Graphical Models

Marco Piastra

Chain Factorization

- **Univariate factorization of a JPD**

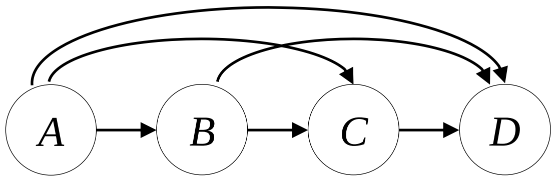
From the definition of conditional probability

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

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



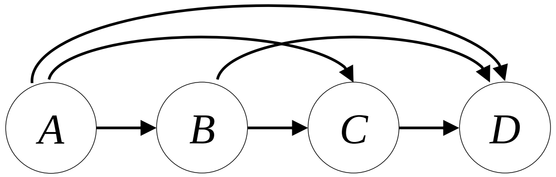
In this <u>oriented</u> graph:

- 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 Factoriaztion

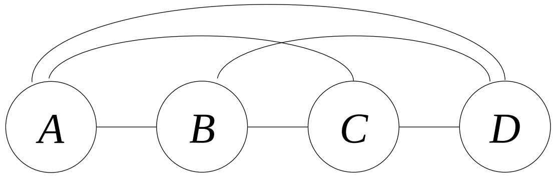
- **Graphical model**

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



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

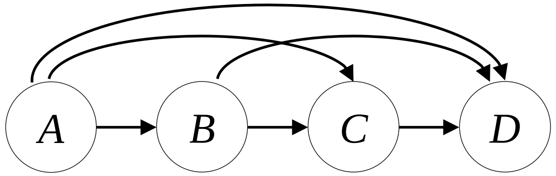


Any *univariate factorization* can be represented by a *graphical model*
Every *completely connected*, *acyclic* and *oriented graph* represents a *univariate factorization*

Chain Factorization and Independence Assumptions

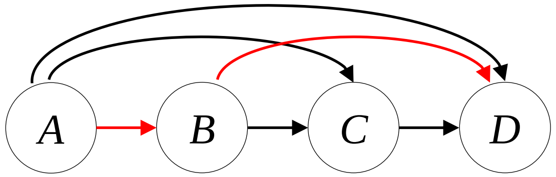
- **Graphical model**

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



- **Independence**

Let's remove <u>a few arcs</u> from the graph and rewrite the factorization accordingly



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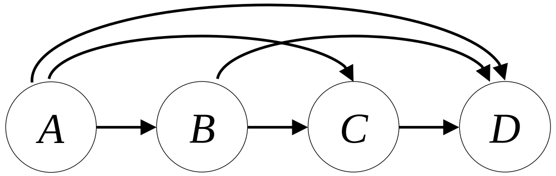

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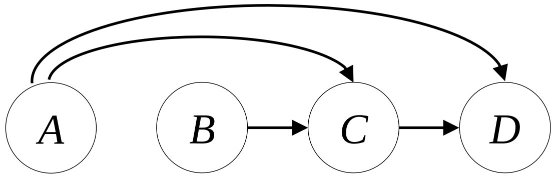


$$P(A,B,C,D) = P(A)\underline{P(B)}P(C|A,B)\underline{P(D|A,C)}$$

The latter holds true only if

$$P(B|A) = P(B) \qquad \langle A \perp B \rangle$$

Independence

$$P(D|A,B,C) = P(D|A,C) \qquad \langle B \perp D \,|A,C\rangle$$

Conditional Independence

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

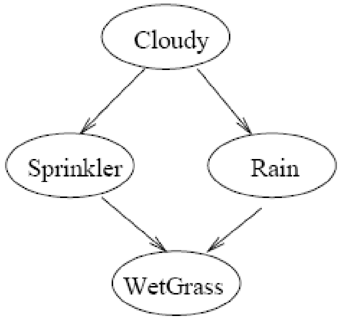
Structure and numbers, instead of just numbers

- A structured, pre-numerical representation of a joint probability

  Each graphical model is an *oriented* graph

  - nodes are *random variables*
  - arcs represent *dependence*

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



C	P(S=F)	P(S=T)
F	0.5	0.5
T	0.9	0.1

C	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
F	T	0.1	0.9
T	T	0.01	0.99

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)

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

Factorization for a graphical model

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

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

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

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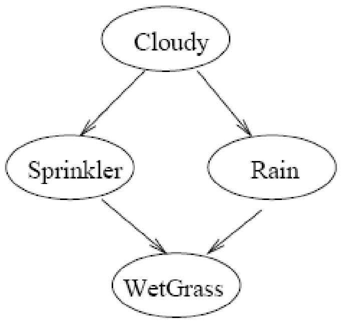

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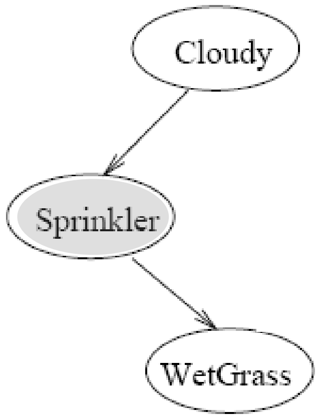
Patterns in Graphical Models

- ***Sequence* or *Chain***

Consider the graph on the right

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

sequence



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

Patterns in Graphical Models

- ***Fork***

Consider the graph on the right

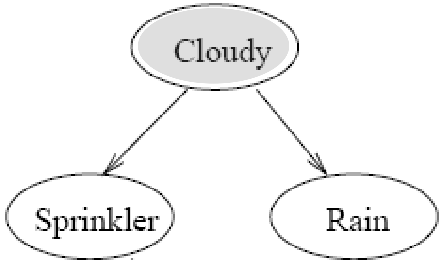
$$P(C, S, R) = P(C)P(S|C)P(R|C)$$

Now suppose you observe C

$$\begin{aligned} P(R, S|C) &= \frac{P(C, S, R)}{P(C)} \\ &= \frac{P(C)P(S|C)P(R|C)}{P(C)} \\ &= \frac{P(C, S)}{P(C)} P(R|C) \\ &= P(S|C)P(R|C) \end{aligned}$$

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

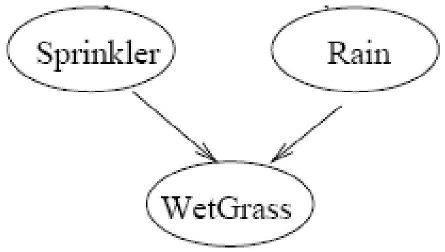
fork



Patterns in Graphical Models

- ***Join* or *Collider*** CAUTION: this case is different from the previous two

join or *collider*



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')*

Now suppose you observe W

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

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

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

No further simplification possible

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

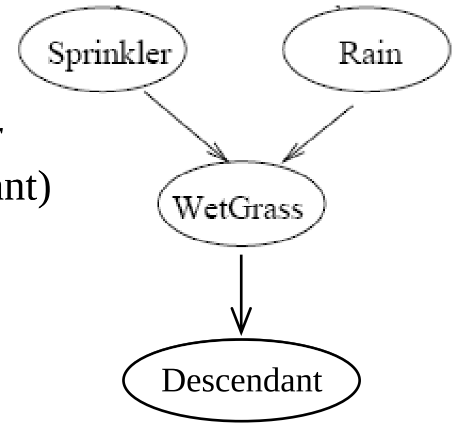
Patterns in Graphical Models

- ***Join or Collider***

The same loss of independence occurs if you observe any of the descendants...

Consider the graph on the right

join or *collider* (with descendant)



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

which is true only if $\langle S \perp R \rangle$

Independence (also 'Marginal Independence')

Now suppose you observe D

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

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

No further simplification possible

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

This implies $\langle S \not\perp R \,|D\rangle$

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

Paths in Graphical Models

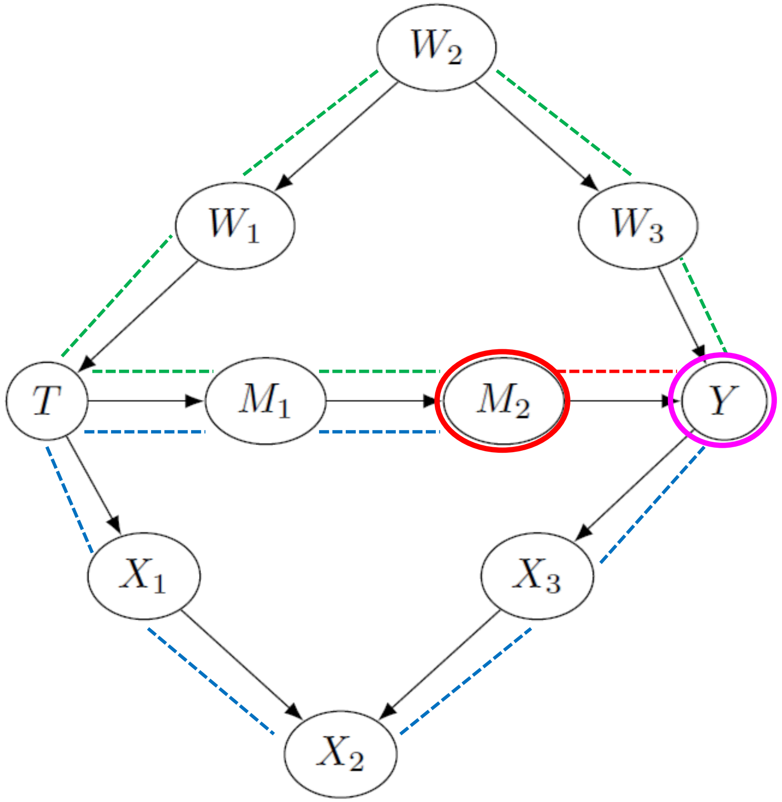
In a graphical model

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



Blocked Paths in Graphical Models

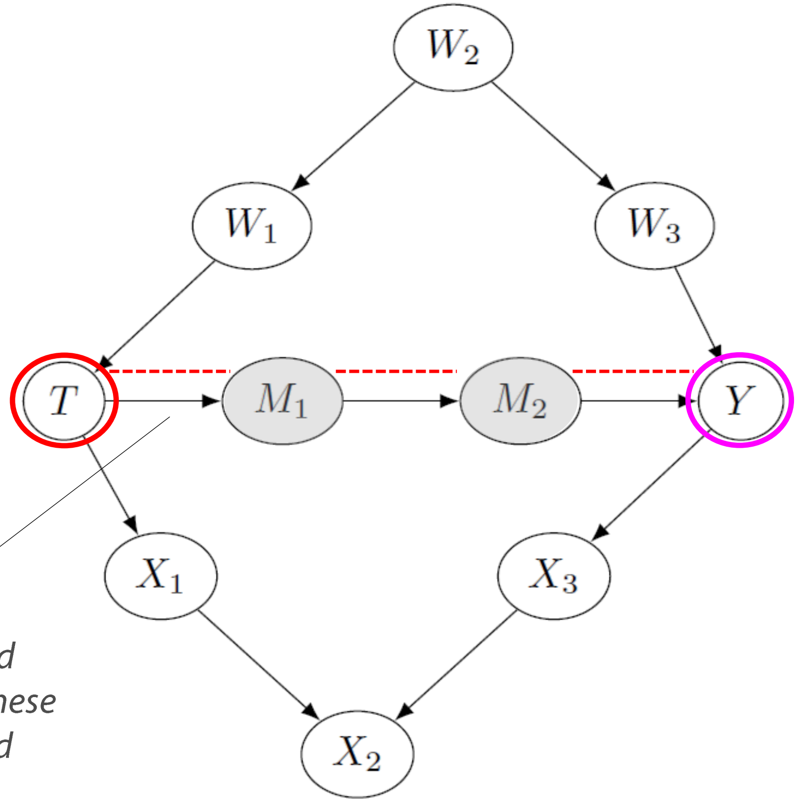
In a graphical model

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 not contain the observation of the join node nor of any of its descendants

This path is blocked whenever any of these nodes are observed



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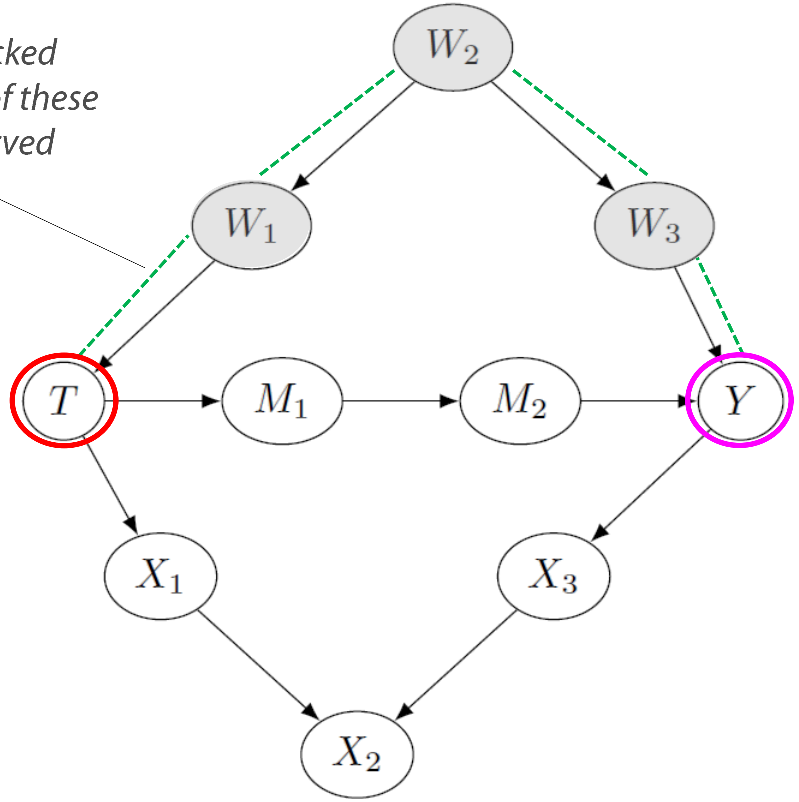

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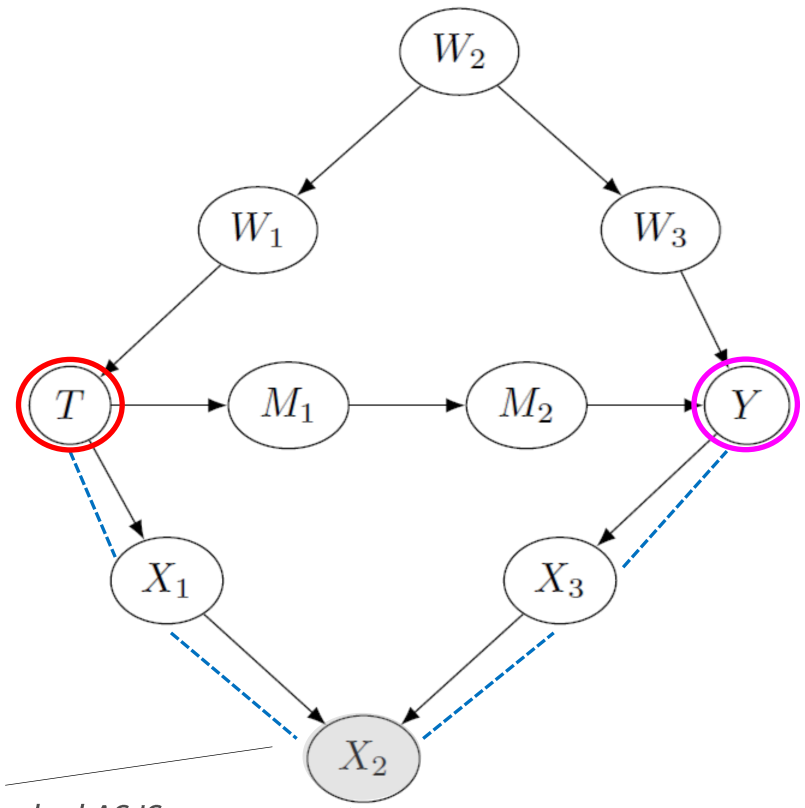

This path is blocked AS IS: the collider blocks it

It becomes unblocked when this node is observed...

Blocked Paths in Graphical Models

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:

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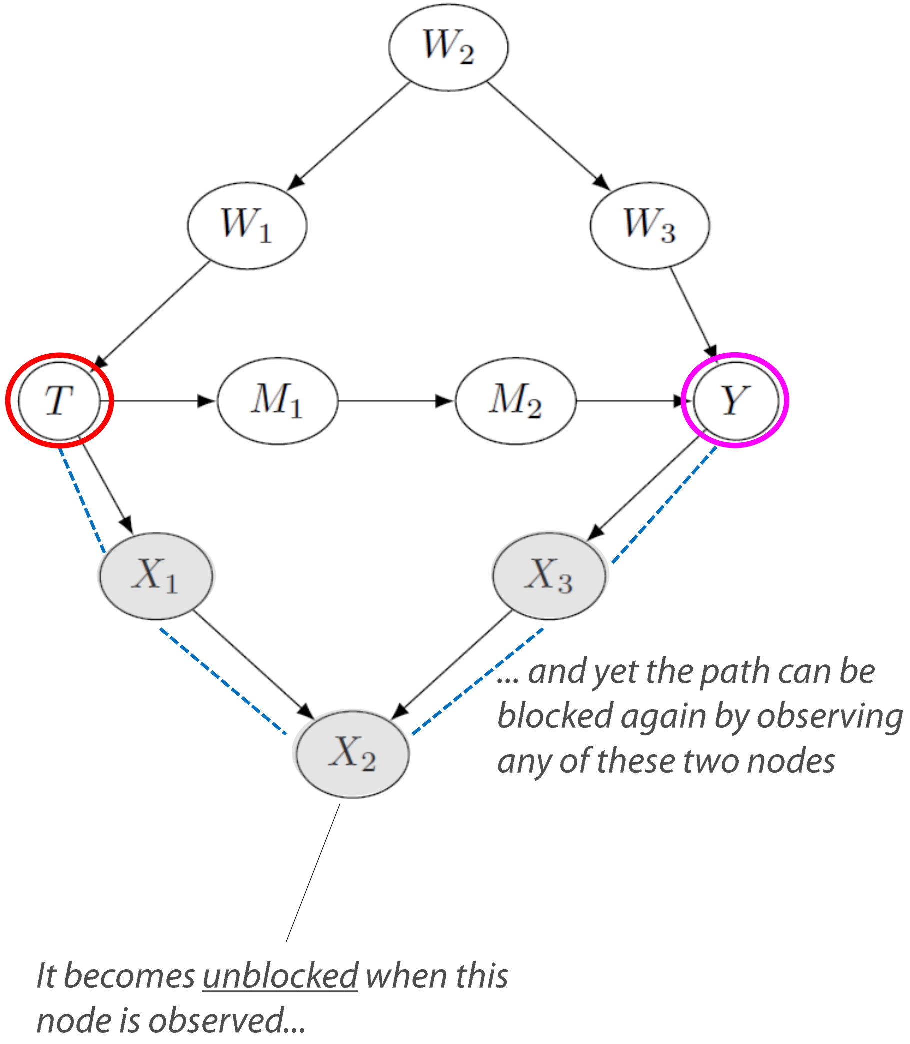


D-Separation in Graphical Models

- **Dependency Separation (d-separation)**

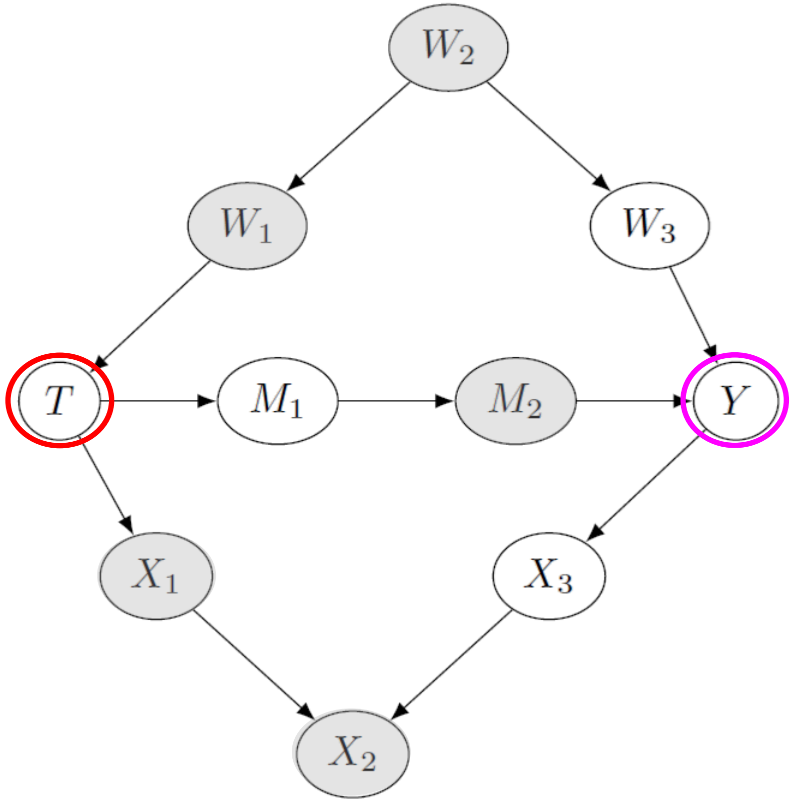
  Any two nodes A and B in a graphical model are ***d-separated*** whenever the observations $\{X_o\}$ are such that all paths between A and B are blocked

  Observed Variables

  In that case we have

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

  But only when all paths are blocked



These observations make the two nodes d-separated

Graphical models: fundamental assumptions

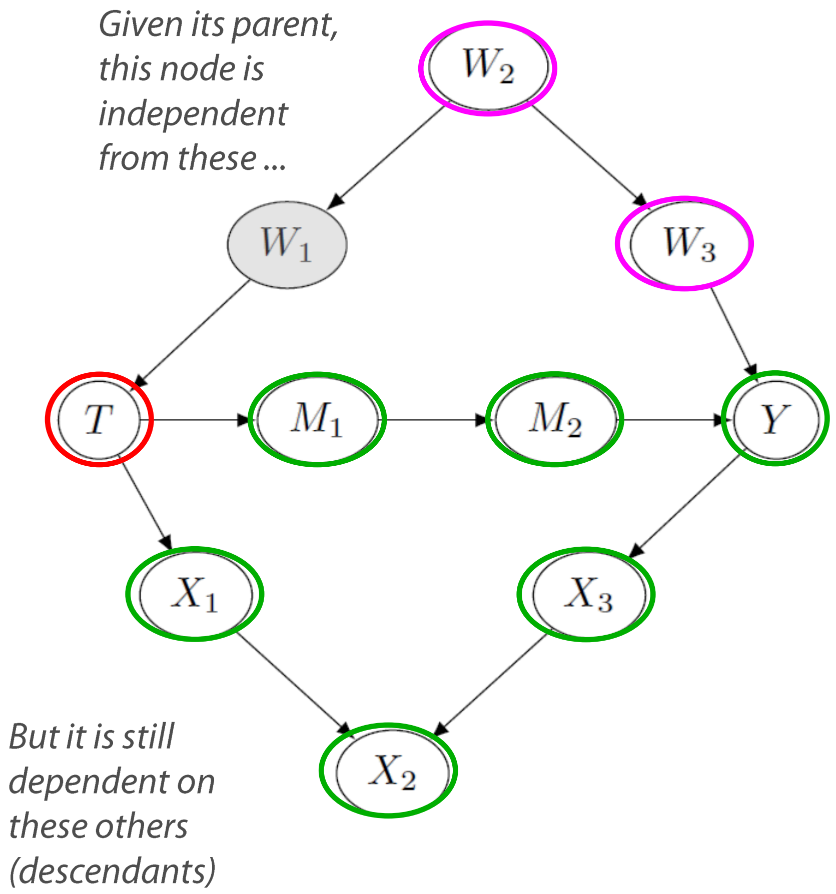
- **Minimality**

  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

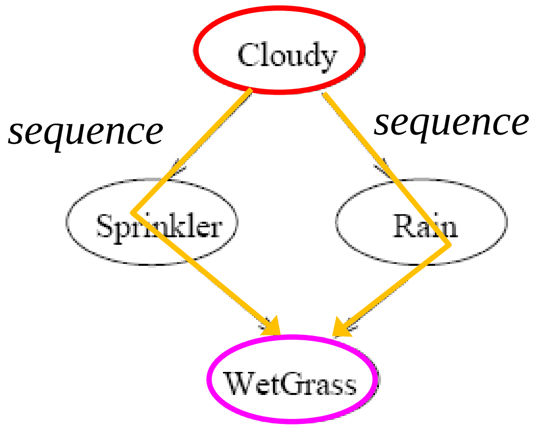
Think it over …



D-Separation in Graphical Models

Example:

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



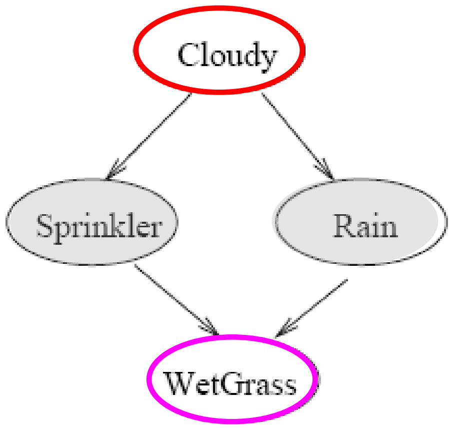
D-Separation in Graphical Models

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>

<Cloudy ⊥ WetGrass | Sprinkler, Rain>



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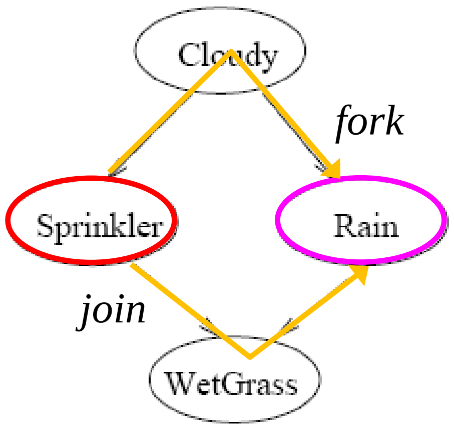


D-Separation in Graphical Models

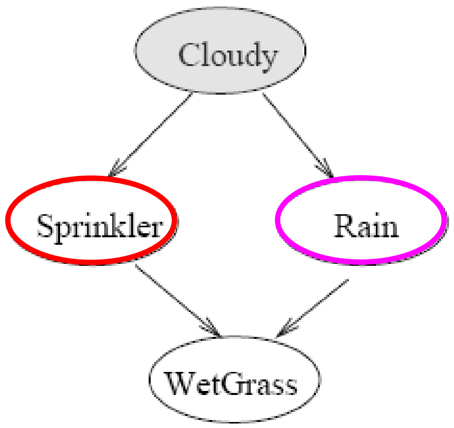
Example:

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>

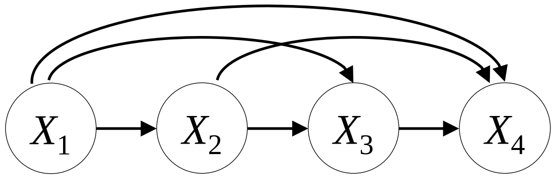
$< \text{Sprinkler} \perp \text{Rain} \mid \text{Cloudy} >$

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



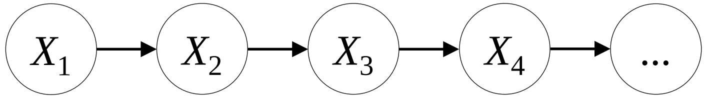
Example of graphical models

- Complete dependency



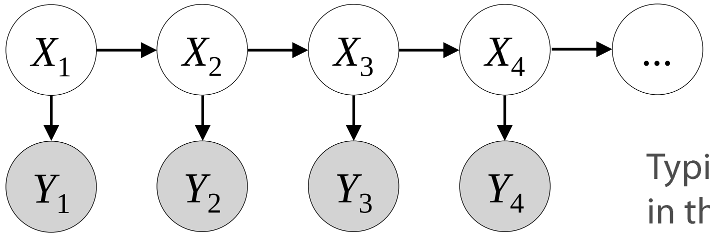
$$P(X_1, X_2, X_3, X_4) = P(X_1)\ P(X_2 \mid X_1)\ P(X_3 \mid X_1, X_2)\ P(X_4 \mid X_1, X_2, X_3)$$

- Markovian model



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

- 'Hidden' Markovian model

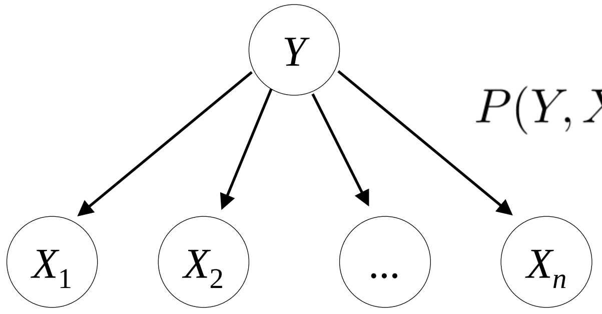


Typically, nodes X_i are *hidden*, in the sense of *non-observable* (see later, about *learning*)

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

Example: *anti-spam filter*

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



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

Anti-spam filter:

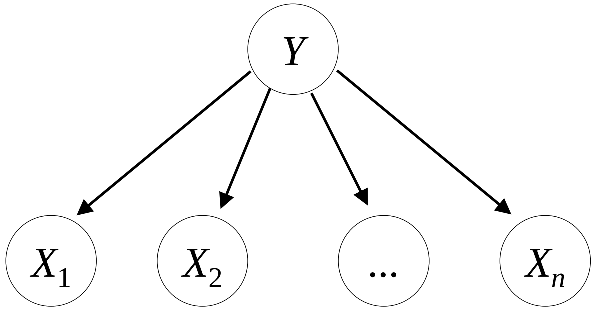
- All random variables are *binomial* (value: either 0 or 1)
- Y represents the class of the message: 1 *spam*, 0 not-*spam*
- Each X_i represents the occurrence of the word i in the message

Assume (*for now*) that the probabilities are given

As we will see, finding the 'right' numbers is a *learning* problem (see after)

Inference in the *anti-spam filter*

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



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:

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

Bayes' Theorem

Conditional independency

Inference in the *anti-spam filter*

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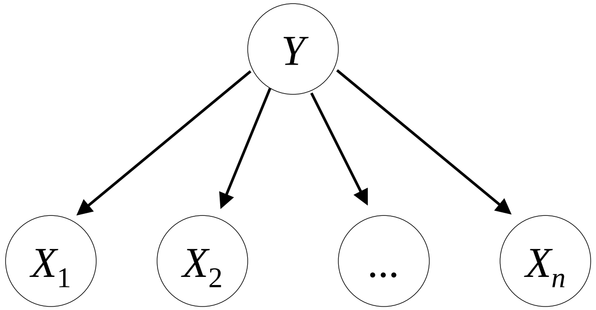

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Conditional independency

Therefore:

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Inference in the *anti-spam filter*

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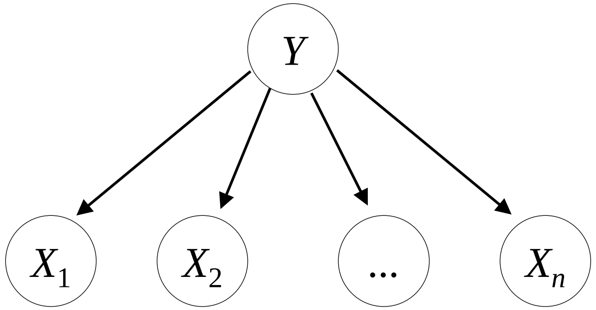

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Bayes' Theorem

Conditional independency

Therefore:

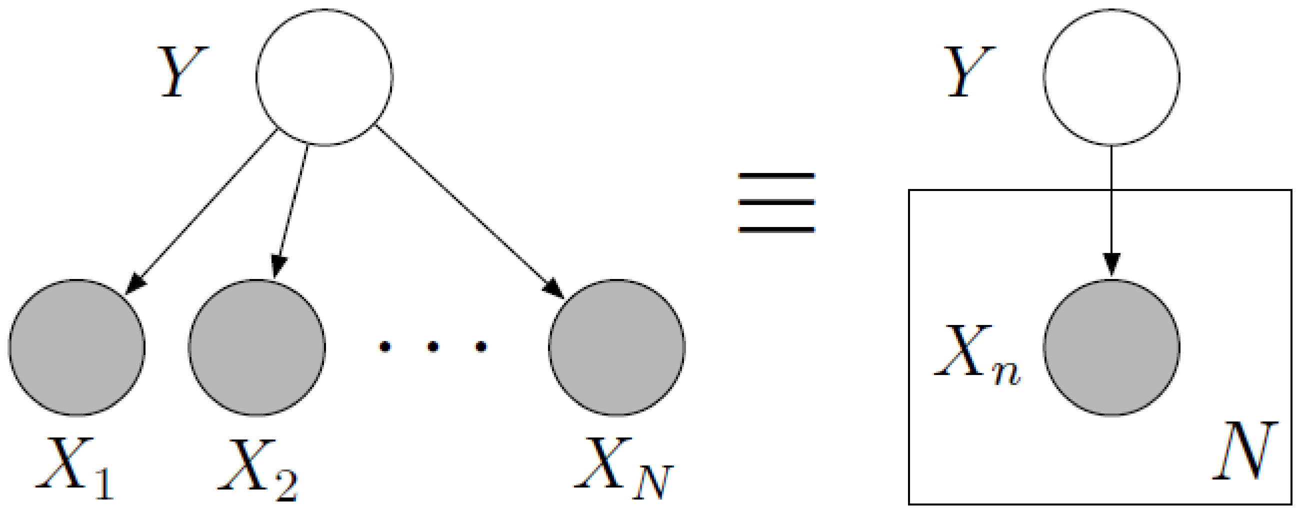
$$\frac{P(Y=1 \mid \{X_k\})}{P(Y=0 \mid \{X_k\})} = \frac{P(Y=1)}{P(Y=0)} \prod_k \frac{P(X_k \mid Y=1)}{P(X_k \mid Y=0)}$$

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



Building a graphical model

- Step 1

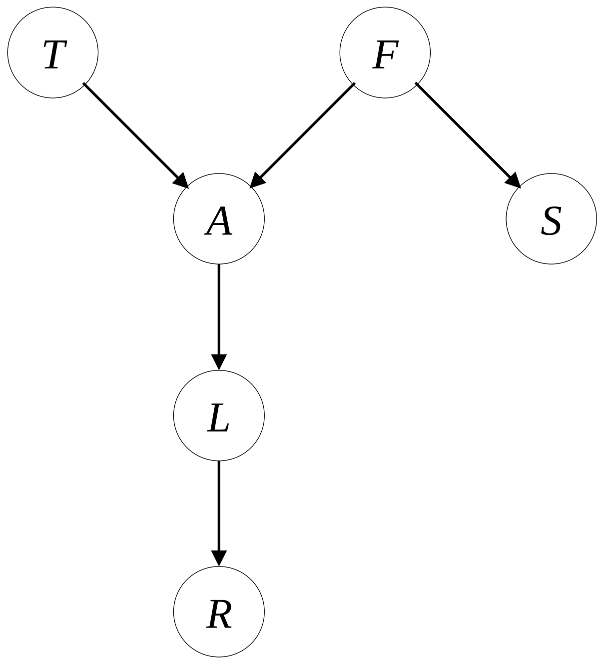
  Defining the nodes, i.e. the random variables

T : (*tampering*)
F : (*fire*)
A : (*alarm*)
S : (*smoke*)
L : (*leaving*)
R : (*report*)

Building a graphical model

- Step 2

  Defining the structure, i.e. the graph



We are thus saying that:

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

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

$\langle L \perp T \mid A \rangle$

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

$\langle A \perp R \mid L \rangle$

T : (*tampering*)

F : (*fire*)

A : (*alarm*)

S : (*smoke*)

L : (*leaving*)

R : (*report*)

Building a graphical model

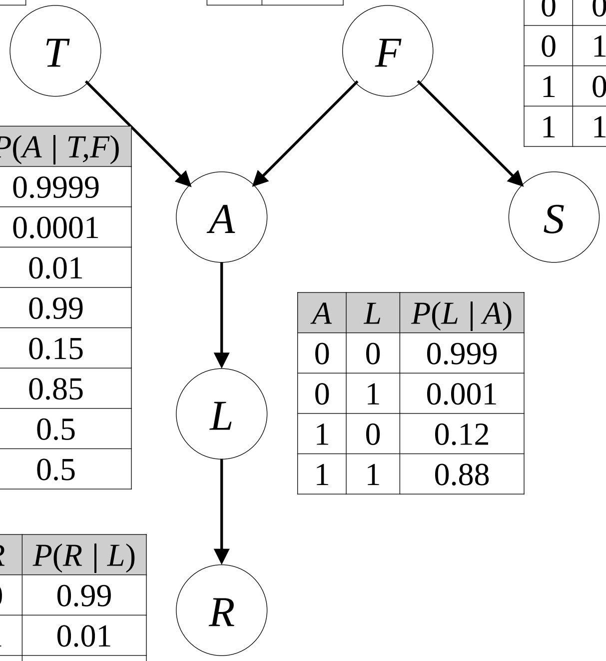
- Step 3

  Defining *conditional probability tables – CPTs*

T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9



T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5

A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

T : (*tampering*)
F : (*fire*)
A : (*alarm*)
S : (*smoke*)
L : (*leaving*)
R : (*report*)

Probabilistic inference

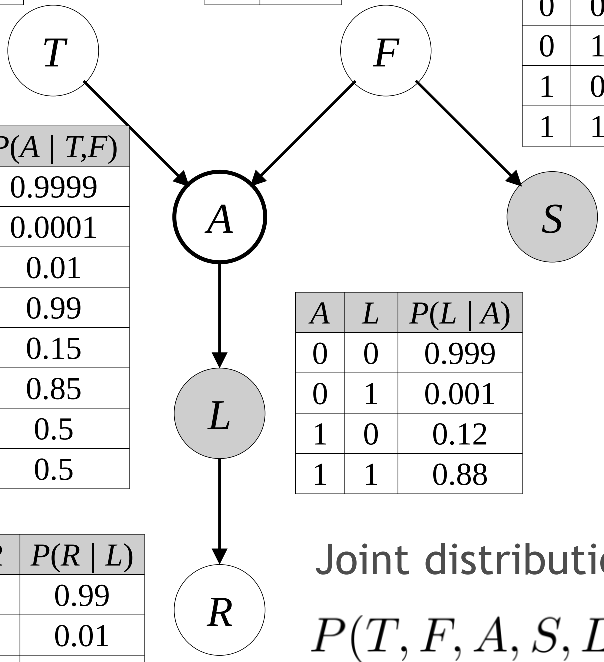
- Step 4

  Consider a specific problem

T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9



T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5

A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

Example: finding A given L=1 e S=0

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

Joint distribution, from the graph:

$$P(T,F,A,S,L,R) = P(T)P(F)P(A|T,F)P(S|F)P(L|A)P(R|L)$$

Probabilistic inference

- Step 5

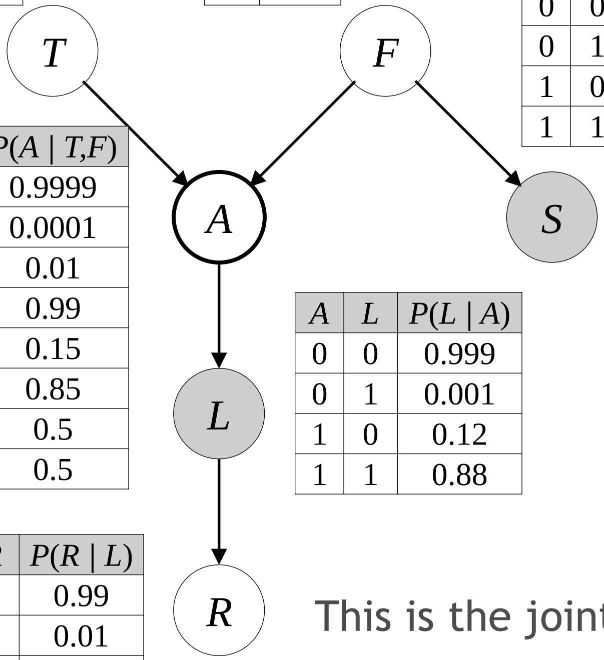
  Computing the answer

T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9

T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5



A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

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:

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

Probabilistic inference

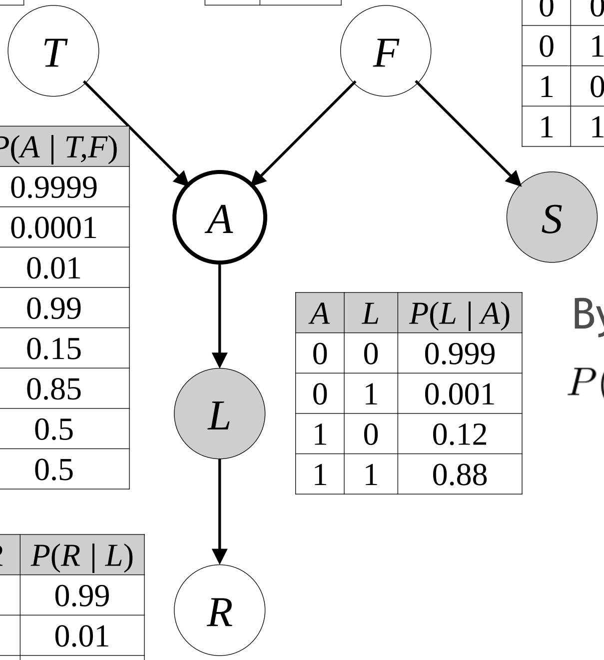
- Step 5

Computing the answer

T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9



T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5

A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

By rewriting the joint distribution:

$$
\begin{aligned}
P(A, L=1, S=0) \\
&= \sum_T \sum_F \sum_R P(L=1|A)P(A|T,F)P(T)P(F)P(S=0|F)P(R|L=1) \\
&= P(L=1|A) \sum_T \sum_F P(A|T,F)P(T)P(F)P(S=0|F) \sum_R P(R|L=1)
\end{aligned}
$$

This sum has value 1
This is not surprising
given that $<A \perp R \mid L>$

- Step 5

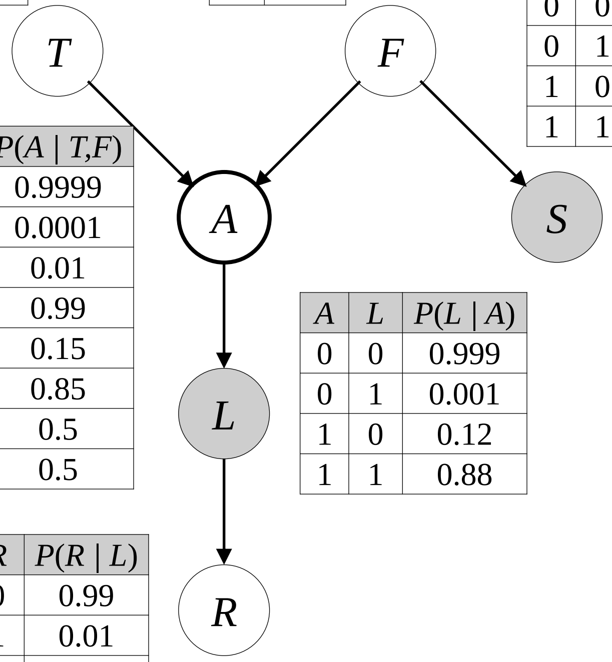
Computing the answer

$$P(A, L=1, S=0) \\ = P(L=1|A) \sum_T \sum_F P(A|T,F)P(T)P(F)P(S=0|F)$$

T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9



T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5

A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

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:*

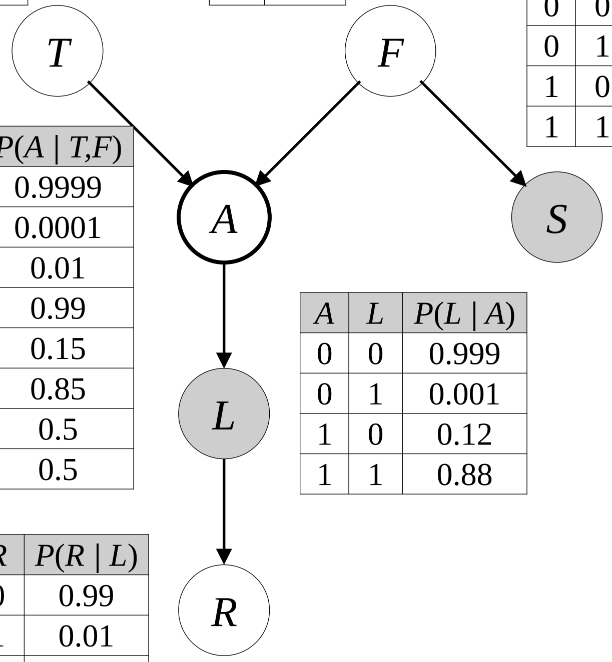
$$f_{T,F,S=0}(A) := \\ \sum_T \sum_F P(A|T,F)P(T)P(F)P(S=0|F)$$

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

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

- Step 5

Computing the answer



T	$P(T)$
0	0.98
1	0.02

F	$P(F)$
0	0.99
1	0.01

F	S	$P(S \mid F)$
0	0	0.99
0	1	0.01
1	0	0.1
1	1	0.9

T	F	A	$P(A \mid T,F)$
0	0	0	0.9999
0	0	1	0.0001
0	1	0	0.01
0	1	1	0.99
1	0	0	0.15
1	0	1	0.85
1	1	0	0.5
1	1	1	0.5

A	L	$P(L \mid A)$
0	0	0.999
0	1	0.001
1	0	0.12
1	1	0.88

L	R	$P(R \mid L)$
0	0	0.99
0	1	0.01
1	0	0.25
1	1	0.75

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*

This factor comes from the *descendants* of *A*

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

Variable elimination for graphical models

- General idea

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

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

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

  Independence in the graph model implies independence in the joint probability distribution

  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

  No *completeness* $\langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{JPD} \not\Rightarrow \langle \{X\} \perp \{Y\} \mid \{Z\} \rangle_{GM}$

  Not all JPDs can be faithfully represented by a graph model

  - *Counterexample: no DAG can represent*

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

    without introducing some further independence relation
    (*no closure under marginalization* - see also https://projecteuclid.org/download/pdf_1/euclid.aos/1031689015)