Discussion0413

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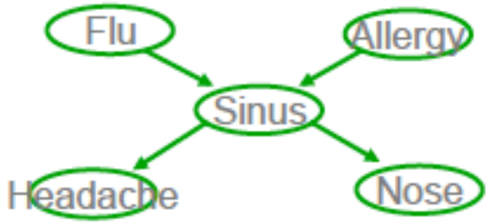
MLE estimate of $\theta_{s|ij}$ from fully observed data



- Maximum likelihood estimate

$$\theta \leftarrow \arg\max_{\theta} \log P(data|\theta)$$

- Our case:

$$P(data|\theta) = \prod_{k=1}^{K} P(f_k, a_k, s_k, h_k, n_k)$$

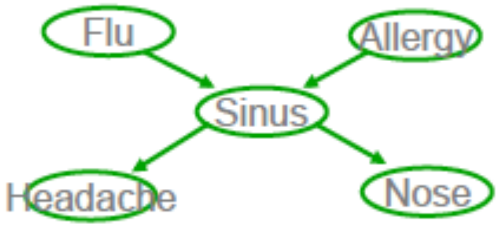
$$P(data|\theta) = \prod_{k=1}^{K} P(f_k)P(a_k)P(s_k|f_k a_k)P(h_k|s_k)P(n_k|s_k)$$

$$\log P(data|\theta) = \sum_{k=1}^{K} \log P(f_k) + \log P(a_k) + \log P(s_k|f_k a_k) + \log P(h_k|s_k) + \log P(n_k|s_k)$$

$$\frac{\partial \log P(data|\theta)}{\partial \theta_{s|ij}} = \sum_{k=1}^{K} \frac{\partial \log P(s_k|f_k a_k)}{\partial \theta_{s|ij}}$$

$$\theta_{s|ij} = \frac{\sum_{k=1}^{K} \delta(f_k = i, a_k = j, s_k = 1)}{\sum_{k=1}^{K} \delta(f_k = i, a_k = j)}$$

Estimate θ from partly observed data



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

$$\theta \leftarrow \arg\max_\theta \log \prod_k P(f_k, a_k, s_k, h_k, n_k|\theta)$$

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

$$\theta \leftarrow \arg\max_\theta \log P(X, Z|\theta)$$

- EM seeks* to estimate:

$$\theta \leftarrow \arg\max_\theta E_{Z|X,\theta}[\log P(X, Z|\theta)]$$

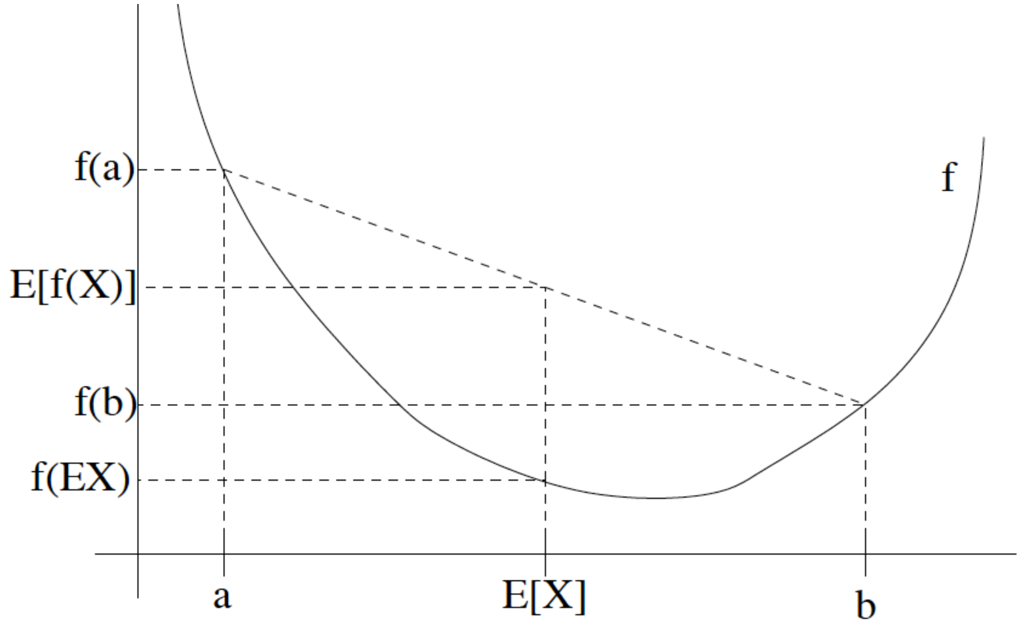
* EM guaranteed to find local maximum

Jensen's Inequality

Theorem. Let f be a convex function, and let X be a random variable. Then:

$$\mathrm{E}[f(X)] \geq f(\mathrm{E}X).$$

Moreover, if f is strictly convex, then $\mathrm{E}[f(X)] = f(\mathrm{E}X)$ holds true if and only if $X = \mathrm{E}[X]$ with probability 1 (i.e., if X is a constant).



Concavity of log function

$$
\begin{aligned}
\sum_i \log p(x^{(i)};\theta) &= \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)};\theta) \\
&= \sum_i \log \sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})} \\
&\geq \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})}
\end{aligned}
$$

EM algorithm

Initialize θ

Repeat

(E-step) For each i, set

$$Q_i(z^{(i)}) := p(z^{(i)}|x^{(i)};\theta).$$

(M-step) Set

$$\theta := \arg\max_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})}.$$

Until convergence

Why EM guaranteed to find local maximum

- We will prove $l(\theta^{t+1}) \geq l(\theta^{t})$

$$
\begin{aligned}
\ell(\theta^{(t+1)}) &\geq \sum_i \sum_{z^{(i)}} Q_i^{(t)}(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta^{(t+1)})}{Q_i^{(t)}(z^{(i)})} \\
&\geq \sum_i \sum_{z^{(i)}} Q_i^{(t)}(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta^{(t)})}{Q_i^{(t)}(z^{(i)})} \\
&= \ell(\theta^{(t)})
\end{aligned}
$$

Why EM not suitable for continuous Z

$$
\begin{aligned}
Q_i(z^{(i)}) &= \frac{p(x^{(i)}, z^{(i)}; \theta)}{\sum_z p(x^{(i)}, z; \theta)} \\
&= \frac{p(x^{(i)}, z^{(i)}; \theta)}{p(x^{(i)}; \theta)} \\
&= p(z^{(i)} | x^{(i)}; \theta)
\end{aligned}
$$

Mixture Distributions

Model joint $P(X_1 \ldots X_n)$ as mixture of multiple distributions.

Use discrete-valued random var Z to indicate which distribution is being use for each random draw

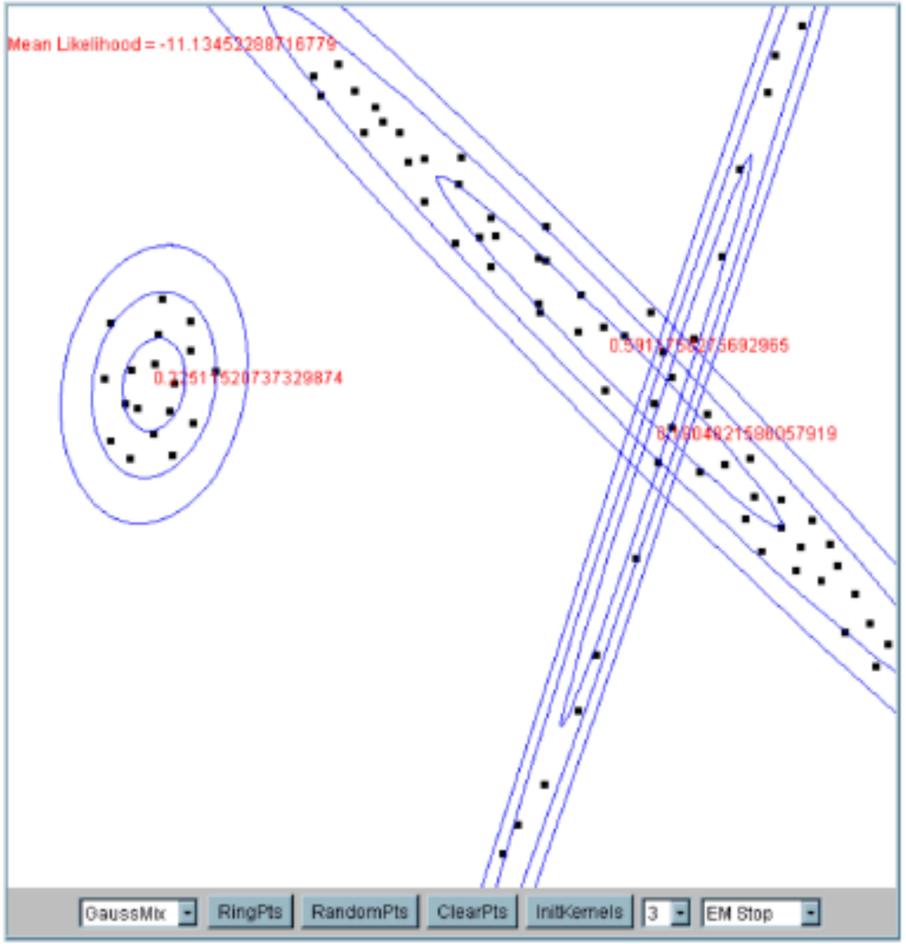
So $$P(X_1 \ldots X_n) = \sum_i P(Z=i) \;\; P(X_1 \ldots X_n|Z)$$

Mixture of *Gaussians*:

- Assume each data point X=<X1, … Xn> 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 <x1,x2 .. xn> according to $N(\mu_i, \Sigma_i)$

Mixture of Gaussians



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.

$$P(X|Z=j)=\prod_i N(X_i|\mu_{ji},\sigma_{ji})$$

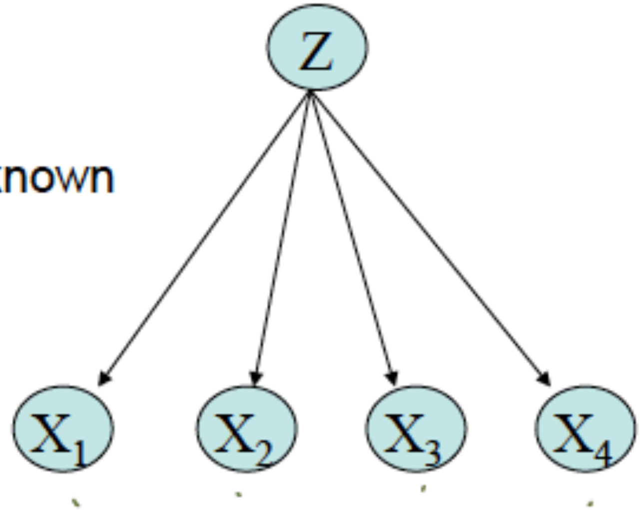
2. assume only 2 clusters (values of Z), and $\forall i,j,\sigma_{ji}=\sigma$

$$P(\mathbf{X})=\sum_{j=1}^{2} P(Z=j|\pi)\prod_i N(x_i|\mu_{ji},\sigma)$$

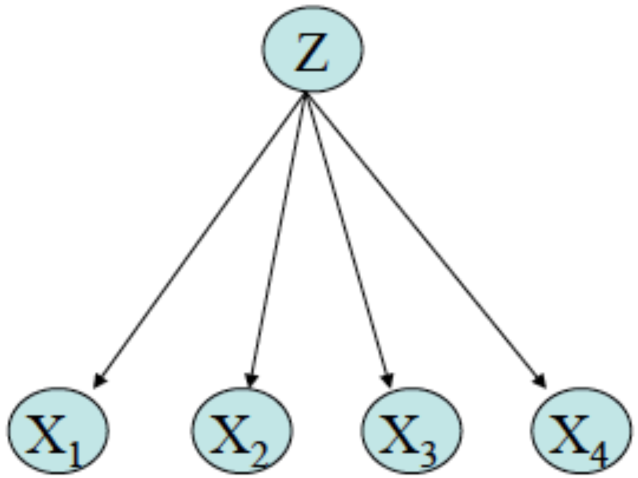
3. Assume σ known, $\pi_1 \ldots \pi_K, \mu_{1i} \ldots \mu_{Ki}$ unknown

Observed: $X=<X_1 \ldots X_n>$

Unobserved: Z



EM



Given observed variables X, unobserved Z

Define $Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')]$

where $\theta = \langle \pi, \mu_{ji} \rangle$

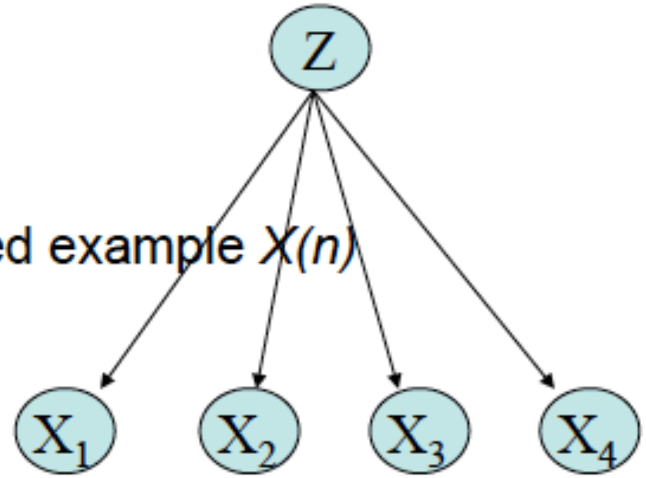
Iterate until convergence:

• E Step: Calculate $P(Z(n)|X(n),\theta)$ for each example $X(n)$. Use this to construct $Q(\theta'|\theta)$

• M Step: Replace current θ by

$$\theta \leftarrow \arg\max_{\theta'} Q(\theta'|\theta)$$

EM – E Step



Calculate $P(Z(n)|X(n),\theta)$ for each observed example $X(n)$

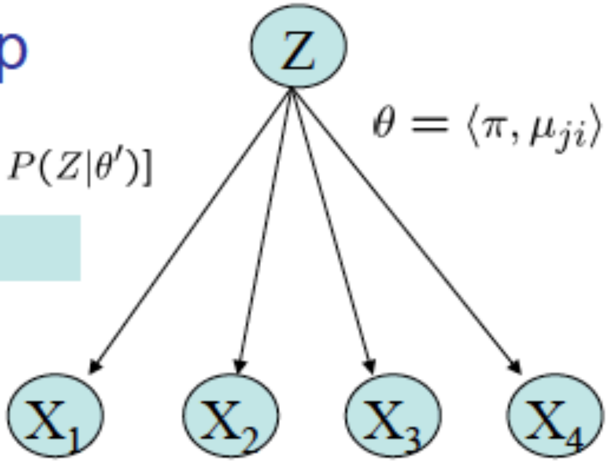
$X(n)=<x_1(n), x_2(n), \ldots x_T(n)>$.

$$P(z(n)=k|x(n),\theta) = \frac{P(x(n)|z(n)=k,\theta) \quad P(z(n)=k|\theta)}{\sum_{j=0}^{1} p(x(n)|z(n)=j,\theta) \; P(z(n)=j|\theta)}$$

$$P(z(n)=k|x(n),\theta) = \frac{\prod_i P(x_i(n)|z(n)=k,\theta)] \quad P(z(n)=k|\theta)}{\sum_{j=0}^{1} \prod_i P(x_i(n)|z(n)=j,\theta) \; P(z(n)=j|\theta)}$$

$$\boxed{P(z(n)=k|x(n),\theta) = \frac{\prod_i N(x_i(n)|\mu_{k,i},\sigma)] \quad (\pi^k(1-\pi)^{(1-k)})}{\sum_{j=0}^{1}[\prod_i N(x_i(n)|\mu_{j,i},\sigma)] \quad (\pi^j(1-\pi)^{(1-j)}))}}$$

EM – M Step



$\theta = \langle \pi, \mu_{ji} \rangle$

First consider update for π

$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

π' has no influence

$$\pi \leftarrow \arg\max_{\pi'} E_{Z|X,\theta}[\log P(Z|\pi')]$$

z=1 for nth example

$$E_{Z|X,\theta}\left[\log P(Z|\pi')\right] = E_{Z|X,\theta}\left[\log\left(\pi'^{\sum_n z(n)}(1-\pi')^{\sum_n (1-z(n))}\right)\right]$$

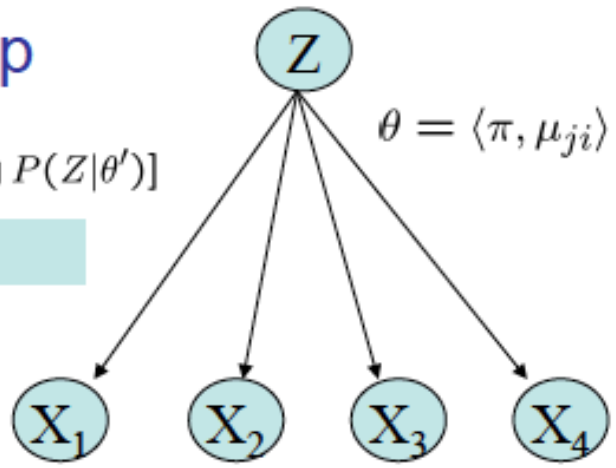
$$= E_{Z|X,\theta}\left[\left(\sum_n z(n)\right)\log \pi' + \left(\sum_n (1-z(n))\right)\log(1-\pi')\right]$$

$$= \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\log \pi' + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\log(1-\pi')$$

$$\frac{\partial E_{Z|X,\theta}[\log P(Z|\pi')]}{\partial \pi'} = \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\frac{1}{\pi'} + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\frac{(-1)}{1-\pi'}$$

$$\boxed{\pi \leftarrow \frac{\sum_{n=1}^N E[z(n)]}{\left(\sum_{n=1}^N E[z(n)]\right) + \left(\sum_{n=1}^N (1 - E[z(n)])\right)} = \frac{1}{N}\sum_{n=1}^N E[z(n)]}$$

EM – M Step



$\theta = \langle \pi, \mu_{ji} \rangle$

First consider update for π

$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X, Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

π' has no influence

$$\pi \leftarrow \arg\max_{\pi'} E_{Z|X,\theta}[\log P(Z|\pi')]$$

z=1 for nth example

$$E_{Z|X,\theta}\left[\log P(Z|\pi')\right] = E_{Z|X,\theta}\left[\log\left(\pi'^{\sum_n z(n)}(1-\pi')^{\sum_n(1-z(n))}\right)\right]$$

$$= E_{Z|X,\theta}\left[\left(\sum_n z(n)\right)\log \pi' + \left(\sum_n (1-z(n))\right)\log(1-\pi')\right]$$

$$= \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\log \pi' + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\log(1-\pi')$$

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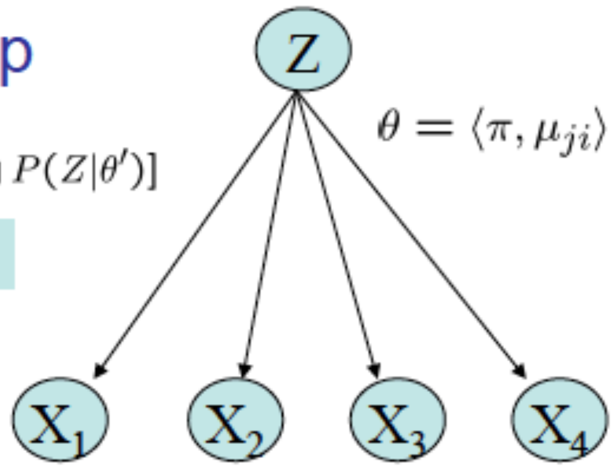
EM – M Step

Now consider update for μ_{ji}

$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X, Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

μ_{ji}' has no influence



$$\mu_{ji} \leftarrow \arg\max_{\mu'_{ji}} E_{Z|X,\theta}[\log P(X|Z,\theta')]$$

…

…

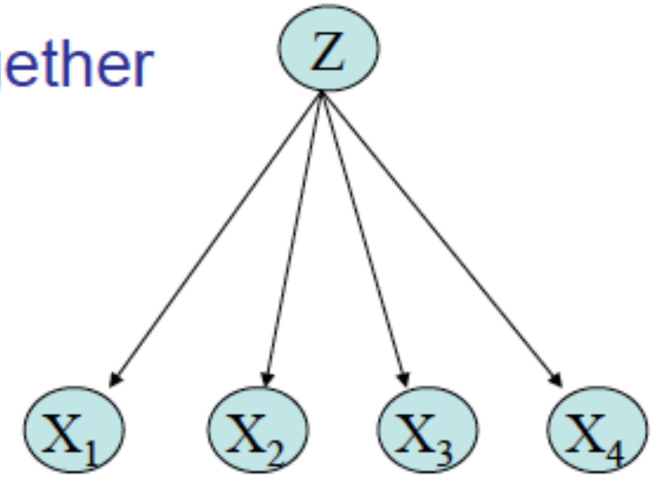
…

$$\boxed{\mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} P(z(n) = j|x(n),\theta) \quad x_i(n)}{\sum_{n=1}^{N} P(z(n) = j|x(n),\theta)}}$$

Compare above to MLE if Z were observable:

$$\mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} \delta(z(n) = j) \quad x_i(n)}{\sum_{n=1}^{N} \delta(z(n) = j)}$$

EM – putting it together



Given observed variables X, unobserved Z

Define $Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')]$

where $\theta = \langle \pi, \mu_{ji} \rangle$

Iterate until convergence:

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

$$P(z(n)=k \mid x(n),\theta) = \frac{[\prod_i N(x_i(n)|\mu_{k,i},\sigma)] \quad (\pi^k(1-\pi)^{(1-k)})}{\sum_{j=0}^{1}[\prod_i N(x_i(n)|\mu_{j,i},\sigma)] \quad (\pi^j(1-\pi)^{(1-j)})}$$

- M Step: Update $\theta \leftarrow \arg\max_{\theta'} Q(\theta'|\theta)$

P(z=1)

$$\pi \leftarrow \frac{1}{N}\sum_{n=1}^{N} E[z(n)] \qquad \mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} P(z(n)=j|x(n),\theta) \quad x_i(n)}{\sum_{n=1}^{N} P(z(n)=j|x(n),\theta)}$$

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(**X**) is true distribution, T(**X**) is our tree-structured network, where **X** = <X_1, … X_n>
  - Chow-Liu minimizes Kullback-Leibler divergence:

$$KL(P(\mathbf{X}) \,||\, T(\mathbf{X})) \equiv \sum_k P(\mathbf{X}=k) \log \frac{P(\mathbf{X}=k)}{T(\mathbf{X}=k)}$$

Chow-Liu Algorithm

<u>Key result</u>: To minimize KL(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 $\mathbf{X} \equiv \langle X_1 \ldots X_n \rangle$

$$\begin{aligned} KL(P(\mathbf{X}) \mid\mid T(\mathbf{X})) &\equiv \sum_k P(\mathbf{X}=k) \log \frac{P(\mathbf{X}=k)}{T(\mathbf{X}=k)} \\ &= -\sum_i I(X_i, Pa(X_i)) + \sum_i H(X_i) - H(X_1 \ldots X_n) \end{aligned}$$

THANKS