Probabilistic Graphical Models

## The Big Objective(s)

In a wide variety of application fields two main problems need to be addressed over and over:

- 1. How can (expert) knowledge of complex domains be efficiently represented?
- 2. How can inferences be carried out within these representations?
- 3. How can such representations be (automatically) extracted from collected data?

We will deal with all three questions during the lecture.

### Example 1: Planning in car manufacturing

#### Available information

"Engine type  $e_1$  can only be combined with transmission  $t_2$  or  $t_5$ ."

"Transmission  $t_5$  requires crankshaft  $c_2$ ."

"Convertibles have the same set of radio options as SUVs."

### Possible questions/inferences:

"Can a station wagon with engine  $e_4$  be equipped with tire set  $y_6$ ?"

"Supplier  $S_8$  failed to deliver on time. What production line has to be modified and how?"

"Are there any peculiarities within the set of cars that suffered an aircondition failure?"

### Example 2: Medical reasoning

#### Available information:

"Malaria is much less likely than flu."

"Flu causes cough and fever."

"Nausea can indicate malaria as well as flu."

"Nausea never indicated pneunomia before."

### Possible questions/inferences

"The patient has fever. How likely is he to have malaria?"

"How much more likely does flu become if we can exclude malaria?"

#### Common Problems

Both scenarios share some severe problems:

#### Large Data Space

It is intractable to store all value combinations, i. e. all car part combinations or inter-disease dependencies.

(Example: VW Bora has  $10^{200}$  theoretical value combinations\*)

### Sparse Data Space

Even if we could handle such a space, it would be extremely sparse, i. e. it would be impossible to find good estimates for all the combinations.

(Example: with 100 diseases and 200 symptoms, there would be about 10<sup>62</sup> different scenarios for which we had to estimate the probability.\*)

<sup>\*</sup> The number of particles in the observable universe is estimated to be between  $10^{78}$  and  $10^{85}$ .

#### Idea to Solve the Problems

**Given:** A large (high-dimensional) distribution  $\delta$  representing the domain knowledge.

**Desired:** A set of smaller (lower-dimensional) distributions  $\{\delta_1, \ldots, \delta_s\}$  (maybe overlapping) from which the original  $\delta$  could be reconstructed with no (or as few as possible) errors.

With such a decomposition we can draw any conclusions from  $\{\delta_1, \ldots, \delta_s\}$  that could be inferred from  $\delta$  — without, however, actually reconstructing it.

## Example: Car Manufacturing

Let us consider a car configuration is described by three attributes:

- Engine E, dom $(E) = \{e_1, e_2, e_3\}$
- $\circ$  Breaks B, dom $(B) = \{b_1, b_2, b_3\}$
- $\circ$  Tires T, dom $(T) = \{t_1, t_2, t_3, t_4\}$

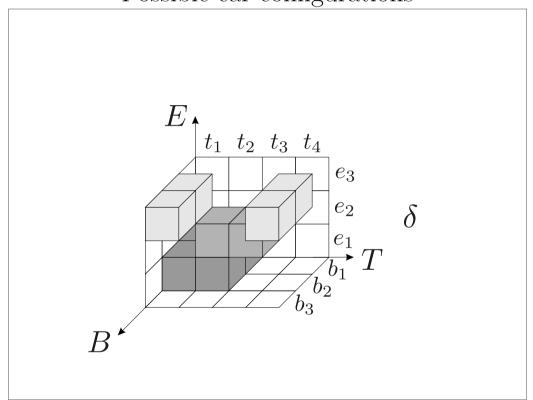
Therefore the set of all (theoretically) possible car configurations is:

$$\Omega = \operatorname{dom}(E) \times \operatorname{dom}(B) \times \operatorname{dom}(T)$$

Since not all combinations are technically possible (or wanted by marketing) a set of rules is used to cancel out invalid combinations.

### Example: Car Manufacturing

#### Possible car configurations

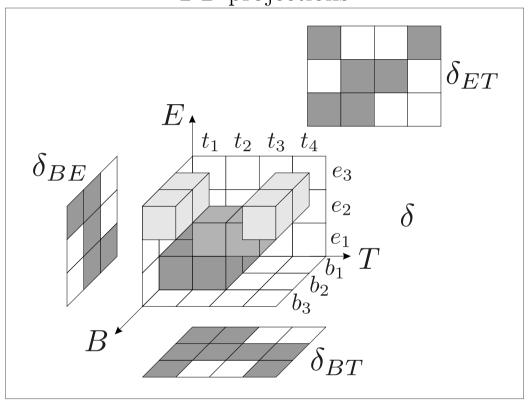


Every cube designates a valid value combination.

10 car configurations in our model.

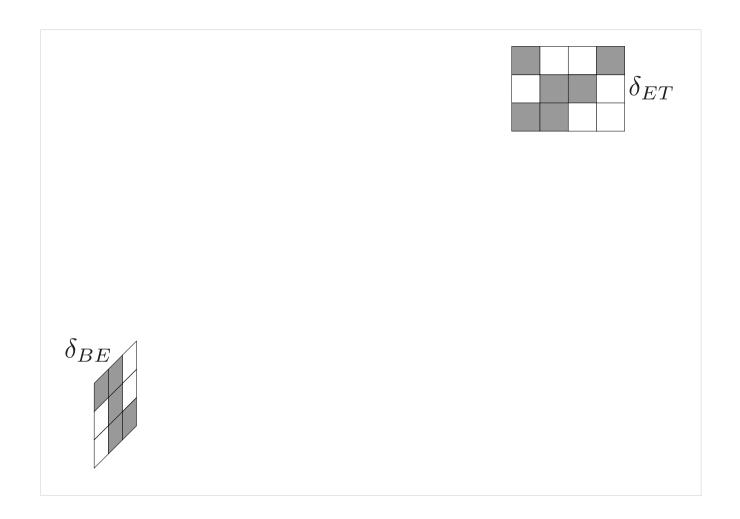
Different colors are intended to distinguish the cubes only.



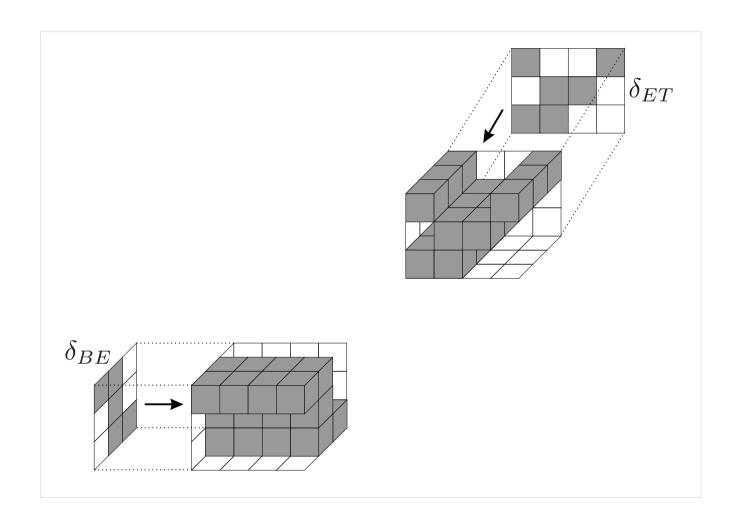


Is it possible to reconstruct  $\delta$  from the  $\delta_i$ ?

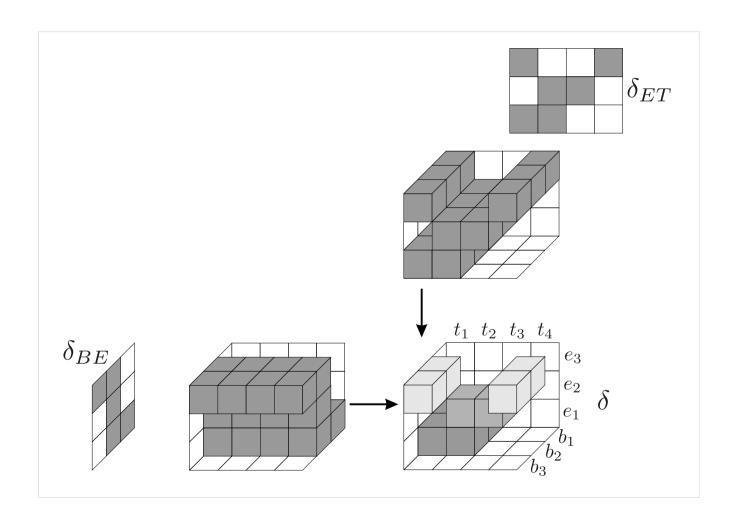
# Example: Reconstruction of $\delta$ with $\delta_{BE}$ and $\delta_{ET}$



# Example: Reconstruction of $\delta$ with $\delta_{BE}$ and $\delta_{ET}$



# Example: Reconstruction of $\delta$ with $\delta_{BE}$ and $\delta_{ET}$



# Causal Dependence vs. Reasoning

Rule: A entails B with certainty x:

$$A \xrightarrow{x} B$$

**Deduction**  $(\rightarrow)$ :

A and  $A \xrightarrow{x} B$ , therefore B more likely as effect (causality)

**Abduction**  $(\leftarrow)$ :

B and  $A \xrightarrow{x} B$ , therefore A more likely as cause (no causality)

For this reason, the notion "dependency model" is to be preferred to "causal network".

### Objective

Is it possible to exploit local constraints (wherever they may come from — both structural and expert knowledge-based) in a way that allows for a decomposition of the large (intractable) distribution  $P(X_1, \ldots, X_n)$  into several sub-structures  $\{C_1, \ldots, C_m\}$  such that:

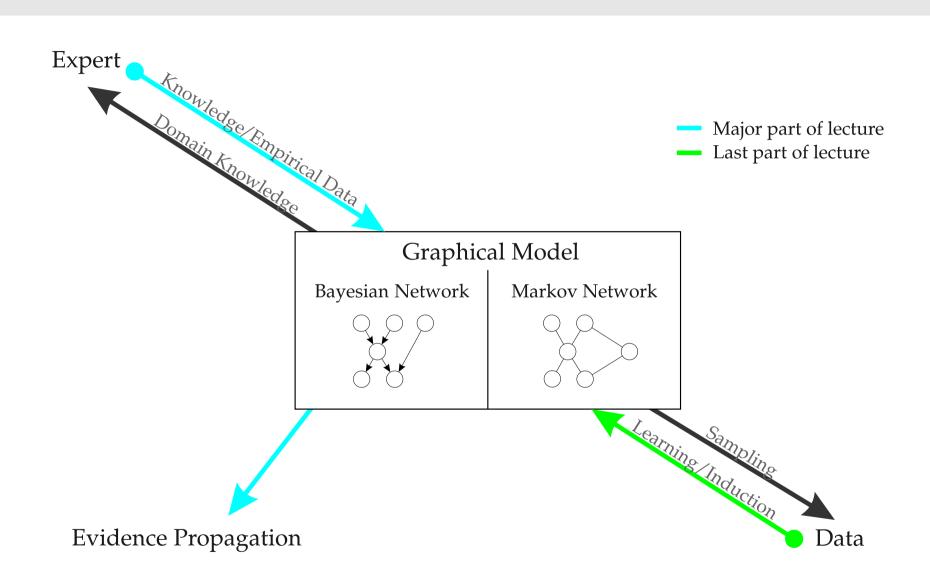
The collective size of those sub-structures is much smaller than that of the original distribution P.

The original distribution P is recomposable (with no or at least as few as possible errors) from these sub-structures in the following way:

$$P(X_1,\ldots,X_n) = \prod_{i=1}^m \Psi_i(c_i)$$

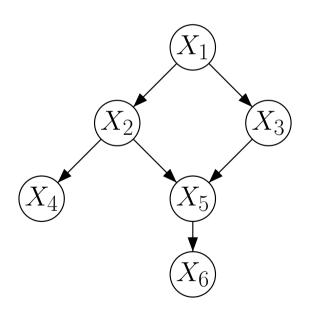
where  $c_i$  is an instantiation of  $C_i$  and  $\Psi_i(c_i) \in \mathbb{R}^+$  a factor potential.

### The Big Picture / Lecture Roadmap



#### Probabilistic Causal Networks

Probabilistic causal networks are directed acyclic graphs (DAGs) where the nodes represent propositions or variables and the directed edges model a direct causal dependence between the connected nodes. The strength of dependence is defined by conditional probabilities.

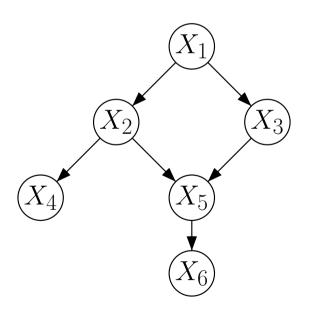


In general (according chain rule):

$$P(X_{1},...,X_{6}) = P(X_{6} | X_{5},...,X_{1}) \cdot P(X_{5} | X_{4},...,X_{1}) \cdot P(X_{4} | X_{3},X_{2},X_{1}) \cdot P(X_{3} | X_{2},X_{1}) \cdot P(X_{2} | X_{1}) \cdot P(X_{1})$$

#### Probabilistic Causal Networks

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According graph (independence structure):

$$P(X_1, \dots, X_6) = P(X_6 \mid X_5) \cdot$$

$$P(X_5 \mid X_2, X_3) \cdot$$

$$P(X_4 \mid X_2) \cdot$$

$$P(X_3 \mid X_1) \cdot$$

$$P(X_2 \mid X_1) \cdot$$

$$P(X_1)$$

#### Formal Framework

Nomenclature for the next slides:

$$X_1,\ldots,X_n$$

Variables

(properties, attributes, random variables, propositions)

$$\Omega_1,\ldots,\Omega_n$$

respective finite domains

(also designated with  $dom(X_i)$ )

$$\Omega = \underset{i=1}{\overset{n}{\times}} \Omega_i$$

Universe of Discourse (tuples that characterize objects

described by  $X_1, \ldots, X_n$ 

$$\Omega_i = \{x_i^{(1)}, \dots, x_i^{(n_i)}\} \quad n = 1, \dots, n, \ n_i \in \mathbb{N}$$

$$n=1,\ldots,n,\ n_i\in\mathbb{N}$$

#### Formal Framework

The product space  $(\Omega, 2^{\Omega}, P)$  is unique iff  $P(\{(x_1, \dots, x_n)\})$  is specified for all  $x_i \in \{x_i^{(1)}, \dots, x_i^{(n_i)}\}, i = 1, \dots, n$ .

When the distribution  $P(X_1, \ldots, X_n)$  is given in tabular form, then  $\prod_{i=1}^n |\Omega_i|$  entries are necessary.

For variables with  $|\Omega_i| \geq 2$  at least  $2^n$  entries.

The application of DAGs allows for the representation of existing (in)dependencies.

### Constructing a DAG

input  $P(X_1, \ldots, X_n)$ output a unique DAG G

- 1: Set the nodes of G to  $\{X_1,\ldots,X_n\}$ .
- 2: Choose a total ordering on the set of variables (e.g.  $X_1 \prec X_2 \prec \cdots \prec X_n$ )
- For  $X_i$  find the smallest (uniquely determinable) set  $S_i \subseteq \{X_1, \ldots, X_n\}$  such that  $P(X_i \mid S_i) = P(X_i \mid X_1, \ldots, X_{i-1})$ .
- 4: Connect all nodes in  $S_i$  with  $X_i$  and store  $P(X_i \mid S_i)$  as quantization of the dependencies for that node  $X_i$  (given its parents).
- $_{5:}$  return G

#### Belief Network

A Belief Network (V, E, P) consists of a set  $V = \{X_1, \ldots, X_n\}$  of random variables and a set E of directed edges between the variables.

Each variable has a finite set of mutual exclusive and collectively exhaustive states.

The variables in combination with the edges form a directed, acyclich graph.

Each variable with parent nodes  $B_1, \ldots, B_m$  is assigned a potential table  $P(A \mid B_1, \ldots, B_m)$ .

Note, that the connections between the nodes not necessarily express a causal relationship.

For every belief network, the following equation holds:

$$P(V) = \prod_{v \in V: P(c(v)) > 0} P(v \mid c(v))$$

with c(v) being the parent nodes of v.

Let  $a_1, a_2, a_3$  be three blood groups and  $b_1, b_2, b_3$  three indications of a blood group test.

Variables: A (blood group) B (indication)

Domains:  $\Omega_A = \{a_1, a_2, a_3\}$   $\Omega_B = \{b_1, b_2, b_3\}$ 

It is conjectured that there is a causal relationship between the variables.

$P(\{(a_i,b_j)\})$				
$\overline{a_1}$	0.64	0.08	0.08	0.8
$a_2$	0.01	0.08	0.01	0.1
$a_3$	0.64 0.01 0.01	0.01	0.08	0.1
$\sum$	0.66	0.17	0.17	1

$$(A)$$
  $B$ 

$$P(A,B) = P(B \mid A) \cdot P(A)$$

We are dealing with a belief network.

#### Expert Knowledge

Metastatic cancer is a possible cause of brain cancer, and an explanation for elevated levels of calcium in the blood. Both phenomena together can explain that a patient falls into a coma. Severe headaches are possibly associated with a brain tumor.

#### Special Case

The patient has severe headaches.

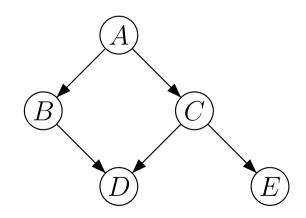
#### Question

Will the patient is go into a coma?

#### Choice of universe of discourse

	Variable	Domain	
$\overline{A}$	metastatic cancer	$\{a_1, a_2\}$	
B	increased serum calcium	$\{b_1,b_2\}$	$(\cdot_1 - \text{present}, \cdot_2 - \text{absent})$
C	brain tumor	$\{c_1,c_2\}$	$\Omega = \{a_1, a_2\} \times \cdots \times \{e_1, e_2\}$
D	coma	$\{d_1,d_2\}$	$ \Omega  = 32$
E	headache	$\{e_1, e_2\}$	

### Analysis of dependencies



#### Choice of probability parameters

$$P(a, b, c, d, e) \stackrel{\text{abbr.}}{=} P(A = a, B = b, C = c, D = d, E = e)$$

$$= P(e \mid c)P(d \mid b, c)P(c \mid a)P(b \mid a)P(a)$$
Shorthand notation

11 values to store instead of 31

Consult experts, textbooks, case studies, surveys, etc.

Calculation of conditional probabilities

Calculation of marginal probabilities

#### Crux of the Matter

Knowledge acquisition (Where do the numbers come from?)

 $\rightarrow$  learning strategies

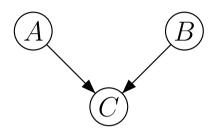
Computational complexities

 $\rightarrow$  exploit independencies

#### Problem:

When does the independency of X and Y given Z hold in (V, E, P)?

How can we determine  $P(X, Y \mid Z) = P(X \mid Z)P(Y \mid Z)$  solely using the graph structure?



### Meal quality

A quality of ingredients

B cook's skill

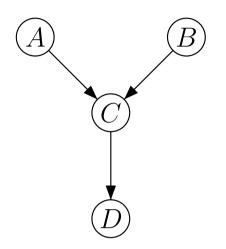
C meal quality

If C is not known, A and B are independent.

If C is known, then A and B become (conditionally) dependent given C.

$$A \not\perp\!\!\!\perp B \mid C$$

## Example (cont.)



#### Meal quality

A quality of ingredients

B cook's skill

C meal quality

D restaurant success

If nothing is known about the restaurant success or meal quality or both, the cook's skills and quality of the ingredients are unrelated, that is, *independent*.

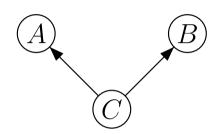
However, if we observe that the restaurant has no success, we can infer that the meal quality might be bad.

If we further learn that the ingredients quality is high, we will conclude that the cook's skills must be low, thus rendering both variables *dependent*.

 $A \not\perp \!\!\!\perp B \mid D$ 

### Dependencies

#### **Diverging Connection**



### Diagnosis

A body temperature

B cough

C disease

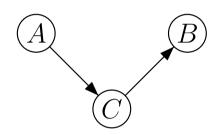
If C is unknown, knowledge about A ist relevant for B and vice versa, i. e. A and B are marginally dependent.

However, if C is observed, A and B become conditionally independent given C.

A influences B via C. If C is known it in a way blocks the information from flowing from A to B, thus rendering A and B (conditionally) independent.

### **Dependencies**

#### **Serial Connection**



#### Accidents

A rain

B accident risk

C road conditions

Analog scenario to case 2

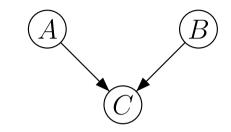
A influences C and C influences B. Thus, A influences B.

If C is known, it blocks the path between A and B.

#### Converging Connection: Marginal Independence

Decomposition according to graph:

$$P(A, B, C) = P(C \mid A, B) \cdot P(A) \cdot P(B)$$



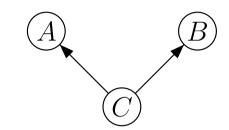
Embedded Independence:

$$P(A, B, C) = \frac{P(A, B, C)}{P(A, B)} \cdot P(A) \cdot P(B)$$
 with  $P(A, B) \neq 0$   
 $P(A, B) = P(A) \cdot P(B)$   
 $\Rightarrow A \perp \!\!\!\perp B \mid \emptyset$ 

#### **Diverging Connection:** Conditional Independence

Decomposition according to graph:

$$P(A, B, C) = P(A \mid C) \cdot P(B \mid C) \cdot P(C)$$



Embedded Independence:

$$P(A, B \mid C) = P(A \mid C) \cdot P(B \mid C)$$
  
 $\Rightarrow A \perp \!\!\!\perp B \mid C$ 

Alternative derivation:

$$P(A, B, C) = P(A \mid C) \cdot P(B, C)$$

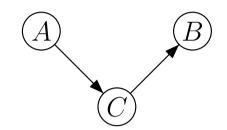
$$P(A \mid B, C) = P(A \mid C)$$

$$\Rightarrow A \perp \!\!\!\perp B \mid C$$

#### Serial Connection: Conditional Independence

Decomposition according to graph:

$$P(A, B, C) = P(B \mid C) \cdot P(C \mid A) \cdot P(A)$$



Embedded Independence:

$$P(A, B, C) = P(B \mid C) \cdot P(C, A)$$

$$P(B \mid C, A) = P(B \mid C)$$

$$\Rightarrow A \perp \!\!\!\perp B \mid C$$

#### Trivial Cases:

Marginal Independence:

$$\bigcirc$$
A



$$P(A,B) = P(A) \cdot P(B)$$

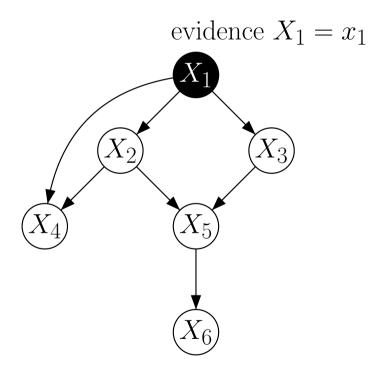
Marginal Dependence:

$$(A)$$
  $\rightarrow (B)$ 

$$P(A, B) = P(B \mid A) \cdot P(A)$$

# Question

**Question:** Are  $X_2$  and  $X_3$  independent given  $X_1$ ?



### d-Separation

Let G = (V, E) a DAG and  $X, Y, Z \in V$  three nodes.

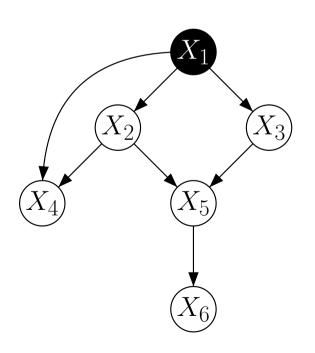
- a) A set  $S \subseteq V \setminus \{X, Y\}$  d-separates X and Y, if S blocks all paths between X and Y. (paths may also route in opposite edge direction)
- b) A path  $\pi$  is d-separated by S if at least one pair of consecutive edges along  $\pi$  is blocked. There are the following blocking conditions:
  - 1.  $X \leftarrow Y \rightarrow Z$  tail-to-tail
  - 2.  $X \leftarrow Y \leftarrow Z$  head-to-tail  $X \rightarrow Y \rightarrow Z$
  - 3.  $X \to Y \leftarrow Z$  head-to-head
- c) Two edges that meet tail-to-tail or head-to-tail in node Y are blocked if  $Y \in S$ .
- d) Two edges meeting head-to-head in Y are blocked if neither Y nor its successors are in S.

## Relation to Conditional independence

If  $S \subseteq V \setminus \{X, Y\}$  d-separates X and Y in a Belief network (V, E, P) then X and Y are conditionally independent given S:

$$P(X, Y \mid S) = P(X \mid S) \cdot P(Y \mid S)$$

Application to the previous example:



Paths: 
$$\pi_1 = \langle X_2 - X_1 - X_3 \rangle$$
,  $\pi_2 = \langle X_2 - X_5 - X_3 \rangle$   
 $\pi_3 = \langle X_2 - X_4 - X_1 - X_3 \rangle$ ,  $S = \{X_1\}$ 

$$\pi_1$$
  $X_2 \leftarrow X_1 \rightarrow X_3$  tail-to-tail  $X_1 \in S \Rightarrow \pi_1$  is blocked by  $S$ 

$$\pi_2$$
  $X_2 \rightarrow X_5 \leftarrow X_3$  head-to-head  $X_5, X_6 \notin S \Rightarrow \pi_2$  is blocked by  $S$ 

$$\pi_3$$
  $X_4 \leftarrow X_1 \rightarrow X_3$  tail-to-tail  $X_2 \rightarrow X_4 \leftarrow X_1$  head-to-head both connections are blocked  $\Rightarrow \pi_3$  is blocked

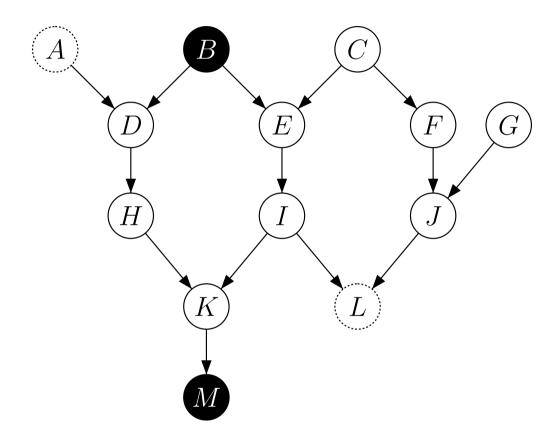
# Example (cont.)

Answer:  $X_2$  and  $X_3$  are d-separated via  $\{X_1\}$ . Therefore  $X_2$  and  $X_3$  become conditionally independent given  $X_1$ .

$$S = \{X_1, X_4\} \implies X_2 \text{ and } X_3 \text{ are d-separated by } S$$

$$S = \{X_1, X_6\} \implies X_2 \text{ and } X_3 \text{ are } not \text{ d-separated by } S$$

## Another Example



Are A and L conditionally independent given  $\{B, M\}$ ?

## Algebraic structure of CI statements

Question: Is it possible to use a formal scheme to infer new conditional independence (CI) statements from a set of initial CIs?

### Repetition

Let  $(\Omega, \mathcal{E}, P)$  be a probability space and W, X, Y, Z disjoint subsets of variables. If X and Y are conditionally independent given Z we write:

$$X \perp \!\!\!\perp_P Y \mid Z$$

Often, the following (equivalent) notation is used:

$$I_P(X \mid Z \mid Y)$$
 or  $I_P(X, Y \mid Z)$ 

If the underlying space is known the index P is omitted.

# (Semi-)Graphoid-Axioms

Let  $(\Omega, \mathcal{E}, P)$  be a probability space and W, X, Y and Z four disjoint subsets of random variables (over  $\Omega$ ). Then the propositions

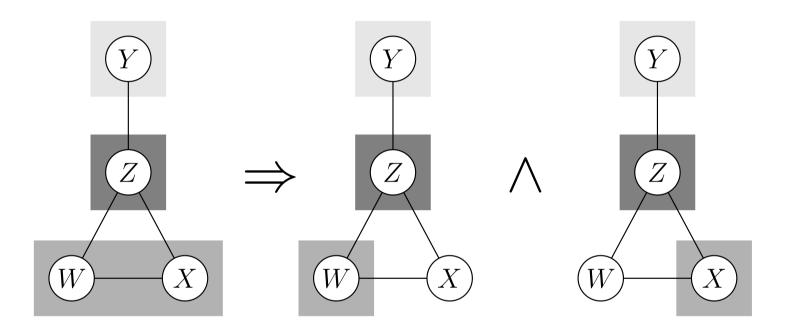
- a) Symmetry:  $(X \perp \!\!\!\perp_P Y \mid Z) \Rightarrow (Y \perp \!\!\!\perp_P X \mid Z)$
- b) Decomposition:  $(W \cup X \perp \!\!\!\perp_P Y \mid Z) \Rightarrow (W \perp \!\!\!\perp_P Y \mid Z) \land (X \perp \!\!\!\perp_P Y \mid Z)$
- c) Weak Union:  $(W \cup X \perp \!\!\!\perp_P Y \mid Z) \Rightarrow (X \perp \!\!\!\perp_P Y \mid Z \cup W)$
- d) Contraction:  $(X \perp\!\!\!\perp_P Y \mid Z \cup W) \wedge (W \perp\!\!\!\perp_P Y \mid Z) \Rightarrow (W \cup X \perp\!\!\!\perp_P Y \mid Z)$

are called the **Semi-Graphoid Axioms**. The above propositions and

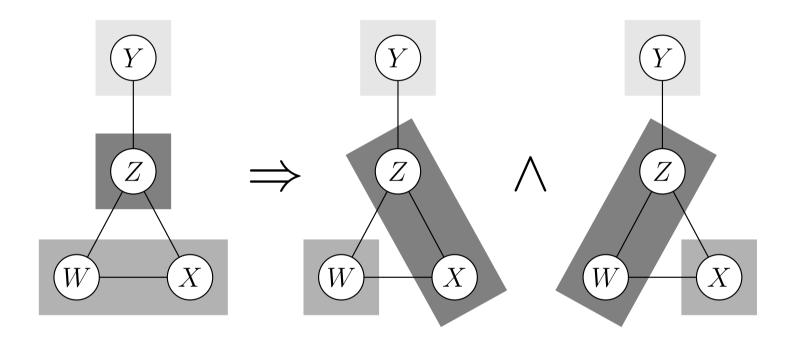
e) Intersection:  $(W \perp \!\!\!\perp_P Y \mid Z \cup X) \land (X \perp \!\!\!\perp_P Y \mid Z \cup W) \Rightarrow (W \cup X \perp \!\!\!\perp_P Y \mid Z)$ 

are called the **Graphoid Axioms**.

# Decomposition

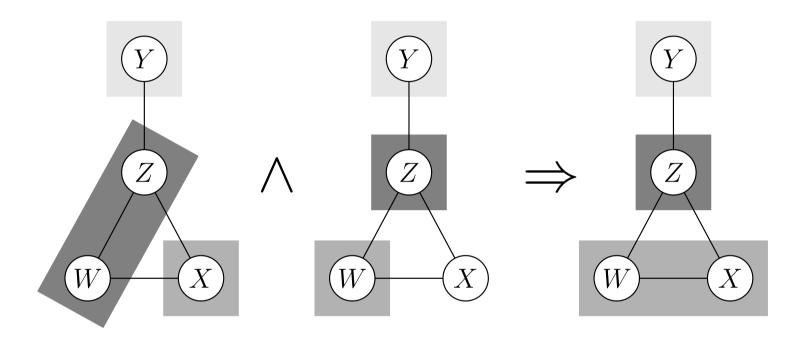


### Weak Union



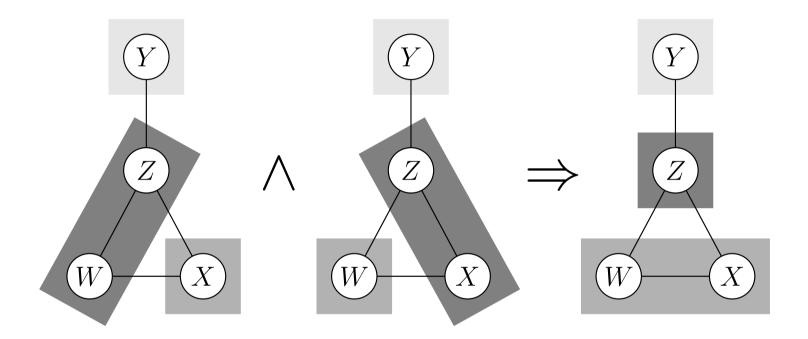
Learning irrelevant information W cannot render irrelevant information X relevant.

#### Contraction



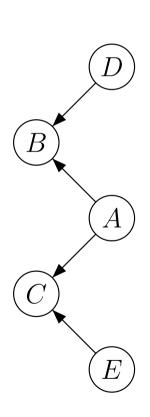
If X is irrelevant (to Y) after having learnt some irrelevant information W, then X must have been irrelevant before.

#### Intersection



Unless W affects Y when X is known or X affects Y when W is known, neither X nor W nor their combination can affect Y.

# Example



Proposition: 
$$B \perp \!\!\! \perp C \mid A$$

Proof: 
$$D \perp \!\!\!\perp A, C \mid \emptyset \quad \land \quad B \perp \!\!\!\perp C \mid A, D$$

$$\stackrel{\text{w. union}}{\Longrightarrow} D \perp \!\!\!\perp C \mid A \wedge B \perp \!\!\!\perp C \mid A, D$$

$$\stackrel{\text{symm.}}{\iff} C \perp\!\!\!\perp D \mid A \quad \land \quad C \perp\!\!\!\perp B \mid A, D$$

$$\stackrel{\text{contr.}}{\Longrightarrow} \quad C \perp \!\!\! \perp B, D \mid A$$

$$\stackrel{\text{decomp.}}{\Longrightarrow} C \perp \!\!\! \perp B \mid A$$

$$\stackrel{\text{symm.}}{\iff} B \perp \!\!\! \perp C \mid A$$

# Conditional (In)Dependence Graphs

**Definition:** Let  $(\cdot \perp \perp_{\delta} \cdot | \cdot)$  be a three-place relation representing the set of conditional independence statements that hold in a given distribution  $\delta$  over a set U of attributes. An undirected graph G = (U, E) over U is called a **conditional dependence graph** or a **dependence map** w.r.t.  $\delta$ , iff for all disjoint subsets  $X, Y, Z \subseteq U$  of attributes

$$X \perp \!\!\! \perp_{\delta} Y \mid Z \Rightarrow \langle X \mid Z \mid Y \rangle_{G},$$

i.e., if G captures by u-separation all (conditional) independences that hold in  $\delta$  and thus represents only valid (conditional) dependences. Similarly, G is called a **conditional independence graph** or an **independence map** w.r.t.  $\delta$ , iff for all disjoint subsets  $X, Y, Z \subseteq U$  of attributes

$$\langle X \mid Z \mid Y \rangle_G \Rightarrow X \perp \!\!\! \perp_{\delta} Y \mid Z,$$

i. e., if G captures by u-separation only (conditional) independences that are valid in  $\delta$ . G is said to be a **perfect map** of the conditional (in)dependences in  $\delta$ , if it is both a dependence map and an independence map.

## Markov Properties of Undirected Graphs

**Definition:** An undirected graph G = (U, E) over a set U of attributes is said to have (w.r.t. a distribution  $\delta$ ) the

### pairwise Markov property,

iff in  $\delta$  any pair of attributes which are nonadjacent in the graph are conditionally independent given all remaining attributes, i.e., iff

$$\forall A, B \in U, A \neq B : (A, B) \notin E \Rightarrow A \perp \!\!\!\perp_{\delta} B \mid U - \{A, B\},\$$

## local Markov property,

iff in  $\delta$  any attribute is conditionally independent of all remaining attributes given its neighbors, i.e., iff

$$\forall A \in U : A \perp \!\!\! \perp_{\delta} U - \operatorname{closure}(A) \mid \operatorname{boundary}(A),$$

### global Markov property,

iff in  $\delta$  any two sets of attributes which are *u*-separated by a third are conditionally independent given the attributes in the third set, i.e., iff

$$\forall X, Y, Z \subseteq U : \langle X \mid Z \mid Y \rangle_G \Rightarrow X \perp \!\!\! \perp_{\delta} Y \mid Z.$$

## Markov Properties of Directed Acyclic Graphs

**Definition:** A directed acyclic graph  $\vec{G} = (U, \vec{E})$  over a set U of attributes is said to have (w.r.t. a distribution  $\delta$ ) the

## pairwise Markov property,

iff in  $\delta$  any attribute is conditionally independent of any non-descendant not among its parents given all remaining non-descendants, i.e., iff

$$\forall A, B \in U : B \in \text{non-descs}(A) - \text{parents}(A) \Rightarrow A \perp \!\!\!\perp_{\delta} B \mid \text{non-descs}(A) - \{B\},$$

### local Markov property,

iff in  $\delta$  any attribute is conditionally independent of all remaining non-descendants given its parents, i.e., iff

$$\forall A \in U : A \perp \perp_{\delta} \text{non-descs}(A) - \text{parents}(A) \mid \text{parents}(A),$$

### global Markov property,

iff in  $\delta$  any two sets of attributes which are d-separated by a third are conditionally independent given the attributes in the third set, i.e., iff

$$\forall X,Y,Z\subseteq U:\quad \langle X\mid Z\mid Y\rangle_{\vec{G}}\ \Rightarrow\ X\perp\!\!\!\perp_{\delta}Y\mid Z.$$