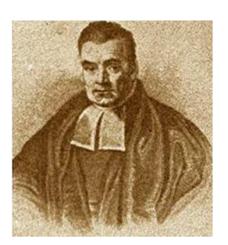
# Part 8: Bayesian Networks

# 8.a Representation and Semantics



Univ.-Prof. Dr. Gerhard Widmer
Department of Computational Perception
Johannes Kepler University Linz

gerhard.widmer@jku.at http://www.cp.jku.at/people/widmer



Reverend Thomas Bayes (1702-1761)

[from the Encyclopaedia Britannica:]

**Bayes, Thomas** (b. 1702, London - d. 1761, Tunbridge Wells, Kent), mathematician who first used probability inductively and established a mathematical basis for probability inference (a means of calculating, from the number of times an event has occurred, the probability that it will occur in future trials).

He set down his findings on probability in "Essay Towards Solving a Problem in the Doctrine of Chances" (1763), published posthumously in the *Philosophical Transactions of the Royal Society of London.* 

The only works he is known to have published in his lifetime are *Divine Benevolence*, or an Attempt to Prove That the Principal End of the Divine Providence and Government is the Happiness of His Creatures (1731) and An Introduction to the Doctrine of Fluxions, and a Defence of the Mathematicians Against the Objections of the Author of the Analyst (1736) which countered attacks by Bishop Berkeley on the logical foundations of Newton's calculus.

#### **Overview**

Representing Knowledge in an Uncertain World: Bayesian Networks

**Conditional Independence in Bayes Nets** 

**Bayes Nets and the Full Joint Distribution** 

An (Informal) Method for Constructing Bayesian Networks

#### **Probabilistic Queries**

#### Remember:

- Every probabilistic query of the form  $P(X \mid E=e)$  can be answered from the *full joint probability distribution* over all domain variables (via Inference by Enumeration)
- BUT (1): Size of full joint is exponential in number of domain variables
- BUT (2): Difficult for system designer to specify probabilities for an exponential number of highly specific atomic events
- Luckily: complexity can be reduced dramatically by independence and conditional independence relationships

#### In this lecture: Bayesian Networks

- Effective, principled way of
  - representing (in)dependencies among variables
  - reconstructing the full joint probability distribution
  - answering arbitrary probabilistic queries
  - → The BN is our agent's **probabilistic knowledge base!**(BNs are a "factorised representation" of the full joint distribution)

# **Bayesian Networks**

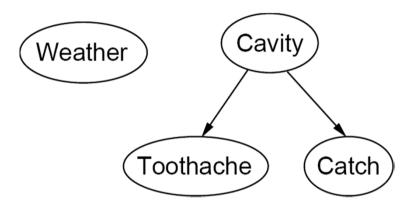
#### A Bayesian Network

- is a directed acyclic graph (DAG)
- Each node is a random variable
- Some nodes are connected via directed links (arrows)
- If there is an arrow from node X to node Y, we say that X is a parent of Y
- Each node  $X_i$  has a conditional probability distribution  $\mathbf{P}(|X_i||Parents(X_i))$  associated with it (in the simplest case: in the form of a conditional probability table)
- The graph has no directed cycles

#### Intuitive interpretation:

 An arrow from X to Y means that X has a direct influence on the probability of Y (or that knowing X gives us information about Y)

# **A Simple Example**



- Cavity causes influences the probability of both Toothache and Catch
- Toothache and Catch are conditionally independent, given Cavity
- Weather is independent of all the other variables

# **A Slightly More Complex Example**

"You have a new burglar alarm installed at home. It is fairly reliable at detecting a burglary, but also sometimes responds to minor earthquakes. You also have two neighbours, John and Mary, who have promised to call you at work when they hear the alarm.

John always calls when he hears the alarm, but sometimes confuses the telephone ringing with the alarm and calls then, too.

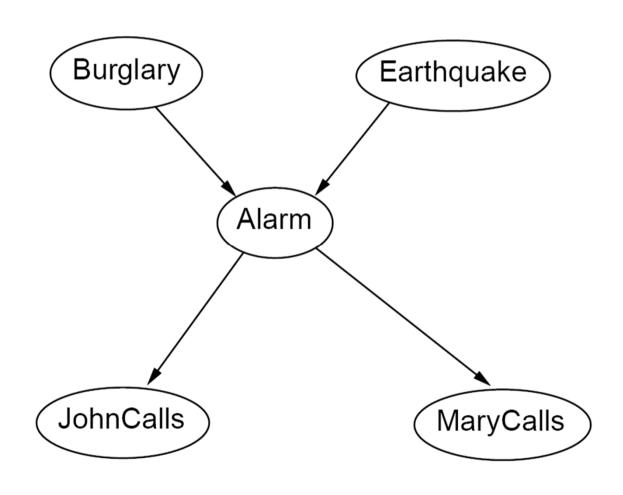
Mary, on the other hand, likes rather loud music and sometimes misses the alarm."

(Russell & Norvig, ch. 14)

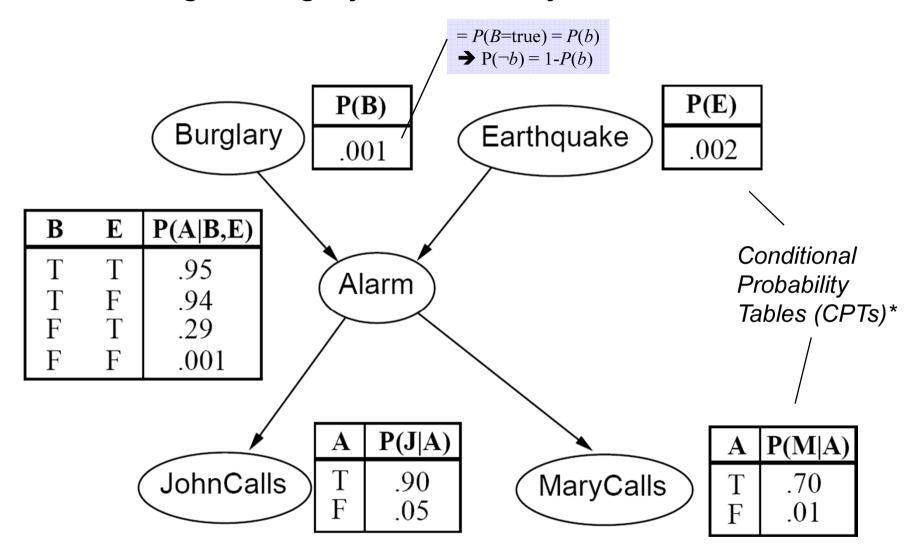
## Typical queries that might be of interest:

- Given that John and/or Mary has / has not called, what is the probability of a burglary, or of an earthquake?
- Given that the alarm goes off, what is the probability that both John and Mary call and that no burglary happened?
- Given a burglary, what is the probability of the alarm going off?
- Given that Mary has just called, how likely is it that John will call, too?

# Modeling the Burglary World as a Bayesian Network



# Modeling the Burglary World as a Bayesian Network

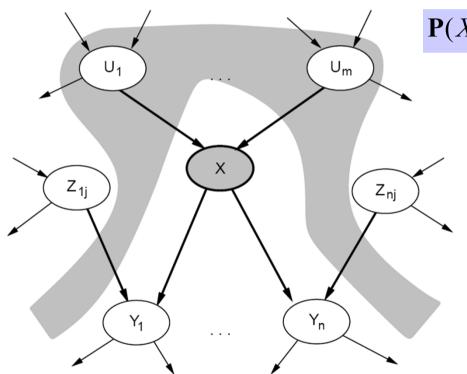


\* Note: Each row in a CPT is a Conditional Probability Distribution

# **Conditional Independence in Bayesian Networks**

#### **Central property of a Bayesian Network:**

Given the values of its parents, each node X is conditionally independent of its non-descendants ("non-descendants": not the children or their children or ...)



$$\mathbf{P}(X | U_1,...,U_m) = \mathbf{P}(X | U_1,...,U_m, Z_{1j},...,Z_{nj})$$

 $\rightarrow$  Parents  $U_i$  separate X from irrelevant variables  $Z_{ij}$ 

But note: *X* is **not** independent of its children and their descendants!

$$\mathbf{P}(X | U_1,...,U_m) \neq \mathbf{P}(X | U_1,...,U_m, Y_{1j},...,Y_n)$$

(because knowing the values of the children permits me to better guess the value of X, even if I know the values of the parents of X)

... consider 
$$P(a \mid \neg b, \neg e)$$
 vs.  $P(a \mid \neg b, \neg e, j, m)$  ...

# **Bayesian Networks and the Full Joint Distribution**

**Remember the full joint distribution:**  $P(X_1, ..., X_n)$  specifies the probability of every possible atomic event  $P(x_1, ..., x_n)$  in the agent's world

#### Remember chain rule:

$$\underline{\mathbf{P}(X_1,...,X_n)} = \mathbf{P}(X_1 \mid X_2,...,X_n)\mathbf{P}(X_2 \mid X_3,...,X_n)\cdots\mathbf{P}(X_n) = \prod_{i=1}^n \mathbf{P}(X_i \mid X_{i+1},...,X_n)$$

## Remember central property of Bayesian Networks (previous slide):

$$\mathbf{P}(X_i | Parents(X_i), Z_1, ..., Z_n) = \mathbf{P}(X_i | Parents(X_i))$$

(where the  $Z_i$  are all other non-descendants of  $X_i$ )

Now: assume variables are ordered according to the graph structure of the BN, "from bottom to top"  $\Rightarrow$  all the children and descendants of node  $X_i$  appear before  $X_i$  in the ordering, all the parents of  $X_i$  appear after  $X_i$ , and any other variables after  $X_i$  are non-descendants of  $X_i$  (is always possible):

$$\underline{\mathbf{P}(X_{1},...,X_{n})} = \prod_{i=1}^{n} \mathbf{P}(X_{i} | X_{i+1},...,X_{n}) = \prod_{i=1}^{n} \mathbf{P}(X_{i} | Parents(X_{i}))$$

parents and non-descendants

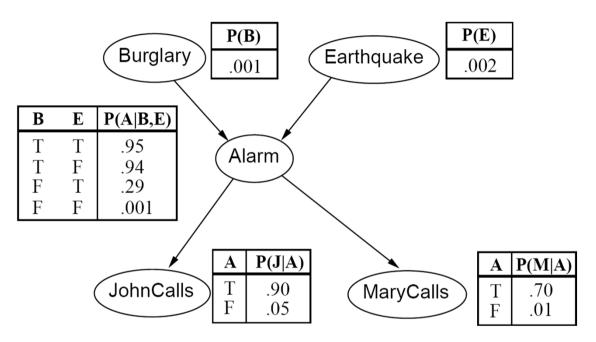
# **Bayesian Networks and the Full Joint Distribution**

$$\mathbf{P}(X_1, X_2, ..., X_n) = \prod_{i=1}^{n} \mathbf{P}(X_i | Parents(X_i))$$
given in CPTs

#### In words:

- Any entry in the full joint distribution can be computed as a product of the conditional probabilities of each variable, given its respective parent values
- Any entry in the full joint distribution can be computed as the product of the appropriate elements of the conditional probability tables (CPTs) in the Bayesian network.
- A Bayesian network is a structured, compact, complete, and non-redundant representation of the full joint distribution, where the compaction is made possible by the explicit knowledge about conditional independencies between variables

# An Example



What is the probability that an alarm has sounded, both John and Mary call, but neither a burglary nor an earthquake has happened? (an atomic event ...)

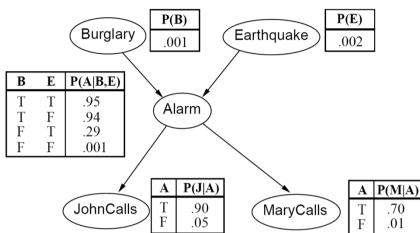
$$P(j \land m \land a \land \neg b \land \neg e) =$$

$$= P(j \mid a)P(m \mid a)P(a \mid \neg b \land \neg e)P(\neg b)P(\neg e) =$$

$$= 0.90 \times 0.70 \times 0.001 \times 0.999 \times 0.998 = 0.00062$$

# **Compactness of the Representation**

• A CPT for a Boolean variable  $X_i$  with k Boolean parents has  $2^k$  rows (one for each combination of parent values)



- Each row requires one number p, for  $X_i = true$  (the number for  $X_i = false$  is just 1-p)
- If each variable has at most k parents, the complete network requires  $O(n \cdot 2^k)$  numbers
- $\rightarrow$  For a fixed k, complexity grows **linearly** with n (number of variables = size of the network), not exponentially  $(O(2^n))$  as with the full joint distribution!
- Burglary network: 1 + 1 + 4 + 2 + 2 = 10 numbers (vs.  $2^5 = 32$ )
- Network with n=30 and k=5: requires 960 numbers (vs.  $2^{30} > 1,000,000,000$ !)

# **Constructing Bayesian Networks**

#### To construct a Bayesian network, we need to do three things:

- Decide on the random variables that define the agent's world
- 2. Specify the structure of the network
- 3. Specify the conditional probability tables for each node
- Step 1: must always be done by the system designer
- Step 2: is often done by the system designer (or an expert in the particular application domain); but there are also algorithms for *automatically learning* the dependency structures (→ machine learning)
  - too complex to be discussed in this class ...
- Step 3: is usually done via *learning* from example observations (estimation of probabilities from a set of observed events)

# Informal Method for Constructing a Bayesian Network Step 2: Specify the Structure of the Network

- 1. Choose some fixed ordering of the variables  $X_1, ..., X_n$
- 2. For i = 1 to n do:

add  $X_i$  to the network;

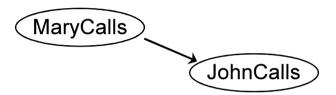
select parents from  $X_1, ..., X_{i-1}$  such that  $P(X_i | Parents(X_i)) = P(X_i | X_1, ..., X_{i-1})$ 

#### **IMPORTANT!**

Must choose all variables as  $Parents(X_i)$  that somehow influence my estimate of the probability of  $X_i$ , or whose prob. somehow correlates with the prob. of  $X_i$ 

- → Guarantees that resulting network really represents the true joint distribution
- Incremental procedure add variables/nodes one by one
- **Optimally:** Choose an ordering such that all the variables that should "logically" be the parents of *X* (i.e., those that "cause" *X*) are added before *X* 
  - → Would guarantee maximal compactness of resulting network

Suppose we choose the ordering M, J, A, B, E (a poor ordering ...)

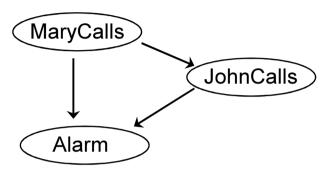


Is JohnCalls independent of MaryCalls?, i.e.,  $P(J \mid M) = P(J)$  (if we don't know anything else)?

Well ... if Mary calls, it is likely that the alarm has gone off, which makes it more likely that John calls (compared to if the alarm had not gone off).

- → The probabilities of *MaryCalls* and *JohnCalls* are somehow related (through a common cause: the alarm)
- $\rightarrow$  **P**( $J \mid M$ )  $\neq$  **P**(J)
- → JohnCalls needs MaryCalls as a parent (or vice versa)

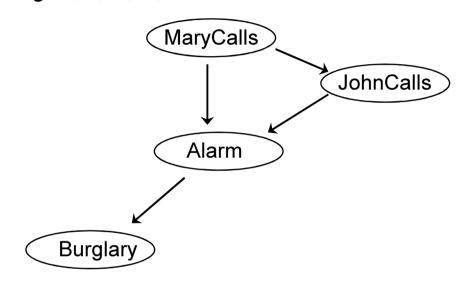
Suppose we choose the ordering *M*, *J*, *A*, *B*, *E* 



$$P(J | M) = P(J)$$
? **NO**

$$P(A | J) = P(A)$$
? NO  $P(A | J, M) = P(A | J)$ ?

Suppose we choose the ordering M, J, A, B, E



NO

$$P(J | M) = P(J)$$
? **NO**

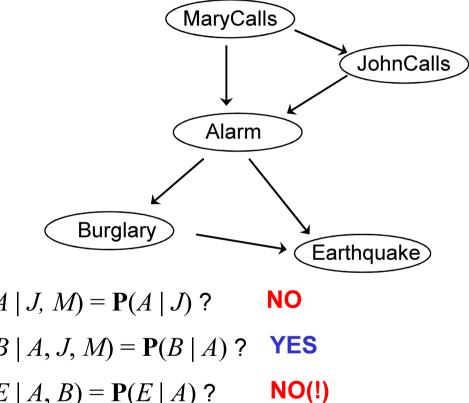
$$P(A \mid J) = P(A)$$
? NO

$$P(B | A) = P(B)$$
? NO

$$P(A | J) = P(A)$$
? NO  $P(A | J, M) = P(A | J)$ ?

$$P(B | A) = P(B)$$
? NO  $P(B | A, J, M) = P(B | A)$ ? YES

Suppose we choose the ordering M, J, A, B, E



$$P(J | M) = P(J)$$
? **NO**

$$P(A | J) = P(A)$$
? NO

$$P(A | J) = P(A)$$
? NO  $P(A | J, M) = P(A | J)$ ?

$$P(B | A) = P(B)$$
 ? **NO**

$$P(B | A) = P(B)$$
? NO  $P(B | A, J, M) = P(B | A)$ ? YES

$$P(E | A) = P(E)$$
 ? **NO**

$$P(E | A) = P(E)$$
? NO  $P(E | A, B) = P(E | A)$ ? NO(!

$$P(E | A, B, J, M) = P(E | A, B)$$
? YES

→ Resulting network is more complex and unintuitive than our previous one ... Why?

# **Node Ordering and Compactness**

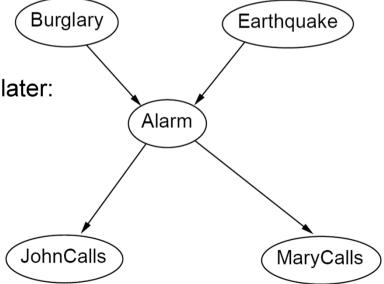
#### Insights:

- Deciding conditional independence in "non-causal" directions is hard
- Guessing conditional probabilities in non-causal directions is even harder ...
- Networks whose nodes are not ordered according to causality tend to be complex (because they need to explicitly encode indirect correlations between variables which are really due to some common cause ..)

#### **Consequence:**

Add variables in "order of causation"

primary causes first, consequences later:

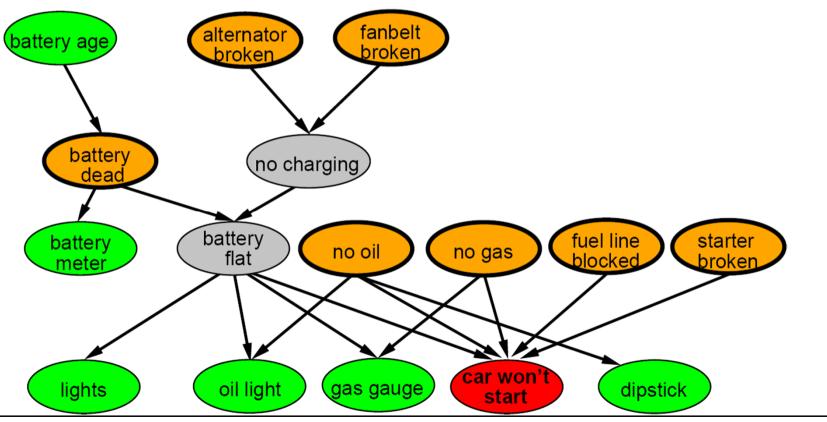


# **Example: Car Diagnosis**

Initial evidence: car won't start

green: observable (testable) variables

orange: possible diagnoses / causes (their probabilities will be determined via probabilistic queries, given the values of some of the testable variables)
 grey: hidden variables – ensure sparse structure, reduce number of parameters



# Part 8: Bayesian Networks

8.b
Inference and (briefly) Learning



Univ.-Prof. Dr. Gerhard Widmer
Department of Computational Perception
Johannes Kepler University Linz

gerhard.widmer@jku.at http://www.cp.jku.at/people/widmer

#### **Overview**

## **Exact inference by enumeration**

Efficient implementation: The Variable Elimination Algorithm

#### **Approximate inference by stochastic sampling:**

- Rejection Sampling
- Likelihood Weighting
- Gibbs Sampling (special case of Markov Chain Monte Carlo (MCMC) sampling)

## Learning Bayesian Networks from Observations (briefly)

→ If you are interested in the omitted topics (and more), consider attending my class "Probabilistic Models" (2 h / 3 ECTS; WS)

→ http://www.cp.jku.at/teaching/current/prob\_models\_introduction\_veryshort.pdf

# **Probabilistic Inference in Bayesian Networks**

#### **Basic task of probabilistic inference:**

- Given the known/observed concrete values of some set of evidence variables)
- Compute the posterior probability distribution for a set of query variables

#### **Notation:**

- X ... query variables
- $\mathbf{E} = \{E_1, ..., E_n\}$  ... evidence variables
- $e = \{e_1, ..., e_n\}$  ... values of the evidence variables in the observed event
- $Y = \{Y_1, ..., Y_m\}$  ... all the other variables ("hidden variables")
- V = X + E + Y ... all variables
- $\rightarrow$  Probabilistic query:  $P(X \mid E=e) = ?$

**Example:** P(Burglary | JohnCalls = true, MaryCalls = true)?

# **Exact Inference by Enumeration**

**Remember:** Any conditional probability can be computed from the full joint distribution by summing over all hidden variables ("inference by enumeration"):

$$P(X | E = e) = \alpha P(X, E = e) = \alpha \sum_{y} P(X, E = e, Y = y)$$

	toothache		¬ toothache	
	catch	¬ catch	catch	¬ catch
cavity	.108	.012	.072	.008
¬ cavity	.016	.064	.144	.576

 $P(cavity \mid toothache) =$ 

$$= \frac{P(cavity \land toothache)}{P(toothache)} = \frac{(.108 + .012)}{(.108 + .012 + .012 + .016 + .064)} = 0.6$$

# **Exact Inference by Enumeration in Bayesian Networks**

#### Remember:

Bayesian network implicitly represents complete joint distribution

$$\mathbf{P}(X_1, X_2, ..., X_n) = \prod_{i=1}^n \mathbf{P}(X_i \mid Parents(X_i))$$

- $\rightarrow$  The probability of any atomic event (i.e., any term of the form  $P(x_1, ..., x_n)$ ) can be computed as a product of conditional probabilities from the network
- → Any query P(X | E=e) can be answered from a Bayesian network by computing sums (over all value combinations of the unseen variables) of products of conditional probabilities (with the values for the E variables fixed)
- → Can sum out over variables from the joint distribution without actually constructing its explicit table representation (which would be exponential in the number of variables)

# Exact Inference by Enumeration in Bayesian Networks: An Example

**Query:** P(Burglary | JohnCalls = true, MaryCalls = true) = ?

- Query variable X = Burglary
- Evidence ( $\mathbf{E} = \mathbf{e}$ ) = {JohnCalls = true, MaryCalls = true} (or {j,m}, in our shorthand notation)
- Hidden variables  $Y = \{Earthquake, Alarm\}$
- Probabilistic query: P(X | E=e) = ?
- → 2 hidden variables
- → Query can be computed via double sum

$$\mathbf{P}(B \mid j, m) = \alpha \mathbf{P}(B, j, m) = \alpha \sum_{x \in \{e, \neg e\}} \sum_{y \in \{a, \neg a\}} \mathbf{P}(B, j, m, E = x, A = y)$$

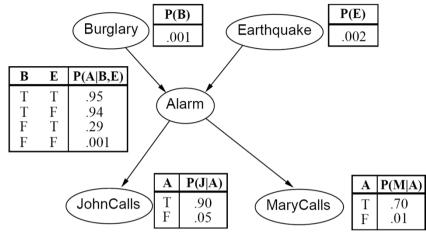
these can be computed from the CPTs of the Bayesian Network

# **Exact Inference by Enumeration**

## **Example computation for**

*Burglary = true*:

$$P(b | j,m) = \alpha \sum_{x \in \{e, \neg e\}} \sum_{y \in \{a, \neg a\}} P(b, j, m, E = x, A = y)$$



$$= \alpha \left[ P(b, j, m, e, a) + P(b, j, m, e, \neg a) + P(b, j, m, \neg e, a) + P(b, j, m, \neg e, \neg a) + P(b, j, m, \neg e, \neg a) + P(b, j, m, \neg e, \neg a) + P(b)P(\neg e)P(\neg a | b, \neg e)P(j | \neg a)P(m | \neg a) + P(b)P(\neg e)P(\neg a | b, \neg e)P(j | \neg a)P(m | \neg a) + P(b)P(\neg e)P(\neg a | b, \neg e)P(j | \neg a)P(m | \neg a) \right]$$

$$P(b \mid j, m) = \alpha \times 0.00059224$$

$$P(\neg b \mid j, m) = \alpha \times 0.0014919$$

$$\alpha = 1/(0.00059224 + 0.0014919) = 479.8142159$$

$$P(B \mid j, m) = \alpha \times [0.00059224, 0.0014919] \approx [0.284, 0.716]$$

→ Probability of burglary, given that both neighbours call, is about 28 %

# **Exact Inference by Enumeration: Optimising the Computation**

$$P(b | j,m)$$
=  $\alpha \sum_{x} \sum_{y} P(b, j, m, E = x, A = y)$ 
=  $\alpha [P(b, j, m, e, a)]$ 
=  $\alpha [P(b)P(e)P(a | b, e)P(j | a)P(m | a)]$ 
+  $P(b, j, m, e, \neg a)$ 
+  $P(b)P(e)P(\neg a | b, e)P(j | \neg a)P(m | \neg a)$ 
+  $P(b)P(\neg e)P(a | b, \neg e)P(j | a)P(m | a)$ 
+  $P(b)P(\neg e)P(\neg a | b, \neg e)P(j | \neg a)P(m | \neg a)$ 
+  $P(b)P(\neg e)P(\neg a | b, \neg e)P(j | \neg a)P(m | \neg a)$ 

**Note:** The product P(j|a)P(m|a) must be computed 2x (for each value of E); and then again 2x, if we also want to compute  $P(\neg b \mid j, m)$  ...

The same goes for  $P(j|\neg a)P(m|\neg a)$ 

**Generally:** In more complex cases, many products must be computed *(exponentially!)* many times

- → Basic Idea: Try to avoid repeated calculations (by doing the calculation only *once* and *storing the result* for later use)
- → A kind of "dynamic programming"

9

# → "Variable Elimination" Algorithm

## **Basic algorithm:**

- 1. Write query computation expression as a sum of products
- 2. Choose an (arbitrary) ordering *L* of the "hidden" variables (i.e., those to be summed out)
- 3. for each variable X in  $m{L}$  :
  - A. "Push in" the sum over *X* as far as possible
  - B. in this innermost sum:
    - a. Compute product of involved terms (CPT entries or stored 'factors') for all possible value combinations of the involved variables
    - b. Sum out the variable to be summed over (X)
    - c. Store resulting factor as a (multi-dimentional) table ('factor')
    - d. Replace the sum by the new factor

**Example:** P(B | j, m) = ?

1. Write query computation expression as a sum of products

$$\mathbf{P}(B \mid j, m) = \alpha \sum_{x=e, \neg e} \sum_{y=a, \neg a} \mathbf{P}(B) P(E = x) P(A = y \mid B, E = x) P(j \mid A = y) P(m \mid E = y)$$

- 2. Choose an (arbitrary) ordering  $\boldsymbol{L}$  of the "hidden" variables e.g., E, A
- 3.A. [1] "Push in" the sum over E as far as possible

$$\mathbf{P}(B \mid j, m) = \alpha \sum_{y=a, \neg a} \mathbf{P}(B) P(j \mid A = y) P(m \mid A = y) \sum_{x=e, \neg e} P(E = x) P(A = y \mid B, E = x)$$

$$\mathbf{P}(B \mid j, m) = \alpha \, \mathbf{P}(B) \sum_{y=a, \neg a} P(j \mid A = y) P(m \mid A = y) \sum_{x=e, \neg e} P(E = x) P(A = y \mid B, E = x)$$

- 3.B. in this innermost sum:
  - a. Compute product of involved terms (CPT entries or stored 'factors') for all possible value combinations of the involved variables
    - $\rightarrow$  compute P(E)P(A|B,E) for all values of E, A, B (entries from CP $\overline{L}$ )
    - $\rightarrow$  gives an intermediate table **T** of dimensionality  $|E| \times |A| \times |B|$
  - b. Sum out over E:
    - $\rightarrow$  for each pair of values of A and B, sum up  $\mathbf{T}(e,A,B) + \mathbf{T}(\neg e,A,B)$
  - c. Store resulting factor as a (multi-dimentional) table
  - $\Rightarrow$  gives a table  $\mathbf{F}_E(A,B)$  of dimensionality  $|A| \times |B|$  (subscript E indicates that E has been summed out)

d. Replace the sum by the new factor

$$\mathbf{P}(B \mid j, m) =$$

$$= \alpha \sum_{y=a,\neg a} \mathbf{P}(B)P(j \mid A = y)P(m \mid A = y) \sum_{x=e,\neg e} P(E = x)P(A = y \mid B, E = x) =$$

$$\mathbf{F}_{E}(A,B)$$

$$= \alpha \sum_{y=a,\neg a} \mathbf{P}(B)P(j \mid A = y)P(m \mid A = y)\mathbf{F}_{E}(A = y, B)$$

 $y=a, \neg a$ 

$$\mathbf{P}(B \mid j, m) = \alpha \sum_{y=a, \neg a} \mathbf{P}(B) P(j \mid A = y) P(m \mid A = y) \mathbf{F}_{E}(A = y, B)$$

#### **Next iteration:**

3.A. [2] "Push in" the sum over A as far as possible

$$\mathbf{P}(B \mid j, m) = \alpha \ \mathbf{P}(B) \sum_{y=a, \neg a} P(j \mid A = y) P(m \mid A = y) \mathbf{F}_E(A = y, B)$$

- 3.B. in this innermost sum:
  - a. Compute products of involved terms (CPT entries or stored 'factors')
  - $\rightarrow$  compute  $P(j|A) P(m|A) \mathbf{F}_E(A,B)$  for all values of A, B
  - $\rightarrow$  gives an intermediate table T of dimensionality  $|A| \times |B|$
  - b. Sum out over A:
  - $\rightarrow$  for each value of B, sum up  $\mathbf{T}(a,B) + \mathbf{T}(\neg a,B)$
  - c. Store resulting factor as table (vector)  $\mathbf{F}_{A}(B)$  of dimensionality |B|

d. replace the sum by the new factor

$$\mathbf{P}(B \mid j, m) =$$

$$= \alpha \ \mathbf{P}(B) \sum_{y=a,\neg a} P(j \mid A = y) P(m \mid A = y) \mathbf{F}_{E}(A = y, B)$$

$$\mathbf{F}_{A}(B)$$

$$= \alpha \ \mathbf{P}(B) \mathbf{F}_{A}(B)$$

# → Final Step:

Compute the result for each value of B (i.e., take point-wise product of P(B) and  $F_A(B)$ ):

$$\mathbf{P}(B \mid j, m) = \begin{bmatrix} P(b \mid j, m) \\ P(\neg b \mid j, m) \end{bmatrix} = \alpha \ \mathbf{P}(B) \cdot \mathbf{F}_{A}(B) = \alpha \begin{bmatrix} P(b)\mathbf{F}_{A}(b) \\ P(\neg b)\mathbf{F}_{A}(\neg b) \end{bmatrix}$$

## The Complexity of Exact Inference in Bayesian Networks

Consider: 
$$P(B | j, m) = \alpha P(B, j, m) = \alpha \sum_{x \in \{e, \neg e\}} \sum_{y \in \{a, \neg a\}} P(B, j, m, E = x, A = y)$$

- → Need to sum over  $2 \times 2 = 2^2 = 4$  value combinations of hidden variables E, A
- → In the worst case, given *n* variables, almost all of these may be hidden and thus must be summed out:
- Worst-case complexity of exact inference in Bayesian Networks is  $O(2^n)$  Can be dramatically improved via clever variable elimination algorithms (see previous slide), *if* 
  - network is sparsely connected (there are many conditional independencies)
  - we happen to pick (guess) a good variable elimination ordering
- → Still: in the *worst case*, no improvement (asymptotically) over full enumeration of joint distribution (and intermediate 'factors' in variable elimination can grow exponentially ...)
- → Need for *approximate* algorithms

# Approximate Inference in Bayesian Networks: Stochastic Sampling

#### Basic idea:

- Randomly generate atomic events (according to the probability distribution defined by the network)
- The frequency with which a certain event occurs gives an estimate of its true probability
- The relative frequencies of all atomic events give an estimate of the full joint distribution
- ightharpoonup Will estimate  $P(X \mid e)$  via a constant (large) number of random samples instead of an exponential summation process

#### Outline of the next slides:

- Estimating the prior (unconditional) probability of events:
  - Sampling without evidence
- 2. Approximately solving probabilistic queries  $\mathbf{P}(\mathbf{X} \mid \mathbf{e})$  :
  - Rejection Sampling
  - Likelihood Weighting
  - Gibbs Sampling
  - more generally: Markov Chain Monte Carlo (MCMC) sampling

# Estimating the Probability of Events: Sampling without Evidence ("Sampling from the Prior Distribution")

Algorithm for randomly generating an atomic event according to the probability distribution represented by the network:

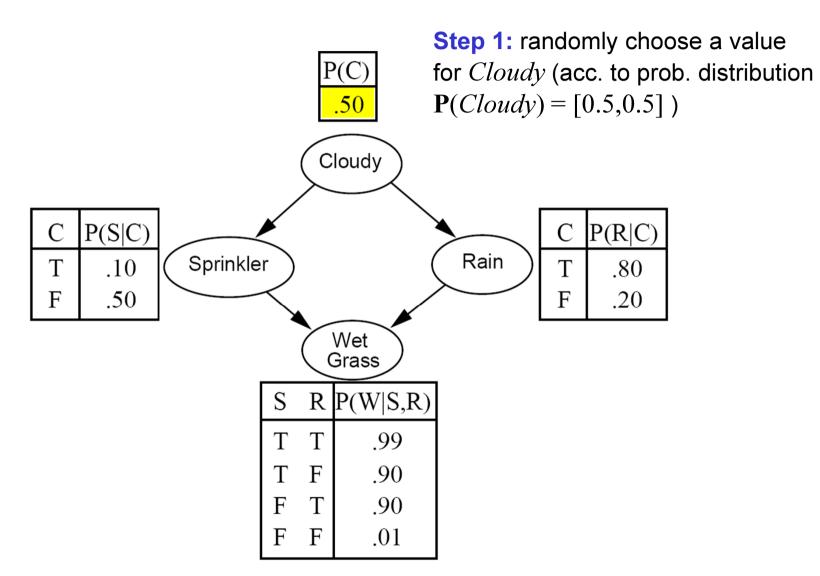
- Sample variables in topological order in the network (from 'top' to 'bottom')
- "Sampling a variable" =
   randomly choosing a value for the variable according to the variable's
   Conditional Probability Table (CPT), taking into account the values of
   the variable's parents (which have already been assigned)
  - → Exercise: Devise an algorithm for choosing values from a set according to a discrete probability distribution (assuming that you have a pseudo-random number generator that returns a random real number uniformly distributed in the interval [0:1])

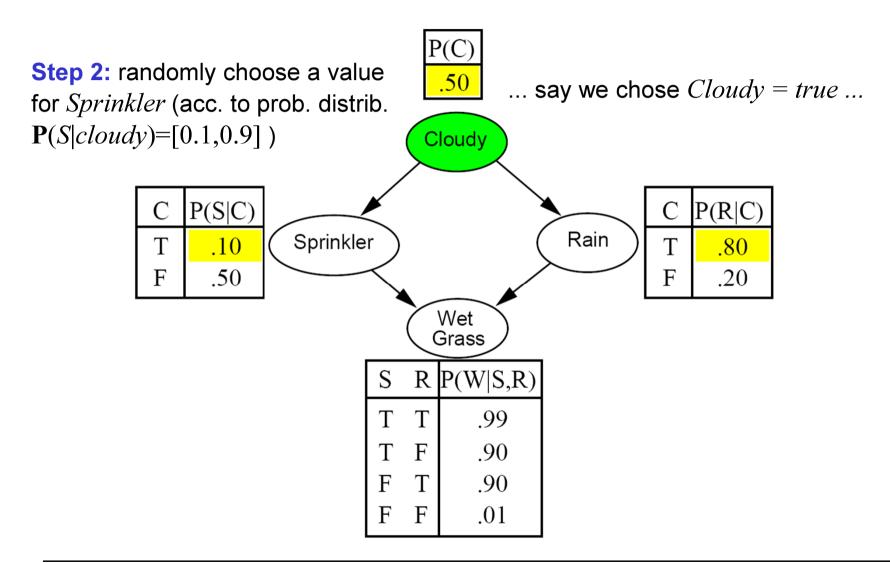
# Estimating the Probability of Events: Sampling without Evidence ("Sampling from the Prior Distribution")

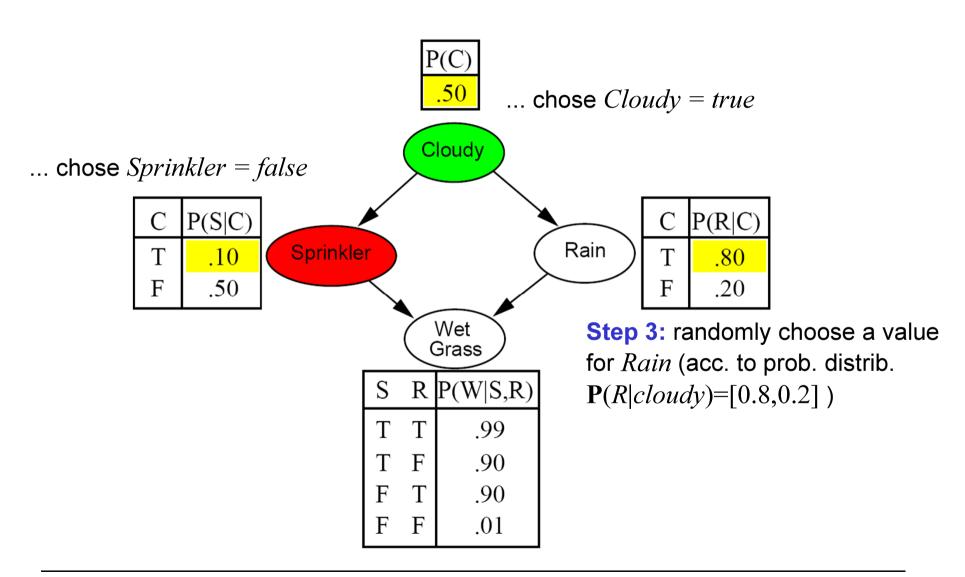
Algorithm for randomly generating an atomic event according to the probability distribution represented by the network:

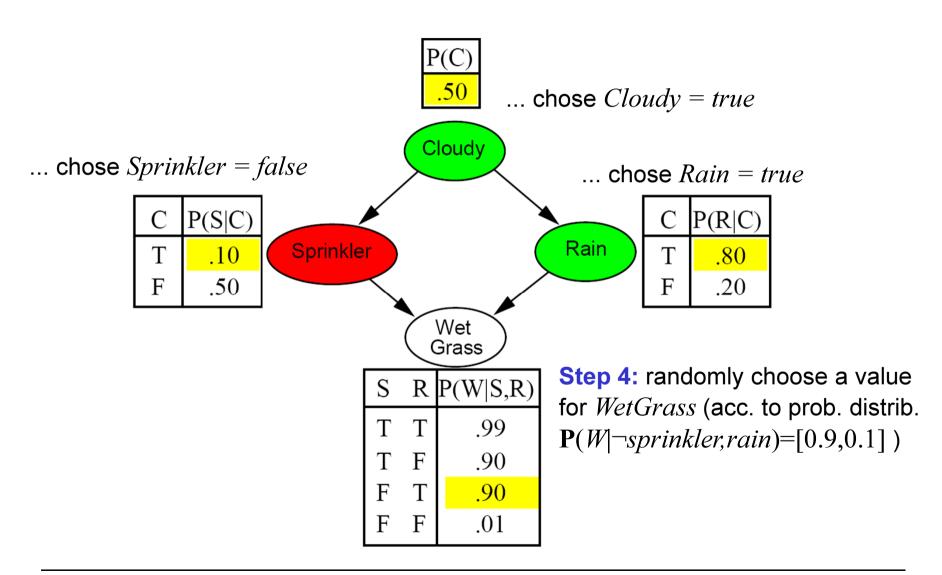
```
function PRIOR-SAMPLE(bn) returns an event sampled from bn inputs: bn, a belief network specifying joint distribution \mathbf{P}(X_1,\ldots,X_n) \mathbf{x}\leftarrow an event with n elements for i=1 to n do x_i\leftarrow a random sample from \mathbf{P}(X_i\mid parents(X_i)) *) given the values of Parents(X_i) in \mathbf{x} return \mathbf{x}
```

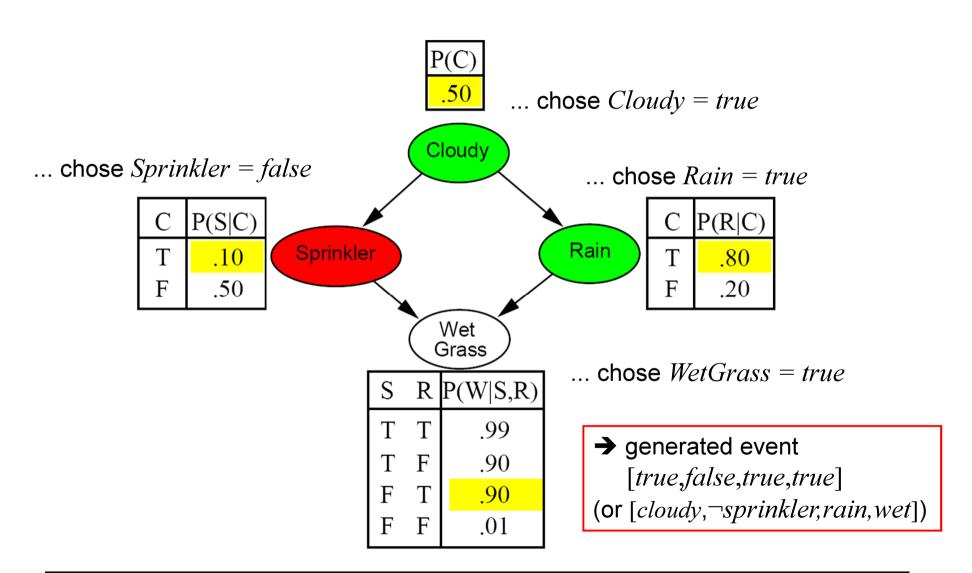
\*) Assumption: Variables  $X_i$  are sorted in topological order ("from top to bottom")











# **Sampling Distribution and Full Joint Distribution**

#### Need to prove that the sampling distribution converges to the true distribution:

Variables are sampled independently (given values of their parents)

 $\rightarrow$  Probability that the sampling algorithm Prior-Sample (PS) generates an event  $(x_1,...,x_n)$  is the product of the probabilities of generating each  $x_i$ :

$$P_{PS}(x_1,...,x_n) = \prod_{i=1}^n P_{PS}(x_i) = \prod_{i=1}^n P(x_i \mid parents(X_i))$$

(because each sampling step depends only on the parent values)

- ightharpoonup As the number of sampled events goes to infinity, the *sampling distribution*  $\mathbf{P}_{PS}$  perfectly approximates the full joint distribution  $\mathbf{P}$  represented by the network
- → Estimates based on this sampling process are said to be *consistent*

# → Estimating the Probability of an Atomic Event

## Estimating the probability of an atomic (i.e., fully specified) event $(x_1,...,x_n)$ :

- Generate N random samples from the network
- Count the number of times K that the specific event appears in these N samples
- Take ratio  $\hat{P} = \frac{K}{N}$  as an estimate of the probability  $P(x_1, ..., x_n)$

#### **Example:**

$$P(cloudy, \neg sprinkler, rain, wet) = P(true, false, true, true) =$$
  
=  $0.5 \times 0.9 \times 0.8 \times 0.9 = 0.324$ 

→ If we take a large number of samples, we can expect around 32.4 % of the samples to be equal to (true, false, true, true)

# Estimating the Probability of a Partially Specified Event

# Estimating the probability of a partially specified event $(x_1, ..., x_m)$ , with m < n:

- Take N random samples (according to the net)
- Count the number of times K of occurrences of atomic events among these samples that  $\mathbf{match}\ (x_1, \ldots, x_m)$  (i.e., that have these specific values for the variables  $X_1, \ldots, X_m$ )
- Take ratio  $\hat{P} = \frac{K}{N}$  as an estimate of the probability  $P(x_1, ..., x_m)$

#### **Example:**

• Assume we generate 1000 samples from the sprinkler network, and 511 of them have Rain = true, then the estimated probability of rain

$$\hat{P}(Rain = true) = \frac{511}{1000} = 0.511$$

# Sampling from the Posterior Distribution – Answering Probabilistic Queries via Sampling (1): Rejection Sampling

**Goal:** compute approximate solution to probabilistic query  $P(X \mid E=e)$  via sampling

**Idea:** use only those samples for estimating P(X) that match the given evidence E=e

#### **Simple Algorithm:**

- Generate N samples from the network
- Keep only those N samples that match the evidence  ${\bf e}$  (i.e., reject those samples with  ${\bf E} \neq {\bf e}$ )
- Count K = number of times that X=x appears in the remaining N samples
- Take ratio  $\hat{P} = \frac{K}{N'}$  as estimate of probability  $P(\mathbf{X} = \mathbf{x} \mid \mathbf{E} = \mathbf{e})$

**Easy to show:** as  $N \to \infty$ , the estimate converges to the true probability

# Sampling from the Posterior Distribution – Answering Probabilistic Queries via Sampling (1): Rejection Sampling

**Goal:** compute approximate solution to probabilistic query  $P(X \mid E=e)$  via sampling **Idea:** use only those samples for estimating P(X) that match the given evidence E=e

### **Simple Algorithm:**

```
function Rejection-Sampling (X, e, bn, N) returns an estimate of P(X|e) local variables: N, a vector of counts over X, initially zero for j=1 to N do \mathbf{x} \leftarrow \text{Prior-Sample}(bn) if \mathbf{x} is consistent with e then \mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1 \text{ where } x \text{ is the value of } X \text{ in } \mathbf{x} return \text{Normalize}(\mathbf{N}[X])
```

**Easy to show:** as  $N \to \infty$ , the estimate converges to the true probability

# **Rejection Sampling: Example**

**Probabilistic query:**  $P(Rain \mid Sprinkler = true)$ 

#### **Assume that**

- we sample N = 100 events
- 73 of these have Sprinkler = false  $\rightarrow$  are rejected
- 27 have  $Sprinkler = true \rightarrow N' = 27$
- of these 27 samples, 8 have Rain = true and 19 have Rain = false

$$\hat{P}(Rain = true \mid Sprinkler = true) = \frac{8}{27} = 0.296$$

$$\hat{P}(Rain = false \mid Sprinkler = true) = \frac{19}{27} = 0.704$$

$$\hat{P}(Rain \mid Sprinkler = true) = [0.296, 0.704]$$

(True answer computed from the network is  $P(Rain \mid Sprinkler = true) = [0.3, 0.7]$ )

# **Rejection Sampling**

#### **Advantage of Rejection Sampling:**

Low computational complexity:
 linear in number of samples and size of network

#### **Problem** with Rejection Sampling:

• Rejects many examples: proportion of samples consistent with evidence E=e drops exponentially with number of evidence variables E!

**Note:** Rejection sampling is very similar to estimating conditional probabilities by observing the real world:

- Would estimate P(Rain | RedSkyAtNight=true) by observing the sky every evening and counting how often it rains after a red sky was observed the previous evening, ignoring those evenings when the sky is not red
  - → the world itself is the sample generation algorithm
- Could take a long time if the sky is red only very rarely ...

# Answering Probabilistic Queries via Sampling (2): Likelihood Weighting

#### Idea:

 Avoid inefficiency of rejection sampling by generating only events that are consistent with the evidence e

#### **Basic algorithm:**

- Fix the values of the evidence variables  $\mathbf{E} = \mathbf{e}$
- Sample only remaining variables  $Z = X \cup Y$ 
  - → guarantees that each generated event is consistent with the evidence
- When collecting the event counts for the query variables X, weight each event by the probability that in an event like this, the evidence variables would actually have these values:

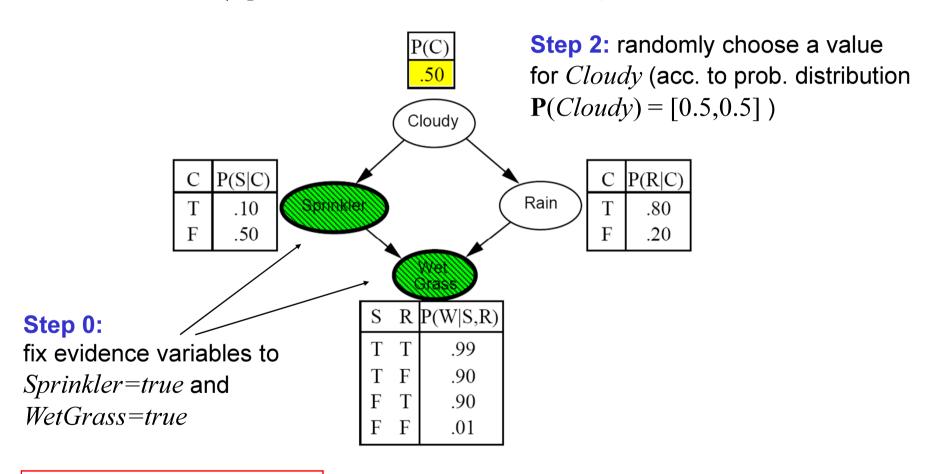
Weight = product of the conditional probabilities of the evidence variables, given their parents' values

**Intuition:** Events in which the actual evidence would be unlikely should be given less weight

# Answering Probabilistic Queries via Sampling (2): Likelihood Weighting

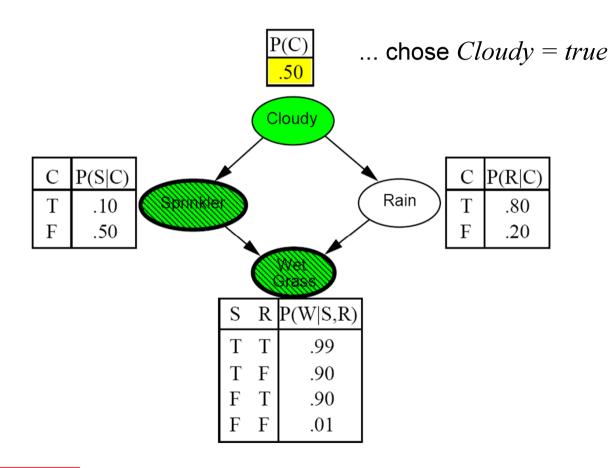
```
function LIKELIHOOD-WEIGHTING(X, e, bn, N) returns an estimate of P(X|e)
   local variables: W, a vector of weighted counts over X, initially zero
   for j = 1 to N do
        \mathbf{x}, w \leftarrow \text{Weighted-Sample}(bn)
        \mathbf{W}[x] \leftarrow \mathbf{W}[x] + w where x is the value of X in \mathbf{x}
   return Normalize(\mathbf{W}[X])
function WEIGHTED-SAMPLE(bn, e) returns an event and a weight
   \mathbf{x} \leftarrow an event with n elements; w \leftarrow 1
   for i = 1 to n do
        if X_i has a value x_i in e
              then w \leftarrow w \times P(X_i = x_i \mid parents(X_i))
              else x_i \leftarrow a random sample from P(X_i \mid parents(X_i))
   return x, w
```

**Query:** P(Rain | Sprinkler = true, WetGrass = true) = ?



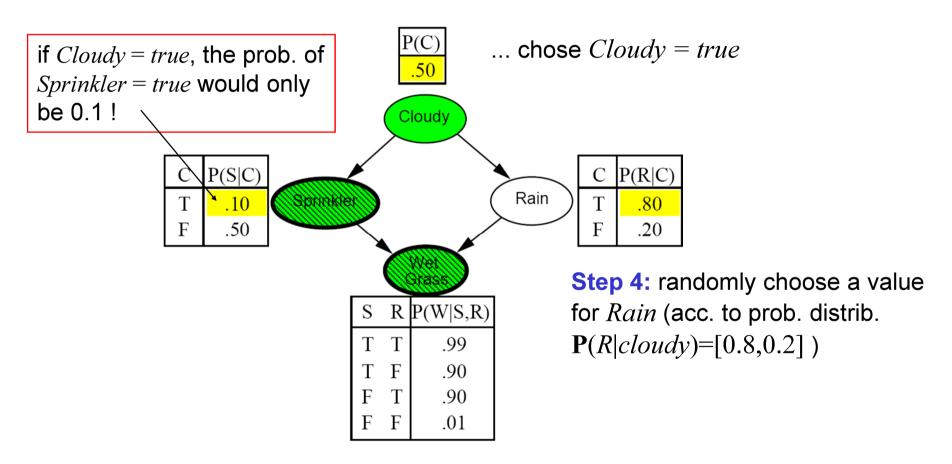
**Step 1:** set weight w = 1.0

**Query:** P(Rain|Sprinkler = true, WetGrass = true) = ?



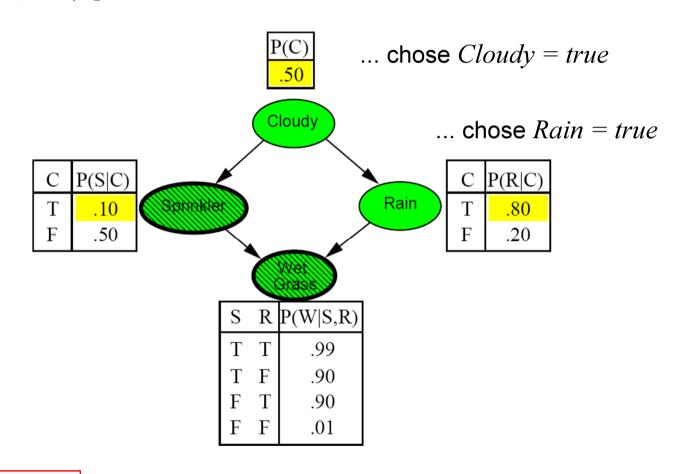
weight w = 1.0

**Query:**  $P(Rain \mid Sprinkler = true, WetGrass = true) = ?$ 



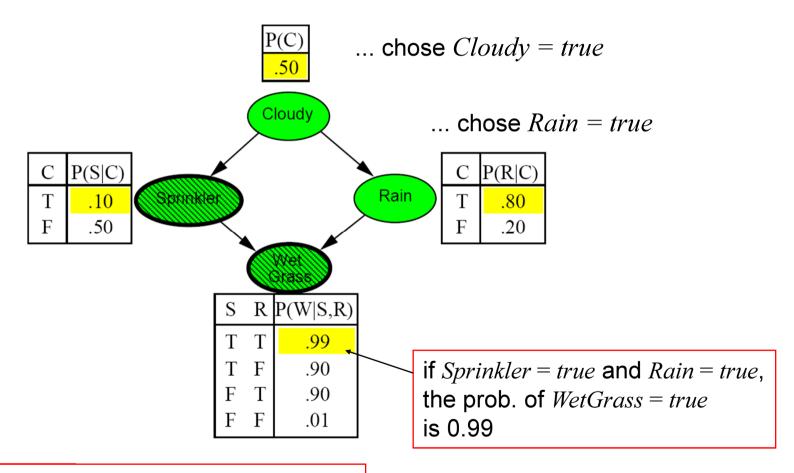
 $\rightarrow$  Step 3: set weight  $w = w \times 0.1 = 0.1$ 

**Query:** P(Rain|Sprinkler = true, WetGrass = true) = ?



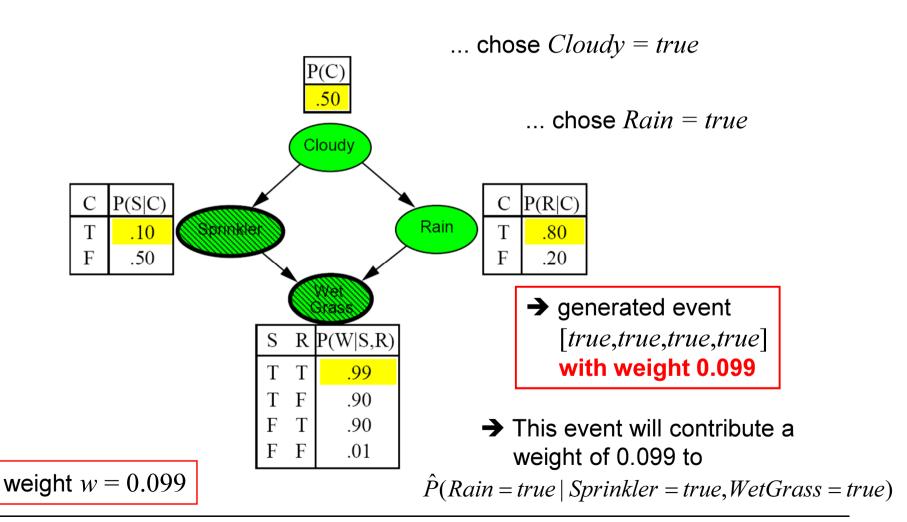
weight w = 0.1

**Query:** P(Rain | Sprinkler = true, WetGrass = true) = ?



→ Step 5: set weight  $w = w \times 0.99 = 0.099$ 

**Query:** P(Rain | Sprinkler = true, WetGrass = true) = ?



# Answering Probabilistic Queries via Sampling (2): Likelihood Weighting

#### **Advantage of Likelihood Weighting:**

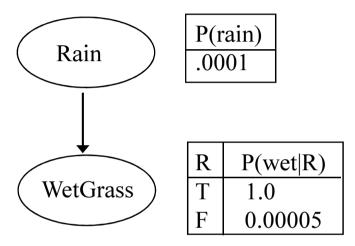
- Generates only samples consistent with given evidence
  - → not as wasteful as rejection sampling

#### **Problem with Likelihood Weighting:**

- Evidence guides the sampling decisions only if it appears among the parents/ancestors of a variable
- Evidence that is "downstream" influences result only through the weight
- Weights decay exponentially with number of downstream evidence variables
- → When a lot of the evidence in the net is "downstream", most of the generated samples will have extremely small weights (i.e., are highly non-representative) → need to sample for a long time until we happen to generate a high-weight sample that is typical of the evidence
- $\Rightarrow$  Essentially, we sample from a distribution that is closer to the prior P(Z) than the posterior  $P(Z \mid E=e)$  ...

# The Problem with Likelihood Weighting: An Example

Consider the following model of the climate in Death Valley:



... and the query P(R|wet) ("what is the probability that it rained or did not rain, given that the grass is wet")

→ LW would start by sampling variable Rain and might produce thousands of samples representing the less probable situation (Rain=false, Wet=true) (and correctly attach the low weight 0.00005 to each of them) before it happens to generate even *one* sample (Rain=true, Wet=true) (with weight 1.0) that is much more likely given the evidence ...

# Answering Probabilistic Queries via Sampling (3): Markov Chain Monte Carlo (MCMC) Sampling

#### **Basic Idea:**

Try to "fix" (improve) a (possibly non-representative) sample by repeaterily re-sampling some of the variables that were generated early in the process, taking into account the current values of all the other variables.

→ iterative process

#### Simplest variant: "Gibbs Sampling"

- Fix the values of the evidence variables  $\mathbf{E} = \mathbf{e}$
- Sample only remaining variables  $Z = X \cup Y$ 
  - → guarantees that each generated event is consistent with the evidence
- Then: iterate N times:
  - · for each  $Z_i$  in  $\mathbf{Z}$  do: \*)

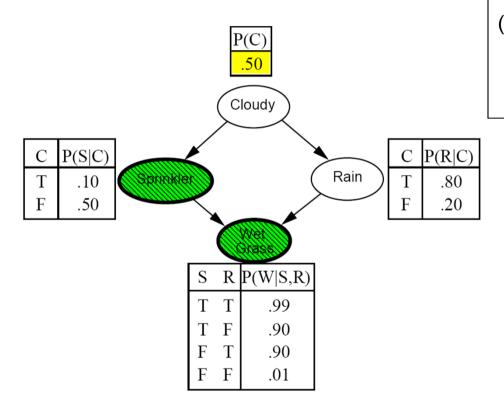
re-sample value of  $Z_i$ , assuming all other values in the net as given

- Return the final sample after N re-sampling iterations
  - \*) Variables can be resampled in an arbitrary (possibly random) order

# **Gibbs Sampling**

#### **Query:**

P(Rain | Sprinkler = true, WetGrass = true) = ?



Assume we sampled the following event in a first pass: [cloudy, sprinkler, ¬ rain, vec]

( rather unlikely given the network:

 $P(\underline{sprinkler} \mid cloudy) = 0.1,$  $P(\underline{wet} \mid \underline{sprinkler}, \neg rain) = 0.9$ 

→ would get weight 0.09 in likelihood v:eighting)

### Gibbs re-sampling step 1:

re-sample (say) *Rain*, given fixed value [cloudy, sprinkler, wet] (see next page):

→ might produce *Rain* = *true* 

#### Gibbs re-sampling step 2:

re-sample *Cloudy*, given fixed values [rain, <u>sprinkler</u>, <u>wet</u>]

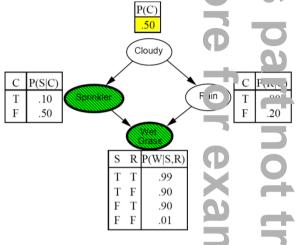
→ might produce *Cloudy* = *false* 

→ new event  $[\neg cloudy, \underline{sprinkler}, rain, \underline{wet}]$  is much more likely given the evidence (would get a weight of  $0.5 \times 0.99 = 0.495$  in likelihood weighting)

# How to re-sample a variable, given fixed values for all others?

**Example:** re-sample *Rain*, given fixed values [cloudy, sprinkler, wet]:

$$\begin{aligned} &\mathbf{P}(R \mid cl, spr, w) = \\ &= \frac{\mathbf{P}(R \land (cl, spr, w))}{P(cl, spr, w)} = \\ &= \frac{\mathbf{P}(R, cl, spr, w)}{\sum_{r^{\pm}} P(r^{\pm}, cl, spr, w)} = \\ &= \frac{P(cl)P(spr \mid cl)\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{\sum_{r^{\pm}} P(cl)P(spr \mid cl)P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ &= \frac{P(cl)P(spr \mid cl)\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{P(cl)P(spr \mid cl) \times \sum_{r^{\pm}} P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ &= \frac{\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{\sum_{r^{\pm}} P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ &= \alpha \times \mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R) \end{aligned}$$



To re-sample Rain:
compute P(R|cl)P(w|spr,R) for all possible values of Rain (i.e., true, false) and probabilistically sample a new value for Rain acc. to the resulting distribution

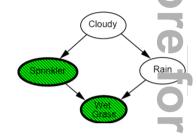
In our case: P(R|cl)P(w|spr,R) = [0.815,0.185]

- → choose value [true,false] probabilistically acc. to ratio 815 : 185
- → might now choose *Rain=true*

# How to re-sample a variable, given fixed values for all others?

**Example:** re-sample *Rain*, given fixed values [cloudy, sprinkler, wet]:

$$\begin{aligned} & \mathbf{P}(R \mid cl, spr, w) = \\ & = \frac{\mathbf{P}(R \land (cl, spr, w))}{P(cl, spr, w)} = \\ & = \frac{\mathbf{P}(R, cl, spr, w)}{\sum_{r^{\pm}} P(r^{\pm}, cl, spr, w)} = \\ & = \frac{P(cl)P(spr \mid cl)\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{\sum_{r^{\pm}} P(cl)P(spr \mid cl)P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ & = \frac{P(cl)P(spr \mid cl)\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{P(cl)P(spr \mid cl) \times \sum_{r^{\pm}} P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ & = \frac{\mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R)}{\sum_{r^{\pm}} P(r^{\pm} \mid cl)P(w \mid spr, r^{\pm})} = \\ & = \alpha \times \mathbf{P}(R \mid cl)\mathbf{P}(w \mid spr, R) \end{aligned}$$



### Insight 1:

- to compute new re-sampling distribution for some variable X, we need only CPTs that contain X;
- the computation depends only on the variables in *X*'s "Markov Blanket":
  - X, its parents, its children, & their parer  $\mathbb{R}$
- → efficiently computable!

#### **Insight 2:**

- (downstream) evidence influences re-sampling (e.g., new value for R is influenced by spr and w)
- → propagation of evidence information
- new distribution we sample from is closer to posterior distribution

# **Why Gibbs Sampling Works**

Intuitive Explanation: See Insight 2 on previous page

#### **Formal Explanation:**

- Gibbs Sampling is a special case of Markov Chain Monte Carlo (MCMC)
   Sampling
- Sequence of Gibbs sampling steps forms a *Markov Process* or *Markov Chain*\*), where each state corresponds to a complete assignment of values to all the variables, and the transition probability is  $P(V \mid all \text{ other } variables)$
- It can be proven (exercise  $\odot$ ) that the chain converges to a "stationary distribution" that is equivalent to the posterior distribution P(X|e) that we ideally wish to sample from
- → Procedure: to obtain a set of samples, first run the Gibbs Sampler for a while (to permit the chain to (nearly) converge to the true posterior distribution), then start collecting samples. Take these as directly representing the distribution P(X | E=e) [→ no weighting necessary as in Likelihood Weighting]

<sup>\*) [</sup>simplified:] A (first-order) Markov chain describes a discrete time process where (the probability of) the system's state at time t depends only on the previous state.

(More about this in "Machine Learning & Pattern Classification" in SS, "Probabilistic Models" in WS)

# Learning Bayesian Networks (just briefly; too complex for this class)

#### **Basic problem:**

- For many tasks, it is impossible to specify an appropriate BN "by hand".
  - experts not available or too expensive
  - required knowledge not available (problem not well enough understood)
  - complex networks need large numbers of parameters

#### → Goal:

- Agent should learn a good network from experience / observations
- Observations (= training examples): specific events observed by the agent (value assignments to random variables that occur at the same time)

### **Assumptions:**

- The random variables used to describe the agent's world are pre-defined by the system designer
- Training examples are "i.i.d." (independent from each other, and identically of distributed [i.e., produced by the same (hidden) process])

## **Learning Bayesian Networks**

#### **Learning Tasks:**

- 1. **Structure Learning:** given a sequence of observations (events) in terms of a set of random variables, infer both the (causal) structure of the domain (i.e., the optimal structure of the BN = factorisation of the joint distribution) and the parameters (conditional probability distributions)
- 2. **Parameter Learning:** given a fixed graph structure of a BN (e.g., provided by a domain expert), and a sequence of observations (events), learn the parameters of the model (i.e., all the conditional probabilities in the CPTs). Two scenarios:
  - A. Learning *from complete data* (fully observed events in each observation, the values of all random variables are known)
  - B. Learning *from incomplete data* (partially observed events the values of some of the random variables are not known)

Centeral Question: what is a "good", "correct", "optimal" network???

→ see next slide: "Maximum Likelihood Principle"

# Parameter Learning (1): Learning from Complete (Fully Observed) Data

#### Task:

• given the graph structure of a BN N (e.g., training observations E (e.g., [¬cloudy,sprinkler,rain,wet], [cloudy,¬sprinkler,¬rain,vet], ...), learn parameters for N (i.e., conditional probabilities for the CPTs) that "fit" the observations.

Sprinkle

#### Criterion: What is a "good" set of parameters?

- Intuitively: A network N is good if the full joint probability distribution it represents is the same as / similar to the empirical distribution implicit in the training examples
- In other words: A network N is good if the probability that it would generate events like the ones in the training set E is high
- Formally: The *likelihood* L(N:E) of a model (network) N relative to a training set E of events is the probability that N would generate E:

$$L(N:E) = P(E \mid N) = (because E are i.i.d.) = \prod_{e \in E} P(e \mid N)$$

- → Goal of parameter learning is to find the parameters that give the maximally likely model
- → Maximum Likelihood Principle

# Parameter Learning (1): Maximising the Likelihood for Complete (Fully Observed) Data

$$L(N:E) = P(E \mid N) = \prod_{e \in E} P(e \mid N) =$$

$$= \prod_{e \in E} \prod_{i} P(x_{i}[e] \mid Parents(X_{i})[e]) =$$

$$= \prod_{i} \left[ \prod_{e \in E} P(x_{i}[e] \mid Parents(X_{i})[e]) \right]$$

 $x_i[e]$  ... value of variable V in evidence example (observation) e

parameters we wish to estimate (CPTs) ...

#### **Consequences:**

- We can maximise the parameters for each random variable  $X_i$  separately
- For each random variable  $X_i$ , we need to find the parameters (conditional probabilities) that maximise the product of  $\mathbf{P}(X_i | Parents(X_i))$  in the given set of training observations
- It is easy to prove that for discrete variables, the estimates that maximise this are the *relative frequencies* as observed in the training data (how often each value of  $X_i$  co-occurs with each value combination of the parents of  $X_i$ )
- In other words: we can estimate all the parameters by counting in E
- → Parameter learning from fully observed data in Bayes Nets is fairly simple

# Parameter Learning (2): Learning from Incomplete (Partially Observed) Data

#### Task:

• given the graph structure of a BN N and a sequence of incomplete training observations E (e.g., [ $\neg$ cloudy,?,?,wet], [cloudy,?,?,wet], ...), learn parameters for N (i.e., conditional probabilities for the CPTs) that "fit" the observations.

#### **Motivation:**

- In many applications, only a subset of the variables used to model the world may be observable (e.g., in robot navigation and sensing)
- Measurements can be missing because of failure of measuring sensor
- → Learning from incomplete observations is a difficult optimisation problem (find parameters that maximise the likelihood relative to incomplete data)
- → Some general-purpose methods exist (Gradient Ascent search, Expectation Maximisation).)
- → Too complex for this class.

# **Structure Learning**

**Task:** Given only a sequence of training observations (events) E (e.g., [ $\neg$ cloudy,sprinkler,rain,wet], [cloudy,  $\neg$ sprinkler,  $\neg$ rain,wet]), infer both

- the (causal) structure of the domain (which variables depend on which others, or should be modelled as depending on which others), and
- the optimal set of parameters for this structure, relative to the training set E

# → Optimisation / search problem:

- Define a quality criterion to be optimised (e.g., the likelihood of a model relative to the training data)
- Search the space of possible graph structures and parameter assignments for a model that maximises this quality criterion
- → huge search space
- → difficult search problem
- → fairly effective search/learning algorithms exist

## **Summary**

**Bayesian Networks (BNs)** are a natural representation for (causally induced) conditional independence relations

BNs represent a full joint probability distribution in a compact way

**Exact inference** with BNs is possible, but costly

Efficient approximate reasoning with BNs: stochastic sampling algorithms

**Automatic learning** of BNs: difficult problem, but a variety of learning algorithms exist

BNs are extensively used in many practical modelling & prediction problems (computer vision, robotics, system diagnosis, ..., ...)

There are many **more types of probabilistic networks** for knowledge representation and inference (for both discrete and continuous domains), with a lot of scientific literature ....