CSCI 5090/7090- Machine Learning

Spring 2018

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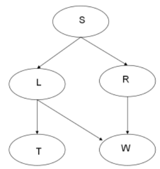
Graphical Models:

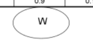
- Inference
- Learning
- EM

(slides borrowed from Tom Mitchell)

Bayesian Networks Definition



Parents	P(W|Pa)	P(¬W|Pa)
L, R	0	1.0
L, ¬R	0	1.0
¬L, R	0.2	0.8
¬L, ¬R	0.9	0.1



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

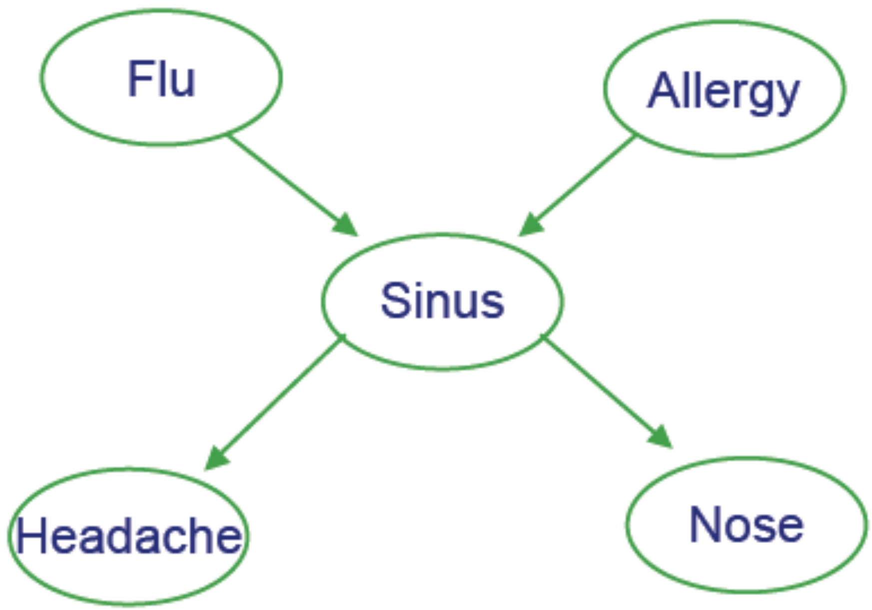
$$P(X_1 \ldots X_n) = \prod_i P(X_i | Pa(X_i))$$

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

- What is the Bayes Net for Naïve Bayes?

Example

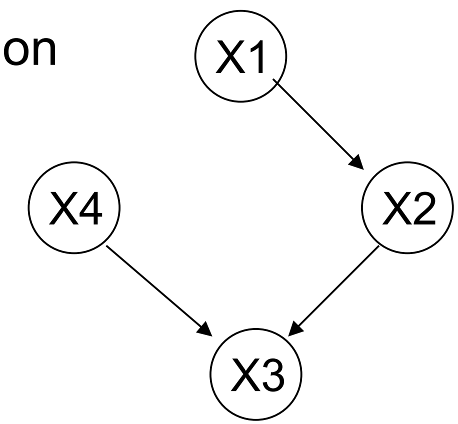
- Bird flu and Allegies both cause Sinus problems
- Sinus problems cause Headaches and runny Nose



Conditional Independence, Revisited

- We said:
  - Each node is conditionally independent of its non-descendents, given its immediate parents.

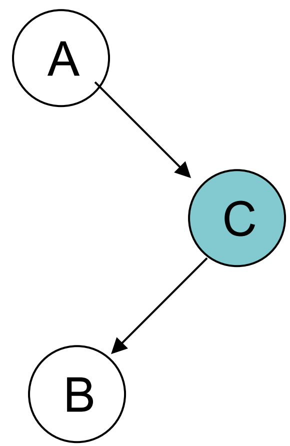
- Does this rule give us all of the conditional independence relations implied by the Bayes network?
  - No!
  - E.g., X1 and X4 are conditionally indep given {X2, X3}
  - But X1 and X4 not conditionally indep given X3
  - For this, we need to understand D-separation



Easy Network 1: Head to Tail

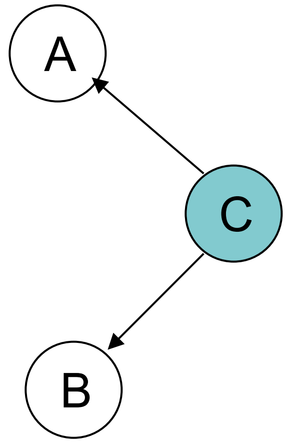
prove A cond indep of B given C?

ie., $p(a,b|c) = p(a|c)\, p(b|c)$

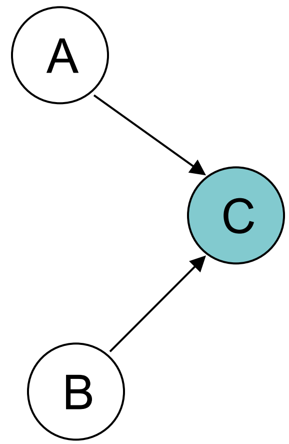


Easy Network 2: Tail to Tail

prove A cond indep of B given C?   ie., $p(a,b|c) = p(a|c)\, p(b|c)$



Easy Network 3: Head to Head



prove A cond indep of B given C?   NO!

Summary:

- p(a,b)=p(a)p(b)
- p(a,b|c) NotEqual p(a|c)p(b|c)

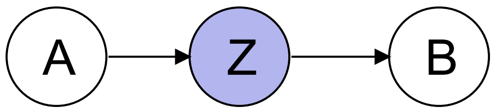
X and Y are conditionally independent given Z, **<u>if and only if</u>** X and Y are D-separated by Z.

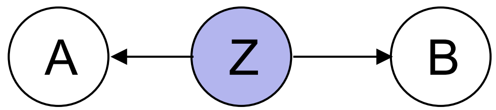
[Bishop, 8.2.2]

Suppose we have three sets of random variables: X, Y and Z

X and Y are **<u>D-separated</u>** by Z (and therefore conditionally indep, given Z) iff every path from every variable in X to every variable in Y is **<u>blocked</u>**

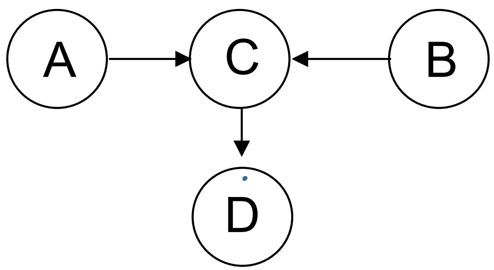
A path from variable X to variable Y is **blocked** if it includes a node in Z such that either





1. arrows on the path meet either head-to-tail or tail-to-tail at the node and this node is in Z

2. or, the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, is in Z



X and Y are **D-separated** by Z (and therefore conditionally indep, given Z) iff every path from every variable in X to every variable in Y is **blocked**

A path from variable A to variable B is **blocked** if it includes a node such that either

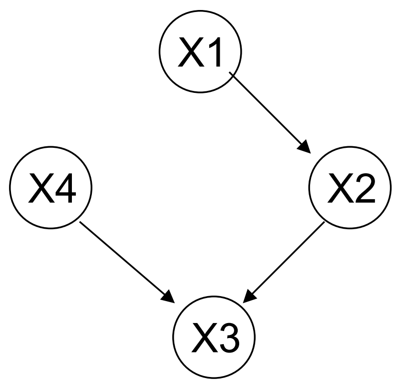
1. arrows on the path meet either head-to-tail or tail-to-tail at the node and this node is in Z

2. or, the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, is in Z

X1 indep of X3 given X2?

X3 indep of X1 given X2?

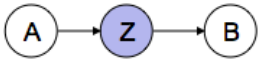
X4 indep of X1 given X2?

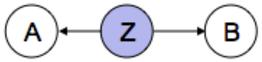


X and Y are **D-separated** by Z (and therefore conditionally indep, given Z) iff every path from any variable in X to any variable in Y is **blocked** by Z

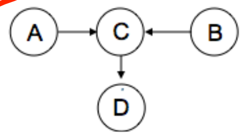
A path from variable A to variable B is **blocked** by Z if it includes a node such that either

1. arrows on the path meet either head-to-tail or tail-to-tail at the node and this node is in Z





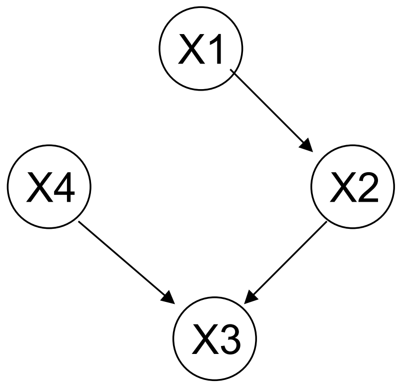
2. the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, is in Z



X4 indep of X1 given X3?

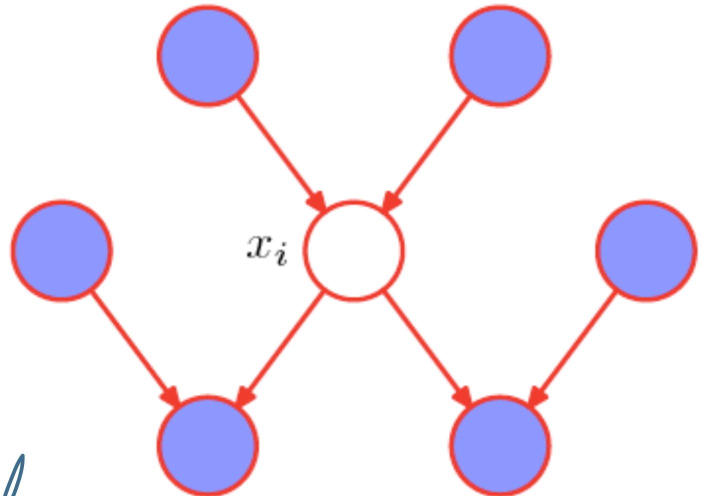
X4 indep of X1 given {X3, X2}?

X4 indep of X1 given {}?



Markov Blanket

The Markov blanket of a node $\mathbf{x}_i$ comprises the set of parents, children and co-parents of the node. It has the property that the conditional distribution of $\mathbf{x}_i$, conditioned on all the remaining variables in the graph, is dependent only on the variables in the Markov blanket.



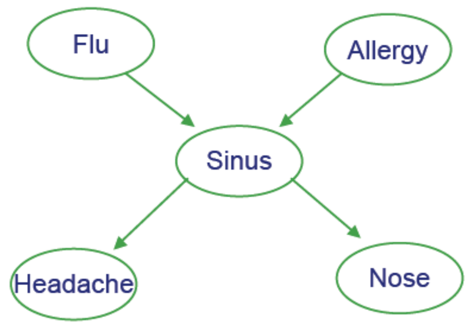
co-parent = other side of X_i's colliders

from [Bishop, 8.2]

What You Should Know

- Bayes nets are convenient representation for encoding dependencies / conditional independence
- BN = Graph plus parameters of CPD's
  - Defines joint distribution over variables
  - Can calculate everything else from that
  - Though inference may be intractable
- Reading conditional independence relations from the graph
  - Each node is cond indep of non-descendents, given only its parents
  - X and Y are conditionally independent given Z if Z D-separates every path connecting X to Y
  - Marginal independence : special case where Z={}

Prob. of joint assignment: easy

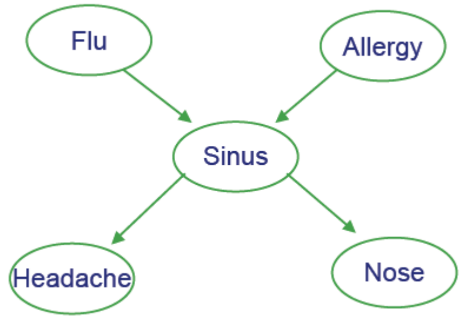


- Suppose we are interested in joint assignment <F=f,A=a,S=s,H=h,N=n>

What is P(f,a,s,h,n)?

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

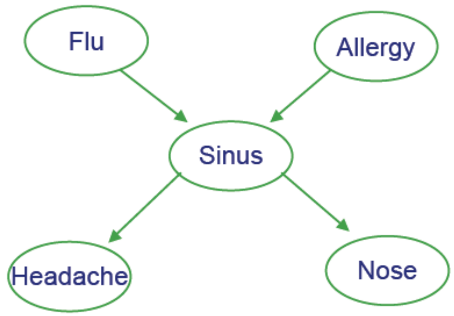
Prob. of marginals: not so easy



- How do we calculate P(N=n) ?

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

Generating a sample from joint distribution: easy



How can we generate random samples drawn according to P(F,A,S,H,N)?

Hint: random sample of F according to $P(F=1) = \theta_{F=1}$:

- draw a value of r uniformly from [0,1]
- if $r<\theta$ then output F=1, else F=0

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

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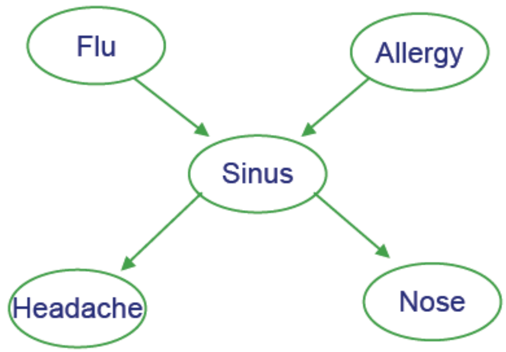


How can we generate random samples drawn according to P(F,A,S,H,N)?

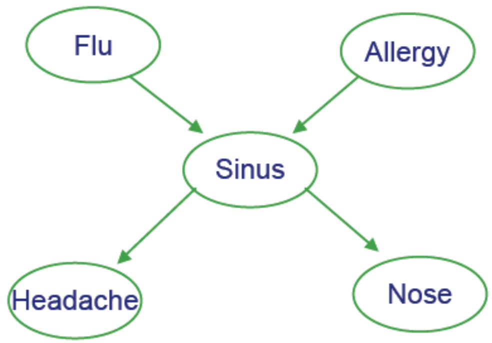
Hint: random sample of F according to $P(F=1) = \theta_{F=1}$:

- draw a value of r uniformly from [0,1]
- if $r<\theta$ then output F=1, else F=0

Solution:

- draw a random value f for F, using its CPD
- then draw values for A, for S|A,F, for H|S, for N|S

Generating a sample from joint distribution: easy



Note we can estimate marginals

like P(N=n) by generating many samples

from joint distribution, then count the fraction of samples for which N=n

Similarly, for anything else we care about

P(F=1|H=1, N=0)

→ weak but general method for estimating <u>any</u> probability term…

Inference in Bayes Nets

- In general, intractable (NP-complete)
- For certain cases, tractable
  - Assigning probability to fully observed set of variables
  - Or if just one variable unobserved
  - Or for singly connected graphs (ie., no undirected loops)
    - Variable elimination
    - Belief propagation
- Often use Monte Carlo methods
  - e.g., Generate many samples according to the Bayes Net distribution, then count up the results
  - Gibbs sampling
- Variational methods for tractable approximate solutions

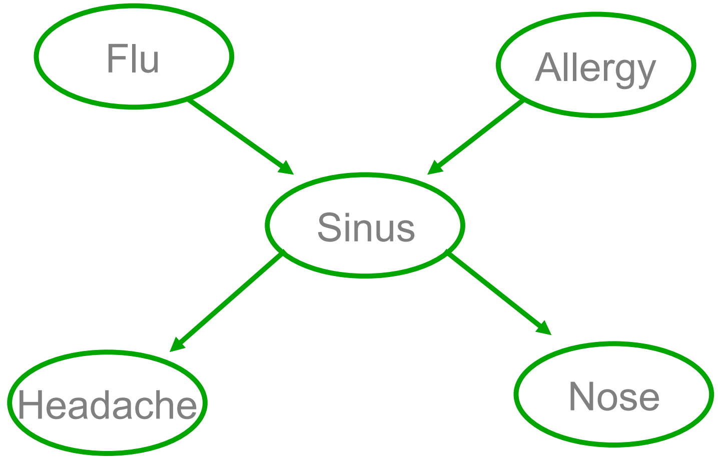
Learning of Bayes Nets

- 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

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

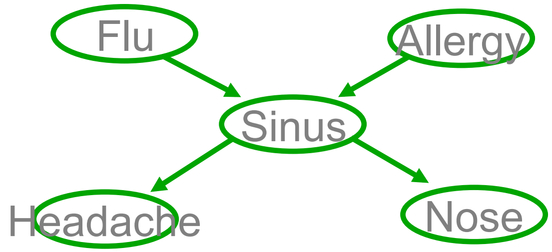
k^{th} training example

$\delta(x) = 1$ 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:

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

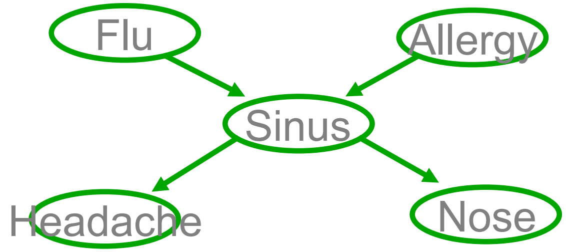
$$P(data|\theta) = \prod_{k=1}^{K} P(f_k)P(a_k)P(s_k|f_k a_k)P(h_k|s_k)P(n_k|s_k)$$

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

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

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

Estimate θ from partly observed data



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

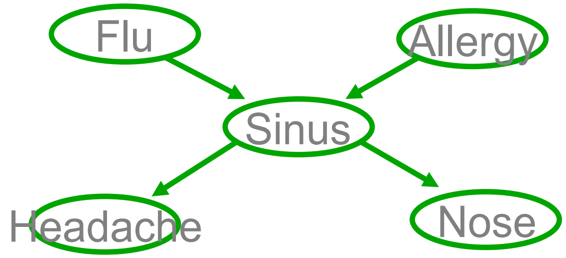
$$\theta \leftarrow \arg\max_\theta \log \prod_k P(f_k, a_k, s_k, h_k, n_k|\theta)$$

- 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



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- Can't calculate MLE:

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

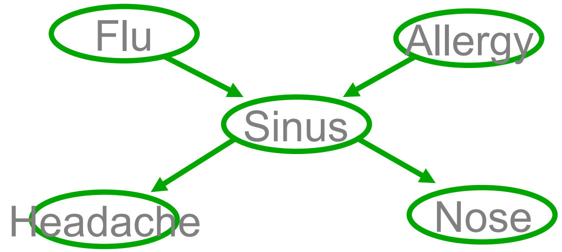
- EM seeks* to estimate:

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

* 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

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

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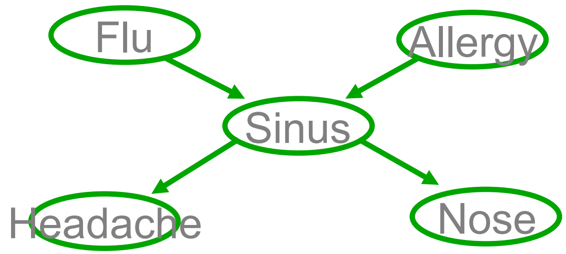
E Step: Use X, θ, to Calculate P(Z|X,θ)

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



- How? Bayes net inference problem.

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

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

observed X={F,A,H,N},
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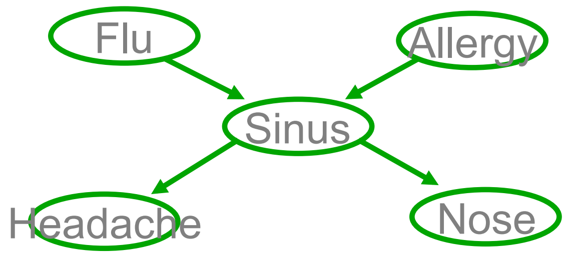
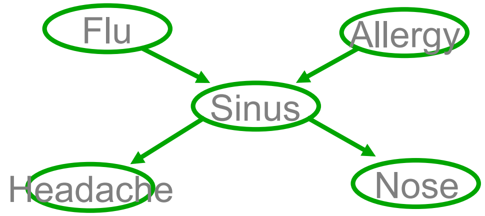


- How? Bayes net inference problem.

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

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

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

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

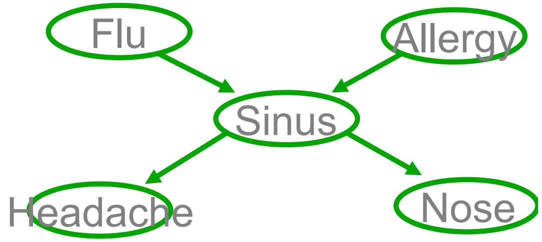
$P(Z|X;\theta)$

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

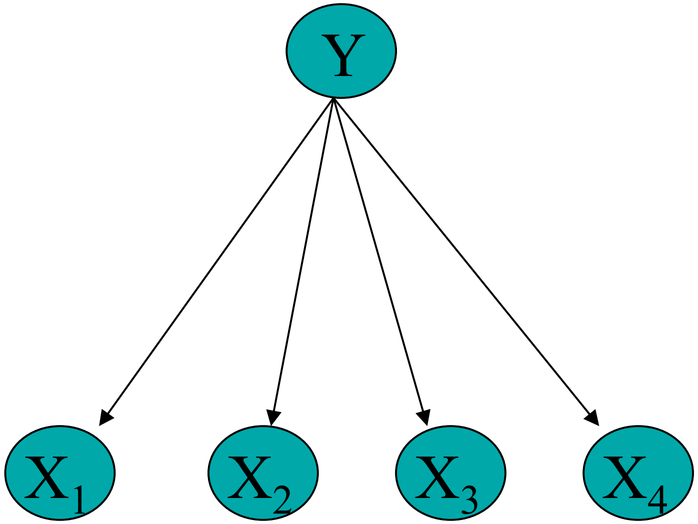
M step:

Calculate estimates similar to MLE, 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

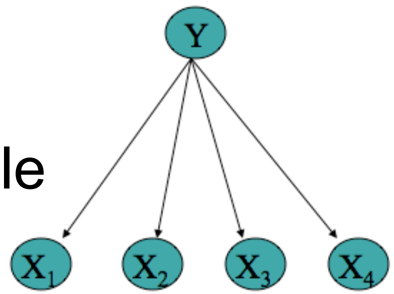
Learn P(Y|X)



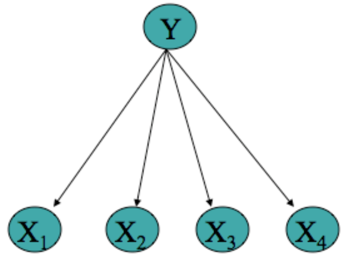
Y	X1	X2	X3	X4
1	0	0	1	1
0	0	1	0	0
0	0	0	1	0
?	0	1	1	0
?	0	1	0	1

E step: Calculate for each training example, k

the expected value of each unobserved variable



EM and estimating θ



Given observed set X, unobserved set Y of boolean values

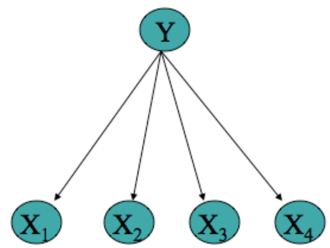
E step: Calculate for each training example, k

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 <u>expected count</u>

EM and estimating θ



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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 <u>expected count</u>

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

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

- **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 $\hat{\theta} = \arg\max_\theta \mathrm{P}(\mathcal{D}|\theta)\mathrm{P}(\theta)$ (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, $\mathrm{P}(c_j|d_i;\hat{\theta})$ (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 $\hat{\theta} = \arg\max_\theta \mathrm{P}(\mathcal{D}|\theta)\mathrm{P}(\theta)$ (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

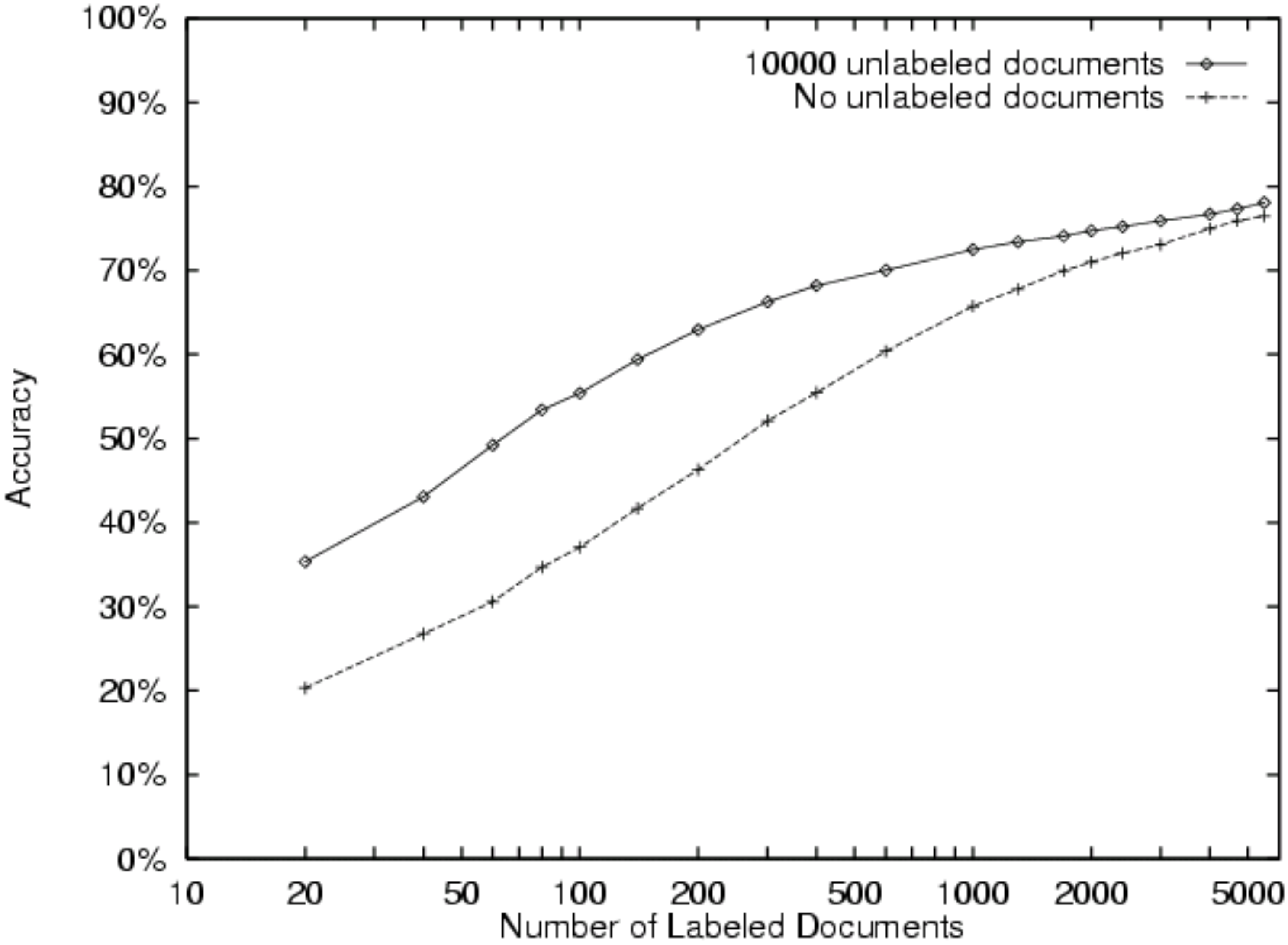


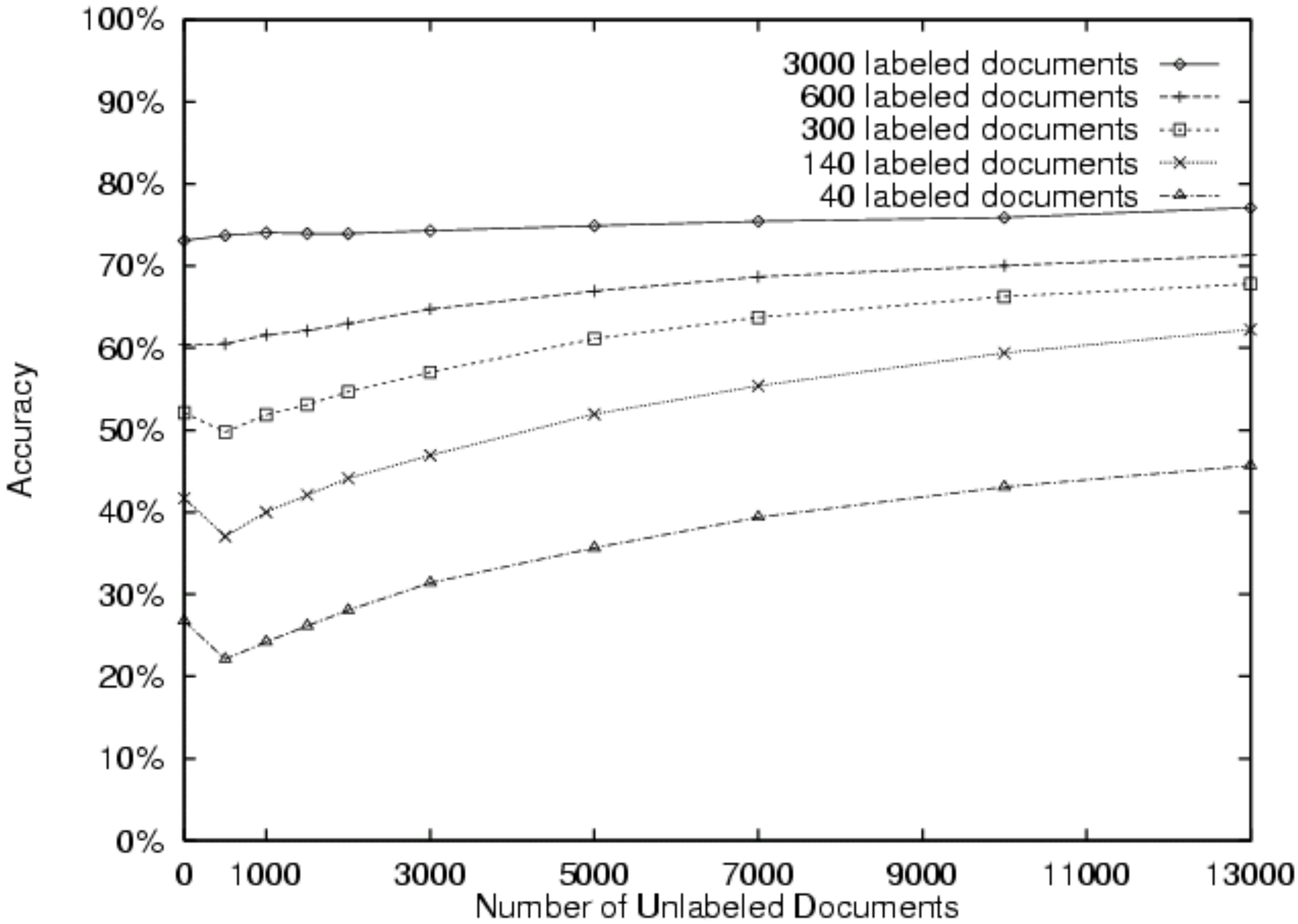
Table 3. Lists of the words most predictive of the course class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common course-related words appear. The symbol D indicates an arbitrary digit.

Iteration 0	Iteration 1	Iteration 2
intelligence	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=course) / P(w|Y ≠ course)

Using one labeled example per class

20 Newsgroups



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, some queries, exact inference is tractable
  - 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