

# CS 4824/ECE 4424: Expectation Maximization

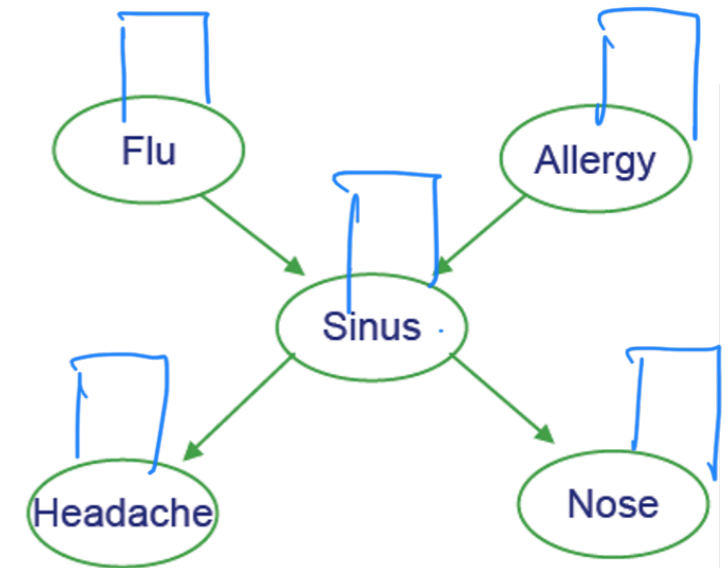
## *Acknowledgement:*

Many of these slides are derived from Tom Mitchell, Pascal Poupart, Pieter Abbeel, Eric Eaton, Carlos Guestrin, William Cohen, and Andrew Moore.

# Estimate $\theta$ from partly observed data — recap

- 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)

$$X = \{F, A, H, N\}$$

- Let  $Z$  be all unobserved variable values

$$Z = \{S\}$$

- Can't calculate MLE

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

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

- Estimate:

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

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

- Maximum likelihood estimate

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

- Our case

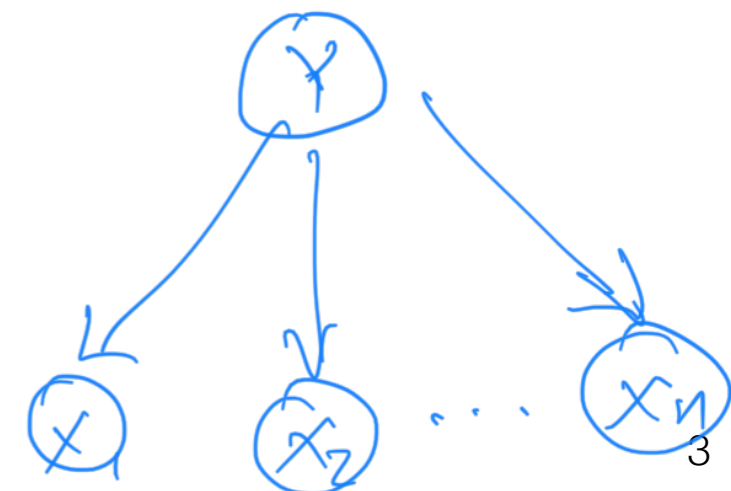
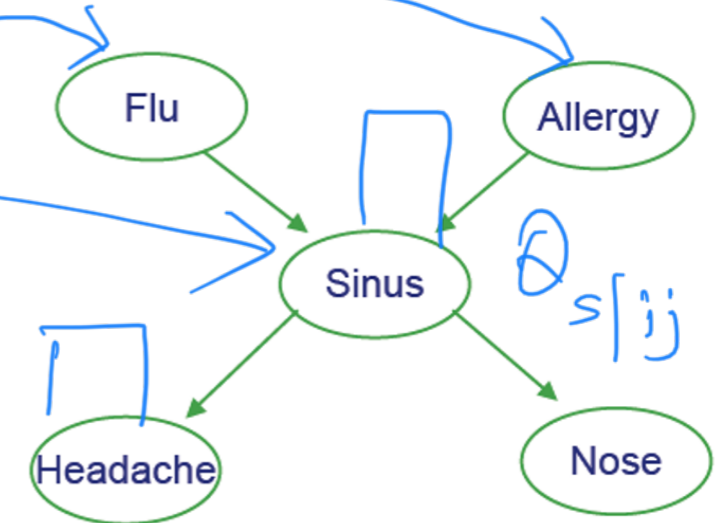
$$P(\text{data}|\theta) = \prod_{k=1}^K P(f_k, a_k, s_k, h_k, n_k)$$

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

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

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

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



# Estimate $\theta$ from partly observed data

- What if FAHN observed, but not S?

- Can't calculate MLE

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

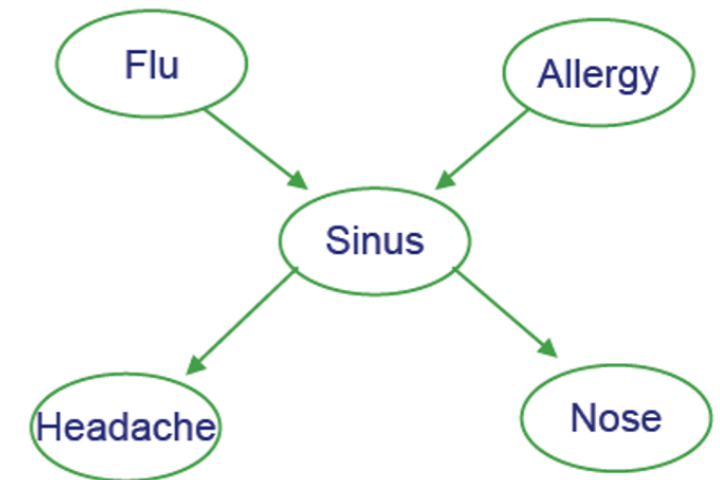
- Let  $X$  be all *observed* variable values (over all examples)

- 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 $\theta$ from partly observed data

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

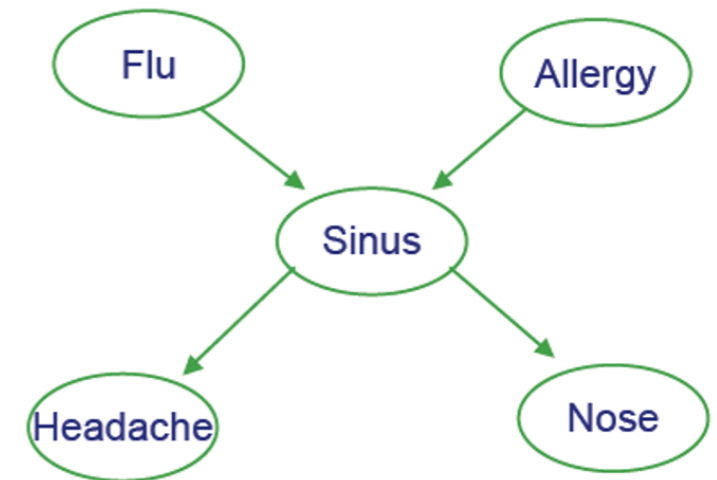
$$\theta \leftarrow \arg \max_{\theta} \log \prod_k P(f_k, a_k, s_k, h_k, n_k | \theta)$$

- 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:

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

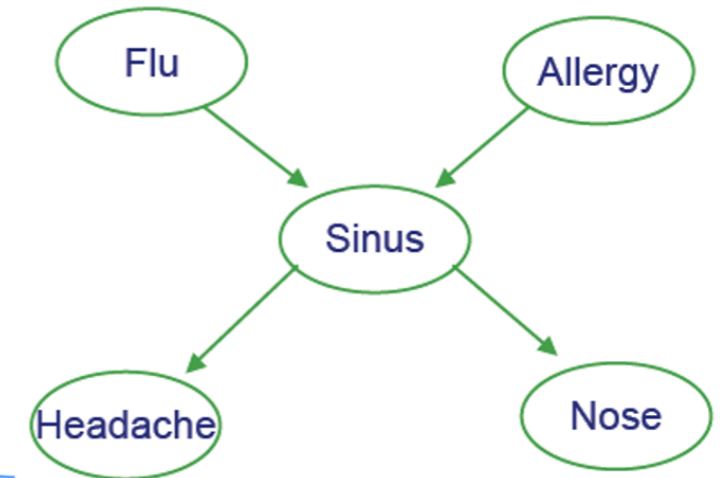


\* EM guaranteed to find local optima

# Estimate $\theta$ from partly observed data

- EM seeks to estimate:

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



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

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

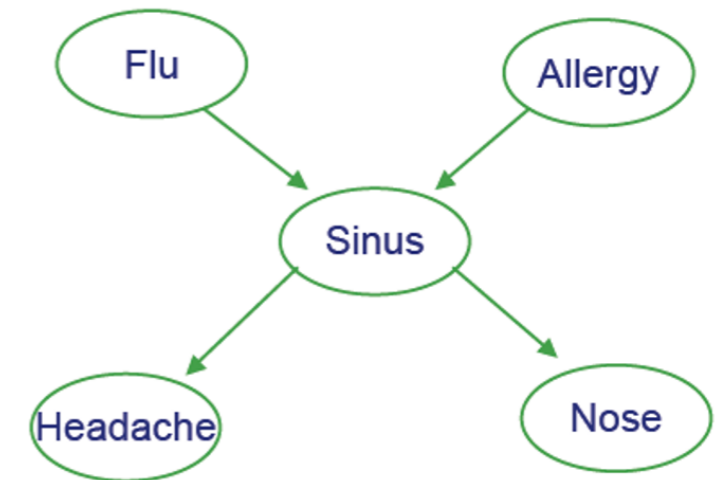
$$E_{P(Z|X,\theta)} \log P(X, Z|\theta) = \sum_{k=1}^K \sum_{i=0}^1 P(S_k = i | f_k, a_k, h_k, n_k) \left[ \log P(f_k) + \log P(a_k) + \log P(s_k | f_k, a_k) + \log P(h_k | s_k) + \log P(n_k | s_k) \right]$$



# Estimate $\theta$ from partly observed data

- EM seeks to estimate:

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



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

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

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

# 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  $\theta$  ←

Iterate until convergence:

- E Step: estimate the values of unobserved  $Z$  conditioned on  $X$  using  $\theta$
- M Step: use observed values plus E-step estimates to derive a better  $\theta$

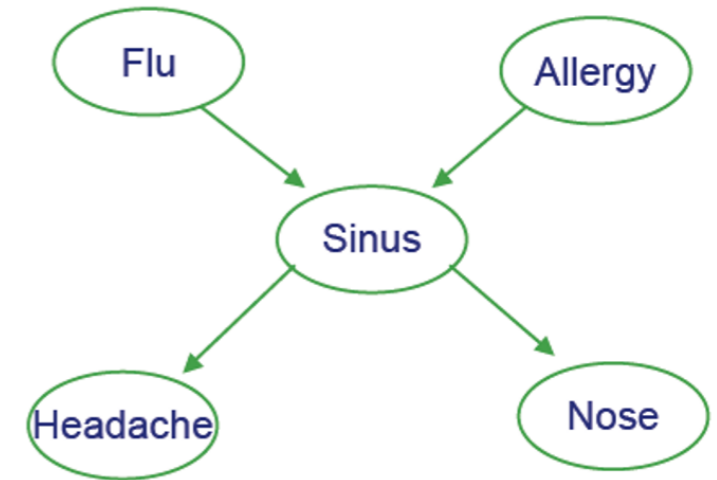
- Guaranteed to find local maximum. Each iteration increases

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



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

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



- How? Bayes net inference problem

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

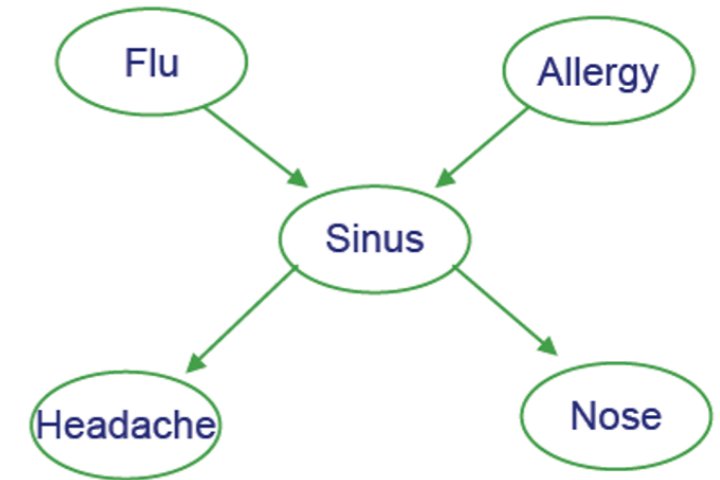
$$\frac{P(S_k = 1, f_k, a_k, h_k, n_k | \theta)}{P(f_k, a_k, h_k, n_k | \theta)}$$

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

$$P(S=1, f_k, a_k, h_k, n_k | \theta) + P(S=0, f_k, a_k, h_k, n_k | \theta)$$

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

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

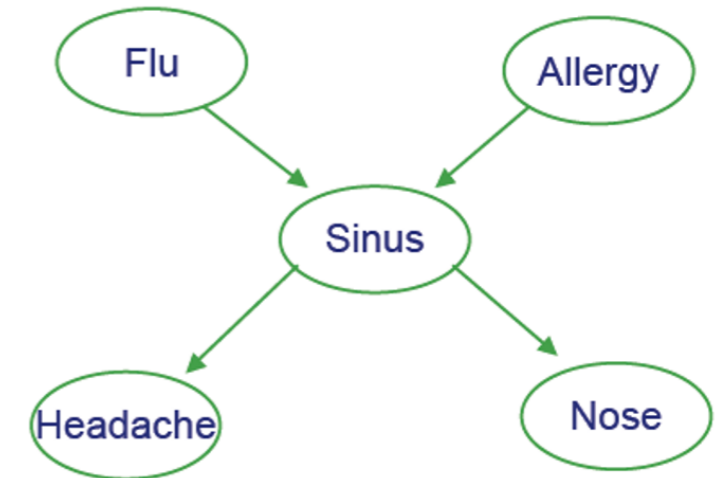


- How? Bayes net inference problem

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

# 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,  $k$

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

- M Step: update all relevant parameters.

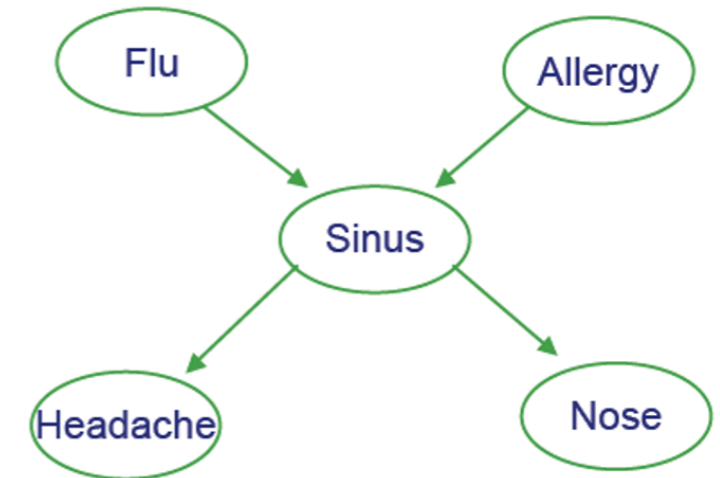
$$\theta_{s|ij} \leftarrow \frac{\sum_{k=1}^K \delta(f_k=i, a_k=j) E[s_k]}{\sum_{k=1}^K \delta(f_k=i, a_k=j)}$$

What was MLE?

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

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

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



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

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

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

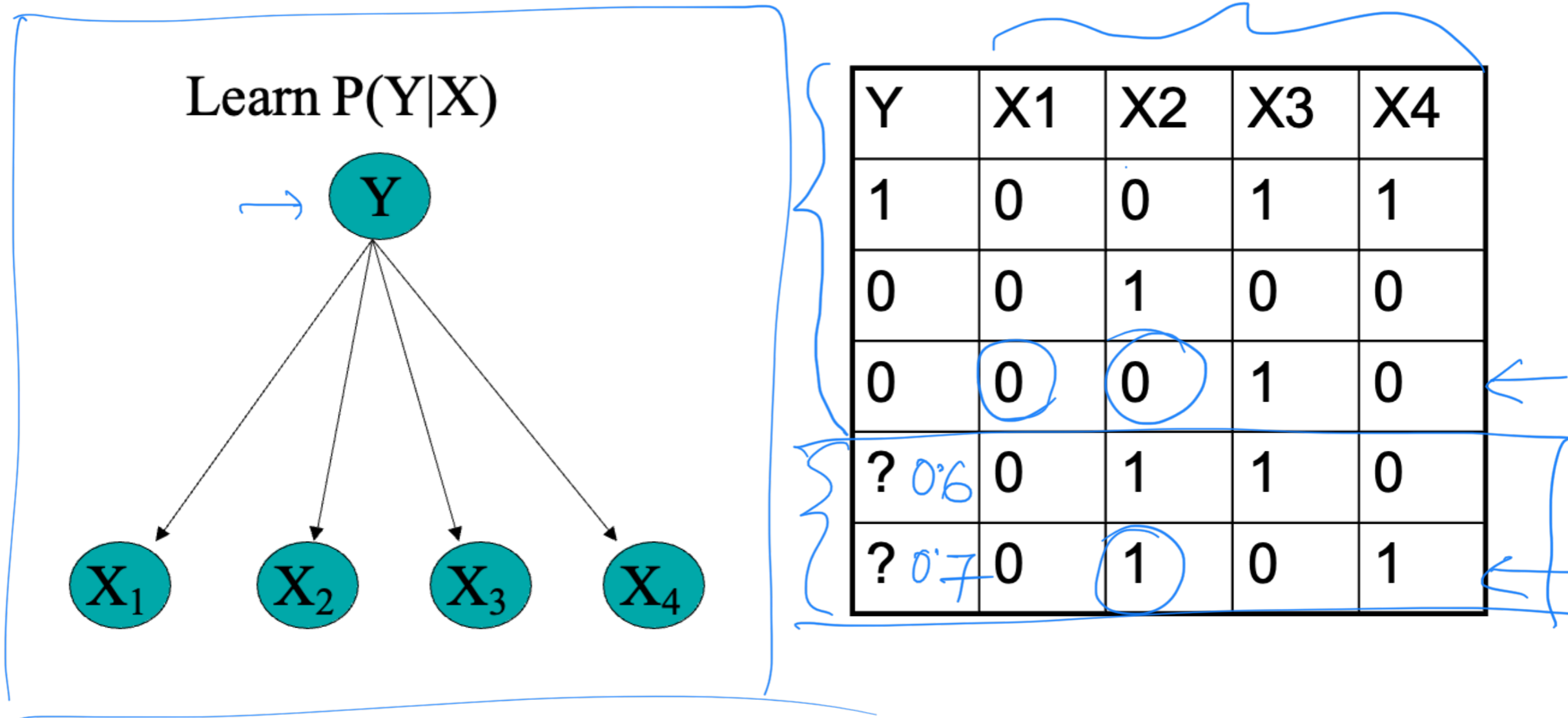
# Generalizing: EM and estimating $\theta$

- 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

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

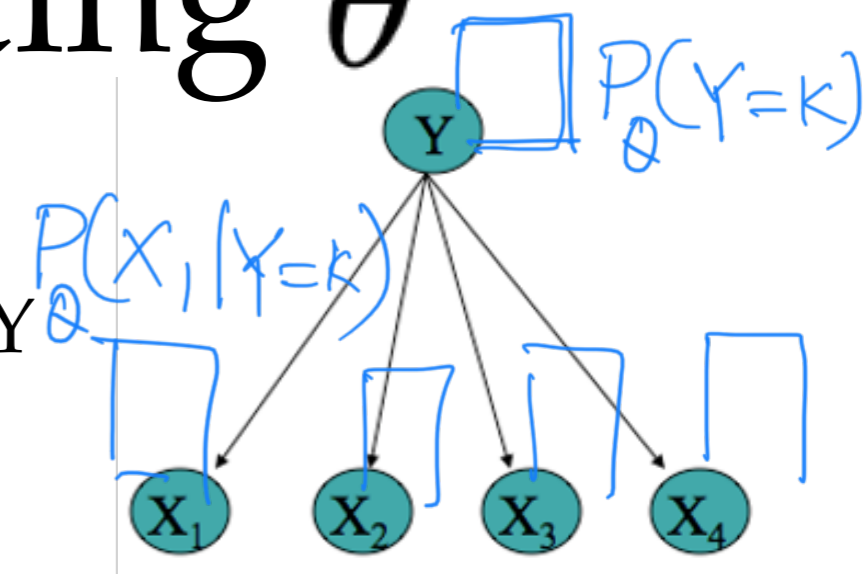
# Using (partially) unlabeled data to help train naïve Bayes classifier



semi-supervised learning

# EM and estimating $\theta$

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



$$\mathbb{E}[Y=k] = P_{\theta}(Y=k | x_1 \dots x_4)$$

$$= \frac{P_{\theta}(x_1 \dots x_4 | Y=k) P_{\theta}(Y=k)}{\sum_j P_{\theta}(x_1 \dots x_4 | Y=j) P_{\theta}(Y=j)}$$

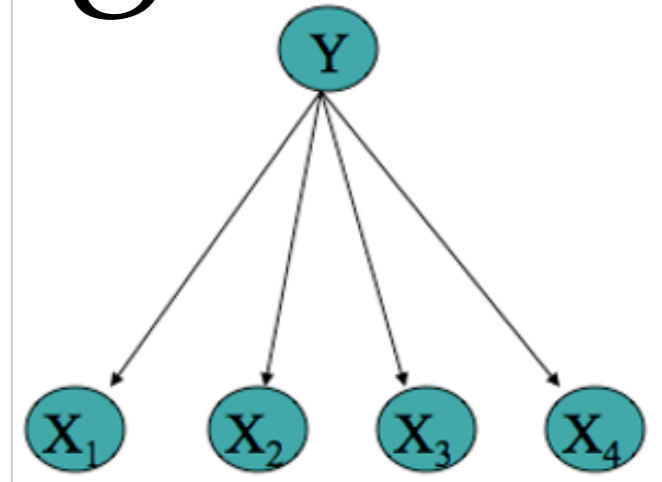
Bayes Rule

$$\prod_{i=1}^4 P(x_i | Y=k)$$



# EM and estimating $\theta$

- Observed set  $X$
- Partially unobserved set  $Y$  of boolean values



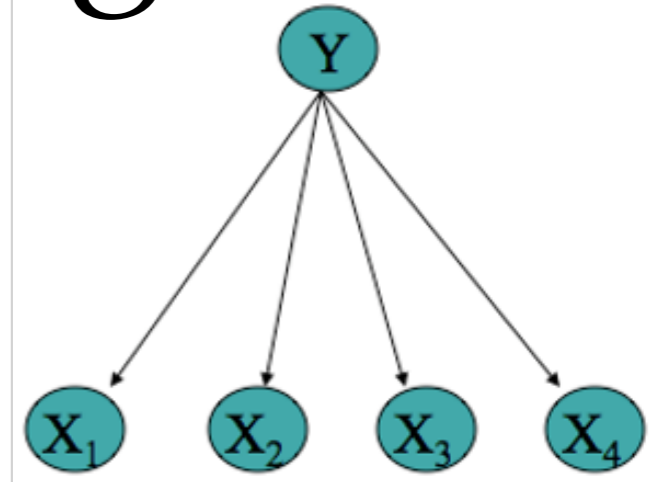
- E step: Calculate for each training example  $k$ , the expected value of each unobserved variable  $Y$

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

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

# EM and estimating $\theta$

- Observed set  $X$
- Partially unobserved set  $Y$  of boolean values



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

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

- 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:

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

# EM algorithm – summary

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

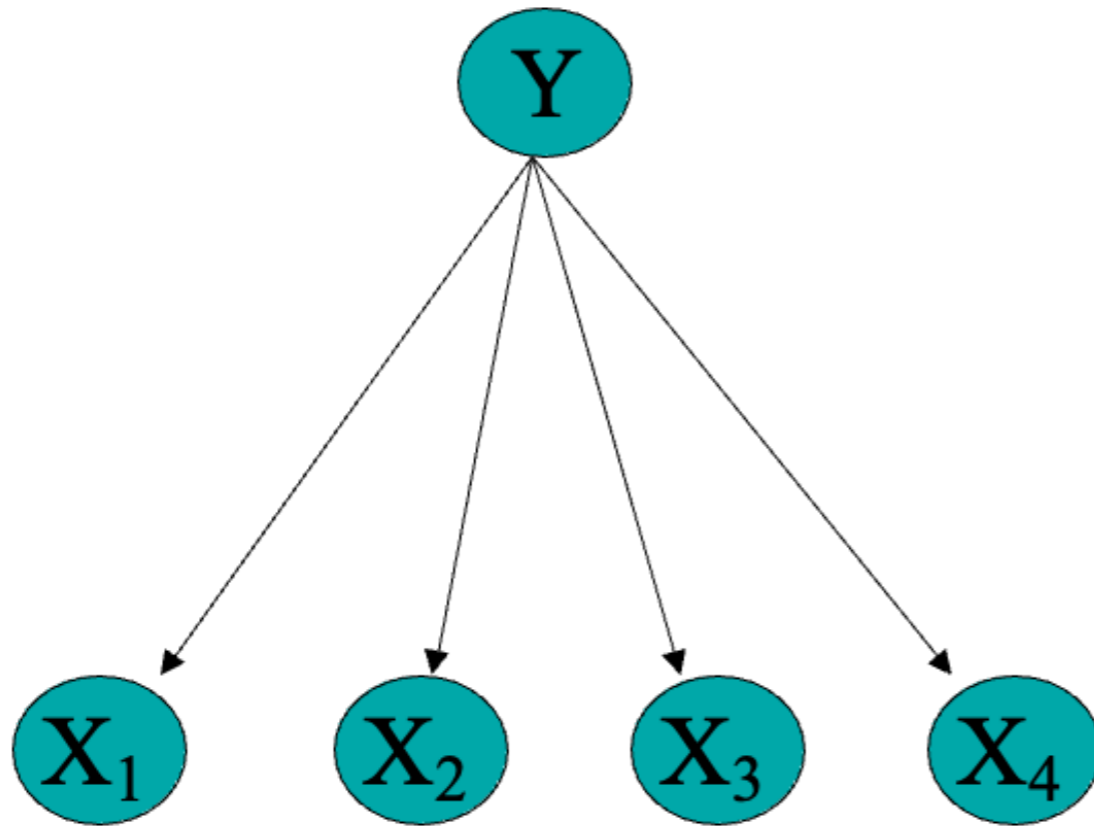
Begin with arbitrary choice for parameters  $\theta$

Iterate until convergence:

- E Step: Use  $X$  and current  $\theta$  to calculate  $P(Z|X,\theta)$
  - M Step: Replace current  $\theta$  by  $\theta \leftarrow \arg \max_{\theta'} Q(\theta'|\theta)$
- Guaranteed to find local maximum. Each iteration increases

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

# What if we have no labeled data at all ?



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

un  
~~semi~~-supervised learning  
^

# Unsupervised clustering

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