## Machine Learning 10-601

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University
October 4, 2012

Today:

- Graphical models
- Bayes Nets:
- Inference
- Learning

Readings:
Required:

- Bishop chapter 8


## Bayesian Networks Definition

A Bayes network represents the joint probability distribution over a collection of random variables

A Bayes network is a directed acyclic graph and a set of conditional probability distributions (CPD's)

- Each node denotes a random variable
- Edges denote dependencies
- For each node $X_{i}$ its CPD defines $P\left(X_{i} \mid P a\left(X_{i}\right)\right)$
- The joint distribution over all variables is defined to be

$$
P\left(X_{1} \ldots X_{n}\right)=\prod_{i} P\left(X_{i} \mid P a\left(X_{i}\right)\right)
$$

$\mathrm{Pa}(\mathrm{X})=$ immediate parents of $X$ in the graph


## What You Should Know

- Bayes nets are convenient representation for encoding dependencies / conditional independence
- BN = Graph plus parameters of CPD's
- Defines joint distribution over variables
- Can calculate everything else from that
- Though inference may be intractable
- Reading conditional independence relations from the graph
- Each node is cond indep of non-descendents, given only its parents

See Bayes Net applet: http://www.cs.cmu.edu/~javabayes/Home/applet.html

## Inference in Bayes Nets

- In general, intractable (NP-complete)
- For certain cases, tractable
- Assigning probability to fully observed set of variables
- Or if just one variable unobserved
- Or for singly connected graphs (ie., no undirected loops)
- Belief propagation
- For multiply connected graphs
- Junction tree
- Sometimes use Monte Carlo methods
- Generate many samples according to the Bayes Net distribution, then count up the results
- Variational methods for tractable approximate solutions


## Example

- Bird flu and Allegies both cause Sinus problems
- Sinus problems cause Headaches and runny Nose



## Prob. of joint assignment: easy

- Suppose we are interested in joint assignment <F=f,A=a,S=s,H=h,N=n>
 What is $P(f, a, s, h, n) ?$

Prob. of marginals: not so easy


Generating a sample from joint distribution: easy

How can we generate random samples drawn according to $\mathrm{P}(\mathrm{F}, \mathrm{A}, \mathrm{S}, \mathrm{H}, \mathrm{N})$ ?


## let's use $p(a, b)$ as shorthand for $p(A=a, B=b)$

Generating a sample from joint distribution: easy

Note we can estimate marginals

like $P(N=n)$ by generating many samples
from joint distribution, then count the fraction of samples for which $\mathrm{N}=\mathrm{n}$

Similarly, for anything else we care about $P(F=1 \mid H=1, N=0)$
$\rightarrow$ weak but general method for estimating any probability term...

## Prob. of marginals: not so easy

But sometimes the structure of the network allows us to be clever $\rightarrow$ avoid exponential work
eg., chain


## Inference in Bayes Nets

- In general, intractable (NP-complete)
- For certain cases, tractable
- Assigning probability to fully observed set of variables
- Or if just one variable unobserved
- Or for singly connected graphs (ie., no undirected loops)
- Variable elimination
- Belief propagation
- For multiply connected graphs
- Junction tree
- Sometimes use Monte Carlo methods
- Generate many samples according to the Bayes Net distribution, then count up the results
- Variational methods for tractable approximate solutions


## Learning of Bayes Nets

- Four categories of learning problems
- Graph structure may be known/unknown
- Variable values may be fully observed / partly unobserved
- Easy case: learn parameters for graph structure is known, and data is fully observed
- Interesting case: graph known, data partly known
- Gruesome case: graph structure unknown, data partly unobserved


## Learning CPTs from Fully Observed Data

- Example: Consider learning the parameter
$\theta_{s \mid i j} \equiv P(S=1 \mid F=i, A=j)$
- MLE (Max Likelihood Estimate) is

$\theta_{s \mid i j}=\frac{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j, s_{k}=1\right)}{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j\right)}$
- Remember why?

MLE estimate of $\theta_{s \mid i j}$ from fully observed data

- Maximum likelihood estimate
$\theta \leftarrow \arg \max _{\theta} \log P($ data $\mid \theta)$
- Our case:


$$
\begin{aligned}
& P(\text { data } \mid \theta)=\prod_{k=1}^{K} P\left(f_{k}, a_{k}, s_{k}, h_{k}, n_{k}\right) \\
& P(\text { data| } \mid \theta)=\prod_{k=1}^{K} P\left(f_{k}\right) P\left(a_{k}\right) P\left(s_{k} \mid f_{k} a_{k}\right) P\left(h_{k} \mid s_{k}\right) P\left(n_{k} \mid s_{k}\right) \\
& \log P(\text { data| } \mid \theta)=\sum_{k=1}^{K} \log P\left(f_{k}\right)+\log P\left(a_{k}\right)+\log P\left(s_{k} \mid f_{k} a_{k}\right)+\log P\left(h_{k} \mid s_{k}\right)+\log P\left(n_{k} \mid s_{k}\right) \\
& \frac{\partial \log P(\text { data| } \mid \theta)}{\partial \theta_{s \mid j}}=\sum_{k=1}^{K} \frac{\partial \log P\left(s_{k} \mid f_{k} a_{k}\right)}{\partial \theta_{s \mid i j}} \\
& \theta_{s \mid i j}=\frac{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j, s_{k}=1\right)}{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j\right)}
\end{aligned}
$$

## Estimate $\theta$ from partly observed data

- What if FAHN observed, but not S?
- Can't calculate MLE

$$
\theta \leftarrow \arg \max _{\theta} \log \prod_{k} P\left(f_{k}, a_{k}, s_{k}, h_{k}, n_{k} \mid \theta\right)
$$



- Let X be all observed variable values (over all examples)
- Let $Z$ be all unobserved variable values
- Can't calculate MLE:

$$
\theta \leftarrow \arg \max _{\theta} \log P(X, Z \mid \theta)
$$

- WHAT TO DO?


## Estimate $\theta$ from partly observed data

- What if FAHN observed, but not S?
- Can't calculate MLE

$$
\theta \leftarrow \arg \max _{\theta} \log \prod_{k} P\left(f_{k}, a_{k}, s_{k}, h_{k}, n_{k} \mid \theta\right)
$$



- Let $X$ be all observed variable values (over all examples)
- Let $Z$ be all unobserved variable values
- Can't calculate MLE:

$$
\theta \leftarrow \arg \max _{\theta} \log P(X, Z \mid \theta)
$$

- EM seeks* to estimate:

$$
\begin{aligned}
\theta \leftarrow \arg \max _{\theta} & E_{Z \mid X, \theta}[\log P(X, Z \mid \theta)] \\
& \quad \text { EM guaranteed to find local maximum }
\end{aligned}
$$

- EM seeks estimate:

$$
\theta \leftarrow \arg \max _{\theta} E_{Z \mid X, \theta}[\log P(X, Z \mid \theta)]
$$



- here, observed $\mathrm{X}=\{\mathrm{F}, \mathrm{A}, \mathrm{H}, \mathrm{N}\}$, unobserved $\mathrm{Z}=\{\mathrm{S}\}$
$\log P(X, Z \mid \theta)=\sum_{k=1}^{K} \log P\left(f_{k}\right)+\log P\left(a_{k}\right)+\log P\left(s_{k} \mid f_{k} a_{k}\right)+\log P\left(h_{k} \mid s_{k}\right)+\log P\left(n_{k} \mid s_{k}\right)$
$E_{P(Z \mid X, \theta)} \log P(X, Z \mid \theta)=\sum_{k=1}^{K} \sum_{i=0}^{1} P\left(s_{k}=i \mid f_{k}, a_{k}, h_{k}, n_{k}\right)$ $\left[\log P\left(f_{k}\right)+\log P\left(a_{k}\right)+\log P\left(s_{k} \mid f_{k} a_{k}\right)+\log P\left(h_{k} \mid s_{k}\right)+\log P\left(n_{k} \mid s_{k}\right)\right]$


## EM Algorithm

EM is a general procedure for learning from partly observed data
Given observed variables X , unobserved $\mathrm{Z}(\mathrm{X}=\{\mathrm{F}, \mathrm{A}, \mathrm{H}, \mathrm{N}\}, \mathrm{Z}=\{\mathrm{S}\}) \vee$
Define $Q\left(\theta^{\prime} \mid \theta\right)=E_{P(Z \mid X, \theta)}\left[\log P\left(X, Z \mid \theta^{\prime}\right)\right]$


Iterate until convergence:

- E Step: Use $X$ and current $\theta$ to calculate $P(Z \mid X, \theta)$
- M Step: Replace current $\theta$ by

$$
\theta \leftarrow \arg \max _{\theta^{\prime}} Q\left(\theta^{\prime} \mid \theta\right)
$$

Guaranteed to find local maximum.
Each iteration increases $E_{P(Z \mid X, \theta)}\left[\log P\left(X, Z \mid \theta^{\prime}\right)\right]$

## E Step: Use X, $\theta$, to Calculate $\mathrm{P}(\mathrm{Z} \mid \mathrm{X}, \theta)$

observed $\mathrm{X}=\{\mathrm{F}, \mathrm{A}, \mathrm{H}, \mathrm{N}\}$, unobserved $Z=\{S\}$


- How? Bayes net inference problem.

$$
\begin{aligned}
& P\left(S_{k}=1 \mid f_{k} a_{k} h_{k} n_{k}, \theta\right)= \\
& P\left(S_{k}=1 \mid f_{k} a_{k} h_{k} n_{k}, \theta\right)=\frac{P\left(S_{k}=1, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)}{P\left(S_{k}=1, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)+P\left(S_{k}=0, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)}
\end{aligned}
$$

EM and estimating $\theta_{s \mid i j}$
observed $X=\{F, A, H, N\}$, unobserved $Z=\{S\}$


E step: Calculate $P\left(Z_{k} \mid X_{k} ; \theta\right)$ for each training example, $k$

$$
P\left(S_{k}=1 \mid f_{k} a_{k} h_{k} n_{k}, \theta\right)=\underset{P\left(z\left(x_{i} \boldsymbol{\theta}\right)\right.}{E}\left[s_{k}\right]=\frac{P\left(S_{k}=1, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)}{P\left(S_{k}=1, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)+P\left(S_{k}=0, f_{k} a_{k} h_{k} n_{k} \mid \theta\right)}
$$

M step: update all relevant parameters. For example:

$$
\theta_{s \mid i j} \leftarrow \frac{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j\right) E\left[s_{k}\right]}{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j\right)}
$$

Recall MLE was: $\theta_{s \mid i j}=\frac{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j, s_{k}=1\right)}{\sum_{k=1}^{K} \delta\left(f_{k}=i, a_{k}=j\right)}$

## EM and estimating $\theta$

More generally,


Given observed set $X$, unobserved set $Z$ of boolean values
E step: Calculate for each training example, $k$
the expected value of each unobserved variable

M step:
Calculate estimates similar to MLE, but replacing each count by its expected count

$$
\delta(Y=1) \rightarrow E_{Z \mid X, \theta}[Y] \quad \delta(Y=0) \rightarrow\left(1-E_{Z \mid X, \theta}[Y]\right)
$$



E step: Calculate for each training example, k the expected value of each unobserved variable


## EM and estimating $\theta$

Given observed set X , unobserved set Y of boolean values
E step: Calculate for each training example, k the expected value of each unobserved variable Y
$E_{P\left(Y \mid X_{1} \ldots X_{N}\right)}[y(k)]=P\left(y(k)=1 \mid x_{1}(k), \ldots x_{N}(k) ; \theta\right)=\frac{P(y(k)=1) \prod_{i} P\left(x_{i}(k) \mid y(k)=1\right)}{\sum_{j=0}^{1} P(y(k)=j) \prod_{i} P\left(x_{i}(k) \mid y(k)=j\right)}$
M step: Calculate estimates similar to MLE, but replacing each count by its expected count

## EM and estimating $\theta$

Given observed set X , unobserved set Y of boolean values
E step: Calculate for each training example, $k$ the expected value of each unobserved variable $Y$
$E_{P\left(Y \mid X_{1} \ldots X_{N}\right)}[y(k)]=P\left(y(k)=1 \mid x_{1}(k), \ldots x_{N}(k) ; \theta\right)=\frac{P(y(k)=1) \prod_{i} P\left(x_{i}(k) \mid y(k)=1\right)}{\sum_{j=0}^{1} P(y(k)=j) \prod_{i} P\left(x_{i}(k) \mid y(k)=j\right)}$
M step: Calculate estimates similar to MLE, but replacing each count by its expected count

$$
\theta_{i j \mid m}=\hat{P}\left(X_{i}=j \mid Y=m\right)=\frac{\sum_{k} P\left(y(k)=m \mid x_{1}(k) \ldots x_{N}(k)\right) \delta\left(x_{i}(k)=j\right)}{\sum_{k} P\left(y(k)=m \mid x_{1}(k) \ldots x_{N}(k)\right)}
$$

MLE would be: $\hat{P}\left(X_{i}=j \mid Y=m\right)=\frac{\sum_{k} \delta\left((y(k)=m) \wedge\left(x_{i}(k)=j\right)\right)}{\sum_{k} \delta(y(k)=m)}$

- Inputs: Collections $\mathcal{D}^{l}$ of labeled documents and $\mathcal{D}^{u}$ of unlabeled documents.
- Build an initial naive Bayes classifier, $\hat{\theta}$, from the labeled documents, $\mathcal{D}^{l}$, only. Use maximum a posteriori parameter estimation to find $\hat{\theta}=\arg \max _{\theta} \mathrm{P}(\mathcal{D} \mid \theta) \mathrm{P}(\theta)$ (see Equations 5 and 6).
- Loop while classifier parameters improve, as measured by the change in $l_{c}(\theta \mid \mathcal{D} ; \mathbf{z})$ (the complete $\log$ probability of the labeled and unlabeled data
- (E-step) Use the current classifier, $\hat{\theta}$, to estimate component membership of each unlabeled document, i.e., the probability that each mixture component (and class) generated each document, $\mathrm{P}\left(c_{j} \mid d_{i} ; \hat{\theta}\right)$ (see Equation 7).
- (M-step) Re-estimate the classifier, $\hat{\boldsymbol{\theta}}$, given the estimated component membership of each document. Use maximum a posteriori parameter estimation to find $\hat{\boldsymbol{\theta}}=$ $\arg \max _{\theta} \mathrm{P}(\mathcal{D} \mid \theta) \mathrm{P}(\theta)$ (see Equations 5 and 6).
- Output: A classifier, $\hat{\theta}$, that takes an unlabeled document and predicts a class label.

From [Nigam et al., 2000]


## Experimental Evaluation

- Newsgroup postings
- 20 newsgroups, 1000/group
- Web page classification
- student, faculty, course, project
- 4199 web pages
- Reuters newswire articles
- 12,902 articles
- 90 topics categories


## 20 Newsgroups



Table 3. Lists of the words most predictive of the course class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common course-related words appear. The symbol $D$ indicates an arbitrary digit.

| Iteration 0 |  | Iteration 1 | Iteration 2 |
| :---: | :---: | :---: | :---: |
| intelligence $D D$ artificial understanding $D D \mathrm{w}$ dist identical rus arrange games dartmouth natural cognitive logic proving prolog knowledge human representation field | word $w$ ranked by $P(w \mid Y=$ course $) / P$ (w\|Y $\neq$ course) <br> Using one labeled example per class | $D D$ $D$ lecture cc $D^{\star}$ $D D: D D$ handout due problem set tay $D D$ am yurttas homework kfoury sec postscript exam solution assaf | $D$ $D D$ lecture cc $D D: D D$ due $D^{\star}$ homework assignment handout set hw exam problem $D D a m$ postscript solution quiz chapter ascii |



## Usupervised clustering

## Just extreme case for EM with zero labeled examples...

## Clustering

- Given set of data points, group them
- Unsupervised learning
- Which patients are similar? (or which earthquakes, customers, faces, web pages, ...)


## Mixture Distributions

Model joint $P\left(X_{1} \ldots X_{n}\right)$ as mixture of multiple distributions.
Use discrete-valued random var $Z$ to indicate which distribution is being use for each random draw
So $P\left(X_{1} \ldots X_{n}\right)=\sum_{i} P(Z=i) P\left(X_{1} \ldots X_{n} \mid Z\right)$

Mixture of Gaussians:


- Assume each data point $X=<X 1, \ldots X n>$ is generated by one of several Gaussians, as follows:

1. randomly choose Gaussian $i$, according to $P(Z=i)$
2. randomly generate a data point $<x 1, x 2$.. xn> according to $N\left(\mu_{i}, \Sigma_{i}\right)$

## EM for Mixture of Gaussian Clustering

Let's simplify to make this easier:

1. assume $X=<X_{1} \ldots X_{n}>$, and the $X_{i}$ are conditionally independent given $Z$.

$$
P(X \mid Z=j)=\prod_{i} N\left(X_{i} \mid \mu_{j i}, \sigma_{j i}\right)
$$

2. assume only 2 clusters (values of $Z$ ), and $\forall i, j, \sigma_{j i}=\sigma$

$$
P(\mathrm{X})=\sum_{j=1}^{2} P(Z=j \mid \pi) \prod_{i} N\left(x_{i} \mid \mu_{j i}, \sigma\right)
$$



Observed: $X=<X_{1} \ldots X_{n}>$ Unobserved: $Z$

Given observed variables $X$, unobserved $Z$
Define $Q\left(\theta^{\prime} \mid \theta\right)=E_{Z \mid X, \theta}\left[\log P\left(X, Z \mid \theta^{\prime}\right)\right]$
where $\theta=\left\langle\pi, \mu_{j i}\right\rangle$


Iterate until convergence:

- E Step: Calculate $P(Z(n) \mid X(n), \theta)$ for each example $X(n)$.

Use this to construct $Q\left(\theta^{\prime} \mid \theta\right)$

- M Step: Replace current $\theta$ by

$$
\theta \leftarrow \arg \max _{\theta^{\prime}} Q\left(\theta^{\prime} \mid \theta\right)
$$

## EM - E Step

Calculate $P(Z(n) \mid X(n), \theta)$ for each observed example $X(n)$ $X(n)=<x_{1}(n), x_{2}(n), \ldots x_{T}(n)>$.

$P(z(n)=k \mid x(n), \theta)=\frac{P(x(n) \mid z(n)=k, \theta) \quad P(z(n)=k \mid \theta)}{\sum_{j=0}^{1} p(x(n) \mid z(n)=j, \theta) P(z(n)=j \mid \theta)}$
$P(z(n)=k \mid x(n), \theta)=\frac{\left[\prod_{i} P\left(x_{i}(n) \mid z(n)=k, \theta\right)\right] P(z(n)=k \mid \theta)}{\sum_{j=0}^{1} \Pi_{i} P\left(x_{i}(n) \mid z(n)=j, \theta\right) P(z(n)=j \mid \theta)}$

$$
P(z(n)=k \mid x(n), \theta)=\frac{\left[\Pi_{i} N\left(x_{i}(n) \mid \mu_{k, i}, \sigma\right)\right]\left(\pi^{k}(1-\pi)^{(1-k)}\right)}{\sum_{j=0}^{1}\left[\Pi_{i} N\left(x_{i}(n) \mid \mu_{j, i}, \sigma\right)\right]\left(\pi^{j}(1-\pi)^{(1-j))}\right)}
$$



| $\begin{aligned} & \text { Now consider update for } \mu_{\mathrm{ji}} \mathrm{EM}-\mathrm{M} \text { Step } \\ & Q\left(\theta^{\prime} \mid \theta\right)=E_{Z \mid X, \theta}\left[\log P\left(X, Z \mid \theta^{\prime}\right)\right]=E\left[\log P\left(X \mid Z, \theta^{\prime}\right)+\log P\left(Z \mid \theta^{\prime}\right)\right] \\ & \mu_{\mathrm{ji}}^{\prime} \text { has no influence } \\ & \mu_{j i} \leftarrow \arg \max _{\mu_{j i}^{\prime}} E_{Z \mid X, \theta}\left[\log P\left(X \mid Z, \theta^{\prime}\right)\right] \\ & \cdots \ldots \\ & \cdots \\ & \mu_{j i} \leftarrow \frac{\sum_{n=1}^{N} P(z(n)=j \mid x(n), \theta) x_{i}(n)}{\sum_{n=1}^{N} P(z(n)=j \mid x(n), \theta)} \\ & \begin{array}{l} \text { Compare above to } \quad \mu_{j i} \leftarrow \frac{\sum_{n=1}^{N} \delta(z(n)=j) x_{i}(n)}{\sum_{n=1}^{N} \delta(z(n)=j)} \\ \text { MLE if } Z \text { were } \\ \text { observable: } \end{array} \end{aligned}$ |
| :---: |
|  |  |
|  |  |
|  |  |

## EM - putting it together

Given observed variables $X$, unobserved $Z$
Define $Q\left(\theta^{\prime} \mid \theta\right)=E_{Z \mid X, \theta}\left[\log P\left(X, Z \mid \theta^{\prime}\right)\right]$ where $\theta=\left\langle\pi, \mu_{j i}\right\rangle$


Iterate until convergence:

- E Step: For each observed example X(n), calculate $P(Z(n) \mid X(n), \theta)$

$$
P(z(n)=k \mid x(n), \theta)=\frac{\left[\Pi_{i} N\left(x_{i}(n) \mid \mu_{k, i}, \sigma\right)\right]\left(\pi^{k}(1-\pi)^{(1-k)}\right)}{\sum_{j=0}^{1}\left[\Pi_{i} N\left(x_{i}(n) \mid \mu_{j, i}, \sigma\right)\right]\left(\pi^{j}(1-\pi)^{(1-j))}\right)}
$$

- M Step: Update $\theta \leftarrow \arg \max _{\theta^{\prime}} Q\left(\theta^{\prime} \mid \theta\right)$


## Mixture of Gaussians applet

Go to: http://www.socr.ucla.edu/htmls/SOCR Charts.html then go to Go to "Line Charts" $\rightarrow$ SOCR EM Mixture Chart - try it with 2 Gaussian mixture components ("kernels")

- try it with 4


## What you should know about EM

- For learning from partly unobserved data
- MLE of $\theta=\quad \arg \max _{\theta} \log P($ data $\mid \theta)$
- EM estimate: $\theta=\arg \max _{\theta} E_{Z \mid X, \theta}[\log P(X, Z \mid \theta)]$ Where X is observed part of data, Z is unobserved
- EM for training Bayes networks
- Can also develop MAP version of EM
- Can also derive your own EM algorithm for your own problem
- write out expression for $E_{Z \mid X, \theta}[\log P(X, Z \mid \theta)]$
- E step: for each training example $\mathrm{X}^{\kappa}$, calculate $\mathrm{P}\left(\mathrm{Z}^{k} \mid \mathrm{X}^{k}, \theta\right)$
- M step: chose new $\theta$ to maximize $E_{Z \mid X, \theta}[\log P(X, Z \mid \theta)]$


## Learning Bayes Net Structure

## How can we learn Bayes Net graph structure?

In general case, open problem

- can require lots of data (else high risk of overfitting)
- can use Bayesian methods to constrain search

One key result:

- Chow-Liu algorithm: finds "best" tree-structured network
- What's best?
- suppose $P(\mathbf{X})$ is true distribution, $T(\mathbf{X})$ is our tree-structured network, where $\mathbf{X}=\left\langle\mathrm{X}_{1}, \ldots \mathrm{X}_{\mathrm{n}}>\right.$
- Chow-Liu minimizes Kullback-Leibler divergence:

$$
K L(P(\mathbf{X}) \| T(\mathbf{X})) \equiv \sum_{k} P(\mathbf{X}=k) \log \frac{P(\mathbf{X}=k)}{T(\mathbf{X}=k)}
$$

## Chow-Liu Algorithm

Key result: To minimize $K L(P \| T)$, it suffices to find the tree network T that maximizes the sum of mutual informations over its edges

Mutual information for an edge between variable $A$ and $B$ :

$$
I(A, B)=\sum_{a} \sum_{b} P(a, b) \log \frac{P(a, b)}{P(a) P(b)}
$$

This works because for tree networks with nodes $\mathbf{X} \equiv\left\langle X_{1} \ldots X_{n}\right\rangle$

$$
\begin{aligned}
K L(P(\mathbf{X}) \| T(\mathbf{X})) & \equiv \sum_{k} P(\mathbf{X}=k) \log \frac{P(\mathbf{X}=k)}{T(\mathbf{X}=k)} \\
& =-\sum_{i} I\left(X_{i}, P a\left(X_{i}\right)\right)+\sum_{i} H\left(X_{i}\right)-H\left(X_{1} \ldots X_{n}\right)
\end{aligned}
$$

## Chow-Liu Algorithm

1. for each pair of vars $A, B$, use data to estimate $P(A, B)$, $P(A), P(B)$
2. for each pair of vars A.B calculate mutual information

$$
I(A, B)=\sum_{a} \sum_{b} P(a, b) \log \frac{P(a, b)}{P(a) P(b)}
$$

3. calculate the maximum spanning tree over the set of variables, using edge weights $I(A, B)$
(given N vars, this costs only $\mathrm{O}\left(\mathrm{N}^{2}\right)$ time)
4. add arrows to edges to form a directed-acyclic graph
5. learn the CPD's for this graph

## Chow-Liu algorithm example Greedy Algorithm to find Max-Spanning Tree


[courtesy A. Singh, C. Guestrin]


## Bayes Nets - What You Should Know

- Representation
- Bayes nets represent joint distribution as a DAG + Conditional Distributions
- D-separation lets us decode conditional independence assumptions
- Inference
- NP-hard in general
- For some graphs, closed form inference is feasible
- Approximate methods too, e.g., Monte Carlo methods, ...
- Learning
- Easy for known graph, fully observed data (MLE's, MAP est.)
- EM for partly observed data, known graph
- Learning graph structure: Chow-Liu for tree-structured networks
- Hardest when graph unknown, data incompletely observed

