Soft Computing

Lecture Notes on Machine Learning

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Unsupervised Learning

– Bayesian Networks –

Beyond Independence . . .

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- It yields optimal classifiers when satisfied
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These models are often referred also as **Graphical Models**

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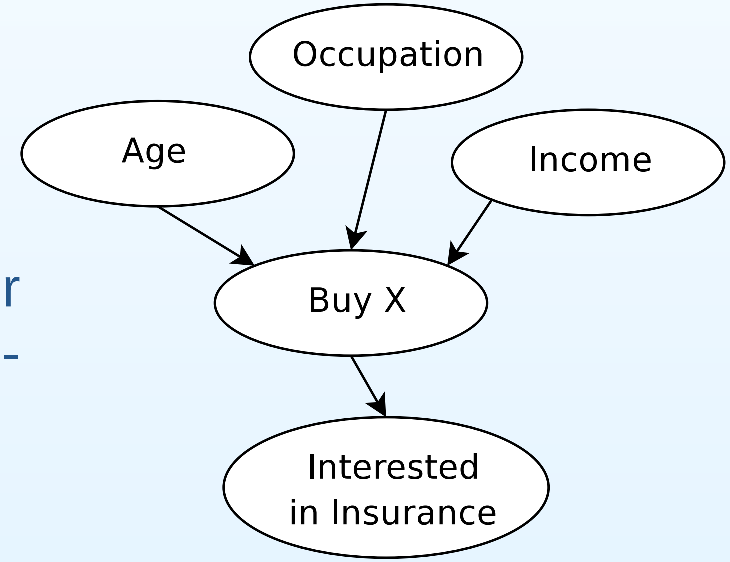
- Age, Occupation and Income determine if customer will buy this product.
- Given that customer buys product, whether there is interest in insurance is now independent of Age, Occupation, Income.



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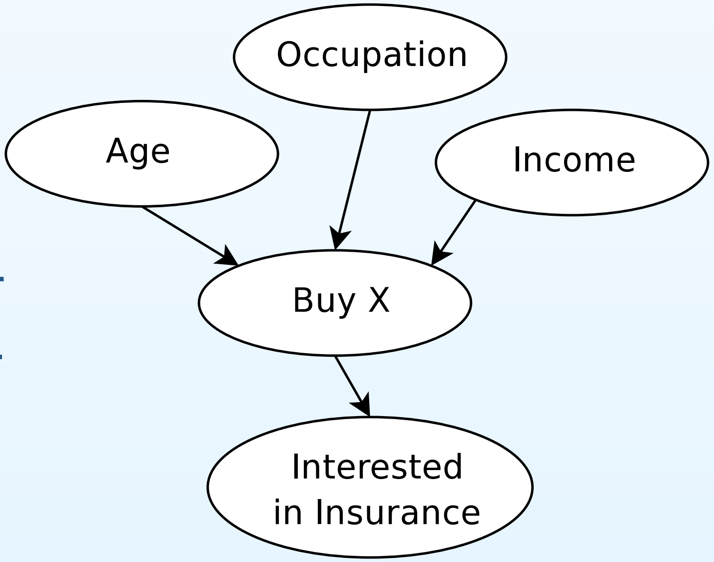

Similar to Naïve Bayes we will make some independence assumptions, but not as strong as the assumption of all variables being independent.

Bayesian Networks

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- A Directed Acyclic Graph (DAG)
  - Nodes - random variables
  - Edges - direct influence

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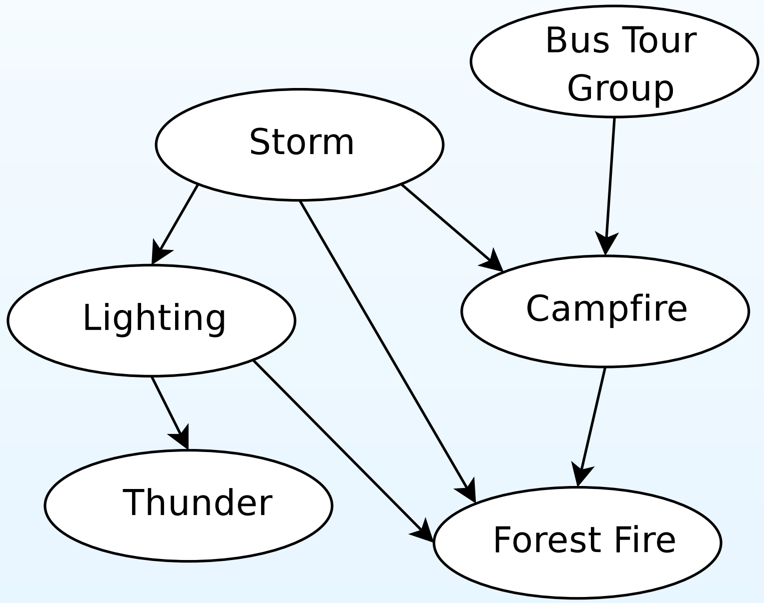
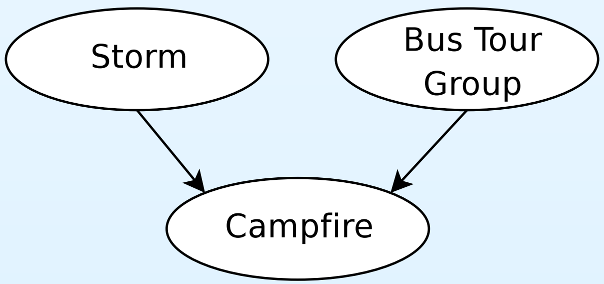
- A Directed Acyclic Graph (DAG)
  - Nodes - random variables
  - Edges - direct influence
- Set of Conditional Probability Distributions (CPD) for "influenced" variables





	S, B	$S, \sim B$	$\sim S, B$	$\sim S, \sim B$
C	0.4	0.1	0.8	0.2
$\sim C$	0.6	0.9	0.2	0.8

Conditional Independence

We say X_1 is conditionally independent of X_2 given X_3 if the probability of X_1 is independent of X_2 given some knowledge about X_3:

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

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The same can be said for a set of variables: X_1, X_2, X_3 is independent of Y_1, Y_2, Y_3 given Z_1, Z_2, Z_3:

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Example: Martin and Norman toss the same coin. Let be A "Norman's outcome", and B "Martin's outcome". Assume the coin might be biased; in this case A and B are not independent: observing that B is Heads causes us to increase our belief in A being Heads.

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Variables A and B are both dependent on C, "the coin is biased towards Heads with probability θ". Once we know for certain the value of C then any evidence about B cannot change our belief about A.

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

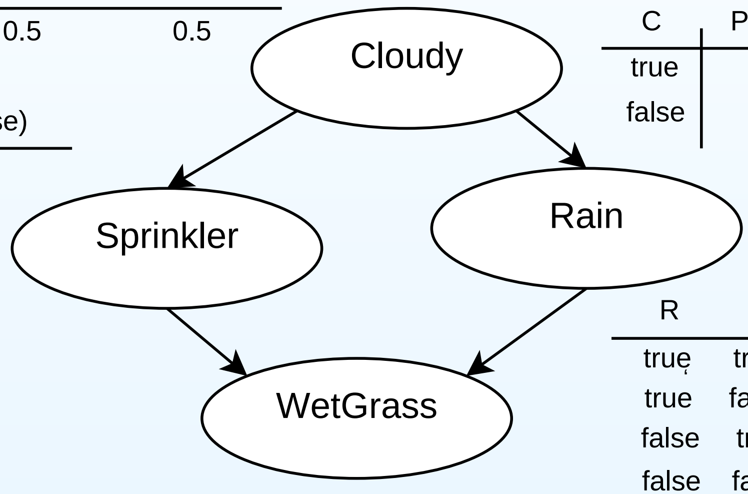
The Sprinkler Example: Modeling

The event “grass is wet” (`W=true`) has two possible causes: either the water *Sprinker* is on (`S=true`) or it is *Raining* (`R=true`).

P(C=true)	P(C=false)
0.5	0.5

C	P(S=true)	P(S=false)
true	0.5	0.5
false	0.9	0.1

C	P(R=true)	P(R=false)
true	0.8	0.2
false	0.2	0.8



R	S	P(W=true)	P(W=false)
true	true	0.99	0.01
true	false	0.9	0.1
false	true	0.9	0.1
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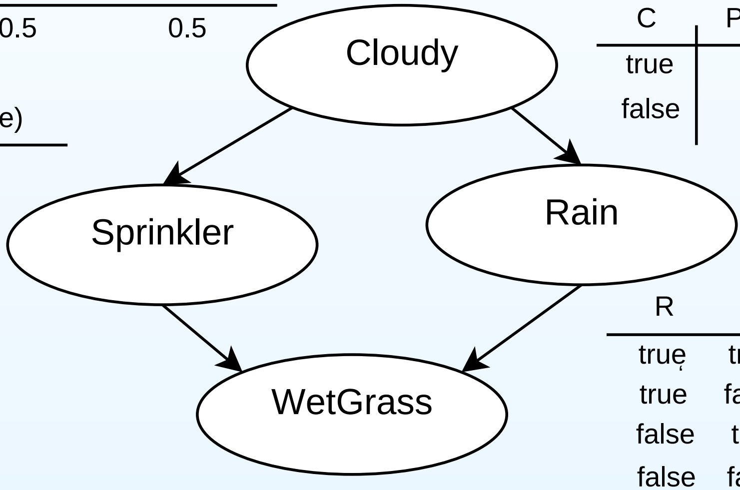

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The strength of this relationship is shown in the tables. For example, on second row, $P(W = true|S = true, R = false) = 0.9$, and, since each row sums up to one, $P(W = false|S = true, R = false) = 1 - 0.9 = 0.1$.

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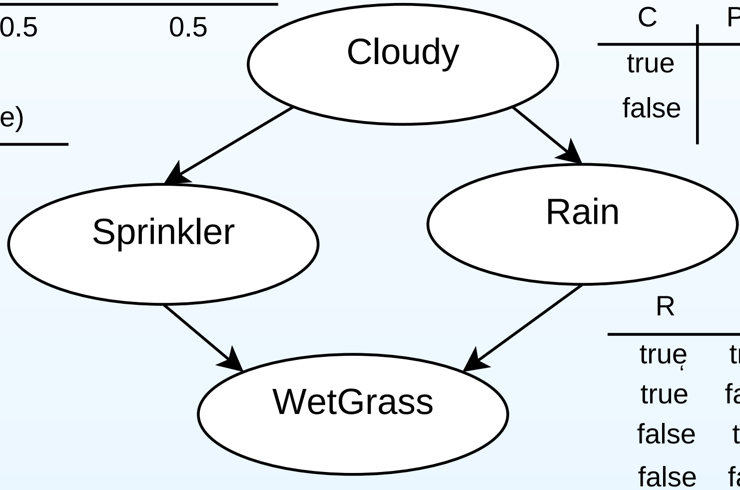

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The C node has no parents, its Conditional Probability Table (CPT) simply specifies the prior probability that it is *Cloudy* (in this case, 0.5).

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The simplest conditional independence encoded in a Bayesian network can be stated as: "a node is independent of its ancestors given its parents."

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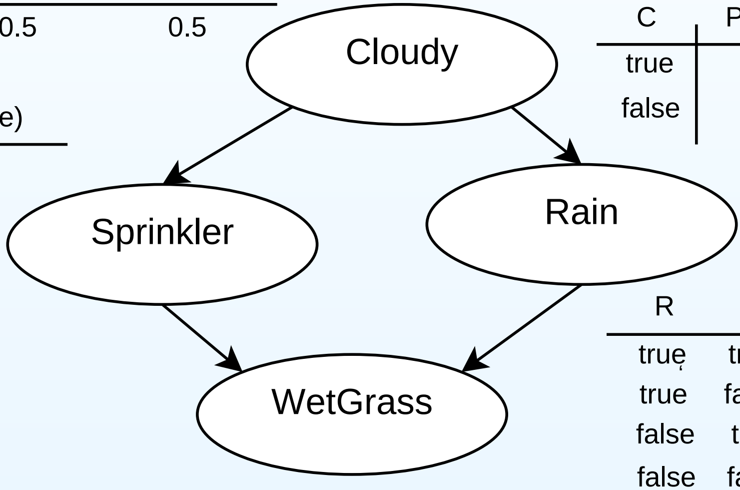

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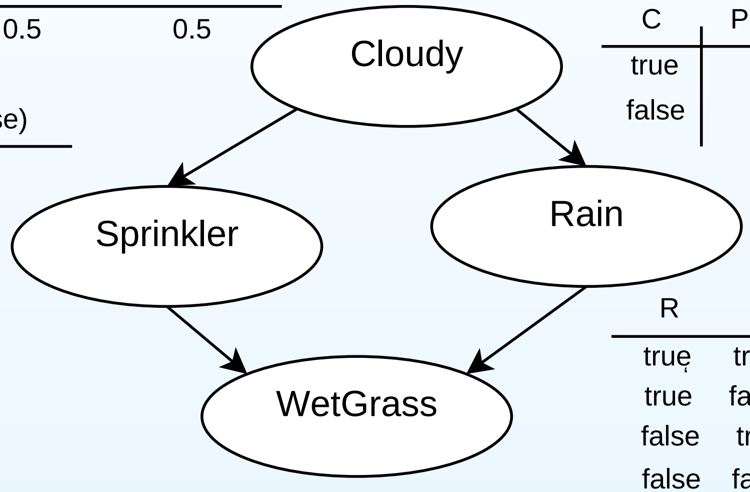

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Using the chain rule we get the joint probability of nodes in the graph

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

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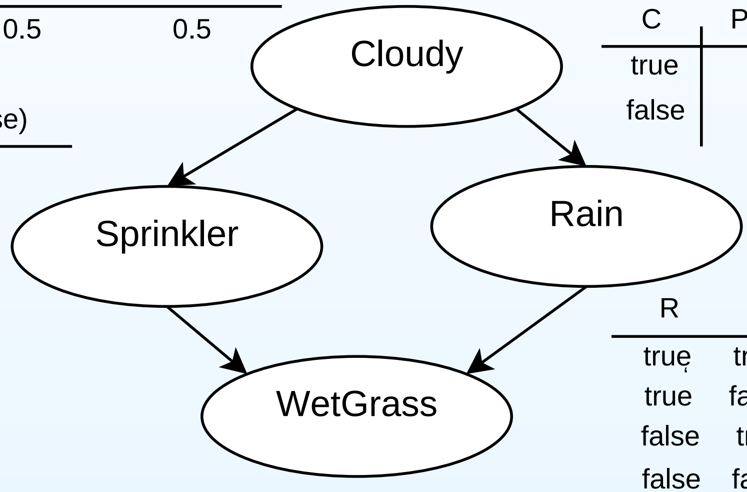

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In general, with N binary nodes and being k the maximum node fan-in, the full joint requires $O(2^N)$ parameters while the factored one $O(N \cdot 2^k)$.

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We observe the fact that the grass is wet. There are two possible causes for this: (a) the sprinkler is on or (b) it is raining. Which is more likely?

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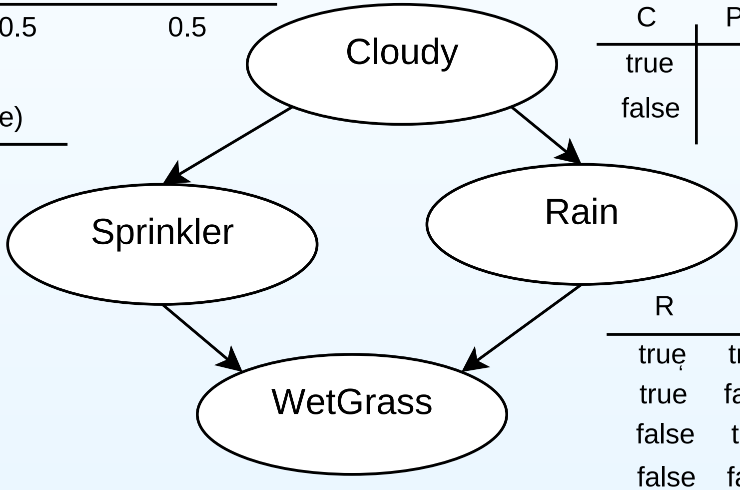

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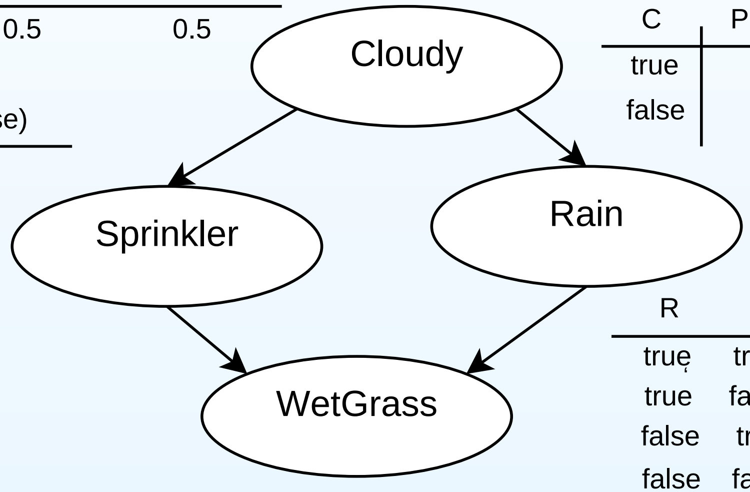

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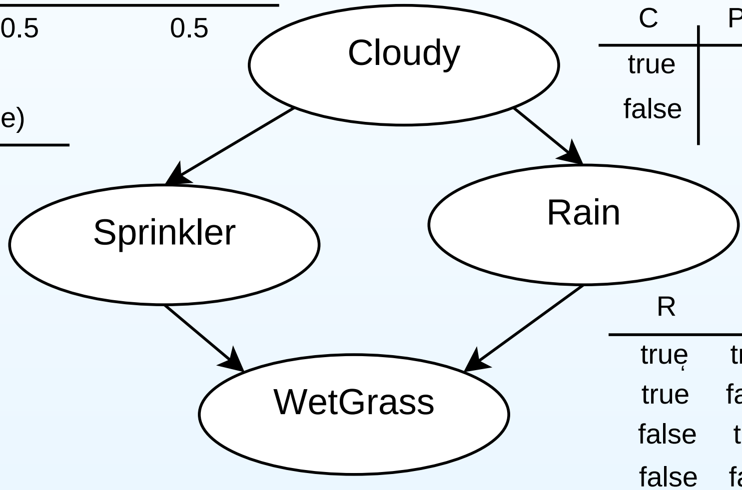

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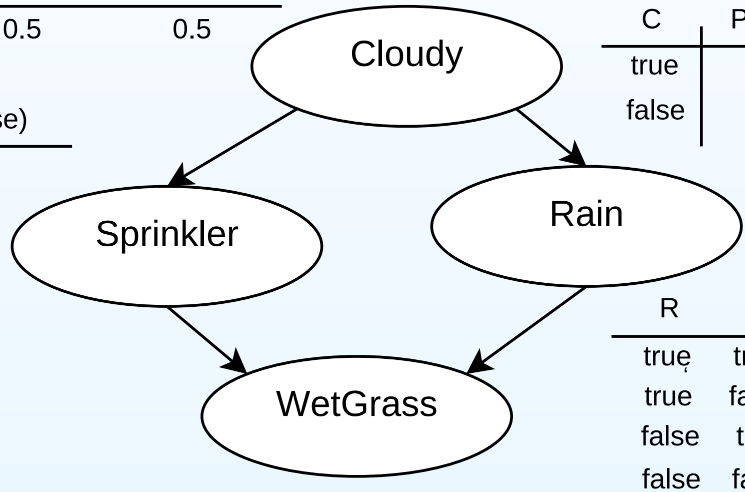

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$P(W)$ is a normalizing constant, equal to the probability (likelihood) of the data; the likelihood ratio is $0.7079/0.4298 = 1.647$.

The Sprinkler Example: Explaining Away

In Sprinkler Example the two causes *"compete"* to *"explain"* the observed data. Hence S and R become conditionally dependent given that their common child, W, is observed.

Example: Suppose the grass is wet, but we know that it is raining. Then the posterior probability of sprinkler being on goes down: $P(S|W, R) = 0.1945$

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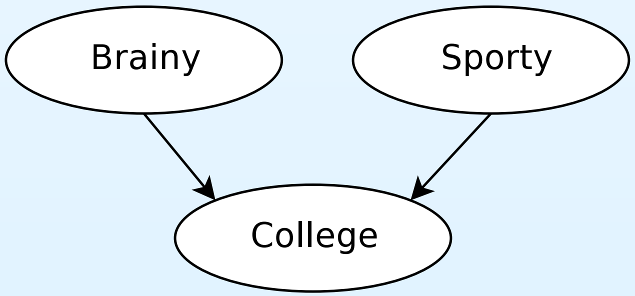
In College population, being Brainy makes you less likely to be Sporty and vice versa, because either property alone is sufficient to explain evidence on C

$$P(S = 1|C = 1, B = 1) \leq P(S = 1|C = 1)$$



Bottom-up and Top-down Reasoning

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The most interesting property of Bayesian Networks is that they can be used to reason about causality on a solid mathematical basis:

Question: Can we distinguish causation from mere correlation? So we don't need to make experiments to infer causality.

Answer: Yes, "sometimes", but we need to measure the relationships between at least three variables.

For details refer to Causality: Models, Reasoning and Inference,Judea Pearl, 2000.

Conditional Independence in Bayesian Networks

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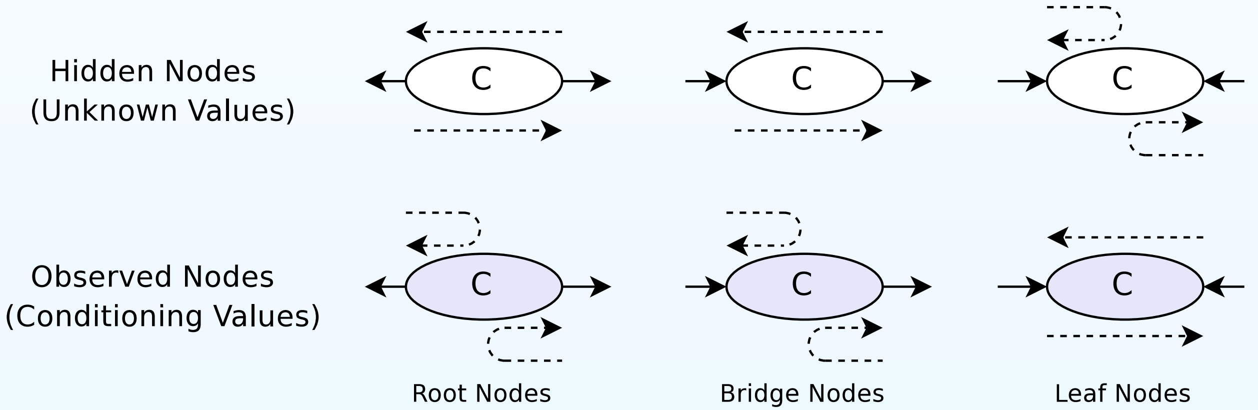

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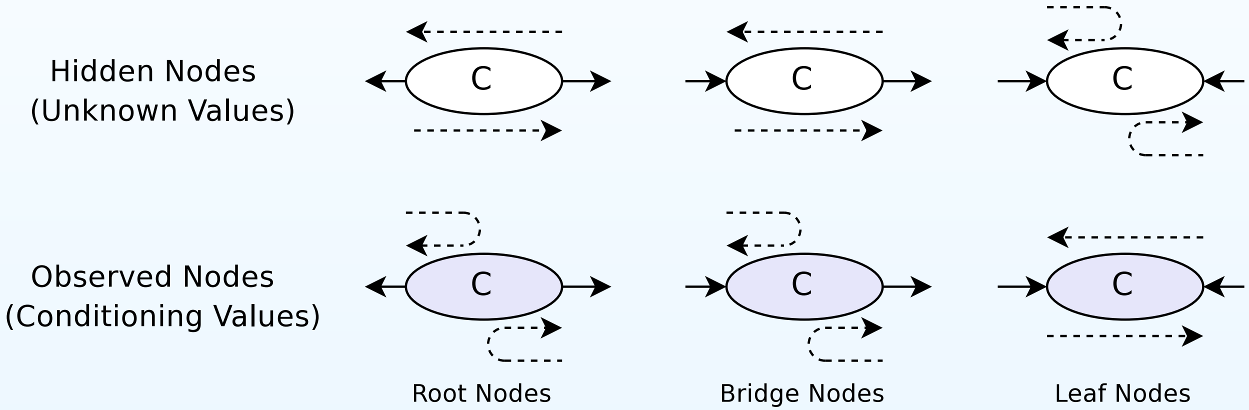

The dotted arcs indicate direction of flow in the path:

- C is a “root”: if C is hidden, children are dependent due to a hidden common cause. If C is observed, they are conditionally independent;

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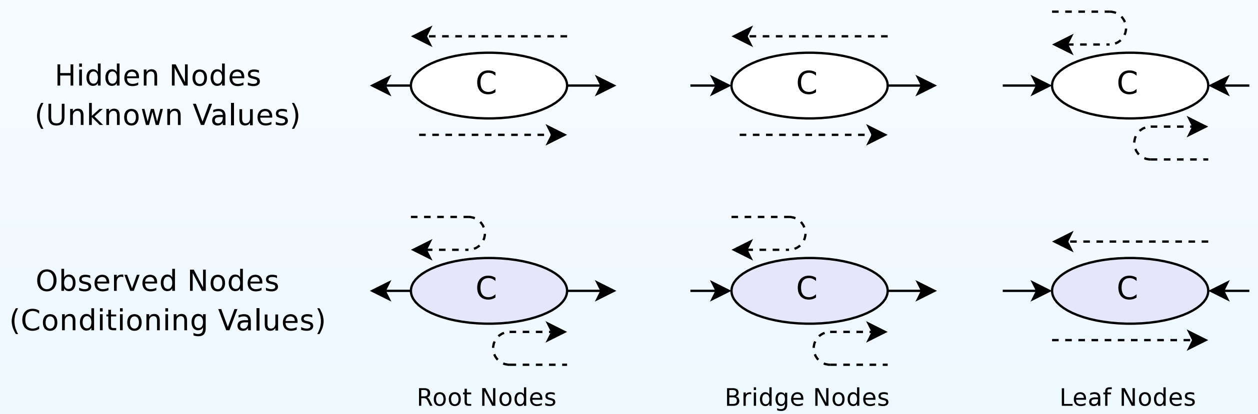

The dotted arcs indicate direction of flow in the path:

- C is a "root": if C is hidden, children are dependent due to a hidden common cause. If C is observed, they are conditionally independent;
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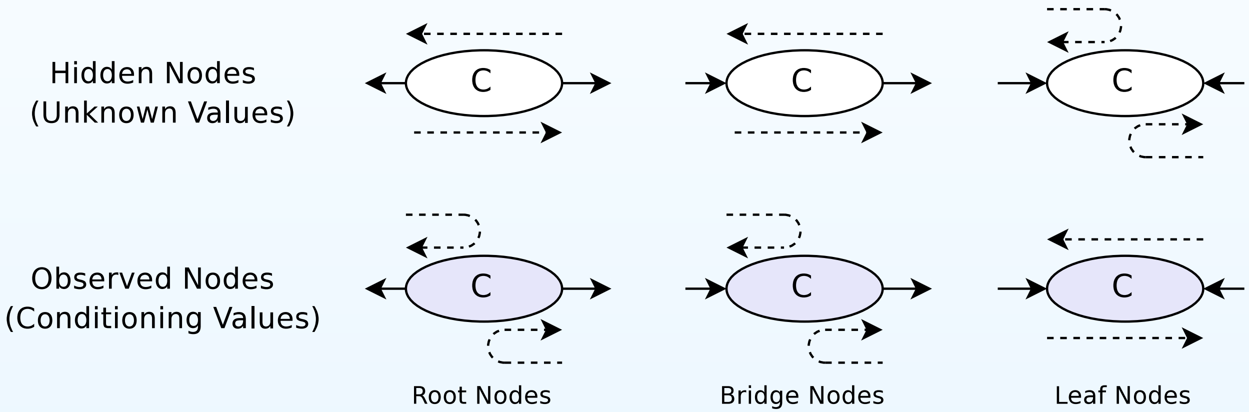

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- C is a “leaf”: if C is hidden, its parents are marginally independent, but if c is observed, the parents become dependent (Explaining Away);
- C is a “bridge”: nodes upstream and downstream of C are dependent iff C is hidden, because conditioning breaks the graph at that point.

Undirected Bayesian Networks

Undirected graphical models, also called **Markov Random Fields** (MRFs) or **Markov Networks**, are more popular with the Physics and Computer Vision communities, and have a simpler definition of independence:

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When converting a directed graph to an undirected graph, we must add links between "unmarried" parents who share a common child (i.e., "**moralize**" the graph) to prevent reading incorrect independences.

Graphical Models with Real Values

We can have Bayesian Networks with real valued nodes:

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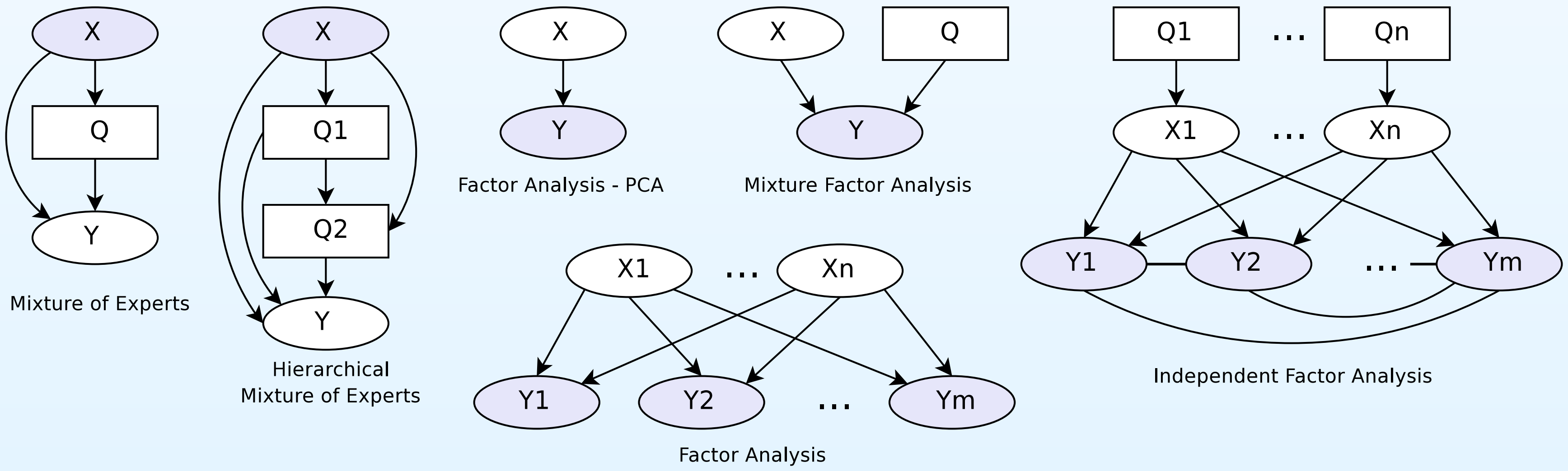

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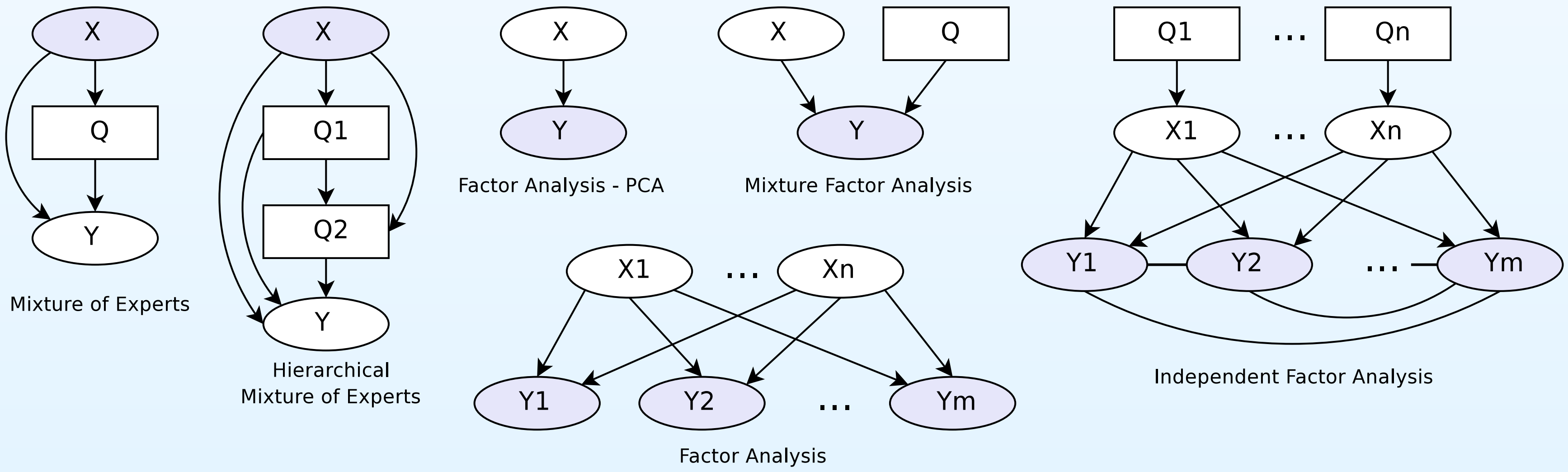

More details in the illuminating paper by Sam Roweis & Zoubin Ghahramani:
A Unifying Review of Linear Gaussian Models, Neural Computation 11(2) (1999) pp.305-345.

Inference Algorithms in Bayesian Networks

A graphical model specifies a complete joint probability distribution:

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We'll see just a few of them ... don't worry!

Inference in Bayes Nets: Variable Elimination

We can sometimes use the factored representation of Joit Probability to do marginalisation efficiently. The key idea is to “push sums in” as far as possible when summing (marginalizing) out irrelevant terms:

$$\begin{aligned} p(W) &= \sum_c \sum_s \sum_r P(C,S,R,W) \\ &= \sum_c \sum_s \sum_r P(W|S,R)P(R|C)P(S|C)P(C) \\ &= \sum_c P(C) \sum_s P(S|C) \sum_r P(W|S,R)P(R|C) \end{aligned}$$

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As we perform the innermost sums we create new terms to be summed:

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Complexity is bounded by the size of the largest term. Finding the optimal order is NP-hard, although greedy algorithms work well in practice.

Inference in Bayes Nets: Local Message Passing (I)

If the underlying undirected graph of the BN is acyclic (i.e., a tree), we can use a local message passing algorithm:

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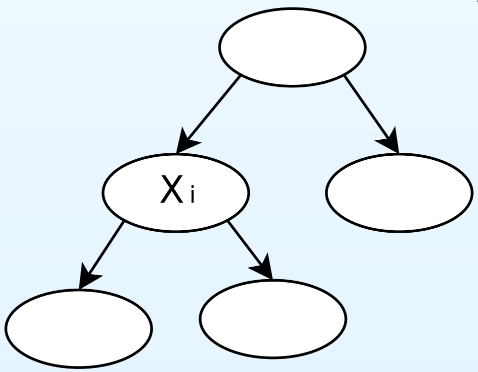

$$\begin{aligned} P(X_i|E) &= P(X_i|E_i^-, E_i^+) \\ &= \frac{P(E_i^-|X_i, E_i^+)P(X_i|E_i^+)}{P(E_i^-|E_i^+)} \\ &= \frac{P(E_i^-|X_i)P(X_i|E_i^+)}{P(E_i^-|E_i^+)} \\ &= \alpha\pi(X_i)\lambda(X_i) \end{aligned}$$

With α independent from X_i, $\pi(X_i) = P(X_i|E_i^+), \lambda(X_i) = P(E_i^-|X_i)$.

Inference in Bayes Nets: Local Message Passing (II)

We can exploit such decomposition to compute $\lambda(X_i) = P(E_i^- | X_i)$ for all X_i recursively as follows:

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$$\lambda(X_i) = P(E_i^-|X_i) = \prod_{X_j \in C} \lambda_j(X_j) = \prod_{X_j \in C} \left(\sum_{X_j} P(X_j|X_i)\lambda(X_j) \right)$$

where $\lambda_j(X_j)$ is the conribution to $P(E_i^-|X_i)$ of subtree rooted at X_j.

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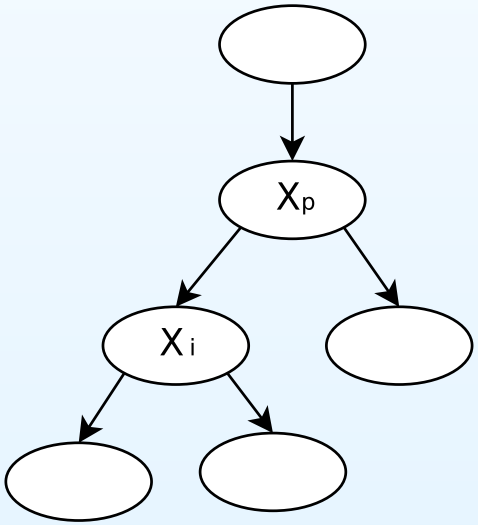

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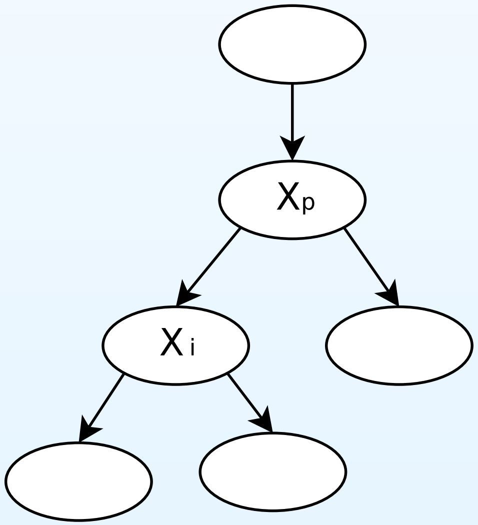

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Having defined $\pi_i(X_p = j)$ equal to $\frac{P(X_p=j|E)}{\lambda_i(X_p=j)}$ we can now compute all $\pi(X_i)$s and then all the $P(X_i|E)$s!

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If we want $P(A, B|C)$ instead of just marginal distrtibutions $P(A|C)$ and $P(B|C)$?

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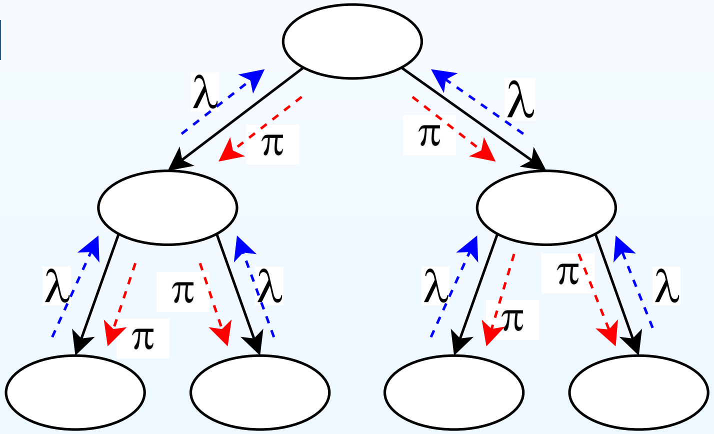

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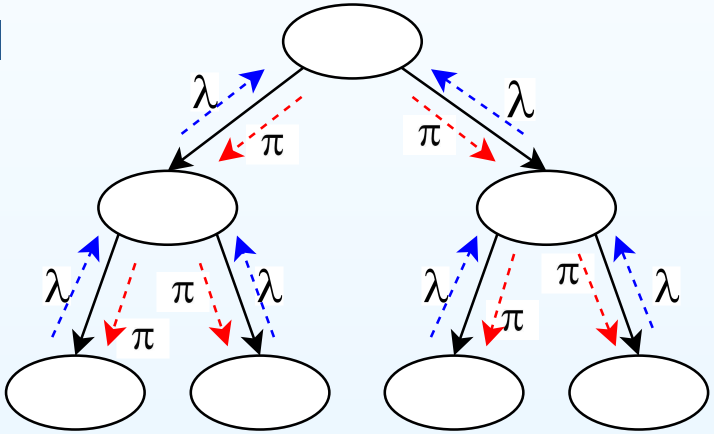
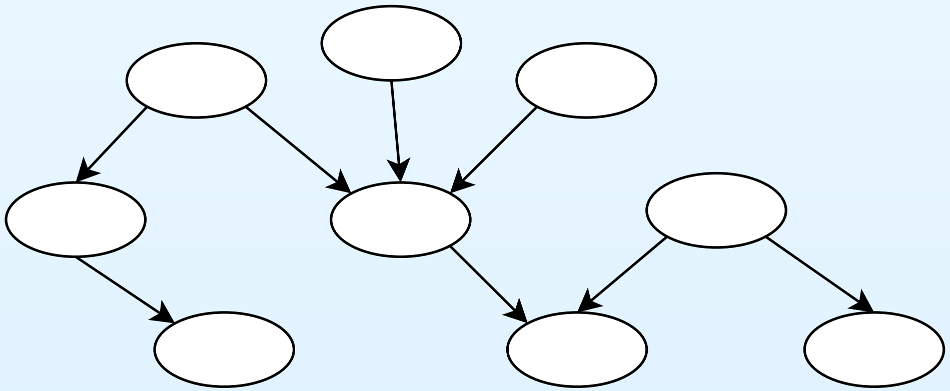


This technique can be generalized to *polytrees*:



Inference in Bayes Nets: Message Passing with Cycles

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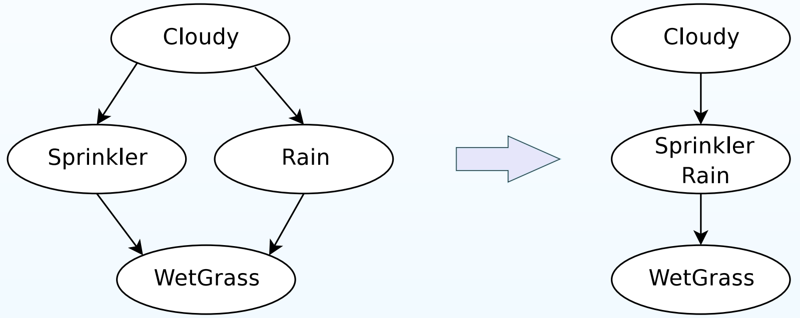
- Clustering variables together:



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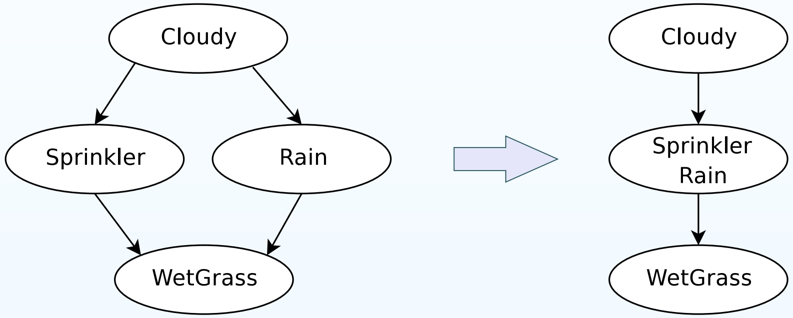

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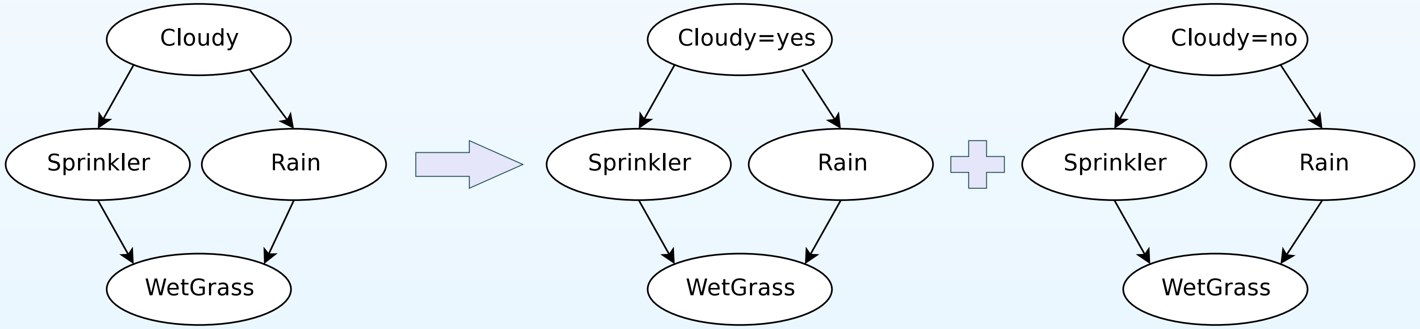

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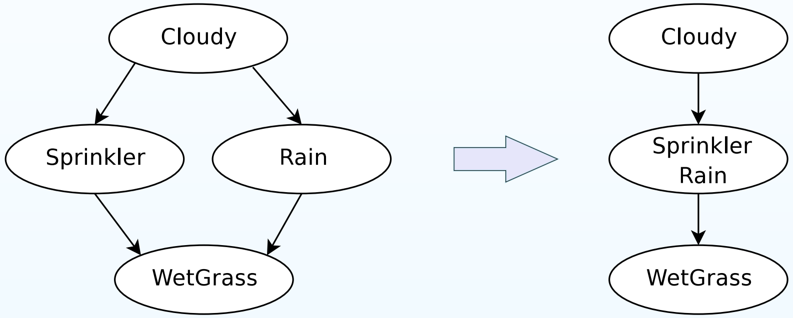

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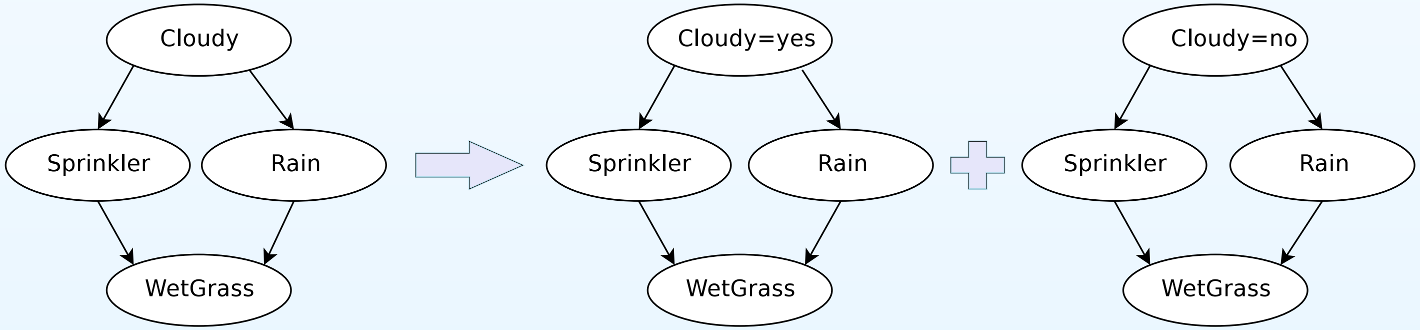
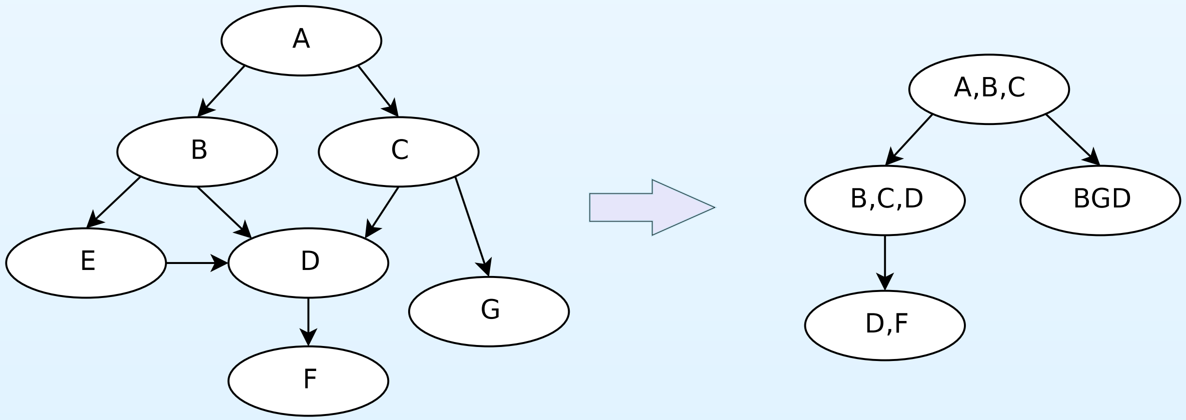


- Join Tree:



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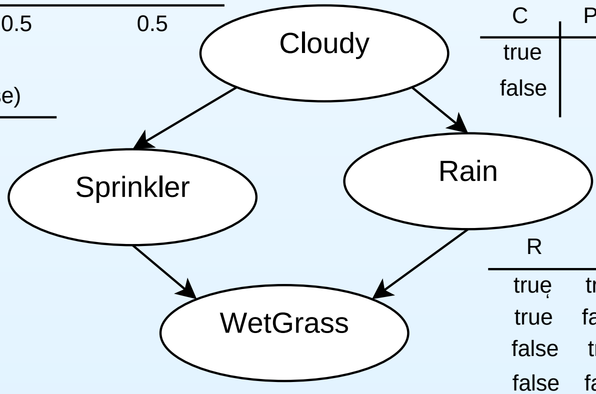
4. Randomly choose a sample w, $w = \texttt{true}$ with prob $P(W|s, r)$

The sample c, s, r, w is a sample from the joint distribution of C, S, R, W.

P(C=true)	P(C=false)
0.5	0.5

C	P(S=true)	P(S=false)
true	0.5	0.5
false	0.9	0.1



C	P(R=true)	P(R=false)
true	0.8	0.2
false	0.2	0.8

R	S	P(W=true)	P(W=false)
true	true	0.99	0.01
true	false	0.9	0.1
false	true	0.9	0.1
false	false	0	1

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- Take a lot of random samples from the joint distributiona and count:
  - N_c: the number of sample in which E_2 is verified.
  - N_s: the number of sample in which both E_1 and E_2 are verified.
  - N:the total number of samples.

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We should use Likelihood Sampling!

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We can exploit a simple idea to improve our sampling strategy

- Suppose in E_2 we have the constraint $X_i = v$
- We are about generating a random value with $P(X_i = v|parents) = w$;
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1. Generate a random assignment for all variables matching E_2;
2. Define w to be the probability that this assignment would have been generated instead of an unmatching assignment (w is the product of all likelihood factors involved in its generation);
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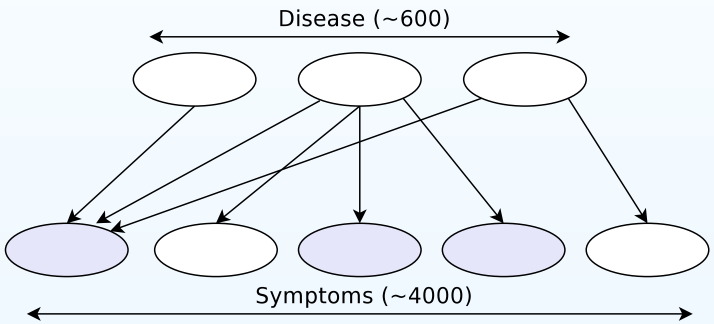
Again the ratio N_s/N_c estimates our query $P(E_1|E_2)$

Bayesian Networks Applications

They originally arose to add probabilities in expert systems; a famous example is the reformulation of the Quick Medical Reference model.



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- Bottom layer represents observed symptoms;
- QMR-DT is so densely connected that exact inference is impossible.

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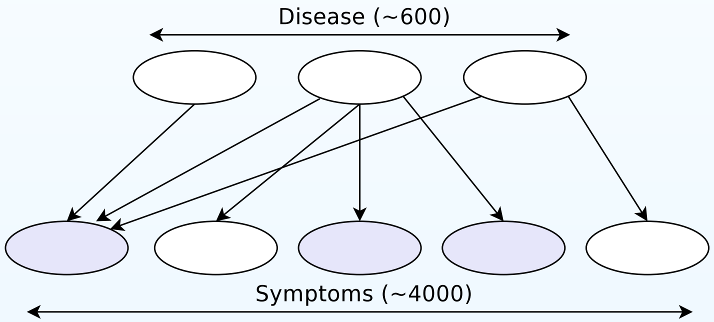

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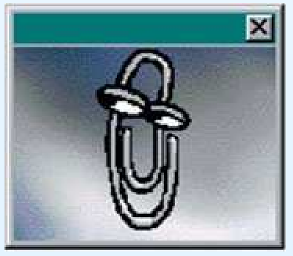
The most widely used Bayes Nets are embedded in Microsoft's products:

- Answer Wizard in Office 95;
- Office Assistant in Office 97;
- Over 30 Technical Support Troubleshooters.



Check the Economist article (22/3/01) about Microsoft's application of BNs.

Learning Bayesian Networks

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This gives rise to 4 approaches:

Structure/Oservability	Full	Partial
Known	Maximum Likelihood Estimation	EM (or gradient ascent)
Unknown	Search through model space	EM + search through model space

Learning: Known Structure & Full Observability

Learning has to find the values of the parameters of each Coditional Probability Distribution which maximizes the likelihood of the training data:

$$\mathcal{L} = \sum_{i=1}^{m} \sum_{r=1}^{R} \log P(X_i | Pa(X_i), \mathcal{D}_r)$$

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Example: For the $WetGrass$ node, from a set of training data, we can just count the number of times the “grass is wet” when it is “raining” and the “sprinler” is on, $N(W = 1, S = 1, R = 1)$, and so on:

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

Learning: Known Structure & Partial Observability

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Example: in the case of *WetGrass* node, we replace the observed counts of the events with the number of times we expect to see each event:

$$P(W|S,R) = \frac{E[N(W,S,R)]}{E[N(S,R)]}$$

where $E[N(x)]$ is the expected number of times x occurs in the training set, given the current guess of the parameters: $E[N(.)] = \sum_k P(.|\mathcal{D}_k)$.

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Last term $c = -\log P(\mathcal{D})$ does not depend on G. We could use structure prior $P(G)$ to penalizes overly complex models, however, this is not necessary since the marginal likelihood term

$$P(\mathcal{D}|G) = \int_\theta P(\mathcal{D}|G, \theta)$$

has already a similar effect; it embodies the Bayesian Occam's razor.

Learning: Unknown Structure & Full Observability (II)

The goal of structure learning is to learn a DAG that best explains the data:

- it is an NP-hard problem, since the number of DAGs on M variables is super-exponential in M
  - there are 543 DAGs on 4 nodes;
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- use multiple restarts to try to find the global optimum, and to learn an ensemble of models.

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- in the fully observable case, dimension of a model is the number of free parameters; in models with hidden variables, it might be less;
- BIC score decomposes into a sum of local terms, but local search is still expensive, because we need to run EM at each step to compute $\hat{\Theta}_G$. We can do local search inside the M-Step (Structural EM).