

## Review

### \* Inference in BNs

evidence node  $E$

query node  $Q$

How to compute  $P(Q|E)$ ?

### \* Polytrees

- singly connected networks
- polynomial time inference

### \* Loopy BNs

Exact inference: node clustering

Approximate inference: stochastic simulation  
[covered later]

## Learning

\* BN = DAG + CPTs not always available from experts

How to learn from examples?

### \* Issues

- structure (DAG) - known or unknown?
- evidence: complete data vs. "incomplete" data  
↳ partial instantiation of nodes in BN
- optimization:  
combinatorial vs. continuous  
(e.g. learning DAG) (e.g. learning CPTs)
- algorithms: non-iterative vs. iterative  
(loop over data many times)
- solution: local vs. global optimum.

- \* Maximum Likelihood (ML) estimation
  - simplest form of learning in ~~BNs~~ BNs
  - choose ("estimate") the model (DAG + CPTs) to maximize  $\underbrace{P(\text{observed data} | \text{model})}_{\text{"likelihood"}}$

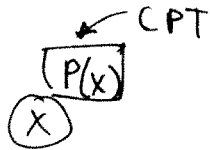
Ex: biased coin

$$X \in \{\text{heads}, \text{tails}\}$$

$$P(X = \text{heads}) = p$$

$$P(X = \text{tails}) = 1 - p$$

Trivial BN



- \* How to estimate  $p$  from observed samples (results of ~~T~~ T coin tosses)?

- \* IID assumptions

Samples are independently, identically distribute to  $P(X)$ .

→  $\{X^{(1)}, X^{(2)}, \dots, X^{(T)}\}$  T samples

- \* Probability of IID data:

$$\begin{aligned} P(\text{data}) &= P(X = x^{(1)}) P(X = x^{(2)}) \dots P(X = x^{(T)}) \\ &= \prod_{t=1}^T P(X = x^{(t)}) \end{aligned}$$

- \* Log-probability  $\mathcal{L}$

$$\mathcal{L} = \log(P(\text{data})) = \log \prod_{t=1}^T P(X = x^{(t)}) = \sum_{t=1}^T \log P(X = x^{(t)})$$

↑  
"log-likelihood"

Let  $N_H = \text{count}(X=\text{heads})$

Let  $N_T = \text{count}(X=\text{tails})$

Clearly:  $N_H + N_T = T \leftarrow \text{total samples}$

In terms of counts:

$$\mathcal{L}(p) = N_H \log(p) + N_T \log(1-p)$$

\* Maximum Likelihood estimation

$$\frac{\partial \mathcal{L}}{\partial p} = \frac{N_H}{p} + \frac{N_T}{1-p} \cdot (-1) = 0$$

$$N_H(1-p) - N_T(p) = 0$$

$$N_H - p(N_H + N_T) = 0$$

$$p = \frac{N_H}{N_H + N_T} = \frac{N_H}{T}$$

intuitively, maximum likelihood estimate of  $p = P(X=\text{heads})$  is relative frequency in observed coin ~~tosses~~ tosses.

Discrete BNs with "completed data"

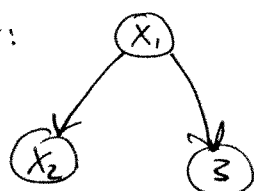
\* Given: fixed DAG over discrete nodes  $\{X_1, X_2, \dots, X_n\}$

\* CPTs enumerate  $P(X_i = x_i \mid \text{pa}(x_i) = \pi)$  as look up tables  
 $\uparrow$  parents of  $X_i$        $\uparrow$  parent configuration

\* Data is  $T$  complete  
 instantiations of nodes in BN

$$\{x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}\}^T$$

Ex:



$$X_i \in \{0, 1\}$$

$$n = 3$$

Data

$t^{\text{th}}$ sample	$X_1$	$X_2$	$X_3$
1	0	0	0
2	1	1	0
3	1	1	0
$\vdots$			
$T$	0	1	3

\* Each  $n$ -tuple of values is called an "example".

Goal: learn from examples;

estimate CPTs  $P(X_i = x \mid \text{pa}_i = \pi)$

that maximize probability of data set  
likelihood

\* I.I.D. Assumption

samples are independently, identically distributed according to  $P(X_1, X_2, \dots, X_n)$ .

\* Probability of I.I.D. set:

$$\cancel{P(\text{data})} P(\text{data}) = \prod_{t=1}^T P(X_1 = x_1^{(t)}, X_2 = x_2^{(t)}, \dots, X_n = x_n^{(t)})$$

↖ probability of  $t^{\text{th}}$  example

\* Work out  $t^{\text{th}}$  term:

$$\begin{aligned} P(X_1 = x_1^{(t)}, \dots, X_n = x_n^{(t)}) &= P(X_1 = x_1^{(t)}) P(X_2 = x_2^{(t)} \mid P(X_1 = x_1^{(t)})) \times \dots \quad \text{product rule} \\ &= \prod_{i=1}^n P(X_i = x_i^{(t)} \mid X_1 = x_1^{(t)}, \dots, X_{i-1} = x_{i-1}^{(t)}) \\ &= \prod_{i=1}^n P(X_i = x_i \mid \text{pa}(x_i) = \text{pa}_i^{(t)}) \quad \text{conditional dependence} \end{aligned}$$

\* Log-likelihood  $\mathcal{L}$

$$\mathcal{L} = \log P(\text{data})$$

$$= \log \prod_{t=1}^T P(X_1^{(t)}, X_2^{(t)}, \dots, X_n^{(t)})$$

$$= \log \prod_{t=1}^T \prod_{i=1}^n P(X_i^{(t)} \mid \text{pa}(X_i) = \text{pa}_i^{(t)})$$

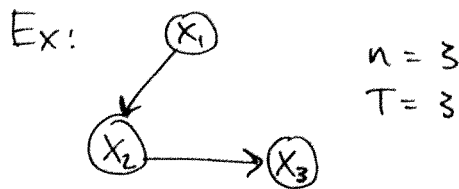
$$= \sum_{t=1}^T \sum_{i=1}^n \log P(X_i = x_i^{(t)} \mid \text{pa}(X_i) = \text{pa}_i^{(t)})$$

$$= \sum_{i=1}^n \sum_{t=1}^T \log P(X_i = x_i^{(t)} \mid \text{pa}(X_i) = \text{pa}_i^{(t)}) \quad \text{swap order of sums}$$

\* Let  $\text{count}(X_i = x, \text{pa}_i = \pi)$  denote examples for which  $X_i = x$  and  $\text{pa}_i(\pi) = \pi$ .

Data set

$t$	$X_1$	$X_2$	$X_3$	$\dots$	$X_n$
1	0	0	1		1
2	1	1	0		0
3	0	1	0		



$$\text{count}(X_2 = 0 \mid X_2 = 1) = 2$$

$$\text{count}(X_3 = 1 \mid X_2 = 0) = 1$$

\* Log-likelihood:

$$\mathcal{L} = \sum_{i=1}^n \sum_{\substack{x \\ \text{values of } X}} \sum_{\substack{\pi \\ \text{parent configuration}}} \text{count}(X_i = x, \text{pa}_i = \pi) \log P(X_i = x \mid \text{pa}_i = \pi)$$

\* ML Estimation

How to choose  $P(X_i = x \mid \text{pa}_i = \pi)$  to maximize  $\mathcal{L}(\text{data})$ ?

\* ML Solution (without proof):

$$P_{ML}(X_i = x \mid \text{pa}_i = \pi) = \frac{\text{count}(X_i = x, \text{pa}_i = \pi)}{\sum_{x'} \text{count}(X_i = x', \text{pa}_i = \pi)}$$

Equivalently:

$$P_{ML}(X_i = x \mid \text{pa}_i = \pi) = \frac{\text{count}(X_i = x, \text{pa}_i = \pi)}{\text{count}(\text{pa}_i = \pi)}$$

\* Properties of MLE

- Asymptotically correct:  $P_{ML}(X_1, X_2, \dots, X_n) \rightarrow P(X_1, X_2, \dots, X_n)$  as  $T \rightarrow \infty$
- Problematic for sparse data:

$$P_{ML}(X_i = x \mid \text{pa}_i = \pi) = 0 \text{ if } \text{count}(X_i = x \mid \text{pa}_i = \pi) = 0$$

$$P_{ML}(X_i = x \mid \text{pa}_i = \pi) \text{ undefined if } \text{count}(\text{pa}_i = \pi) = 0$$

- Other useful notation:

Indicator function:

$$I(x, x') = \begin{cases} 0 & \text{if } x \neq x' \\ 1 & \text{if } x = x' \end{cases}$$

$$\text{count}(pa_i = \pi) = \sum_{t=1}^T I(pa_i^{(t)}, \pi)$$

$$\text{count}(X_i = x, pa_i = \pi) = \sum_{t=1}^T I(pa_i^{(t)}, \pi) I(X_i^{(t)}, x)$$