

Machine Learning 10-601, 10-301

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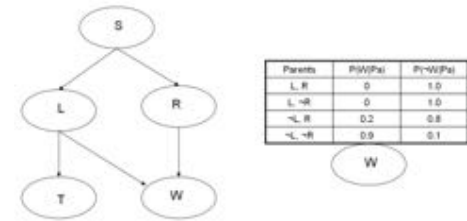
Today:

- Graphical models 3
 - Learning Bayesian Networks

Readings:

- Bishop chapter 8
<https://www.microsoft.com/en-us/research/wp-content/uploads/2016/05/Bishop-PRML-sample.pdf>

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 $P(X_i | Pa(X_i))$
- The joint distribution over all variables is defined to be

$$P(X_1 \dots X_n) = \prod_i P(X_i | Pa(X_i))$$

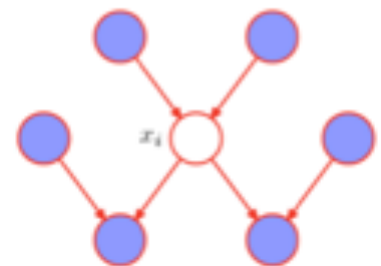
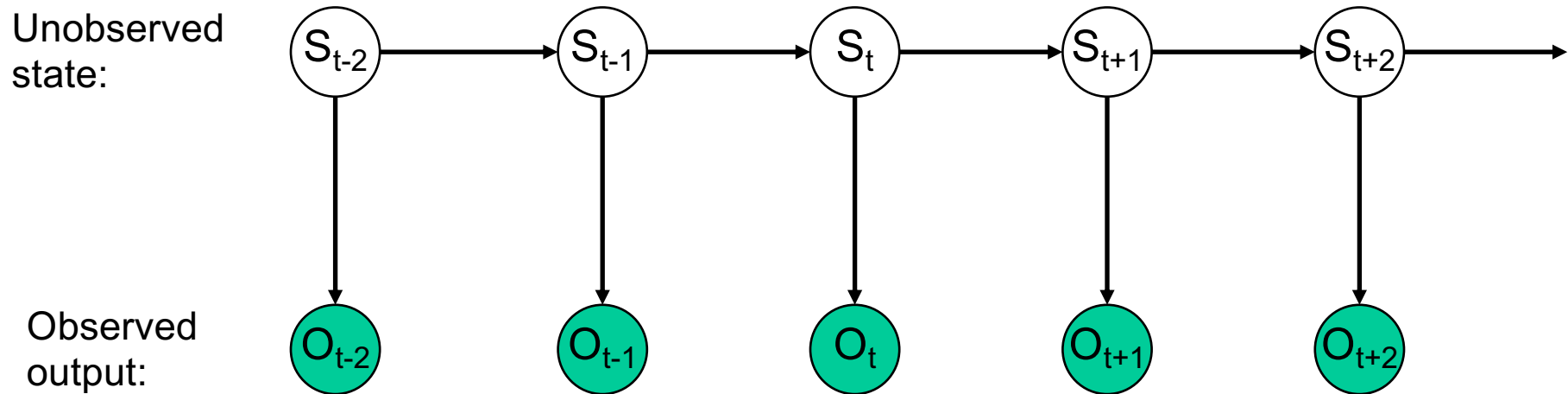
$Pa(X)$ = immediate parents of X in the graph

Poll: Answer Question 1

What is the graphical model for a Naïve Bayes classifier?

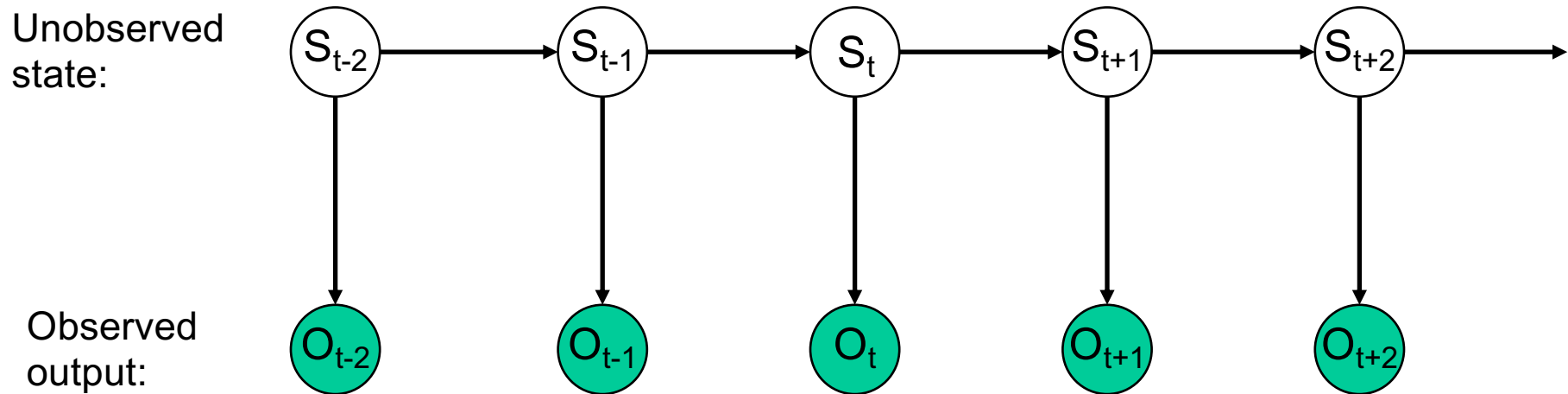
Bayes Network for a Hidden Markov Model

Implies the future is conditionally independent of the past, given the present



Bayes Network for a Hidden Markov Model

Implies the future is conditionally independent of the past, given the present



$$P(S_{t-2}, O_{t-2}, S_{t-1}, \dots, O_{t+2}) =$$

Learning of Bayes Nets

Four types of learning problems

- Graph structure may be known/unknown
 - Variable values may be fully observed / partly unobserved
1. Easy case: learn parameters when graph structure is *known*, and training data is *fully observed*
 2. Interesting case: graph *known*, data *partly observed*
 3. Interesting case: graph *unknown*, data *fully observed*
 4. Gruesome case: graph structure *unknown*, data *partly unobserved*

Easy: Graph Known, Fully Observed Data

- Example: Consider learning the parameter

$$\theta_{K=1|S=0,A=1} \equiv P(K = 1|S = 0, A = 1)$$



- Max Likelihood Estimate is

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

S	A	K	E	H
1	0	1	1	0
0	1	0	0	1
0	1	1	0	0
0	0	0	1	0
1	1	1	1	1

$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M \delta(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M \delta(s_m = i, a_m = j)}$$

m^{th} training example

$\delta(X) = 1$ if X is true
0 otherwise

let's use a_m to represent value of A on the m^{th} example

Easy: Graph Known, Fully Observed Data

- Example: Consider learning the parameter

$$\theta_{K=1|S=0,A=1} \equiv P(K = 1|S = 0, A = 1)$$



S	A	K	E	H
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0	1	0	0	1
0	1	1	0	0
0	0	0	1	0
1	1	1	1	1

Poll: Answer Question 2

What is the Maximum Likelihood estimate of $P(K=1|S=0,A=1)$

let's use a_m to represent value of A on the m th example

Easy: Graph Known, Fully Observed Data

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$$\theta_{K=1|S=0,A=1} \equiv P(K = 1|S = 0, A = 1)$$



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0	0	0	1	0
1	1	1	1	1

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Fully Observed

S	A	K	E	H
1	0	1	1	0
0	1	0	0	1
0	1	1	0	0
0	0	0	1	0
1	1	1	1	1

Partially Observed

S	A	K	E	H
1	0	1	1	0
0	1	?	0	1
0	1	1	0	0
0	?	0	1	0
1	1	1	1	1



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0	1	1	0	0
0	?	0	1	0
1	1	1	1	1

EM Approach

Pr	S	A	K	E	H
1.0	1	0	1	1	0
0.6	0	1	1	0	1
0.4	0	1	0	0	1
1.0	0	1	1	0	0
0.2	0	1	0	1	0
0.8	0	0	0	1	0
1.0	1	1	1	1	1

- Max Likelihood Estimate is

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$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M \delta(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M \delta(s_m = i, a_m = j)}$$

m^{th} training example

$\delta(X) = 1$ if X is true
0 otherwise

- EM Estimate is:

$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j)}$$

let's use a_m to represent value of A on the m^{th} example

Fully Observed

S	A	K	E	H
1	0	1	1	0
0	1	0	0	1
0	1	1	0	0
0	0	0	1	0
1	1	1	1	1

$$\theta_{K=1|S=0,A=1} =$$

Partially Observed

S	A	K	E	H
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- EM Estimate

$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j)}$$

$$\theta_{K=1|S=0,A=1} =$$

let's use a_m to represent value of A on the m^{th} example

Fully Observed

S	A	K	E	H
1	0	1	1	0
0	1	0	0	1
0	1	1	0	0
0	0	0	1	0
1	1	1	1	1

$$\theta_{K=1|S=0,A=1} = \frac{1}{1+1}$$

Partially Observed

S	A	K	E	H
1	0	1	1	0
0	1	?	0	1
0	1	1	0	0
0	?	0	1	0
1	1	1	1	1

EM Approach

Pr	S	A	K	E	H
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m^{th} training example

$\delta(X) = 1$ if X is true
0 otherwise

- EM Estimate $\theta_{K=1|S=0,A=1} = \frac{0.6 + 1 + 0.2}{0.6 + 0.4 + 1 + 0.2}$

$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j)}$$

- Fractional examples
- Replace $\delta(X)$ by $P(X)$
- Replaces counts by expected values
- iterate!

let's use a_m to represent value of A on the m^{th} example

EM algorithm



- Let X be all *observed* variable values (over all examples)
- Let Z be all *unobserved* variable values

EM algorithm:

- Iterate until convergence:
 - E step: use current Bayes net parameters θ to estimate unobserved Z values

S	A	K	E	H
1	0	1	1	0
0	1	?	0	1
0	1	1	0	0
0	?	0	1	0
1	1	1	1	1

Pr	S	A	K	E	H
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1.0	0	1	1	0	0
0.2	0	1	0	1	0
0.8	0	0	0	1	0
1.0	1	1	1	1	1

- M step: use estimated values of Z to retrain Bayes net params θ

$$\theta_{K=1|S=i,A=j} = \frac{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j, k_m = 1)}{\sum_{m=1}^M P_{\theta}(s_m = i, a_m = j)}$$

Expected value =
probability weighted average

$$E_{P(X)}[f(X)] = \sum_x P(X = x) f(x)$$

Expected value =
probability weighted average

$$E_{P(X)}[f(X)] = \sum_x P(X = x) f(x)$$

Let X be all *observed* variable values (over all examples)

Let Z be all *unobserved* variable values over all examples

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

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

* EM guaranteed to find local maximum

- EM seeks estimate:

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



- suppose for every example, observed $X=\{S,A,E,H\}$, unobserved $Z=\{K\}$
- how do we calculate $E_{P(Z|X,\theta)} \log P(X, Z|\theta)$ over our M training examples?

$$\log P(X, Z|\theta) = \sum_{m=1}^M \log P(s_m) + \log P(a_m) + \log P(k_m|s_m, a_m) + \log P(e_m|k_m) + \log P(h_m|k_m)$$

$$E_{P(Z|X,\theta)} \log P(X, Z|\theta)$$

$$= \sum_{m=1}^M \sum_{i=0}^1 P(k=i|s_m, a_m, e_m, h_m) [\log P(s_m) + \log P(a_m) + \log P(k=i|s_m, a_m) + \log P(e_m|k=i) + \log P(h_m|k=i)]$$

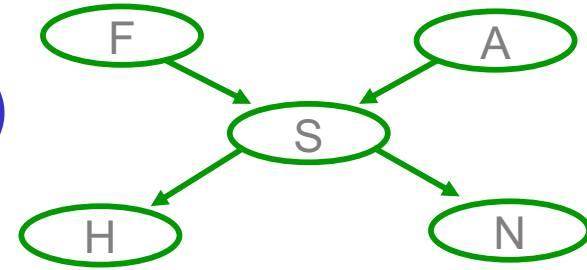
m^{th} training example

This corresponds to splitting each training example into two probabilistically weighted examples

let's use a_m to represent value of A on the m^{th} example

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

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



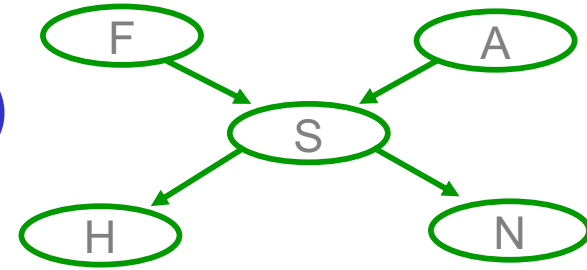
How? Bayes net inference problem.

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

let's use a_k to represent value of A on the k th example

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

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



How? Bayes net inference problem.

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

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

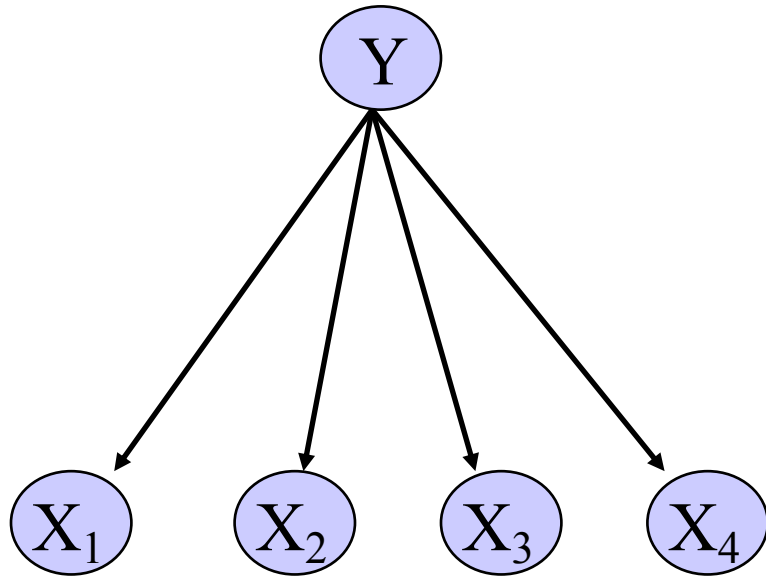
let's use a_k to represent value of A on the k th example

EM in general

- Unobserved data points can be any combination of variables sometimes observed , sometimes not
- You can build a MAP version instead of MLE version of EM
- Basis for many important algorithms
 - Hidden markov models
 - Unsupervised clustering

Using Unlabeled Data to Help Train Naïve Bayes Classifier

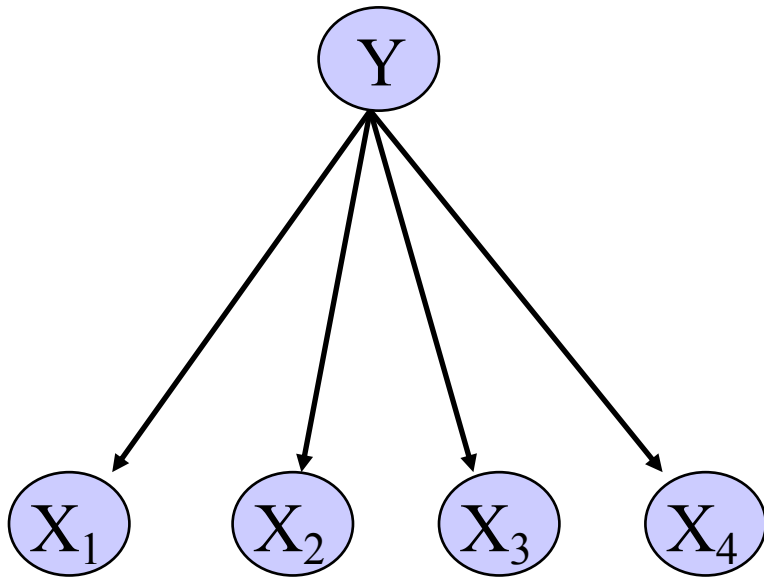
Learn $P(Y|X)$



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

Using Unlabeled Data to Help Train Naïve Bayes Classifier

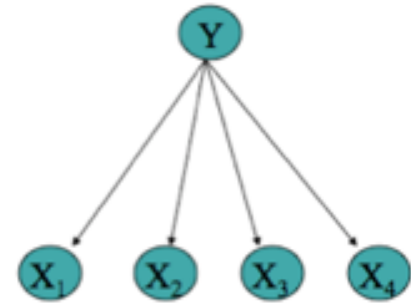
Learn $P(Y|X)$



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

$$P(Y=1 | x_1, x_2, x_3, x_4) = \frac{P(Y=1) \prod_i P(x_i | Y=1)}{\sum_k P(Y=k) \prod_i P(x_i | Y=k)}$$

EM and estimating θ



Given observed set X , unobserved set Y of boolean values

E step: Calculate for each training example, k

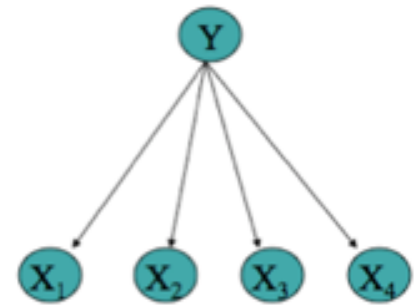
the expected value of each unobserved value of variable Y

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

k^{th} training example

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

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

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

k^{th} training example

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

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

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

-
- **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 $\hat{\theta} = \arg \max_{\theta} P(\mathcal{D}|\theta)P(\theta)$ (see Equations 5 and 6).
 - Loop while classifier parameters improve, as measured by the change in $l_c(\theta|\mathcal{D}; \mathbf{z})$ (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, $P(c_j|d_i; \hat{\theta})$ (see Equation 7).
 - **(M-step)** Re-estimate the classifier, $\hat{\theta}$, given the estimated component membership of each document. Use maximum a posteriori parameter estimation to find $\hat{\theta} = \arg \max_{\theta} P(\mathcal{D}|\theta)P(\theta)$ (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

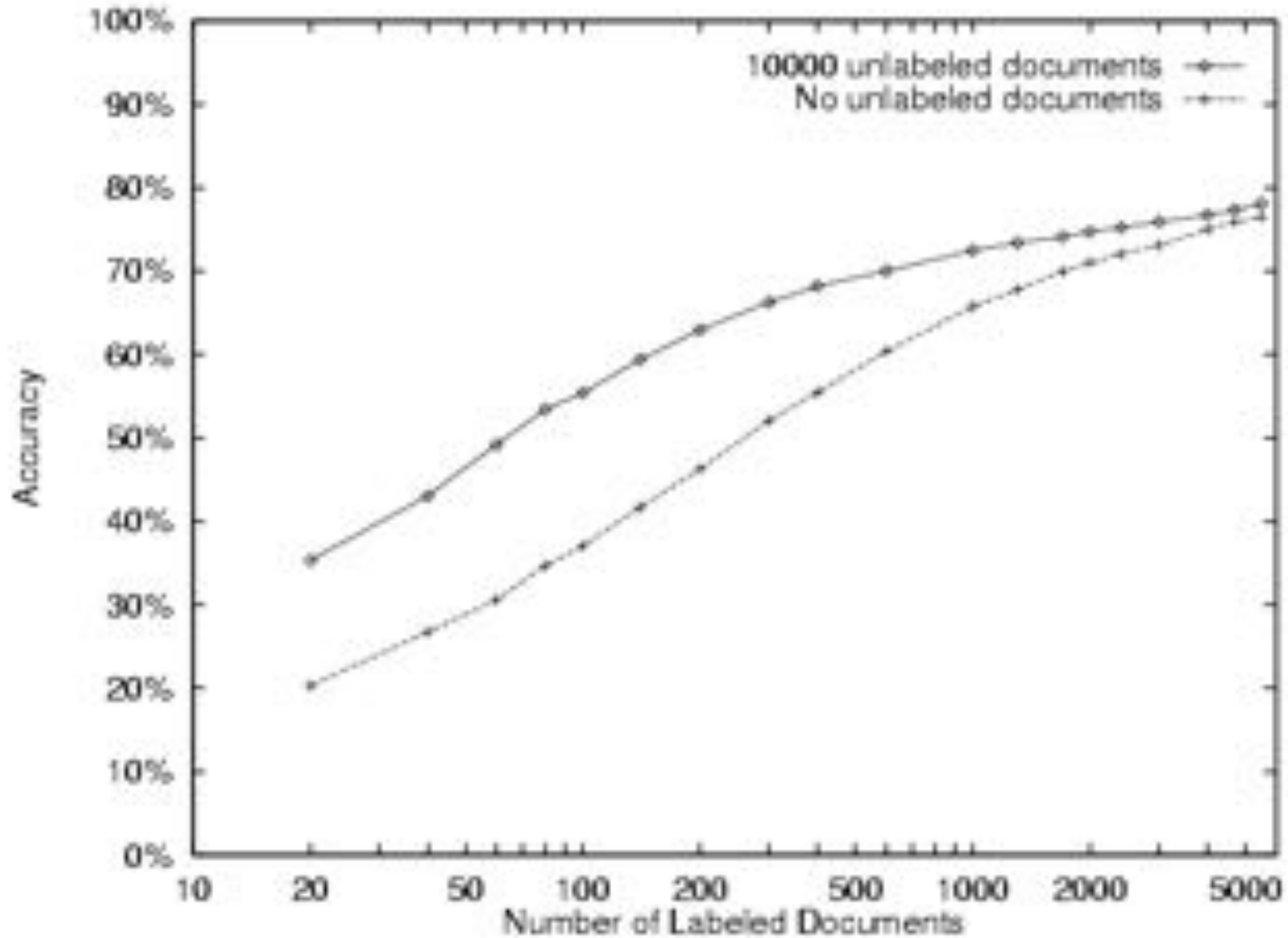


Table 3. Lists of the words most predictive of the course class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common course-related words appear. The symbol D indicates an arbitrary digit.

Iteration 0		Iteration 1	Iteration 2
intelligence	word w ranked by $P(w Y=\text{course})$ $/P(w Y \neq \text{course})$	DD	D
DD		D	DD
artificial		lecture	lecture
understanding		cc	cc
DDw		D^*	$DD:DD$
dist		$DD:DD$	due
identical		handout	D^*
rus		due	homework
arrange		problem	assignment
games		set	handout
dartmouth		lay	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	aseaf	ascii	

Using one labeled example per class

What you should know about EM

- For learning from partly unobserved data
- MLE of $\theta = \arg \max_{\theta} \log P(\text{data}|\theta)$
- EM estimate: $\theta = \arg \max_{\theta} E_{Z|X,\theta}[\log P(X, Z|\theta)]$
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 $E_{Z|X,\theta}[\log P(X, Z|\theta)]$
 - E step: for each training example X^k , calculate $P(Z^k | X^k, \theta)$
 - M step: chose new θ to maximize $E_{Z|X,\theta}[\log P(X, Z|\theta)]$

Unsupervised clustering

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

Clustering

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

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

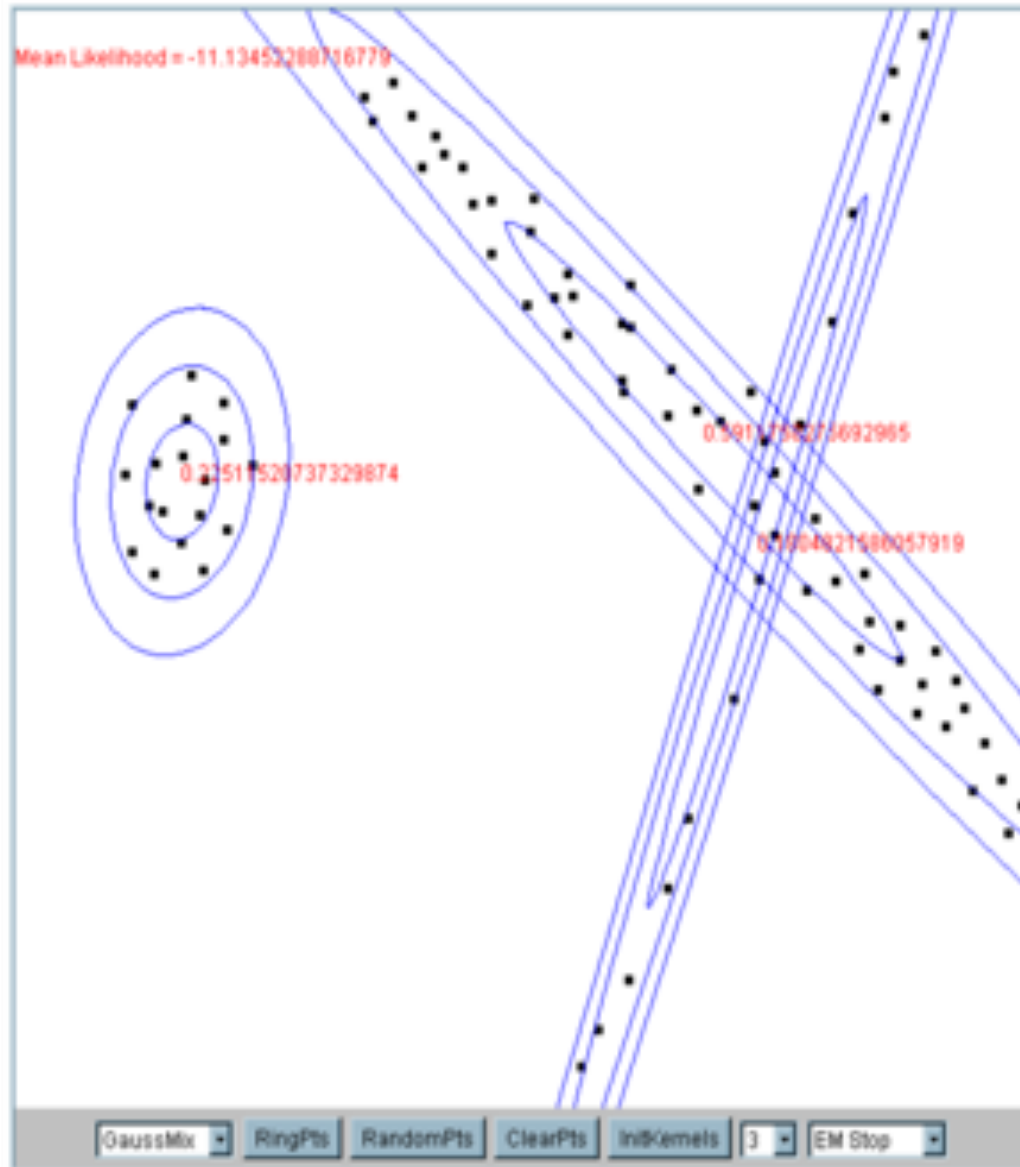
So

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

Mixture of *Gaussians*:

- Assume each data point $X = \langle X_1, \dots, X_n \rangle$ 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 $\langle x_1, x_2 \dots x_n \rangle$ 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 $X = \langle X_1 \dots X_n \rangle$, and the X_i are conditionally independent given Z .

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

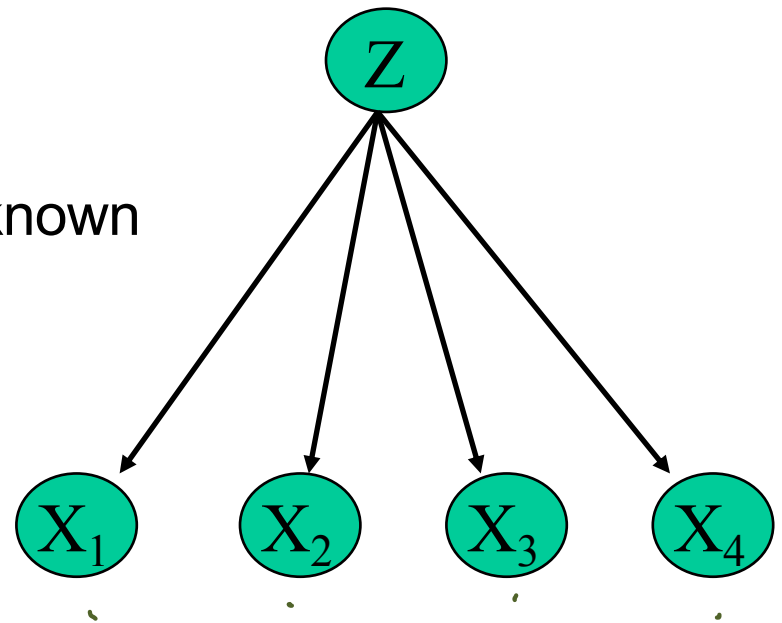
2. assume only 2 clusters (values of Z), and $\forall i, j, \sigma_{ji} = \sigma$

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

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

Observed: $X = \langle X_1 \dots X_n \rangle$

Unobserved: Z

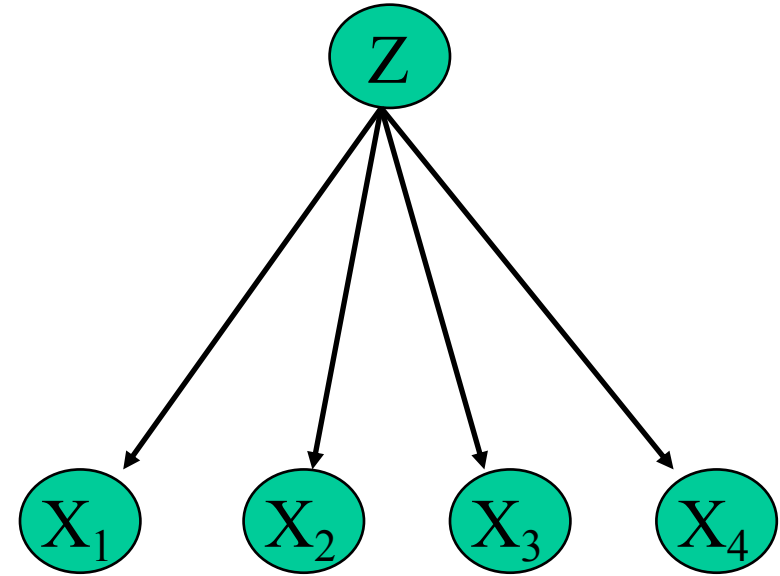


EM

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:

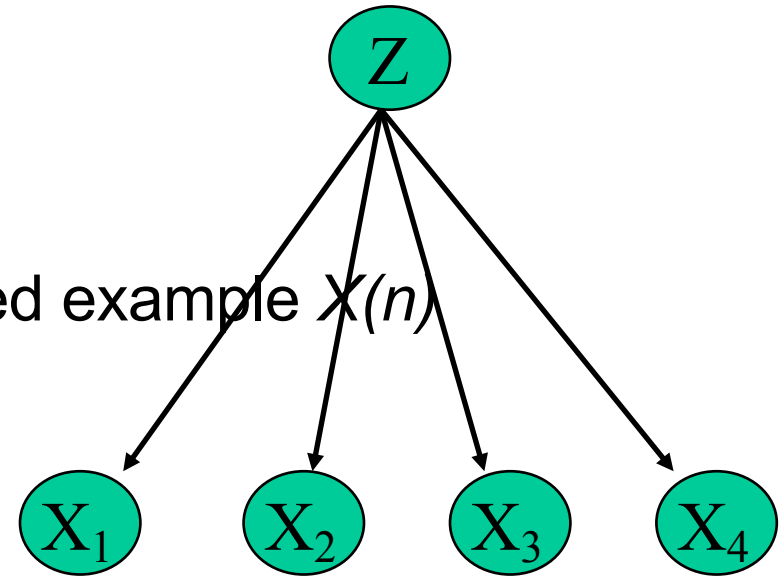
- E Step: Calculate $P(Z(n)|X(n), \theta)$ for each example $X(n)$. Use this to construct $Q(\theta'|\theta)$

- 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 $X(n)$

$X(n) = \langle x_1(n), x_2(n), \dots, x_T(n) \rangle$.



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

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

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

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 n th example

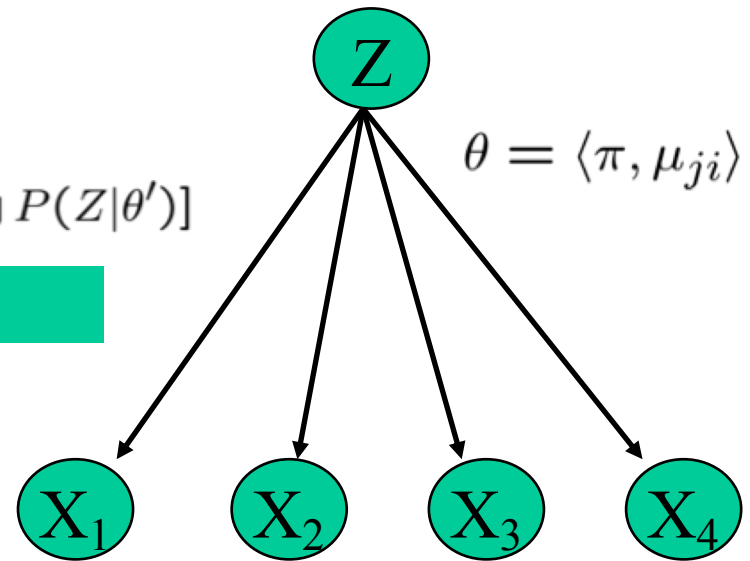
$$E_{Z|X,\theta}[\log P(Z|\pi')] = E_{Z|X,\theta}[\log (\pi'^{\sum_n z(n)} (1 - \pi')^{\sum_n (1 - z(n))})]$$

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

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

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

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

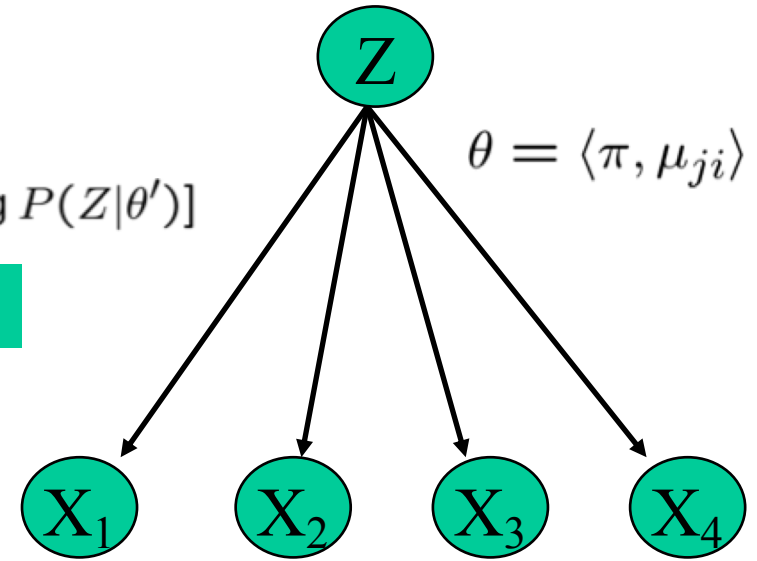


EM – M Step

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



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

...

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

Compare above to MLE if Z were observable:

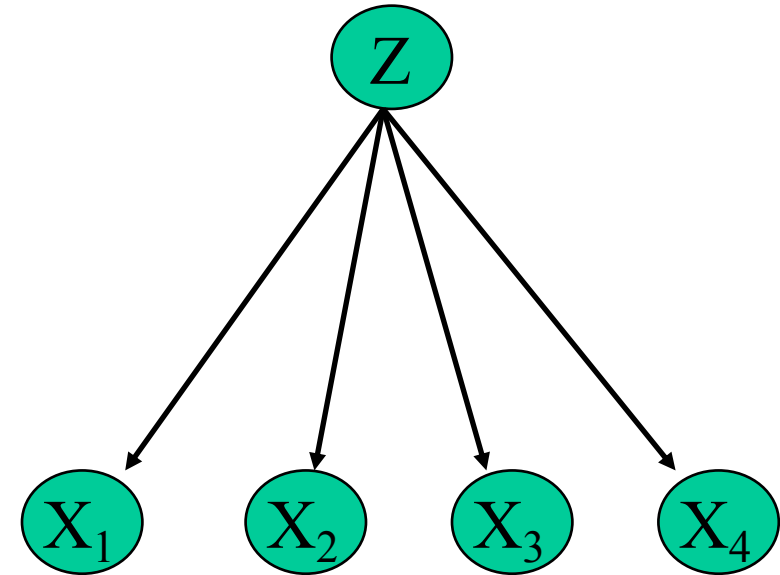
$$\mu_{ji} \leftarrow \frac{\sum_{n=1}^N \delta(z(n) = j) x_i(n)}{\sum_{n=1}^N \delta(z(n) = j)}$$

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 $P(Z(n)|X(n), \theta)$

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

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

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

(Handwritten note: $P(z=1)$ with an arrow pointing to π)

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