

## Graphical Probabilistic Models

## Graphical Models Show Dependencies



## Consider More Complex Barking Story




## Bayes Network Allows Reconstruction of Probability Tables

- $P(p, d, b, t, r)=P(p \mid d, b, t, r) P(d \mid b, t, r) P(b \mid t, r) P(t \mid r) P(r)$ by the chain rule
- But by conditional independence in the graph,
$P(p, d, b, t, r)=P(p \mid d, b, t, r) P(d \mid b, \notin, r) P(b \mid t, r) P(t \mid r) P(r)$

$$
=P(p \mid d) P(d \mid b, r) P(b) P(t \mid r) P(r)
$$

. $P\left(x_{1}, \ldots, x_{n}\right)=\prod_{i=n}^{1} P\left(x_{i} \mid \operatorname{Par}\left(x_{i}\right)\right)$
where Par gives the parents of a node


## A Very Large Bayes Net <br> David Heckerman, Pathfinder/Intellipath, around 1990



## How (not) to do Inference

- So, we can reconstruct the probability of any particular scenario
- But, normally we want to know the probabilities of some nodes given that we have observed some others
- E.g., what is the probability of a burglar given that the police were called and the trash can was not knocked over?
- By abuse of notation, we write a variable $x$ to represent whatever its value is, and $x^{+}, x^{-}$if its value is known to be T or F (binary case)

$$
\begin{gathered}
P\left(b^{+} \mid p^{+}, t^{-}\right)=\frac{P\left(b^{+}, p^{+}, t^{-}\right)}{P\left(b^{+}, t^{-}\right)} \\
\frac{\sum_{d, r} P\left(p^{+}, d, b^{+}, t^{-}, r\right)}{\sum_{b, d, r} P\left(p^{+}, d, b, t^{-}, r\right)}
\end{gathered}
$$

- Downside: exponential number of terms in the "don't care" variables


## Rules and Probabilities

- Many have wanted to put a probability on assertions and on rules, and compute with likelihoods
- E.g., Mycin's certainty factor framework
$-A(p=.3) \& B(p=.7)==(p=.8)==>C(p=?)$
- Problems:
- How to combine uncertainties of preconditions and of rule
- How to combine evidence from multiple rules
- Theorem: There is NO such algebra that works when rules are considered independently.
- Need BN for a consistent model of probabilistic inference


## For Poly-Trees, simple propagation

- Suppose we observe B
- Reduce c.p. table of its children (D) to the $\mathrm{B}=\mathrm{T}$ or $\mathrm{B}=\mathrm{F}$ cases
- Propagate
- Suppose we observe $P$
- Use Bayes' Rule to update D
- Propagate
- Suppose we observe D
- Do both of the above
- Because everything is singly connected, one pass updates all probabilities
- Much more complex if the network is multiply connected! Propagation doesn't work.



## Exact Solution of BN's

(non-poly-trees)

- $P(a, b, c, d, e)=P(a) P(b \mid a) P(c \mid a) P(d \mid b, c) P(e \mid c)$
- What is the probability of a specific state, say $A=T, B=F$, $\mathrm{C}=\mathrm{T}, \mathrm{D}=\mathrm{T}, \mathrm{E}=\mathrm{F}$ ?
$P\left(a^{+}, b^{-}, c^{+}, d^{+}, d^{-}\right)=P\left(a^{+}\right) P\left(b^{-} \mid a^{+}\right) P\left(c^{+} \mid a^{+}\right) P\left(d^{+} \mid b^{-}, a^{+}\right) P\left(e^{-} \mid c^{+}\right)$

- What is the probability that $\mathrm{E}=\mathrm{t}$ given $\mathrm{B}=\mathrm{t}$ ?
$P\left(e^{+} \mid b^{+}\right)=P\left(e^{+}, b^{+}\right) / P\left(b^{+}\right)$
- Consider the term $P\left(e^{+}, b^{+}\right)$
$P\left(e^{+}, b^{+}\right)=\sum_{a c d} P\left(a, b^{+}, c, d, e^{+}\right)$
$=\sum_{a, c, d} P(a) P\left(b^{+} \mid a\right) P(c \mid a) P\left(D \mid b^{+}, c\right) P\left(e^{+} \mid c\right)$
$=\sum_{c} P\left(e^{+} \mid c\right)\left(\sum_{a} P(a) P(c \mid a) P\left(b^{+} \mid a\right)\right)\left(\sum_{d} P\left(d, b^{+} \mid c\right)\right)$
- 12 instead of 32 multiplications (even in this small example)

Alas, optimal
factoring is NP-hard

## Other Exact Methods



- Join-tree: Merge variables into (small!) sets of variables to make graph into a poly-tree. Most commonly-used; aka Clustering, Junction-tree, Potential)
- Cutset-conditioning: Instantiate a (small!) set of variables, then solve each residual problem, and add solutions weighted by probabilities of the instantiated variables having those values
-...
- All these methods are essentially equivalent; with some time-space tradeoffs.


## We don't want to model high-arity dependence



- $p\left(c \mid a_{1}, a_{2}, \ldots\right)$
- too many probabilities needed in conditional probability table
- Can we simplify?
- Noisy or
- noisy and
- noisy max/min
- ?


## Simplifying Conditional Probability Tables via Noisy-OR

- Do we know any structure in the way that $\operatorname{Par}(x)$ "cause" $x$ ?
- If each destroyer can sink the ship with probability $P\left(s \mid d_{i}\right)$, what is the probability that the ship will sink if it's attacked by both?
$1-P\left(s \mid d_{1}, d_{2}\right)=\left(1-P\left(s \mid d_{1}\right)\right)\left(1-P\left(s \mid d_{2}\right)\right)(1-l)$
- For $|\operatorname{Par}(x)|=n$, this requires $O(n)$ parameters, not $O\left(k^{n}\right)$

$d_{1}$

$s$

$d_{2}$


## Approximate Inference in BN's

- Direct Sampling
- Rejection Sampling
- Likelihood Weighting
- Markov chain Monte Carlo
- Gibbs and other similar sampling methods


## Direct Sampling

function Prior-Sample(bn) returns an event sampled from bn
inputs: bn, a Bayes net specifying the joint distribution $\mathbf{P}\left(\mathrm{X}_{1}, \ldots \mathrm{X}_{\mathrm{n}}\right)$
$x:=$ an event with $n$ elements
for $i=I$ to $n$ do
$\mathrm{x}_{\mathrm{i}}:=\mathrm{a}$ random sample from $\mathrm{P}\left(\mathrm{X}_{\mathrm{i}} \mid \operatorname{Par}\left(\mathrm{X}_{\mathrm{i}}\right)\right)$
return $x$
$\lim _{n \rightarrow \infty} \frac{N_{P S}\left(x_{1}, \ldots, x_{n}\right)}{N}=P\left(x_{1}, \ldots, x_{n}\right) \quad P\left(x_{1}, \ldots, x_{m}\right) \approx \frac{N_{P S}\left(x_{1}, \ldots, x_{m}\right)}{N}$

- From a large number of samples, we can estimate all joint probabilities
- The probability of an event is the fraction of all complete events generated by PS that match the partially specified event - hence we can compute all conditionals, etc.


## Likelihood Weighting

- In trying to compute $P(X \mid e)$, where $e$ is the evidence (variables with known, observed values),
- Sample only the variables other than those in e
- Weight each sample by how well it predicts e

```
\(\begin{aligned} S_{W S}(\boldsymbol{z}, \boldsymbol{e}) w(\boldsymbol{z}, \boldsymbol{e}) & =\prod_{i=1}^{l} P\left(z_{i} \mid \operatorname{Par}\left(Z_{i}\right)\right) \prod_{i=1}^{m} P\left(e_{i} \mid \operatorname{Par}\left(E_{i}\right)\right) \\ & =P(\boldsymbol{z}, \boldsymbol{e})\end{aligned}\)
```


## Likelihood Weighting <br> ```SWS(\boldsymbol{z},\boldsymbol{e})w(\boldsymbol{z},\boldsymbol{e})```

inputs: bn, a Bayes ne
$X$, the query variable
e, evidence specified as an event
N , the number of samples to be generated
local:W, a vector of weighted counts over values of X , initially 0
for $\mathrm{j}=1$ to N do
$\mathbf{y}, \mathrm{w}:=$ WeightedSample(bn)
if $\mathbf{y}$ is consistent with e then
$W[v]:=W[v]+w$ where $v$ is the value of $X$ in $y$
return Normalize(W[X])
function Weighted-Sample(bn,e) returns an event and a weigh
$x:=$ an event with $n$ elements; $w:=1$
for $i=1$ to $n$ do
if $X_{i}$ has a value $x_{i}$ in $e$
then $w:=w * P\left(X_{i}=x_{i} \mid \operatorname{Par}\left(X_{i}\right)\right)$
else $x_{i}:=$ a random sample from $P\left(X_{i} \mid \operatorname{Par}\left(X_{i}\right)\right)$
return $\mathrm{x}, \mathrm{w}$

## Markov chain Monte Carlo

function $\operatorname{MCMC}(\mathrm{X}, \mathrm{e}, \mathrm{bn}, \mathrm{N})$ returns an estimate of $\mathrm{P}(\mathrm{X} \mid \mathrm{e})$ local: $\mathrm{K}[\mathrm{X}]$, a vector of counts over values of X , initially 0
$Z$, the non-evidence variables in bn (includes $X$ )
$\mathbf{x}$, the current state of the network, initially a copy of e
initialize $\mathbf{x}$ with random values for the vars in $\mathbf{Z}$

for $\mathrm{j}=\mathrm{I}$ to N do
for each Zi in Z do
sample the value of $\mathrm{Zi}_{\mathrm{i}}$ in x from $\mathrm{P}\left(\mathrm{Zi}_{\mathrm{i}} \mid \mathrm{mb}\left(\mathrm{Z}_{\mathrm{i}}\right)\right)$, given the values of $\mathrm{mb}\left(\mathrm{Zi}_{\mathrm{i}}\right)$ in $x$
$K[v]:=K[v]+I$ where $v$ is the value of $X$ in $\mathbf{x}$
return Normalize( $K[X]$ )

- Wander incrementally from the last state sampled, instead of re-generating a completely new sample
- For every unobserved variable, choose a new value according to its probability given the values of vars in it Markov blanket (remember, it's independent of all other vars)
- After each change, tally the sample for its value of $X$; this will only change sometimes
- Problem: "narrow passages"


## Learning Probabilistic Models: A Simple Example

- Surprise Candy Corp. makes two flavors of candy: cherry and lime
- Both flavors come in the same opaque wrapper
- Candy is sold in large bags, which have one of the following distributions of flavors, but are visually indistinguishable:
- $h_{1}: 100 \%$ cherry
- $h_{2}: 75 \%$ cherry, $25 \%$ lime
- $h_{3}: 50 \%$ cherry, $50 \%$ lime
- $h_{4}: 25 \%$ cherry, $75 \%$ lime
- $h_{5}: 100 \%$ lime
- Relative prevalence of these types of bags is (.1, .2, .4, .2,.I)
- As we eat our way through a bag of candy, predict the flavor of the next piece; actually a probability distribution.


## Bayesian Learning about a Fixed Simple Set of Hypotheses

- Calculate the probability of each hypothesis given the data $P\left(h_{i} \mid \mathbf{d}\right)=\alpha P\left(\mathbf{d} \mid h_{i}\right) P\left(h_{i}\right)$
- To predict the probability distribution over an unknown quantity, $X$,
$P(X \mid \mathbf{d})=\sum_{i} P\left(X \mid \mathbf{d}, h_{i}\right) P\left(h_{i} \mid \mathbf{d}\right)=\sum_{i} P\left(X \mid h_{i}\right) P\left(h_{i} \mid \mathbf{d}\right)$
- If the observations $\mathbf{d}$ are independent, then $P\left(\mathbf{d} \mid h_{i}\right)=\prod_{j} P\left(d_{j} \mid h_{i}\right)$
- E.g., suppose the first 10 candies we taste are all lime $P\left(\mathbf{d} \mid h_{3}\right)=0.5^{10} \approx 0.001$


## Learning Hypotheses and Predicting from Them

- (a) probabilities of $\boldsymbol{h}_{\boldsymbol{i}}$ after $\boldsymbol{k}$ lime candies; (b) prob. of next lime

- MAP prediction: predict just from most probable hypothesis - After 3 limes, $\boldsymbol{h}_{5}$ is most probable, hence we predict lime -Even though, by (b), it's only 80\% probable


## Observations

- Bayesian approach asks for prior probabilities on hypotheses!
- Natural way to encode bias against complex hypotheses: make their prior probability very low
- Choosing $h_{\mathrm{MAP}}$ to maximize $P\left(h_{i} \mid \mathbf{d}\right)=\alpha P\left(\mathbf{d} \mid h_{i}\right) P\left(h_{i}\right)$
- is equivalent to minimizing $-\log P\left(\mathbf{d} \mid h_{i}\right)-\log P\left(h_{i}\right)$
- but from our earlier discussion of entropy as a measure of information, these two terms are
- \# of bits needed to describe the data given hypothesis
- \# bits needed to specify the hypothesis
- Thus, MAP learning chooses the hypothesis that maximizes compression of the data; Minimum Description Length principle
- Assuming uniform priors on hypotheses makes MAP yield $h_{\mathrm{ML}}$, the maximum likelihood hypothesis, which maximizes
$P\left(h_{i} \mid \mathbf{d}\right)=\alpha P\left(\mathbf{d} \mid h_{i}\right)$


## How to Build a Bayes Network

- Human expertise
- E.g., like building the Acute Renal Failure program, Pathfinder, Alarm, ...
- Human expertise to determine structure, data to determine parameters
- Point parameter estimation
- Smoothing
- Useful distributions:
- Common: Beta (binomial), Dirichlet (multinomial)
- Any of the "exponential family", e.g., normal, Poisson, Gamma, etc.
- Automated methods to discover structure and parameters
- "Best" model is the one that predicts the highest probability for the data actually observed.


## Learning Structure

- In general, we are trying to determine not only parameters for a known structure but in fact which structure is best
- or the probability of each structure, so we can average over them to make a prediction


## Structure Learning

- Recall that a Bayes Network is fully specified by
- a DAG $G$ that gives the (in)dependencies among variables
- the collection of parameters $\theta$ that define the conditional probability tables for each of the $P\left(x_{i} \mid \operatorname{Par}\left(x_{i}\right)\right)$
. Then $P(G \mid D)=\frac{P(D \mid G) P(G)}{P(D)} \propto P(D \mid G) P(G)$
- We define the Bayesian score as $\log P(D \mid G)+\log (P(G))$
$P(D \mid G)=\int_{\theta_{G}} P\left(D \mid \theta_{G}, G\right) P\left(\theta_{g} \mid G\right) P(G) d \theta_{G}$
- But
-First term: usual marginal likelihood calculation
- Second term: parameter priors
-Third term: "penalty" for complexity of graph
- Define a search problem over all possible graphs \& parameters


## Searching for Models

- How many possible DAGs are there for $n$ variables?
$-<3^{n^{2}}=$ all possible directed graphs on $n$ vars
- Not all are DAGs
- To get a closer estimate, imagine that we order the variables so that the parents of each var come before it in the ordering. Then
- there are $n$ !possible ordering, and
-the $i$-th var can have any of the previous vars as a parent

$$
n!\prod_{i=1}^{n} 2^{i-1}=n!\cdot 2^{\sum_{i=1}^{n}(i-1)}=O\left(n!\cdot 2^{n^{2}}\right)
$$

- If we can choose a particular ordering, say based on prior knowledge, then we need consider "merely" $O\left(2^{n}\right)$ models
. If we restrict $|\operatorname{Par}(\mathrm{X})|$ to no more than $k$, consider $\leq \sum_{i=1}^{n}\binom{n}{k}$ models
- this is actually practical
- Search actions: add, delete, reverse an arc
- Hill-climb on $P(D \mid G)$ or on $P(G \mid D)$
- All "usual" tricks in search: simulated annealing, random restart, ...


## Caution about Hidden Variables (Confounders)

- Suppose you are given a dataset containing data on patients' smoking, diet, exercise, chest pain, fatigue, and shortness of breath
- You would probably learn a model like the one below left
- If you can hypothesize a "hidden" variable (not in the data set), e.g., heart disease, the learned network might be much simpler, such as the one below right
- But, there are potentially infinitely many such variables


