Machine Learning 10-601

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Today:

- Graphical models
- Bayes Nets:
  - EM
  - Mixture of Gaussian clustering
  - Learning Bayes Net structure (Chow-Liu)

Readings:

- Bishop chapter 8
- Mitchell chapter 6

⊗ → ⊕ : $P_\theta(x,y) = P_{\theta_Y}(y) P_{\theta_X}(y|x)$

MLE: $l(\theta) = \mathbb{E}_{P_{data}}[\ln P_\theta(x,y)]$

$\approx \frac{1}{N}\sum_{i=1}^{N} \ln P_{\theta_Y}(y_i) P_{\theta_X}(x_i|y_i)$

$= \frac{1}{N}\sum_{i=1}^{N} (\ln P_{\theta_Y}(y_i) + \ln P_{\theta_X}(x_i|y_i))$

若存在隐变量 (存在于概率模型中但没有任何数据观测) $\Rightarrow$ MLE.

↳ z

$l(\theta) = \max_\theta \mathbb{E}_{P_{data}}[\ln P_\theta(x)]$, $P(x) = \int p(x,z)\,dz$.

$\Rightarrow$ 估计下界:

$$\ln P_\theta(x) = \ln \int P_\theta(x,z)\,dx$$

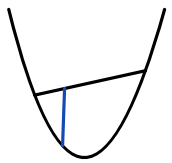
$$= \ln \int q(z) \frac{P_\theta(x,z)}{q(z)}\,dx$$

$q(x)$ $\mathbb{E}(x)$

$$= \ln \mathbb{E}_{q(z)}\left[\frac{P_\theta(x,z)}{q(z)}\right]$$ 詹森不等式.

$$\geq \mathbb{E}_{q(z)}[\ln P_\theta(x,z) - \ln q(z)]$$

$f(x)$: convex



$\Rightarrow \mathbb{E}(f(x)) \geq f(\mathbb{E}(x))$

If $f(x)$ is concave : 相反

$\mathbb{E}[f(x)] \leq f(\mathbb{E}[x])$

↳ 当 $q(x) \propto P_\theta(x,z)$, 即

$q(x) = P_\theta(z|x) = \frac{P_\theta(x,z)}{\sum_z P(x,z)}$

时, 等号成立.

取最小值时, 等号成立, 即有.

$$\min_\theta \ln P_\theta(x) = \mathbb{E}_{P_\theta(z|x)}\left[\ln \frac{P_{\theta'}(x,z)}{\sum_z P_\theta(x,z)}\right]$$

使用 Expectation Maximization 进行估计 (MLE)

Learning of Bayes Nets

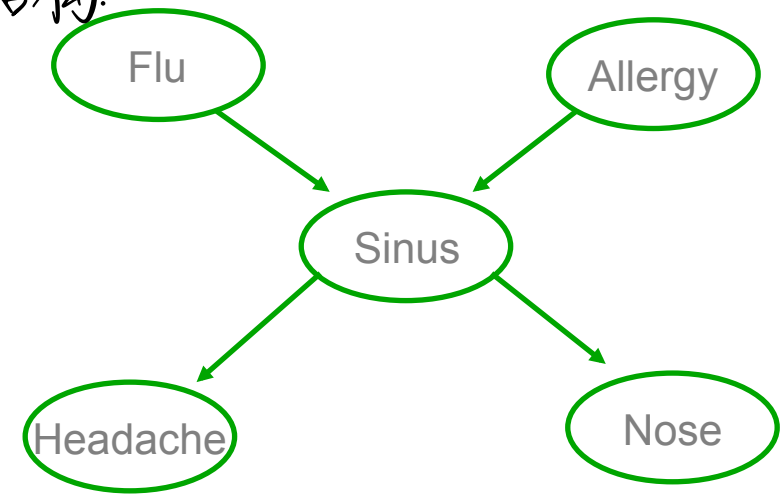
- Four categories of learning problems
  - Graph structure may be known/unknown 学习图的拓扑结构
  - Variable values may be fully observed / partly unobserved
    有无隐变量.
- Easy case: learn parameters for graph structure is *known*, and data is *fully observed*
- Interesting case: graph *known*, data *partly known*
- Gruesome case: graph structure *unknown*, data *partly unobserved*

Learning CPTs from Fully Observed Data

给定观测数据与图的结构.

- Example: Consider learning the parameter

$$\theta_{s|ij} \equiv P(S = 1 | F = i, A = j)$$



- Max Likelihood Estimate is

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

k[th] training example

δ(x) = 1 if x=true,
= 0 if x=false

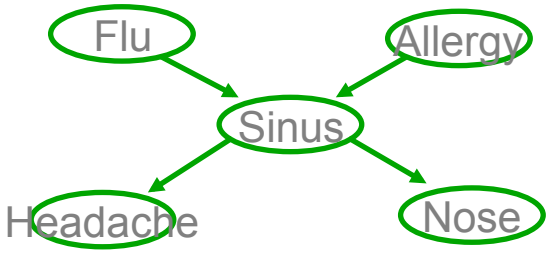
- Remember why?

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

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

- Maximum likelihood estimate

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



- Our case:

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

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

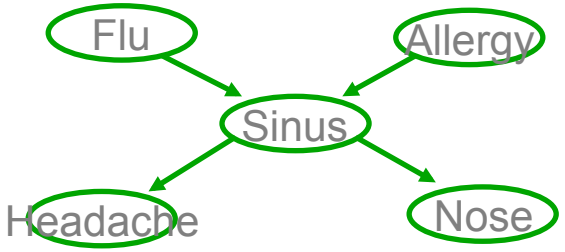
$$\log P(data|\theta) = \sum_{k=1}^{K} \log P(f_k) + \log P(a_k) + \log P(s_k|f_k a_k) + \log P(h_k|s_k) + \log P(n_k|s_k)$$

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

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

Estimate θ from partly observed data

假设有隐变量h.



- 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:

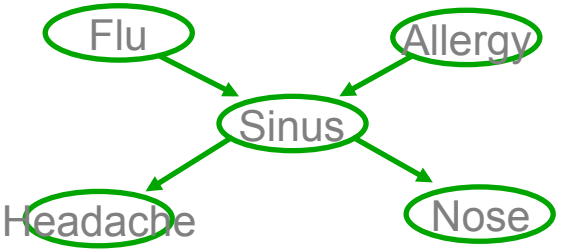
$$\theta \leftarrow \arg\max_{\theta} \log P(X, Z|\theta)$$

- WHAT TO DO?

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:

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

可观测 / 不可观测

- EM seeks* to estimate:

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

是迭代求解，故可以在线迭代计算，时间复杂度不高。

* EM guaranteed to find local maximum

$E_{P(x|y)}[x]$

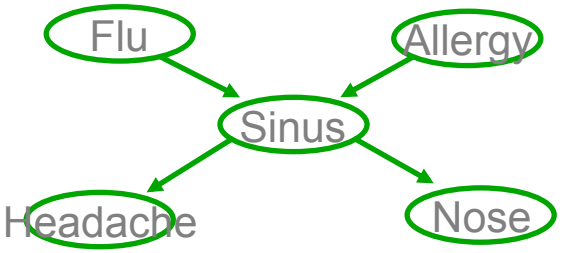
$= \int x p(x|y) dx$

$P(Z|X) = \frac{P(X,Z)}{P(X)}$

$= \frac{P(X,Z)}{\sum_z P(X, Z=z)}$

- EM seeks estimate:

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



- here, observed X={F,A,H,N}, unobserved Z={S}

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

$$E_{P(Z|X,\theta)} \log P(X, Z|\theta) = \sum_{k=1}^{K} \sum_{i=0}^{1} P(s_k = i|f_k, a_k, h_k, n_k)$$

$$[logP(f_k) + \log P(a_k) + \log P(s_k|f_k a_k) + \log P(h_k|s_k) + \log P(n_k|s_k)]$$

EM Algorithm - Informally

EM is a general procedure for learning from partly observed data

Given observed variables X, unobserved Z (X={F,A,H,N}, Z={S})

Begin with arbitrary choice for parameters θ

Iterate until convergence:

- E Step: estimate the values of unobserved Z, using θ
- M Step: use observed values plus E-step estimates to derive a better θ

Guaranteed to find local maximum.

Each iteration increases $E_{P(Z|X,\theta)}[\log P(X, Z|\theta')]$

EM Algorithm - Precisely

EM is a general procedure for learning from partly observed data

Given observed variables X, unobserved Z (X={F,A,H,N}, Z={S})

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

Iterate until convergence:

- E Step: Use X and current θ to calculate P(Z|X,θ)
- M Step: Replace current θ by

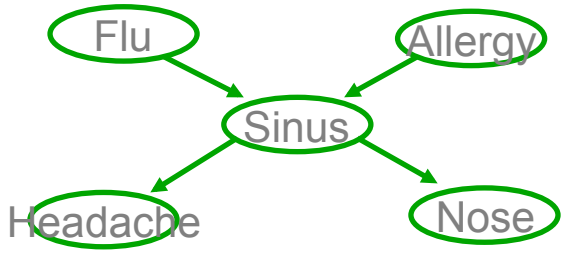
$$\theta \leftarrow \arg\max_{\theta'} Q(\theta'|\theta)$$

Guaranteed to find local maximum.

Each iteration increases $E_{P(Z|X,\theta)}[\log P(X, Z|\theta')]$

E Step: Use X, θ, to Calculate P(Z|X,θ)

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



- How? Bayes net inference problem.

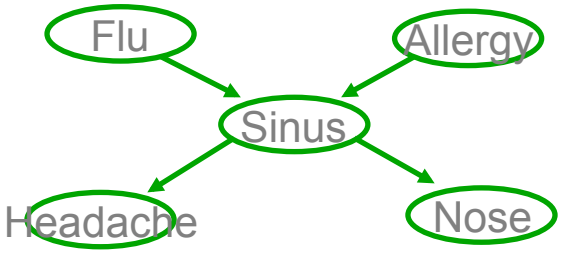
$$P(S_k = 1 | f_k a_k h_k n_k, \theta) =$$

$$P(S_k = 1 | f_k a_k h_k n_k, \theta) = \frac{P(S_k = 1, f_k a_k h_k n_k | \theta)}{P(S_k = 1, f_k a_k h_k n_k | \theta) + P(S_k = 0, f_k a_k h_k n_k | \theta)}$$

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

EM and estimating $\theta_{s|ij}$

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



E step: Calculate $P(Z_k|X_k; \theta)$ for each training example, k

$$P(S_k = 1|f_k a_k h_k n_k, \theta) = E[s_k] = \frac{P(S_k = 1, f_k a_k h_k n_k|\theta)}{P(S_k = 1, f_k a_k h_k n_k|\theta) + P(S_k = 0, f_k a_k h_k n_k|\theta)}$$

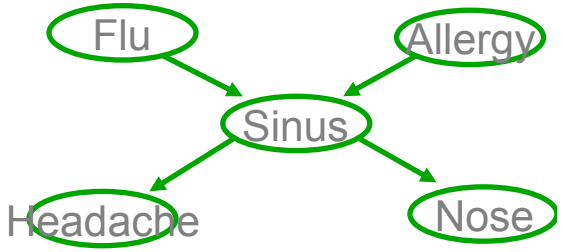
$P(z|x;\theta)$

M step: update all relevant parameters. For example:

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

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

EM and estimating θ



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 in each training example

M step:

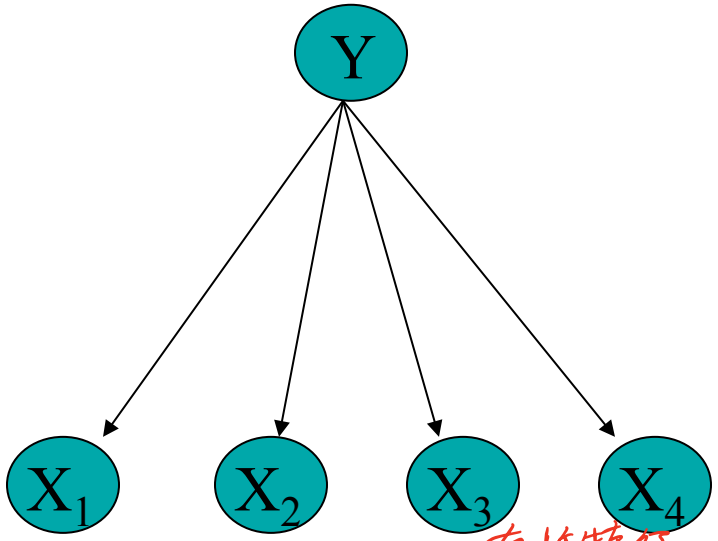
Calculate θ similar to MLE estimates, but replacing each count by its expected count

$$\delta(Y = 1) \rightarrow E_{Z|X,\theta}[Y] \qquad \delta(Y = 0) \rightarrow (1 - E_{Z|X,\theta}[Y])$$

Using Unlabeled Data to Help Train Naïve Bayes Classifier

Learn P(Y|X)

半监督学习. semi-Supervised



Y	X1	X2	X3	X4
1	0	0	1	1
0	0	1	0	0
0	0	0	1	0
?	0	1	1	0
?	0	1	0	1

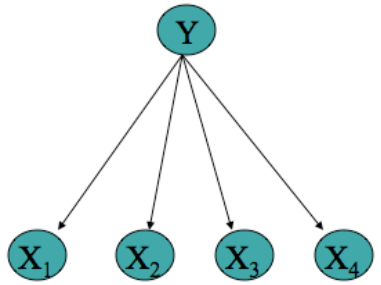
$E_{P(Y|X,\theta)}[\ln P(X,Y,\theta)]$

$P_{\theta_y}(Y)\prod_{j=1}^{d} P_{\theta_x}(X_j|Y)$ → d有d个特征

E-step: $P(X,Y|\theta) = \frac{P_\theta(X,Y)}{\sum_y P_\theta(X,Y=y)}$

↳ 分母要对第四、五个样本进行估计

EM and estimating θ



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

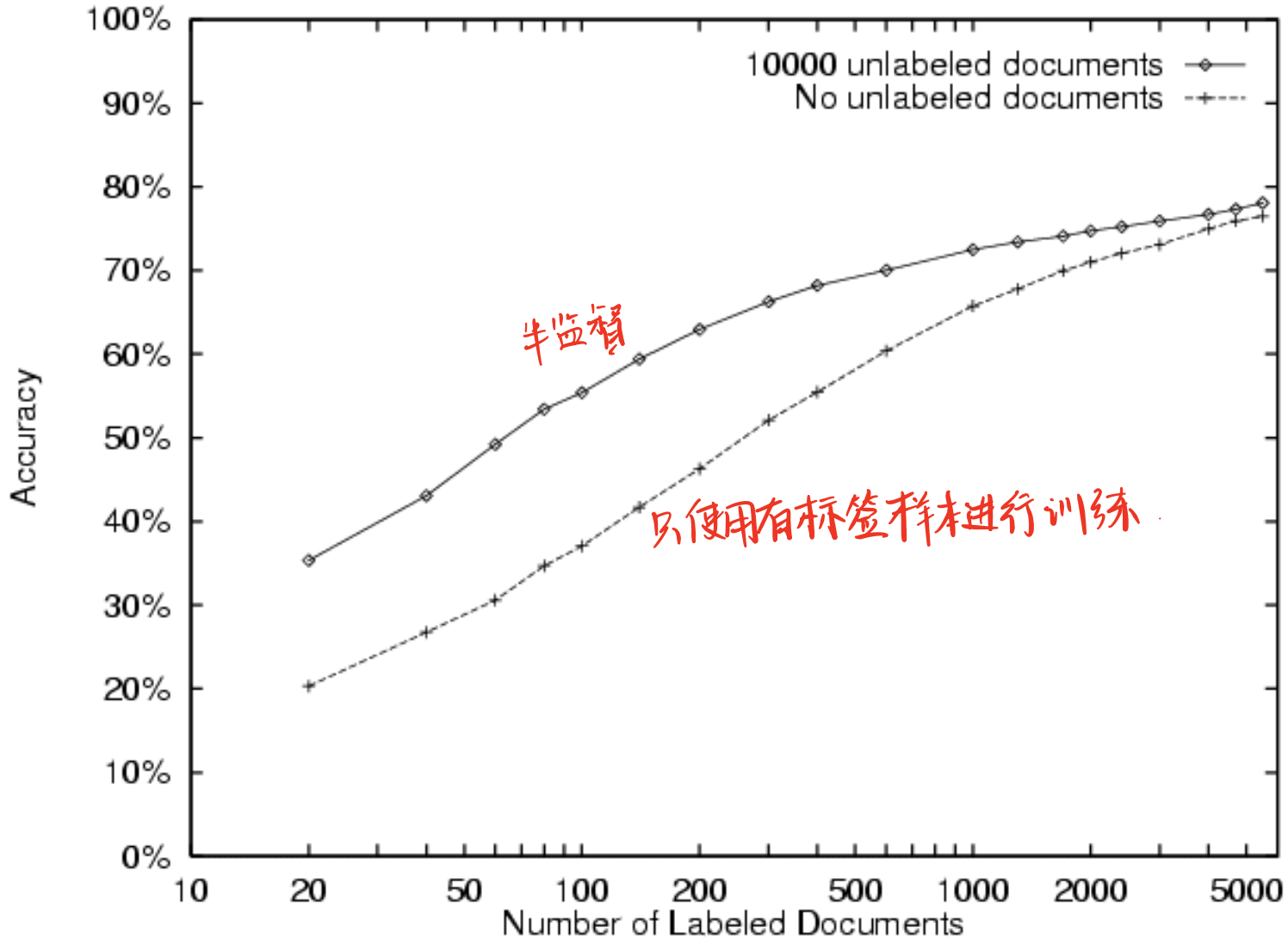
$$E_{P(Y|X_1 \ldots X_N)}[y(k)] = P(y(k)=1|x_1(k), \ldots x_N(k); \theta) = \frac{P(y(k)=1)\prod_i P(x_i(k)|y(k)=1)}{\sum_{j=0}^{1} P(y(k)=j)\prod_i P(x_i(k)|y(k)=j)}$$

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

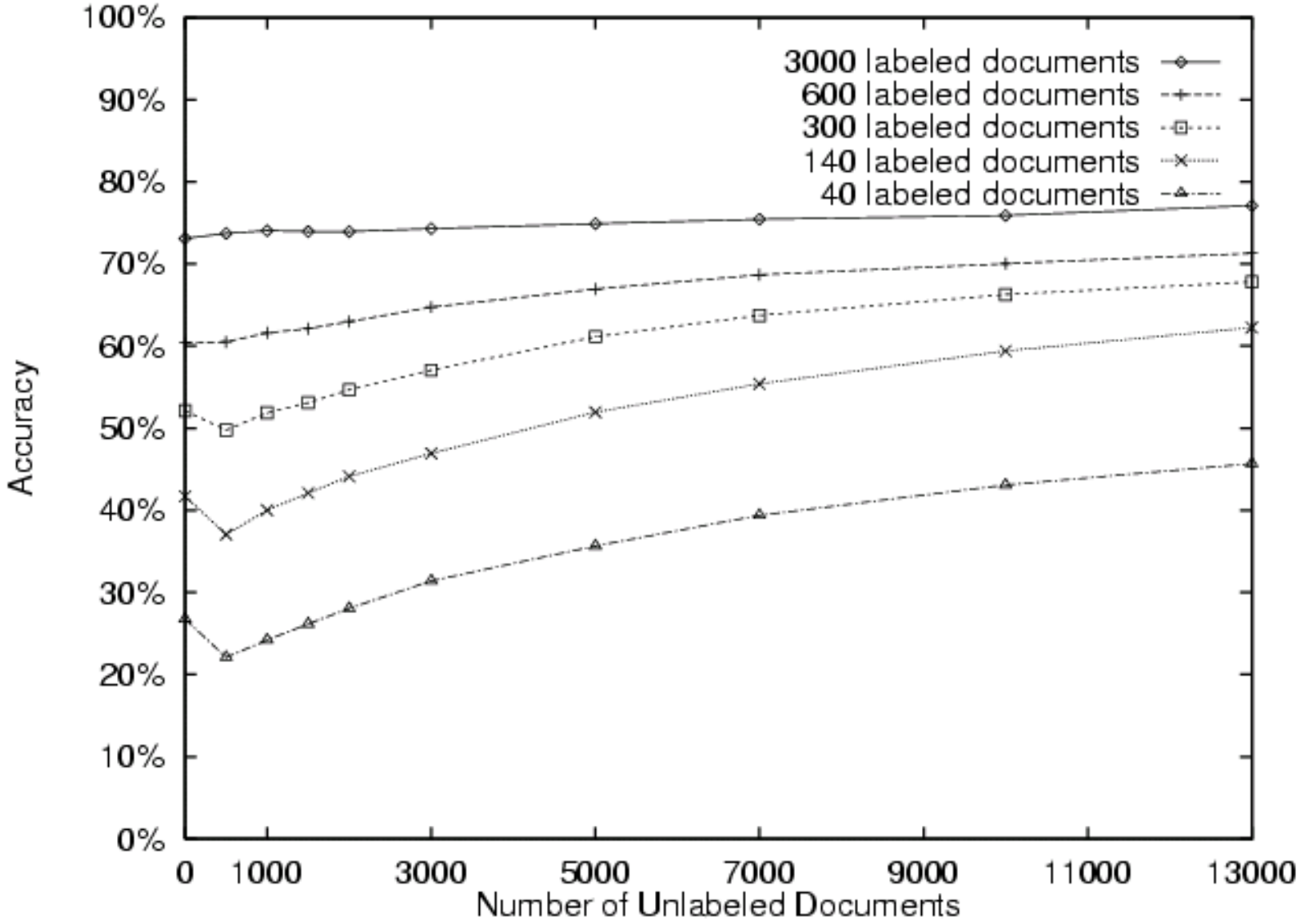
$$\theta_{ij|m} = \hat{P}(X_i = j|Y = m) = \frac{\sum_k P(y(k)=m|x_1(k)\ldots x_N(k))\ \delta(x_i(k)=j)}{\sum_k P(y(k)=m|x_1(k)\ldots x_N(k))}$$

MLE would be: $\hat{P}(X_i = j|Y = m) = \frac{\sum_k \delta((y(k)=m) \wedge (x_i(k)=j))}{\sum_k \delta(y(k)=m)}$

20 Newsgroups



20 Newsgroups



Unsupervised clustering

Just extreme case for EM with zero labeled examples…

参数来自多个高斯分布 ⇒ 聚类（没有任何有标注的样本）

Clustering

- Given set of data points, group them 按相似度分组
- Unsupervised learning
- Which patients are similar? (or which earthquakes, customers, faces, web pages, …)

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

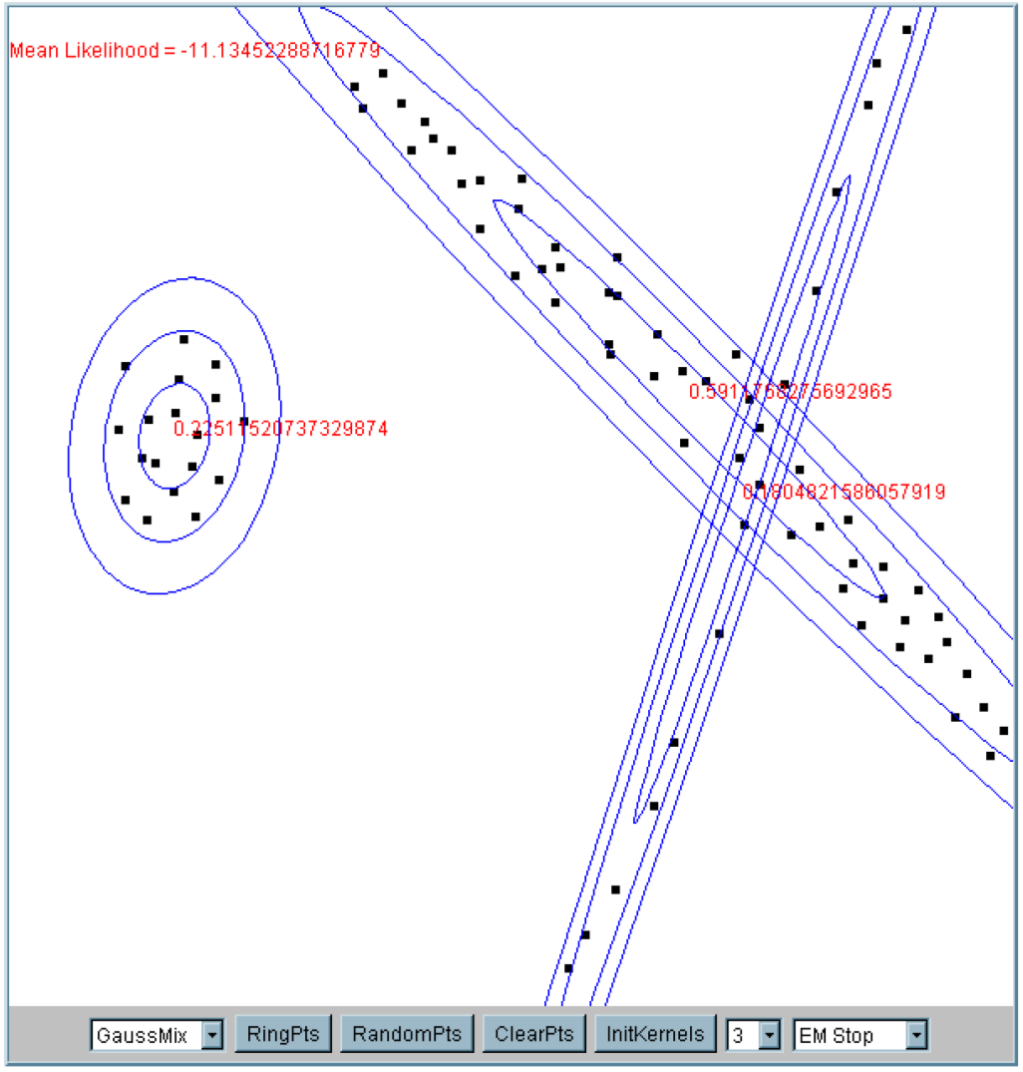
Mixture of *Gaussians*:

- 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 $N(\mu_i, \Sigma_i)$

假设 $X=(x_1,x_2)$ 是由3个高斯分布生成的

Mixture of Gaussians



EM for Mixture of Gaussian Clustering

Let's simplify to make this easier:

高斯的Naïve Bayes.

1. assume $X=<X_1 \ldots X_n>$, and the X_i are conditionally independent given Z.

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

简化

⇒ 协方差矩阵从 nxn 变成对角矩阵

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

假设只有2个类.

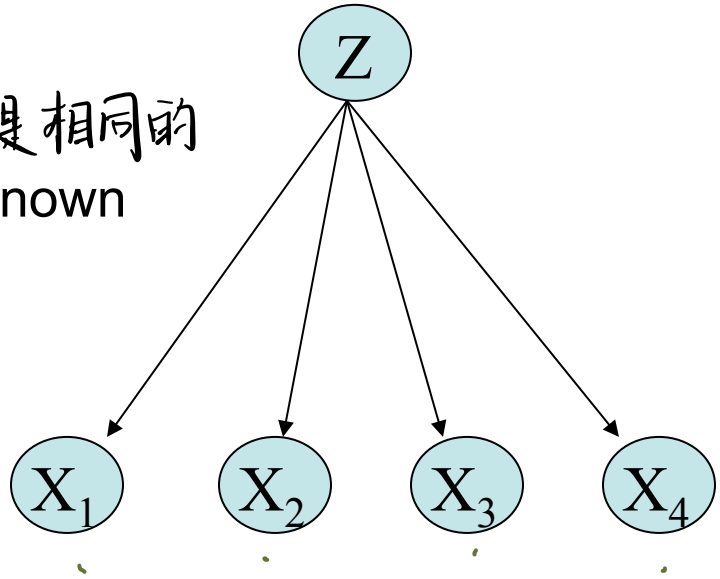
$$P(\mathbf{X}) = \sum_{j=1}^{2} P(Z=j|\pi) \prod_i N(x_i|\mu_{ji}, \sigma)$$

假设3每个协方差矩阵是相同的

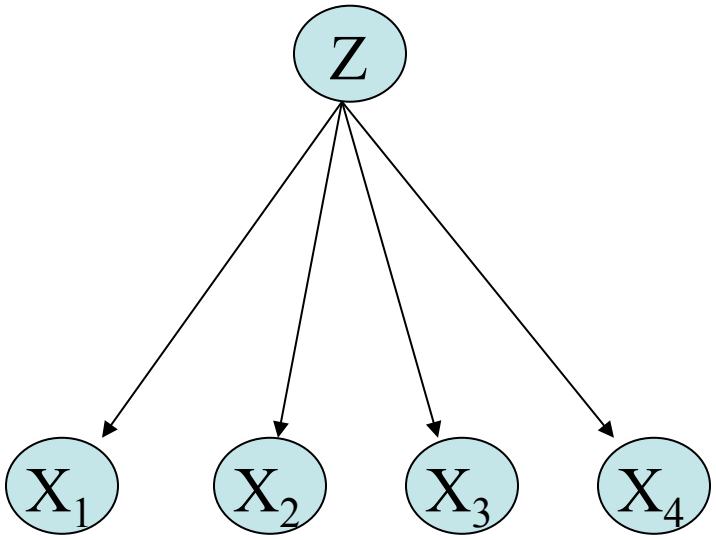
3. Assume σ known, $\pi_1 \ldots \pi_K, \mu_{1i} \ldots \mu_{Ki}$ unknown

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

Unobserved: Z



EM



Given observed variables X, unobserved Z

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

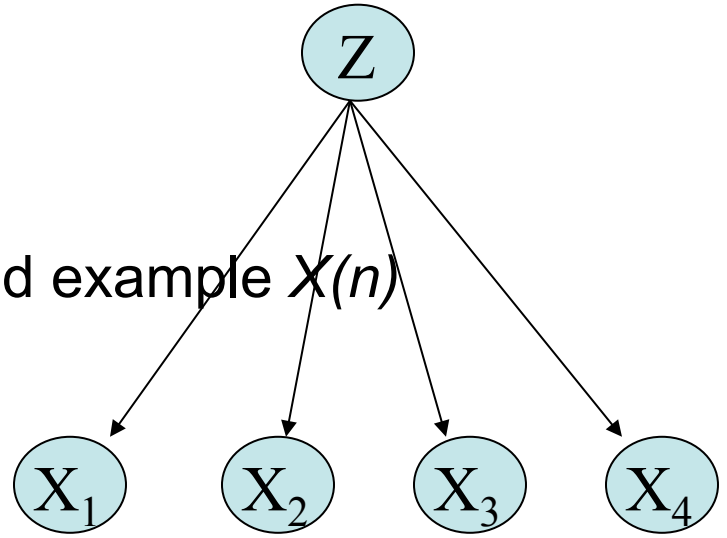
where $\theta = \langle \pi, \mu_{ji} \rangle$

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 $X(n)$

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

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

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

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

EM – M Step

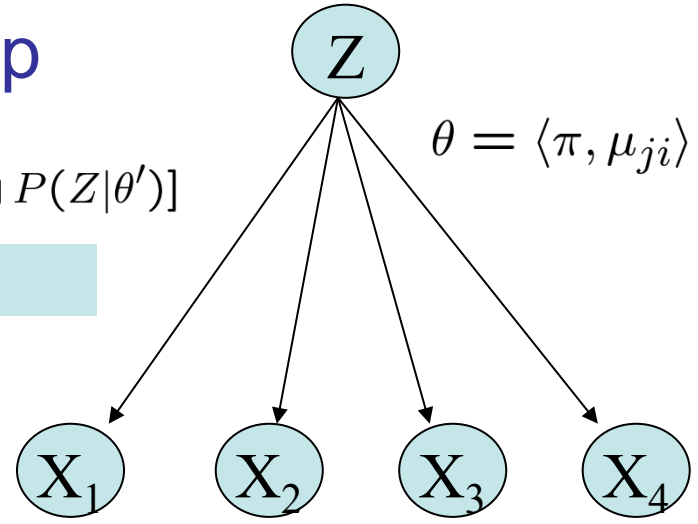
First consider update for π

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

π' has no influence

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

z=1 for nth example



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

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

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

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

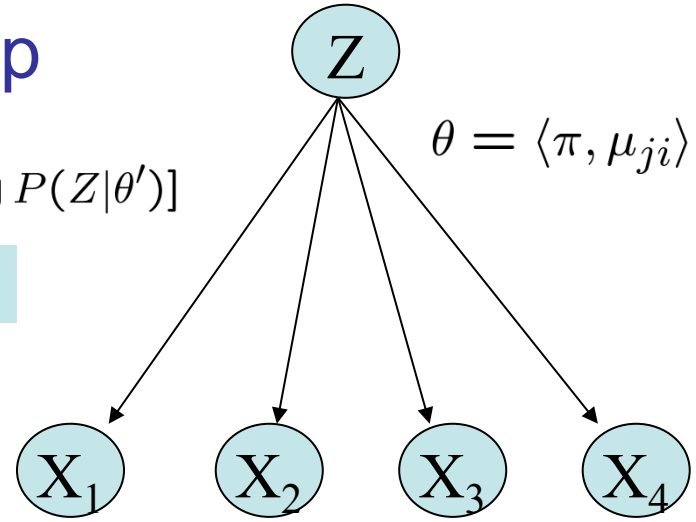
$$\pi \leftarrow \frac{\sum_{n=1}^N E[z(n)]}{\left(\sum_{n=1}^N E[z(n)]\right) + \left(\sum_{n=1}^N (1 - E[z(n)])\right)} = \frac{1}{N}\sum_{n=1}^N E[z(n)]$$

EM – M Step

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



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

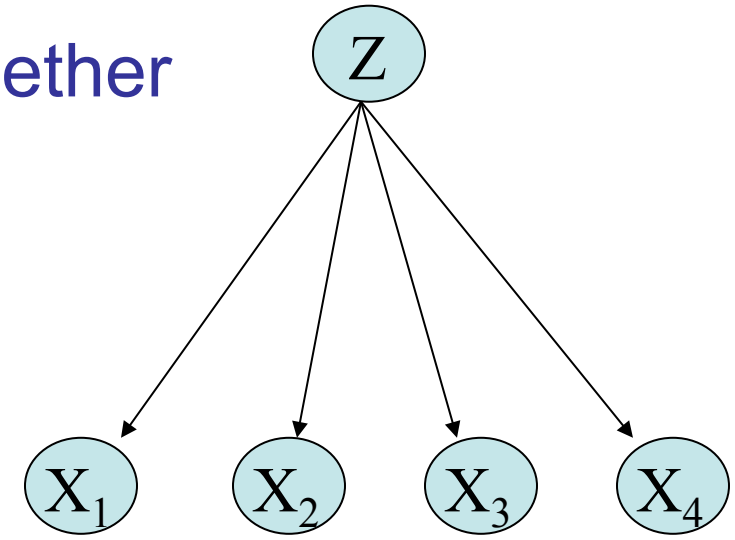
…
…
…

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

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

$$\pi \leftarrow \frac{1}{N} \sum_{n=1}^{N} E[z(n)]$$

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

What you should know about EM

- For learning from partly unobserved data
- MLE of θ = $\arg\max_{\theta} \log P(data|\theta)$
- EM estimate: θ = $\arg\max_{\theta} E_{Z|X,\theta}[\log P(X, Z|\theta)]$

  Where X is observed part of data, Z is unobserved
- Nice case is Bayes net of boolean vars:
  - M step is like MLE, with with unobserved values replaced by their expected values, given the other observed values
- 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 $E_{Z|X,\theta}[\log P(X, Z|\theta)]$
  - E step: for each training example X^k, calculate $P(Z^k \mid X^k, \theta)$
  - M step: chose new θ to maximize

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(**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

Key result: 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:

AB边缘相对于联合概率分布的KL散度

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

$I(A,B) = KL\left(P(A,B) \,\|\, P(A)P(B)\right)$

This works because for tree networks with nodes $\mathbf{X} \equiv \langle X_1 \ldots X_n \rangle$

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

$$= -\sum_i I(X_i, Pa(X_i)) + \sum_i H(X_i) - H(X_1 \ldots X_n)$$

对于树形结构，$|Pa(X_i)| \le 1$（父节点个数）

$\min_T KL(P(X) \,\|\, T(X)) = \int P(x) \ln \frac{P(x)}{T(x)} dx = \int P(x) \ln P(x) dx - \int P(x) \ln T(x) dx$

这个是n个变量组成的多元变量

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

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

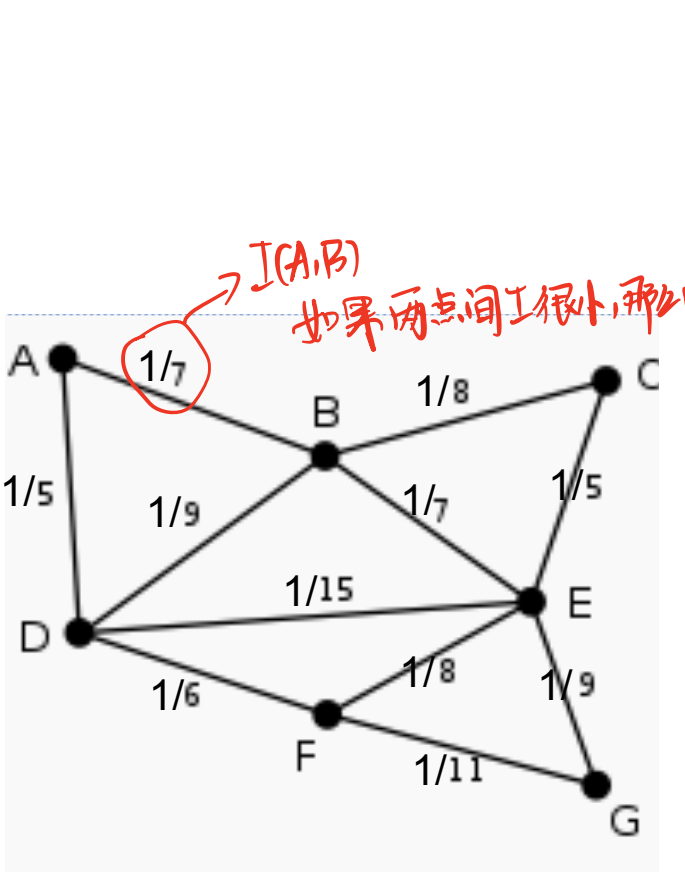
3. calculate the maximum spanning tree over the set of variables, using edge weights $I(A,B)$

   (given N vars, this costs only $O(N^2)$ time)

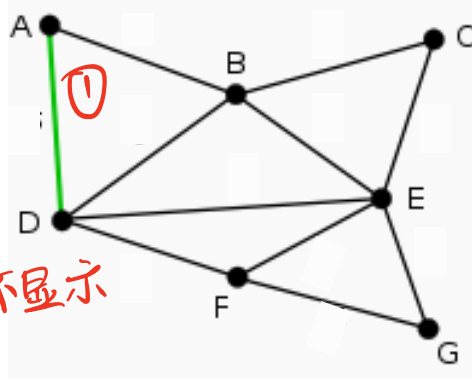
4. add arrows to edges to form a directed-acyclic graph

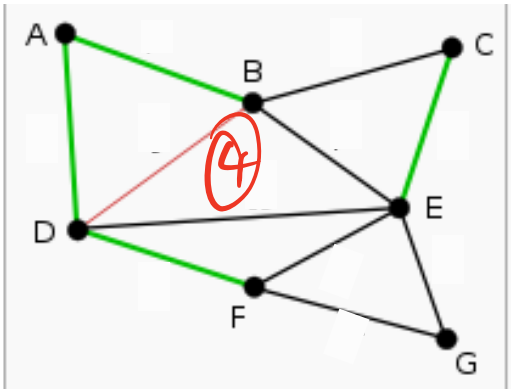
5. learn the CPD's for this graph

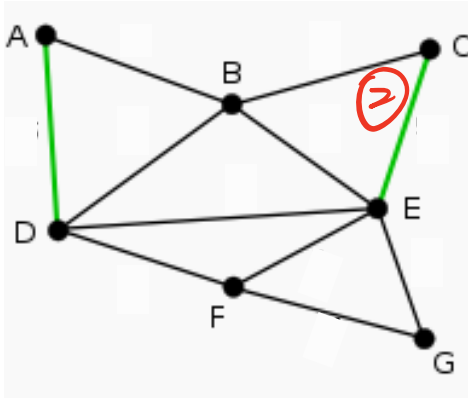
Chow-Liu algorithm example
Greedy Algorithm to find Max-Spanning Tree

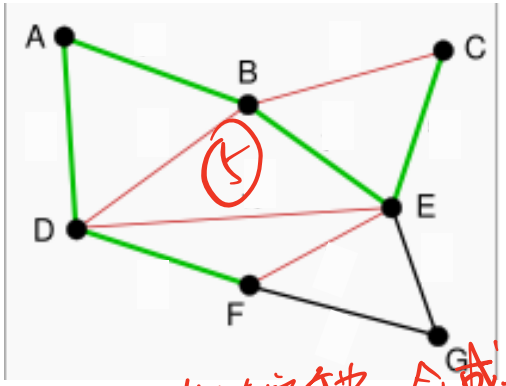


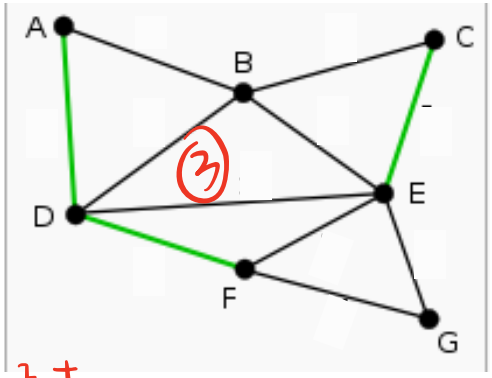
I(A,B) 如果两点间I很小，那么不显示



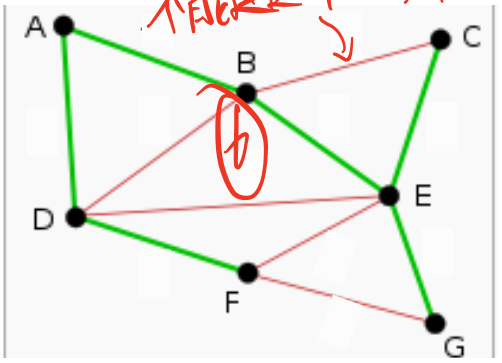








不能选这个边，会成环。



[courtesy A. Singh, C. Guestrin]

通过最大化ΣI来构建一颗树。

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