparse BN.
- The two classes of criteria used to learn the structure of the DAG are:
 - *constraint-based*
 - *score-based*

Conditional Independence Tests

- **Most common:** exact test for *partial correlations*.
- $H_0: C \perp\!\!\!\perp_P W \mid N \rightarrow$ no edge
- $H_1: C \not\perp\!\!\!\perp_P W \mid N \rightarrow$ edge between **C** and **W**



Conditional Independence Tests using bnlearn package

- ✓ Using “bnlearn” package

- ✓ Test for partial correlations

- ✓ Computing the corresponding statistics.

- ✓ P-value

- ✓ The null hypothesis ***is not*** rejected :

p-value > α ---- there is no edge.

- ✓ The null hypothesis is rejected:

p-value < α ----- there is an edge.

- ✓ We will discuss this in practical.

Network Scores

Same as Discrete BN:

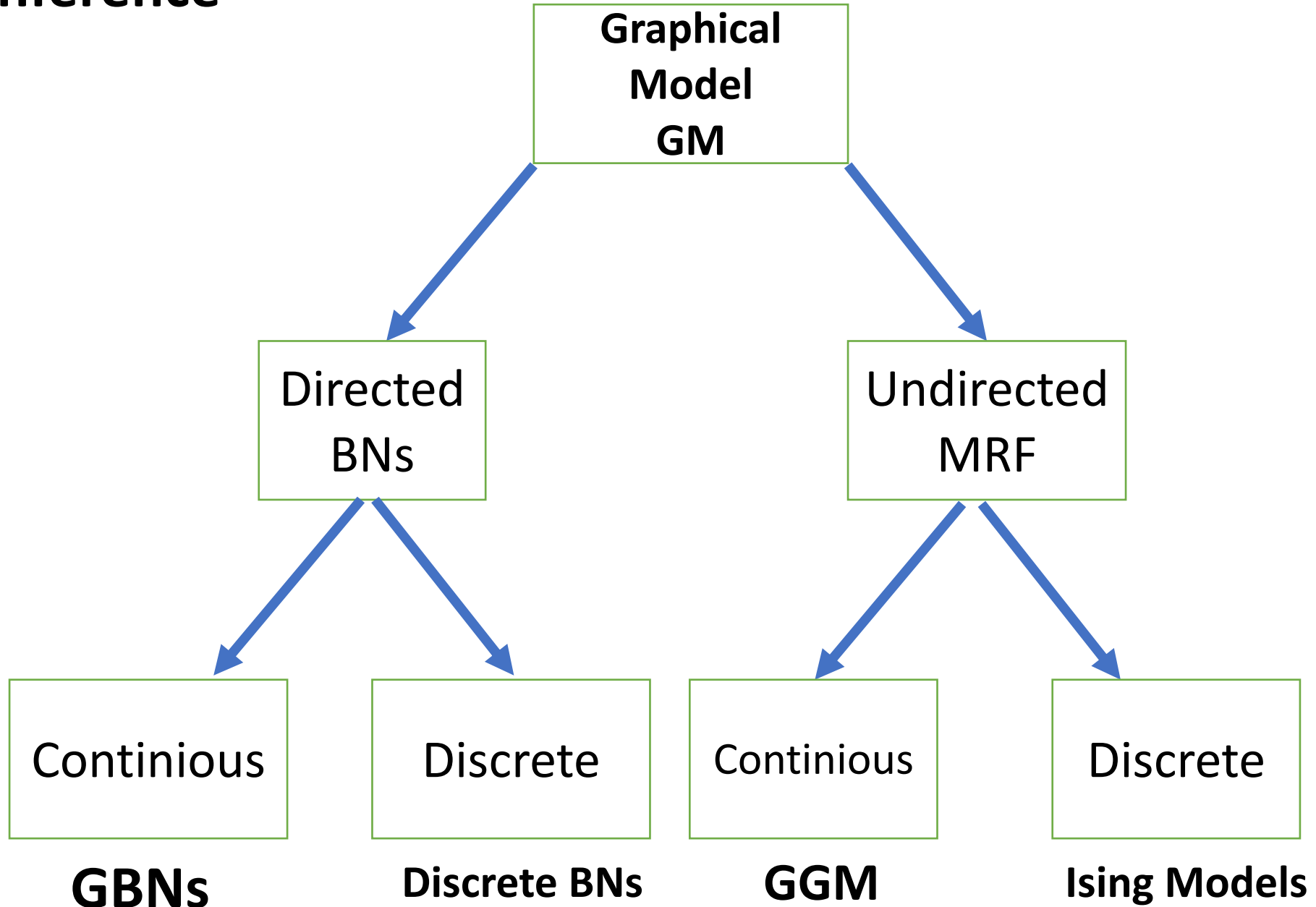
- **BIC**
- **BGe** (Bayesian Gaussian equivalent score)

✓ Search for the best network structure.

Summary

- Bayesian networks
- are a combination of a DAG and a global distribution, both defined on the same variables.
- Provide a systematic decomposition of the global distribution into lower-dimensional local distributions, in a divide-and-conquer way.
- Provide a principled solution to the problem of feature selection using Markov blankets.
- Can be a very useful tool for Network reconstruction.

Network Inference



Finally, practically: MRFs vs BNs

- **MRFs** have more power than **BNs**, but are more difficult to interpret and deal with computationally.
- A general rule of thumb is to use **Bayesian networks** whenever possible, and only switch to MRFs if there is no natural way to model the problem with a directed graph.

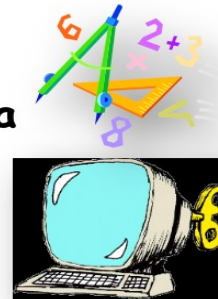
In a nutshell



Raw data



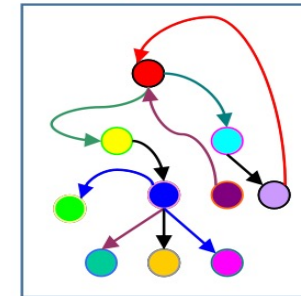
Cleaned data



Machine Learning



Statistical Methods



Network inference

- Think about the application of this concept in your field for a few minutes and discuss that in pairs.
- Consider the following questions for reflection in your field:
 - ✓ What variables are present in your project?
 - ✓ Why are these variables important?
 - ✓ What motivates your interest in understanding their interdependencies?
 - ✓ How does this understanding contribute to your work or goals?

References

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