Machine Learning

CS60050

E-M Algorithm and

Gaussian Mixture Model

Machine Learning 10-601

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

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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

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

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

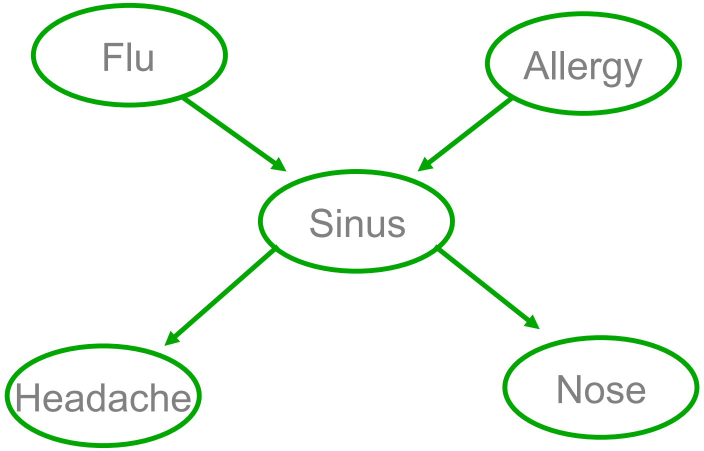
- Max Likelihood Estimate is

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

k^th training example

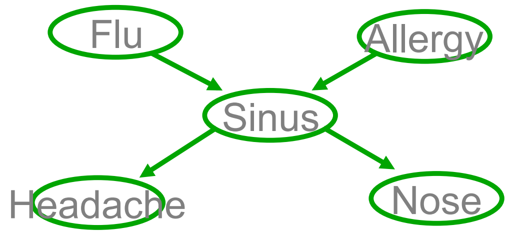
δ(x) = 1 if x=true,
= 0 if x=false

- 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:

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

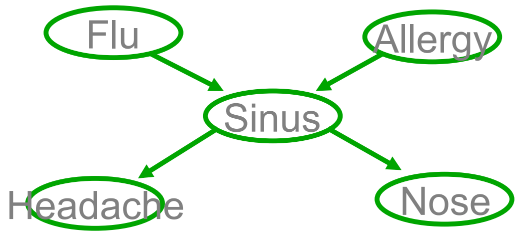
$$P(data|\theta) = \prod_{k=1}^{K} P(f_k)P(a_k)P(s_k|f_k a_k)P(h_k|s_k)P(n_k|s_k)$$

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

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

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

Estimate θ from partly observed data



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

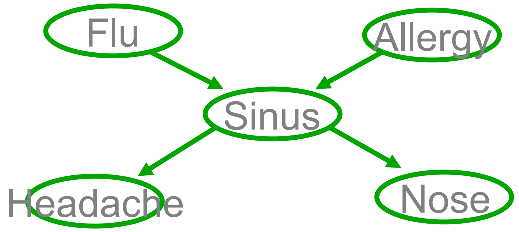
$$\theta \leftarrow \arg\max_\theta \log \prod_k P(f_k, a_k, s_k, h_k, n_k|\theta)$$

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

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

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

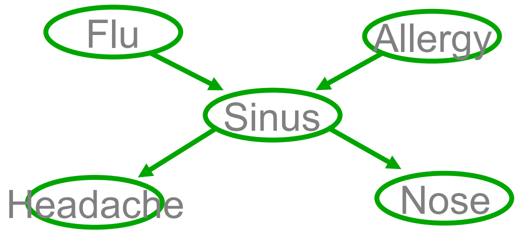
- EM seeks* to estimate:

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

* EM guaranteed to find local maximum

- 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}

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

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

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

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

current

M step new

Iterate until convergence:

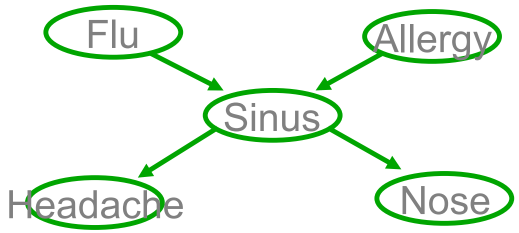
- E Step: Use X and current θ to calculate P(Z|X,θ)
- M Step: Replace current θ by

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

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}



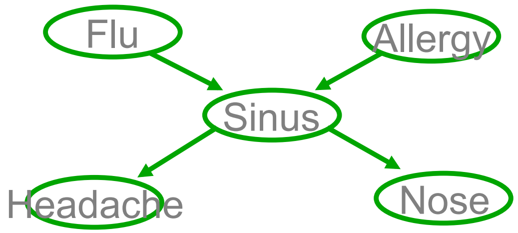
- How? Bayes net inference problem.

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

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

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

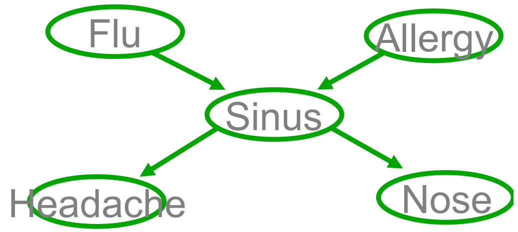
$$P(S_k = 1|f_k a_k h_k n_k, \theta) = \underbrace{E[s_k]}_{P(Z|X;\theta)} = \frac{P(S_k = 1, f_k a_k h_k n_k|\theta)}{P(S_k = 1, f_k a_k h_k n_k|\theta) + P(S_k = 0, f_k a_k h_k n_k|\theta)}$$

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

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

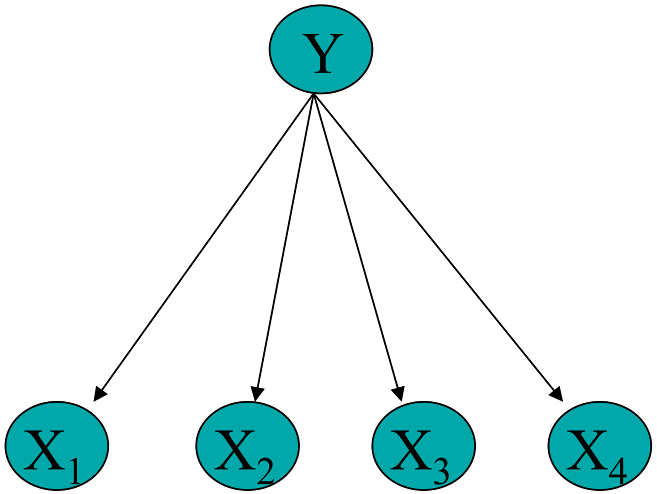
M step:

Calculate θ similar to MLE estimates, but replacing each count by its <u>expected count</u>

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

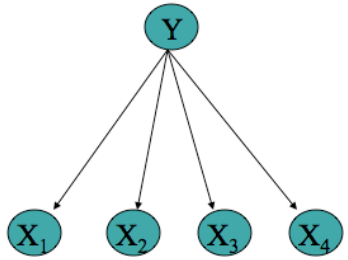
Using Unlabeled Data to Help Train Naïve Bayes Classifier

Learn P(Y|X)



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

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

Experimental Evaluation

From [Nigam et al., 2000]

- 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

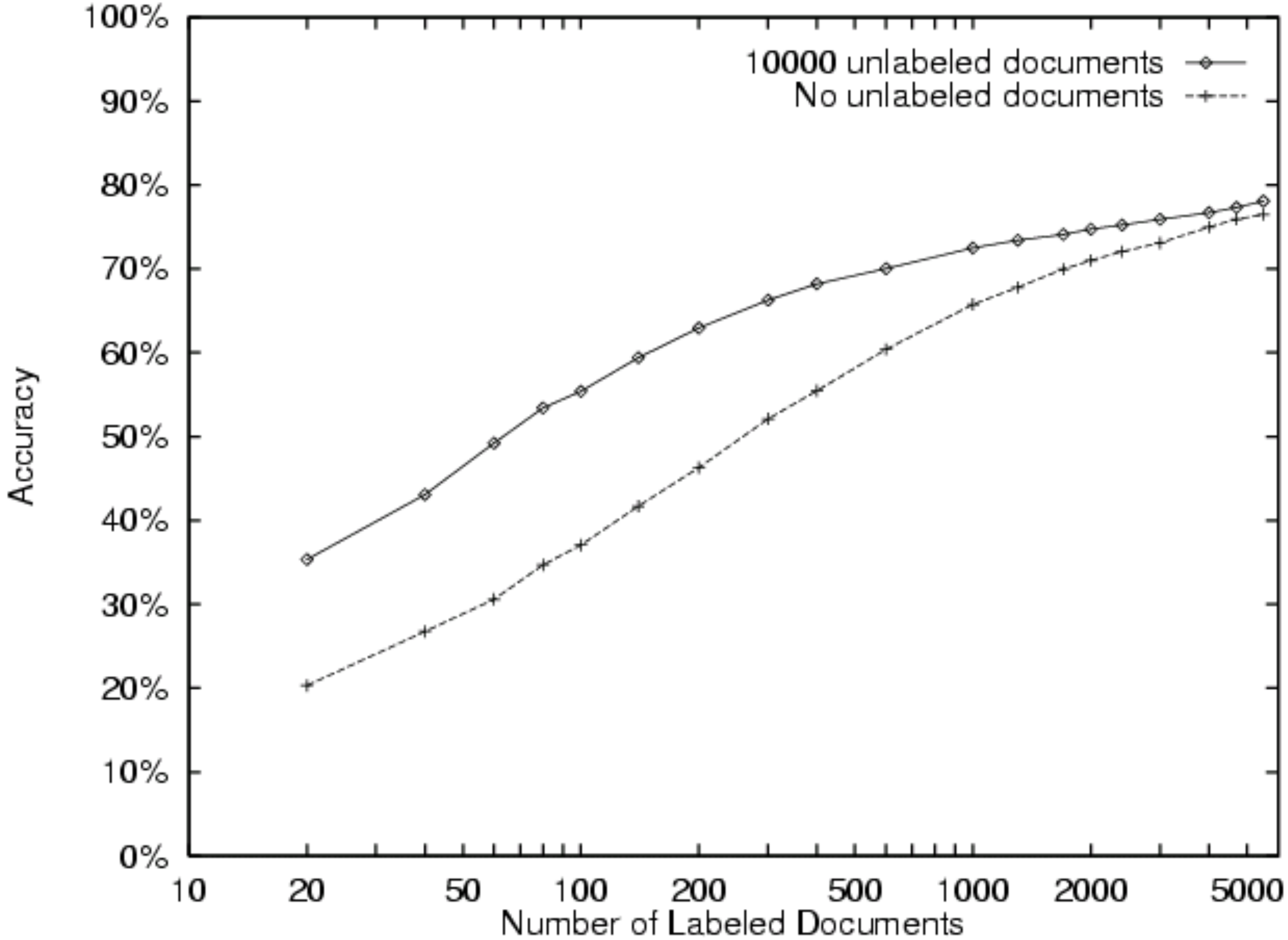


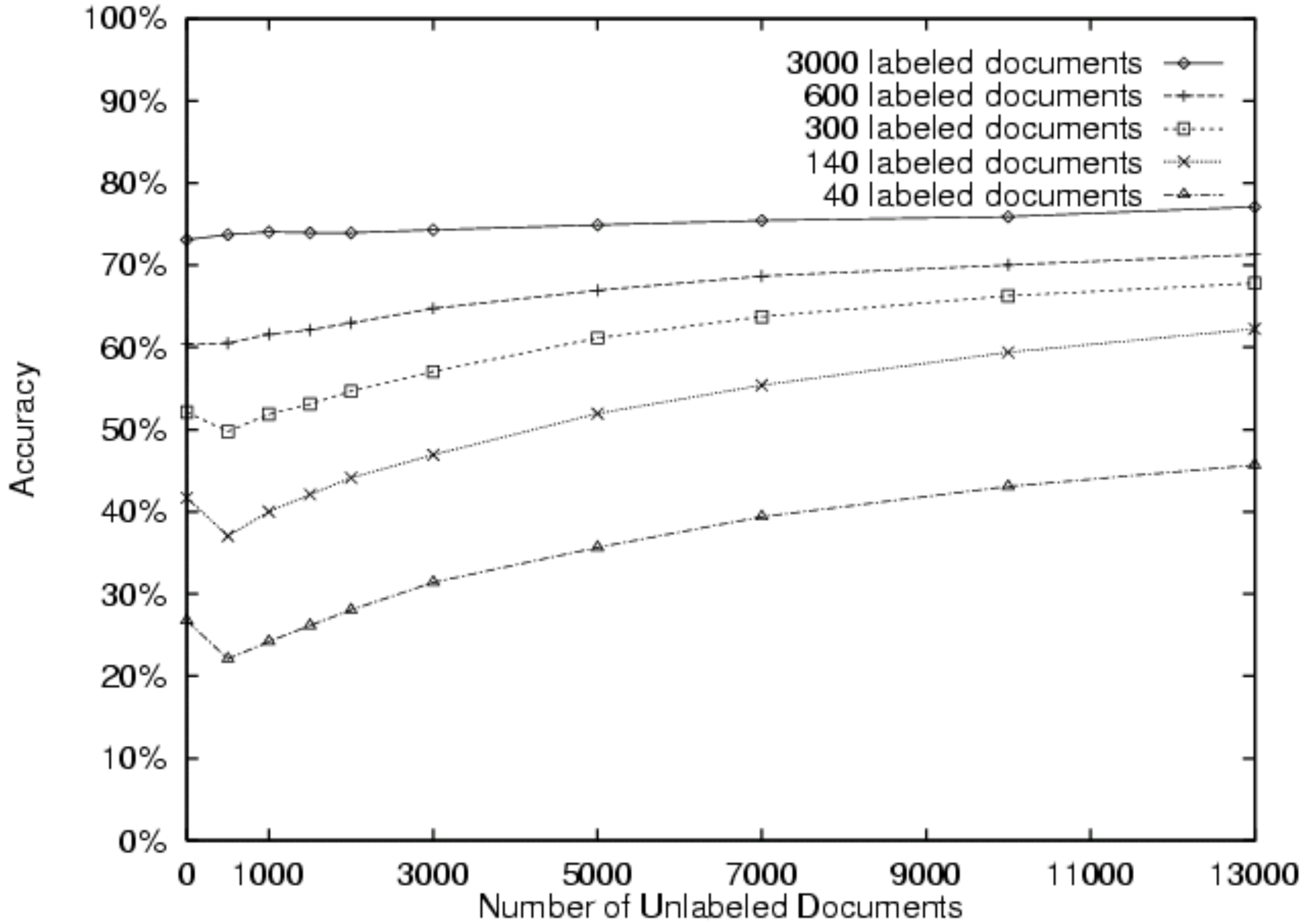
Table 3. Lists of the words most predictive of the course class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common course-related words appear. The symbol D indicates an arbitrary digit.

Iteration 0	Iteration 1	Iteration 2
intelligence	DD	D
DD	D	DD
artificial	lecture	lecture
understanding	cc	cc
DDw	$D^{\star}$	$DD{:}DD$
dist	$DD{:}DD$	due
identical	handout	$D^{\star}$
rus	due	homework
arrange	problem	assignment
games	set	handout
dartmouth	tay	set
natural	DDam	hw
cognitive	yurttas	exam
logic	homework	problem
proving	kfoury	DDam
prolog	sec	postscript
knowledge	postscript	solution
human	exam	quiz
representation	solution	chapter
field	assaf	ascii

word w ranked by $P(w|Y{=}\text{course}) / P(w|Y \neq \text{course})$

Using one labeled example per class

20 Newsgroups



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 $P(X_1 \dots X_n)$ as mixture of multiple distributions.

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

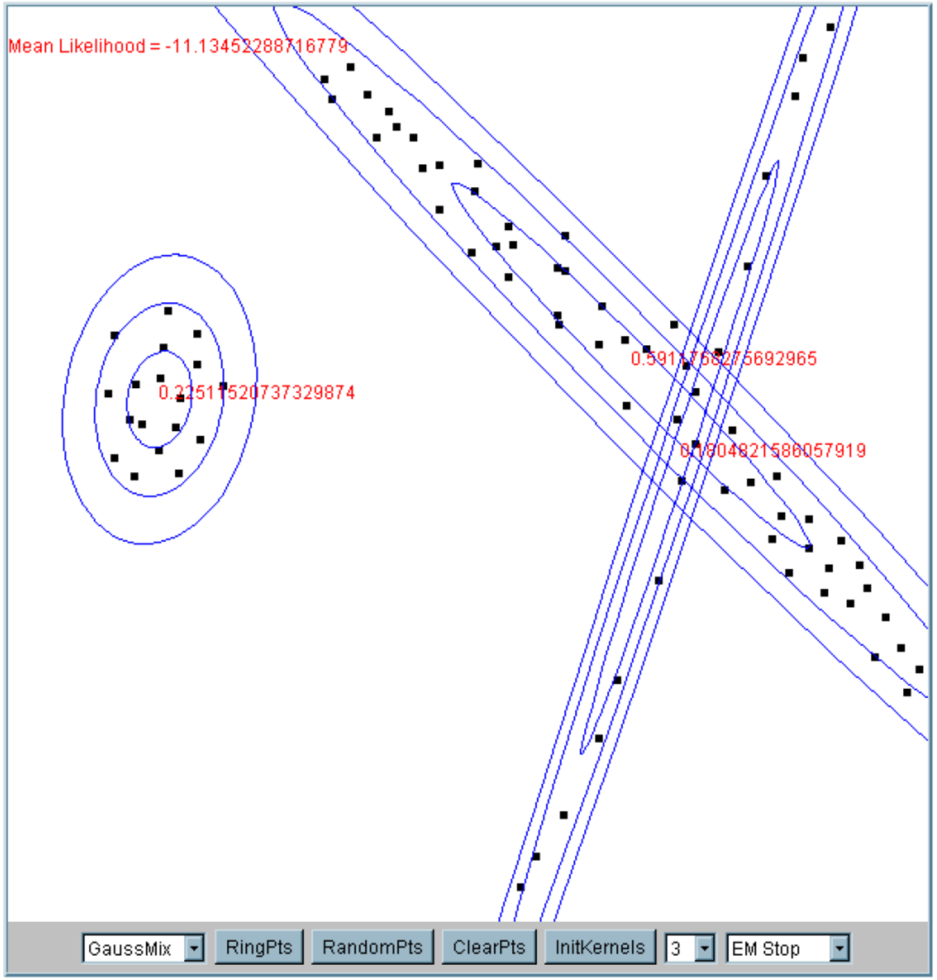
So $$P(X_1 \dots X_n) = \sum_i P(Z=i) \;\; P(X_1 \dots X_n | Z)$$

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 ... X_n>, and the X_i are conditionally independent given Z.

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

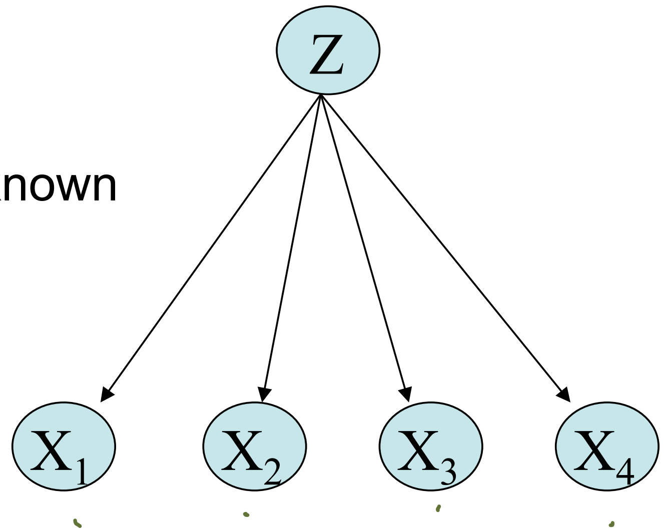
2. assume only 2 clusters (values of Z), and $\forall i, j, \sigma_{ji} = \sigma$

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

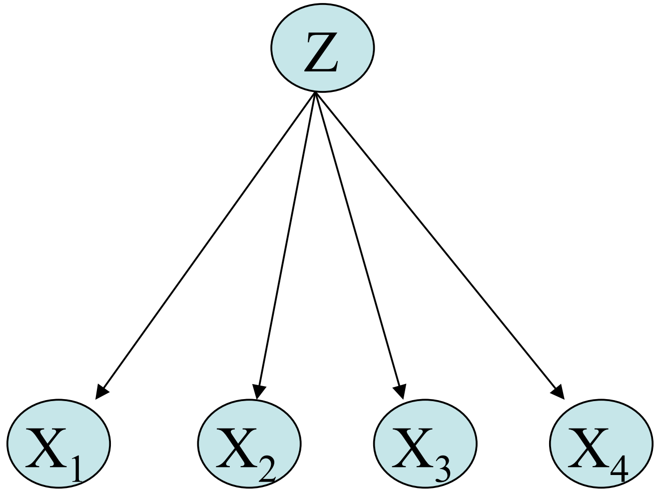
3. Assume σ known, π_1 ... π_K, μ_{1i} ...μ_{Ki} unknown

Observed: X=<X_1 ... 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 $\theta = \langle \pi, \mu_{ji} \rangle$

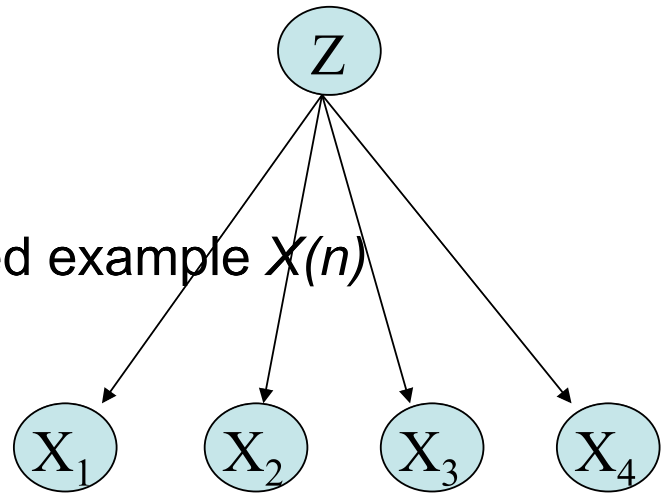
Iterate until convergence:

• 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),θ)* for each observed example *X(n)*

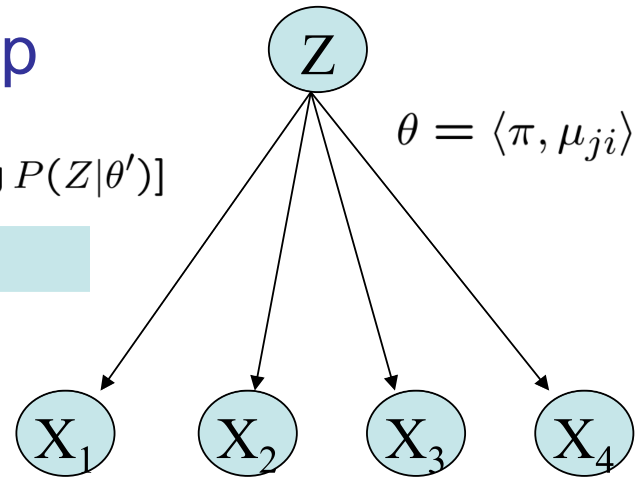
$X(n)=<x_1(n), x_2(n), \ldots x_T(n)>$.

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

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

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

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

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

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

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

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

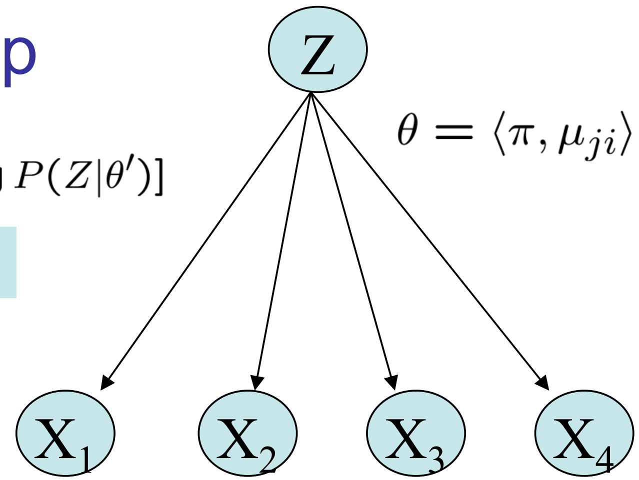
$$\boxed{\pi \leftarrow \frac{\sum_{n=1}^N E[z(n)]}{\left(\sum_{n=1}^N E[z(n)]\right) + \left(\sum_{n=1}^N (1-E[z(n)])\right)} = \frac{1}{N}\sum_{n=1}^N E[z(n)]}$$

EM – M Step

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



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

…

…

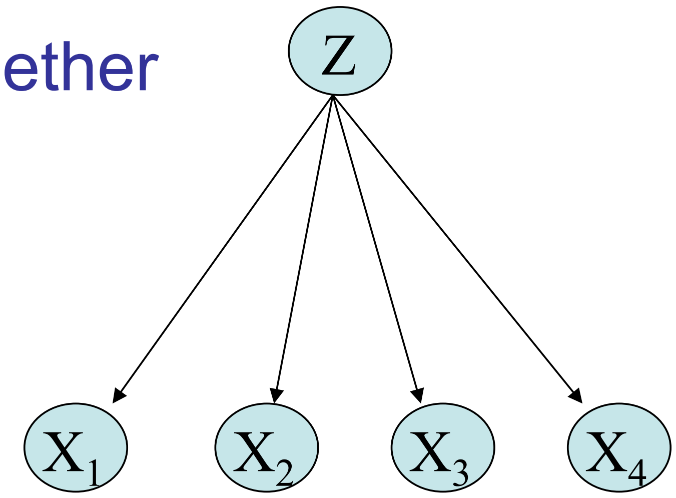
…

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

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), θ)*

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

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

P(z=1)

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

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

Mixture of Gaussians applet

Go to: http://www.socr.ucla.edu/htmls/SOCR_Charts.html

then go to Go to “Line Charts” → 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 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 $P(\mathbf{X})$ is true distribution, $T(\mathbf{X})$ is our tree-structured network, where $\mathbf{X} = \langle X_1, \ldots X_n \rangle$
  - Chow-Liu minimizes Kullback-Leibler divergence:

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

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:

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

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

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

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

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

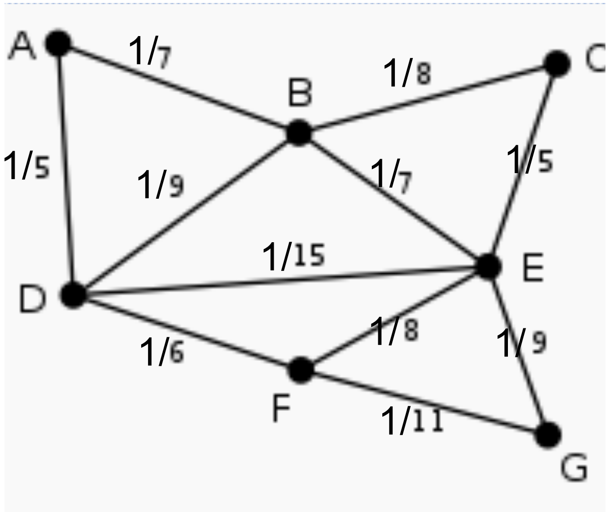
3. calculate the maximum spanning tree over the set of variables, using edge weights *I(A,B)*

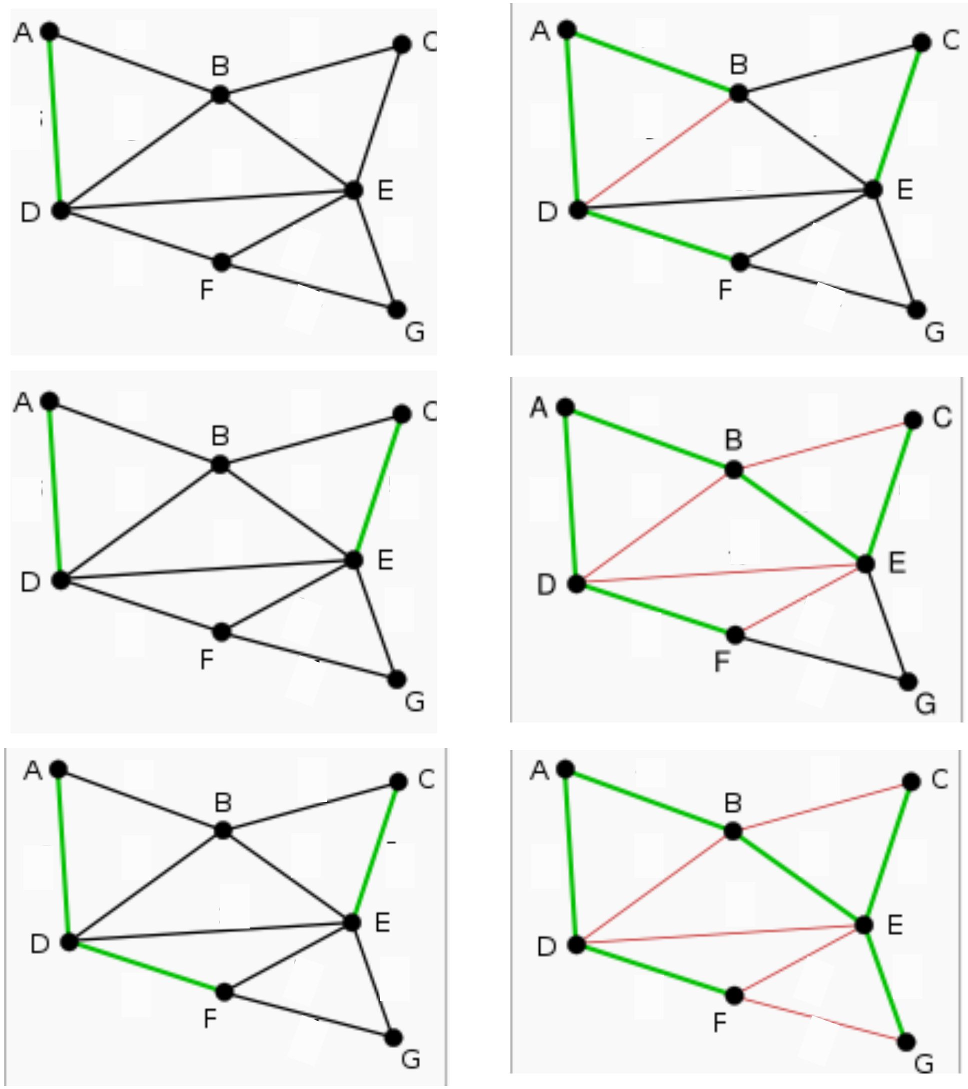
   (given N vars, this costs only $O(N^2)$ time)

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





[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

Thank You!