# Artificial Intelligence

A course about foundations



#### Probabilistic Reasoning: Graphical Models

Marco Piastra

Artificial Intelligence 2023-2024 Graphical Models [1]

# Factorizations & Graphs

Artificial Intelligence 2023-2024 Graphical Models [2]

#### Chain Factorization

#### Univariate factorization of a JPD

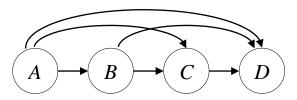
From the definition of conditional probability

$$P(A, B, C, D) = P(A)P(B|A)P(C|A, B)P(D|A, B, C)$$

Any joint probability distribution can be factorized in a way such that each factor is *univariate* (i.e. one random variable as independent) conditional distribution.

- Each factorization depends on an arbitrary sequence of the random variables
- Hence factorizations are not unique: any sequence produces a legitimate factorization of the same kind

#### Graphical equivalent



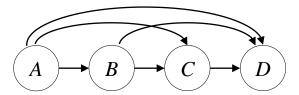
In this <u>oriented</u> graph:

- each node represents a random variable (and the corresponding *univariate* factor)
- each arc represents a conditioning of a random variable over another one (i.e. dependence)

#### Chain Factorization

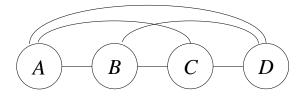
#### Graphical model

$$P(A, B, C, D) = P(A)P(B|A)P(C|A, B)P(D|A, B, C)$$



#### This graph:

- is *acyclic*: if you follow the arrows, you will never return to the same node
- is completely connected: if you ignore arc orientations, every node is connected to any other node



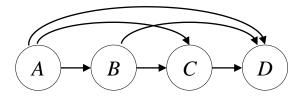
Any univariate factorization can be represented by a graphical model Every completely connected, acyclic and oriented graph represents a univariate factorization

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### Chain Factorization and Independence Assumptions

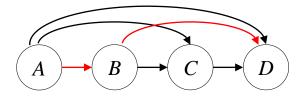
#### Graphical model

$$P(A, B, C, D) = P(A)P(B|A)P(C|A, B)P(D|A, B, C)$$



#### Independence

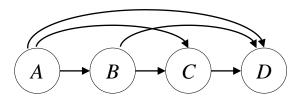
Let's remove a few arcs from the graph and rewrite the factorization accordingly



### Chain Factorization and Independence Assumptions

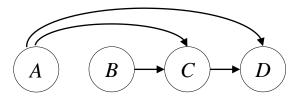
#### Graphical model

$$P(A, B, C, D) = P(A)P(B|A)P(C|A, B)P(D|A, B, C)$$



#### Independence

Let's remove a few arcs from the graph and rewrite the factorization accordingly



$$P(A, B, C, D) = P(A)P(B)P(C|A, B)P(D|A, C)$$

The latter holds true only if

$$P(B|A) = P(B)$$

$$P(D|A, B, C) = P(D|A, C)$$

Independence 
$$\langle A \perp B \rangle$$
 Conditional Independence 
$$\langle B \perp D \mid A, C \rangle$$

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# Determining Independence from Graphs

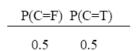
### Graphical models (a.k.a. Bayesian Networks)

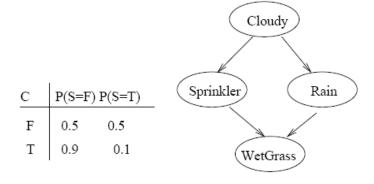
Structure and numbers, instead of just numbers

A structured, pre-numerical representation of a joint probability

Each graphical model is an *oriented* graph

- nodes are random variables
- arcs represent dependence





С	P(R=F) P(R=T)	
F	0.8	0.2
T	0.2	0.8

S R	P(W=F)	P(W=T)
F F	1.0	0.0
T F	0.1	0.9
FΤ	0.1	0.9
ТТ	0.01	0.99

Artificial Intelligence 2023–2024 Graphical Models [8]

## From graphical models to joint probability

#### Joint probability factorization

A chain factorization like the following is always allowed

$$P(C, S, R, W) = P(C)P(S|C)P(R|C, S)P(W|C, S, R)$$

Hint: apply the definition of conditional probability repeatedly (such factorization is not unique)

#### Factorization for a graphical model

$$P(X_1, X_2, \dots, X_n) = \prod_i P(X_i \mid parents(X_i))$$

where  $parents(X_i)$  are the nodes from which there is an entry arc to  $X_i$ 

С	P(S=F) P(S=T)	
F	0.5	0.5
T	0.9	0.1

For this example, the above rule produces:

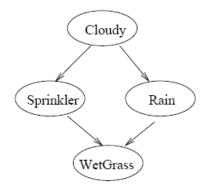
$$P(C, S, R, W) = P(C)P(S|C)P(R|C)P(W|S, R)$$

Note the difference from above

Independence assumptions:  $\langle R \perp S \mid C \rangle$ ,  $\langle W \perp C \mid R, S \rangle$ 

A complete specification of a joint probability would require  $2^4 = 16$  values
The values in figure are just 9

P(C=F)	P(C=T)
0.5	0.5



С	P(R=F)	P(R=T)
F	0.8	0.2
T	0.2	0.8

S R	P(W=F)	P(W=T)
F F	1.0	0.0
T F	0.1	0.9
FΤ	0.1	0.9
ТТ	0.01	0.99

#### Sequence or Chain

Consider the graph on the right

$$P(C, S, W) = P(C)P(S|C)P(W|S)$$

Now suppose you observe S

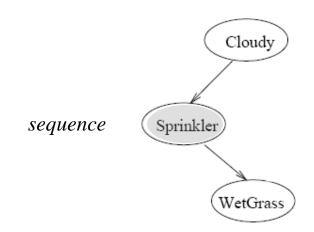
$$P(C, W|S) = \frac{P(C, S, W)}{P(S)}$$

$$= \frac{P(C)P(S|C)P(W|S)}{P(S)}$$

$$= \frac{P(C, S)}{P(S)}P(W|S)$$

$$= P(C|S)P(W|S)$$

This implies  $\langle C \perp W \mid S \rangle$ 



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#### Fork

Consider the graph on the right

$$P(C, S, R) = P(C)P(S|C)P(R|C)$$

Now suppose you observe C

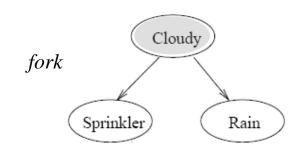
$$P(R, S|C) = \frac{P(C, S, R)}{P(C)}$$

$$= \frac{P(C)P(S|C)P(R|C)}{P(C)}$$

$$= \frac{P(C, S)}{P(C)}P(R|C)$$

$$= P(S|C)P(R|C)$$

This implies  $\langle R \perp S \mid C \rangle$ 



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Join or Collider

CAUTION: this case is different from the previous two

Consider the graph on the right

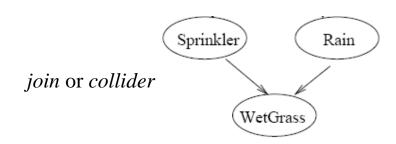
$$P(R,S,W) = P(S)P(R)P(W|S,R)$$
 which is true only if  $\langle S \perp R \rangle$  \_\_\_\_\_\_\_\_ Independence (also 'Marginal Independence')

 $\neq P(S|W)P(R|W)$ 

Now suppose you observe W

$$\begin{split} P(R,S|W) &= \frac{P(R,S,W)}{P(W)} \\ &= \frac{P(S)P(R)P(W|S,R)}{P(W)} & \text{No further simplification possible} \end{split}$$

This implies  $\langle S \not\perp R | W \rangle$ 



#### Join or Collider

The same loss of independence occurs if you observe any of the <u>descendants</u>...

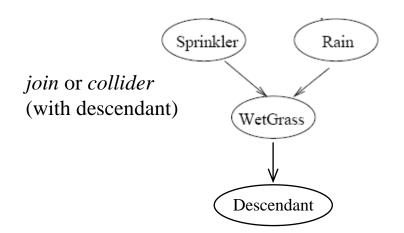
Consider the graph on the right

Now suppose you observe D

$$\begin{split} P(R,S,W|D) &= \frac{P(R,S,W,D)}{P(D)} \\ &= \frac{P(S)P(R)P(W|S,R)P(D|W)}{P(D)} \quad \substack{\text{No further simplification} \\ possible} \\ &\neq P(S|D)P(R|D) \end{split}$$

This implies  $\langle S \not\perp \!\!\! \perp R \mid \!\! D \rangle$ 

... at any subsequent level of descendance (try yourself)



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# d-Separation

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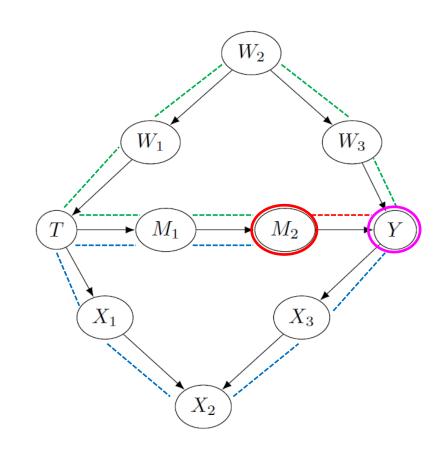
In a graphical model

Consider any two nodes A and B

A *path* between *A* and *B* is a path in the graph ignoring orientation (i.e. arrows)

#### Example:

In the graph on the right, consider <u>all</u> paths between  $M_2$  and Y



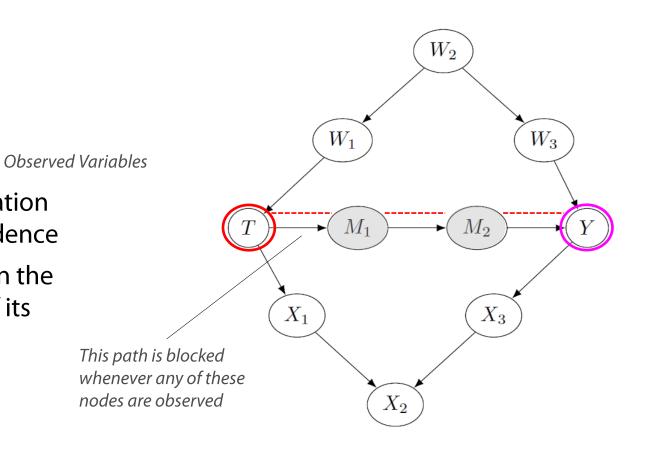
Artificial Intelligence 2023–2024 Graphical Models [15]

In a graphical model

A *path* between any two nodes A and B is **blocked** whenever the observations  $\{X_o\}$  are such that the path contains either:

1) a sequence or a fork for which one observation  $X \in \{X_o\}$  creates a condition of independence

2) a collider for which  $\{X_o\}$  does <u>not</u> contain the observation of the join node nor of any of its descendants



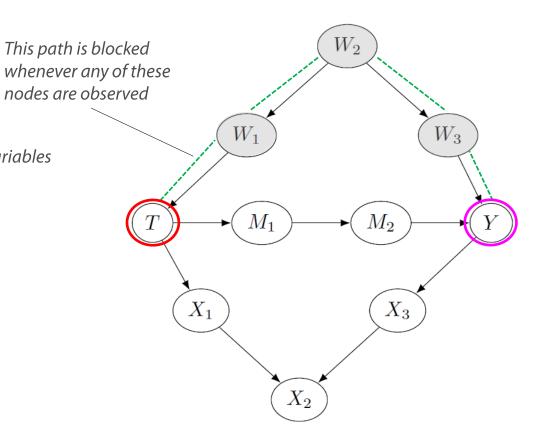
Artificial Intelligence 2023–2024 Graphical Models [16]

In a graphical model

A *path* between any two nodes A and B is **blocked** whenever the observations  $\{X_o\}$  are such that the path contains either:

Observed Variables

- 1) a sequence or a fork for which one observation  $X \in \{X_o\}$  creates a condition of independence
- 2) a collider for which  $\{X_o\}$  does <u>not</u> contain the observation of the join node nor of any of its descendants

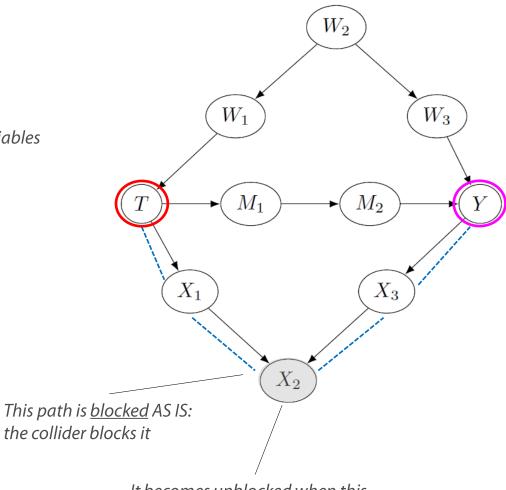


Artificial Intelligence 2023-2024 Graphical Models [17]

In a graphical model

A path between any two nodes A and B is **blocked** whenever the observations  $\{X_o\}$  are such that the path contains either: Observed Variables

- 1) a sequence or a fork for which one observation  $X \in \{X_o\}$  creates a condition of independence
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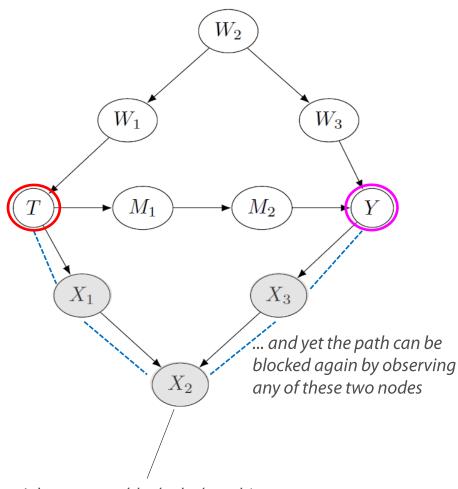
It becomes <u>unblocked</u> when this node is observed...

Artificial Intelligence 2023–2024 Graphical Models [18]

In a graphical model

A path between any two nodes A and B is **blocked** whenever the observations  $\{X_o\}$  are such that the path contains either: Observed Variables

- 1) a sequence or a fork for which one observation  $X \in \{X_o\}$  creates a condition of independence
- 2) a collider for which  $\{X_o\}$  does <u>not</u> contain the observation of the join node nor of any of its descendants



It becomes <u>unblocked</u> when this node is observed...

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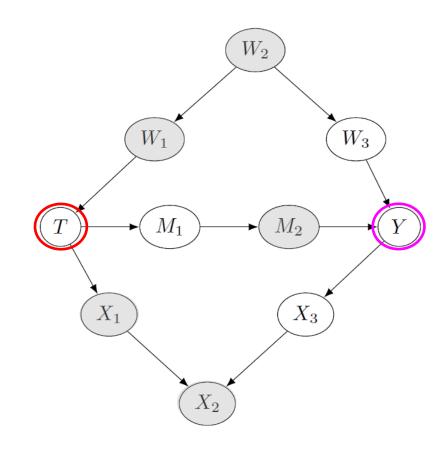
#### Dependency Separation (d-separation)

Any two nodes A and B in a graphical model are  $\emph{d-separated}$  whenever the observations  $\{X_o\}$  are such that all paths between A and B are blocked

In that case we have

 $\langle A \perp B | \{X_o\} \rangle$ 

But only when <u>all</u> paths are blocked



These observations make the two nodes <u>d-separated</u>

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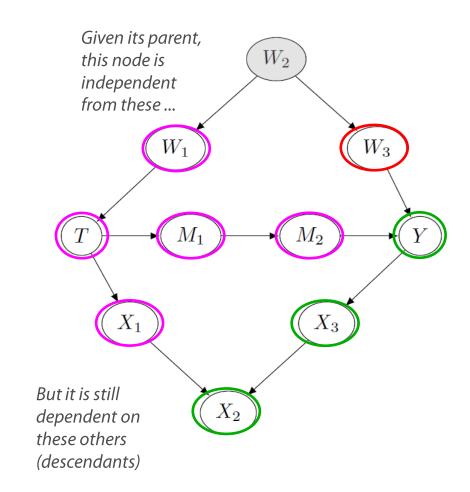
# Graphical models: fundamental assumptions

#### Minimality

Adjacent nodes in the graph are dependent.

#### Local Markov Assumption

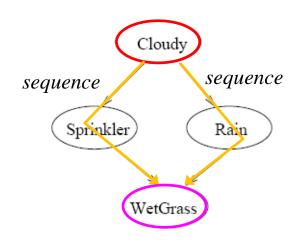
Given its parents in the graph, a node A is independent of all its non-descendants



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#### Example:

Cloudy and WetGrass are independent when both paths in color are blocked

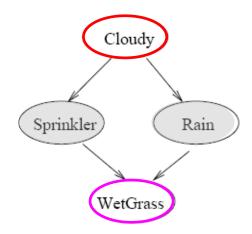


Artificial Intelligence 2023-2024 Graphical Models [22]

#### Example:

Cloudy and WetGrass are independent when both paths in color are blocked

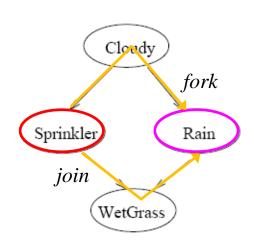
These are two *sequences*:
Sprinkler and Rain must be <u>known</u>



Artificial Intelligence 2023-2024 Graphical Models [23]

#### Example:

Sprinkler and Rain are independent when both paths in color are blocked



Artificial Intelligence 2023-2024 Graphical Models [24]

#### Example:

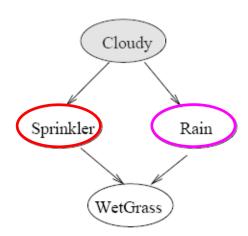
Sprinkler and Rain are independent when both paths in color are blocked

One *fork* and one *collider*: Cloudy must be <u>known</u> whereas WetGrass must be <u>unknown</u>

< Sprinkler 

L Rain | Cloudy >

Check more examples and quiz with Bayes program (see course webpage)!



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# Inference in a Graphical Model

# Building a graphical model

Step 1

Defining the nodes, i.e. the random variables

T: (tampering)

*F* : (*fire*)

A: (alarm)

*S* : (*smoke*)

L: (leaving)

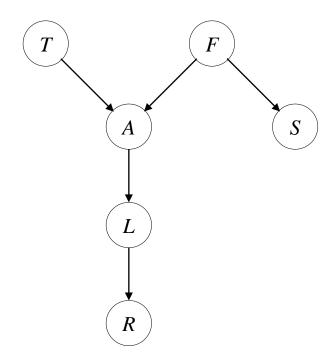
*R* : (*report*)

Artificial Intelligence 2023-2024 Graphical Models [27]

# Building a graphical model

Step 2

Defining the structure, i.e. the graph



We are thus saying that:

 $< T \perp F >$  (but they become dependent when any of A, L or R are known)

 $\langle A \perp S \mid F \rangle$ 

 $< L \perp T \mid A>$ 

< $L \perp F \mid A>$ 

 $<A \perp R \mid L>$ 

*T* : (tampering)

*F* : (*fire*)

A: (alarm)

*S* : (*smoke*)

L: (leaving)

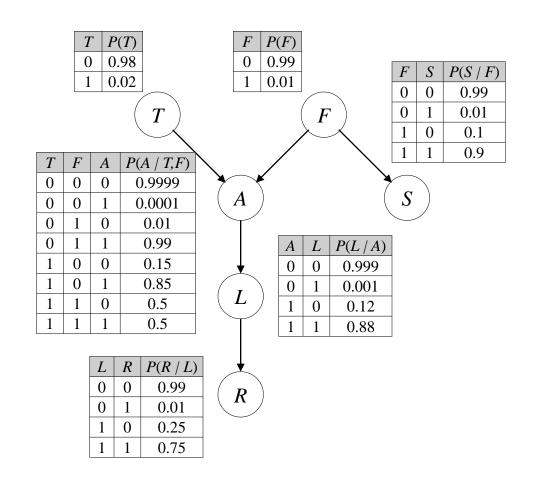
*R* : (*report*)

Artificial Intelligence 2023-2024 Graphical Models [28]

# Building a graphical model

#### Step 3

Defining conditional probability tables – CPTs



*T* : (tampering)

*F* : (*fire*)

A: (alarm)

S: (smoke)

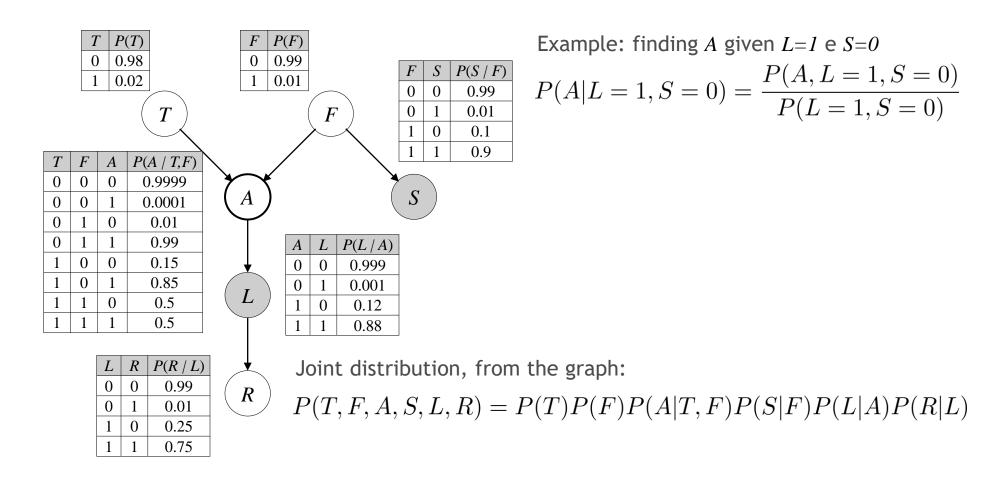
L: (leaving)

R:(report)

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#### Step 4

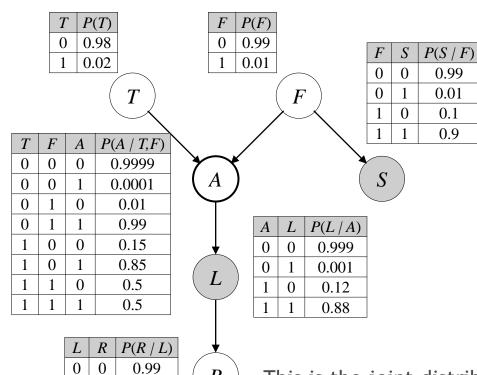
Consider a specific problem



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#### Step 5

Computing the answer



0.01

0.25

0.75

 $1 \mid 0$ 

Note that:

$$P(A|L=1, S=0) = \frac{P(A, L=1, S=0)}{P(L=1, S=0)}$$

This is a normalizing term: it can be computed from

$$P(A, L = 1, S = 0)$$

In fact:

$$P(L=1, S=0) = \sum_{A} P(A, L=1, S=0)$$

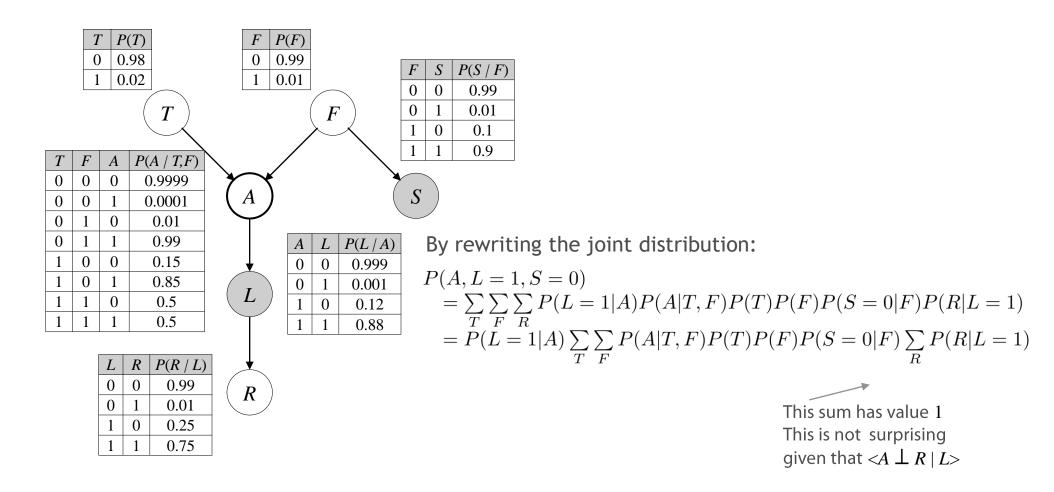
Typically, the most time-consuming computations in an inference problem are marginalizations

This is the joint distribution to be computed:

$$P(A, L = 1, S = 0) = \sum_{T, F, R} P(T)P(F)P(A|T, F)P(S = 0|F)P(L = 1|A)P(R|L = 1)$$

#### Step 5

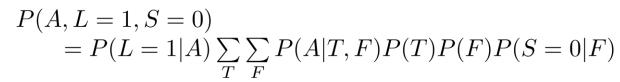
Computing the answer

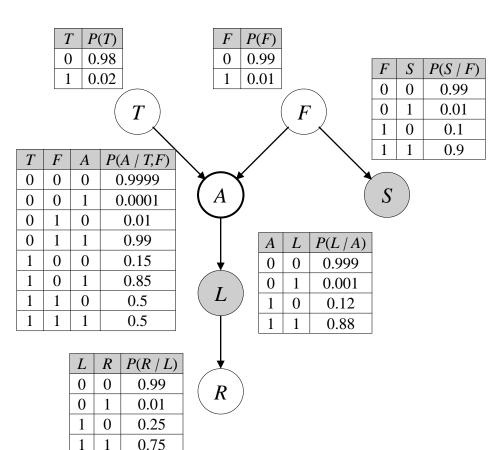


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Step 5

Computing the answer





By convention, we write:

$$P(A, L = 1, S = 0) = f_{T,F,S=0}(A)f_{L=1}(A)$$

where the f are the factors of the method also known as elimination of variables:

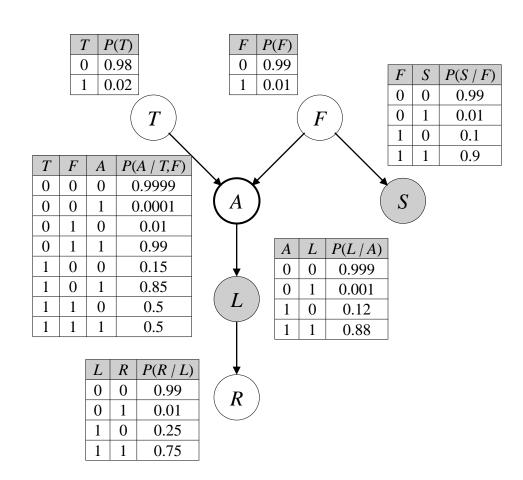
$$f_{T,F,S=0}(A) := \sum_{T} \sum_{F} P(A|T,F)P(T)P(F)P(S=0|F)$$

$$f_{L=1}(A) := P(L=1|A)$$

Note in passing that factors f are not probabilities (i.e. they do not sum to 1).

#### Step 5

Computing the answer



Note that:

$$P(A,L=1,S=0) = f_{T,F,S=0}(A)f_{L=1}(A)$$
 This factor comes from the parents of  $A$  The descendants of  $A$ 

This is true for any node *A* that *d-separates* the graph

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# Variable elimination for graphical models

#### General idea

Write the marginal joint probability from the query in the form:

$$P(\lbrace X_r \rbrace, \lbrace X_o \rbrace) = \sum_{\lbrace X_i \rbrace} \prod_{X} P(X \mid parents(X))$$

- 1) Find the best ordering of terms for the marginalization of irrelevant variables:
- 2) Move summations 'inside' the product as much as possible (i.e. find *factors f*)
- 3) Compute factors (i.e. by sum of products) and obtain numbers (i.e. terms)
- 4) Plug these *terms* into the product and obtain a simpler form for

$$P(\{X_r\}, \{X_o\})$$

5) Wrap it up and compute the response:

$$P(\{X_r\}|\{X_o\}) = \frac{P(\{X_r\}, \{X_o\})}{\sum_{\{X_r\}} P(\{X_r\}, \{X_o\})}$$

Remember: the method is NP-complete (anyway)

### Graphical models as a probabilistic method

#### Advantages

*Correctness* (of representation)

$$\langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{GM} \Rightarrow \langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{JPD}$$

In a *finitary setting*, they are always *computable* 

Graph models are easy to read (compared to JPDs)

#### Limitations

#### No abstraction over multiplicity

(i.e. no First-order Logic equivalent – see also http://www.pr-owl.org/basics/bn.php#reasoning)

- Consider you receive multiple reports (random variable *R*) of fire: do they support each other? Which ones are reliable?
- Time sequences or specific patterns of variable size

$$\langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{JPD} \Rightarrow \langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{GM}$$

Counterexample: no DAG can represent

$$\langle X_1 \perp \{X_2, Y_2\} \rangle$$
,  $\langle X_2 \perp \{X_1, Y_1\} \rangle$ 

Not all JPDs can be faithfully represented by a graph model

without introducing some further independence relation

(no closure under marginalization - see also https://projecteuclid.org/download/pdf\_1/euclid.aos/1031689015)

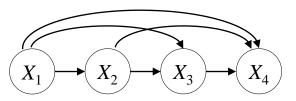
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# Graphical Models in Action

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## Example of graphical models

Complete dependency



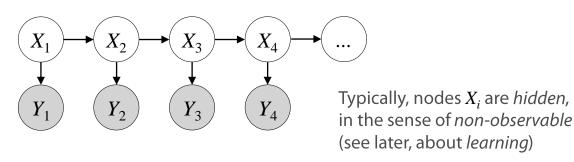
$$P(X_1, X_2, X_3, X_4) = P(X_1) P(X_2 \mid X_1) P(X_3 \mid X_1, X_2) P(X_4 \mid X_1, X_2, X_3)$$

Markovian model

$$X_1 \longrightarrow X_2 \longrightarrow X_3 \longrightarrow X_4 \longrightarrow \dots$$

$$P(X_1, ..., X_n) = P(X_1) \prod_{i=2}^n P(X_i \mid X_{i-1})$$

'Hidden' Markovian model

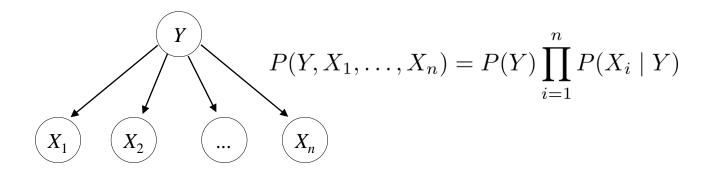


$$P(X_1, \dots, X_n Y_1, \dots, Y_n) = P(X_1) P(Y_1 | X_1) \prod_{i=2}^n P(X_i | X_{i-1}) P(Y_i | X_i)$$

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## Example: anti-spam filter

a.k.a. 'Naïve (Discrete) Bayesian Classifier'



#### Anti-spam filter:

- All random variables are binomial (value: either 0 or 1)
- *Y* represents the class of the message: 1 *spam*, 0 not-*spam*
- Each  $X_i$  represents the occurrence of the word i in the message

Assume (*for now*) that the probabilities are given
As we will see, finding the 'right' numbers is a *learning* problem (see after)

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# Inference in the anti-spam filter

Given a message with occurrence values  $\{X_k\}$ , the class with the highest conditional probability is determined

The message is spam if

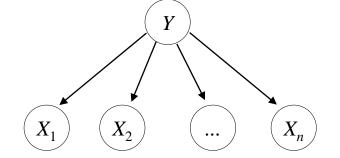
$$\frac{P(Y = 1 \mid \{X_k\})}{P(Y = 0 \mid \{X_k\})} > \lambda$$

Note that:

$$P(Y = 1 \mid \{X_k\}) = \frac{P(\{X_k\} \mid Y = 1)P(Y = 1)}{\sum\limits_{Y} P(\{X_k\} \mid Y)P(Y)} = \frac{P(Y = 1)\prod\limits_{k} P(X_k \mid Y = 1)}{\sum\limits_{Y} P(Y)\prod\limits_{k} P(X_k \mid Y)}$$

 $P(Y, X_1, \dots, X_n) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y)$ 

Conditional independency



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# Inference in the anti-spam filter

Given a message with occurrence values  $\{X_k\}$ , the class with the highest conditional probability is determined

The message is spam if

$$\frac{P(Y = 1 \mid \{X_k\})}{P(Y = 0 \mid \{X_k\})} > \lambda$$

 $X_1$   $X_2$  ...  $X_n$ 

 $P(Y, X_1, \dots, X_n) = P(Y) \prod^n P(X_i \mid Y)$ 

Note that:

$$P(Y = 1 \mid \{X_k\}) = \frac{P(\{X_k\} \mid Y = 1)P(Y = 1)}{\sum_{Y} P(\{X_k\} \mid Y)P(Y)} = \frac{P(Y = 1) \prod_{k} P(X_k \mid Y = 1)}{\sum_{Y} P(Y) \prod_{k} P(X_k \mid Y)}$$
Conditional independency

Therefore:

$$\frac{P(Y=1 \mid \{X_k\})}{P(Y=0 \mid \{X_k\})} = \frac{P(Y=1)}{P(Y=0)} \prod_k \frac{P(X_k \mid Y=1)}{P(X_k \mid Y=0)}$$

Bayes' Theorem

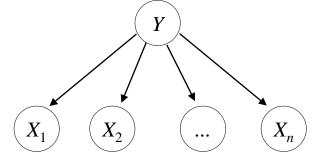
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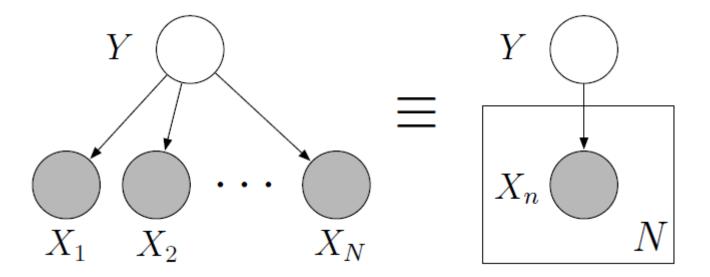
Bayes' Theorem

The logarithm is used to simplify computations:

$$\log \frac{P(Y=1|\{X_k\})}{P(Y=0|\{X_k\})} = \log \frac{P(Y=1)}{P(Y=0)} + \sum_{k} \log \frac{P(X_k|Y=1)}{P(X_k|Y=0)}$$

# An aside: plate notation

A shorthand notation for graphical models



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