Machine Learning 10-701

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

February 17, 2011

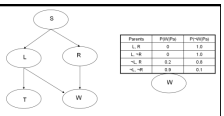
Today:

- Graphical models
- Learning from fully labeled data
- Learning from partly observed data
- EM

Readings:

Required:
- Bishop chapter 8, through 8.2

Bayes Network 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 CPD's

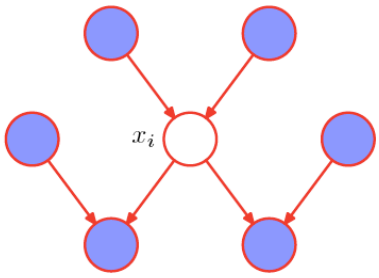
- Each node denotes a random variable
- Edges denote dependencies
- CPD for each node X_i defines $P(X_i \mid Pa(X_i))$
- The joint distribution over all variables is defined as

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

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

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.



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 its immediate parents
  - D-separation
  - 'Explaining away'

Java Bayes Net Applet

http://www.pmr.poli.usp.br/ltd/Software/javabayes/Home/applet.html

by **Fabio Gagliardi Cozman**

Learning of Bayes Nets

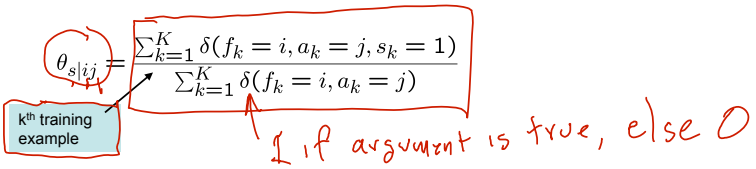
- Four categories of learning problems
  - Graph structure may be known/unknown
  - Variable values may be fully observed / partly unobserved
- Easy case: learn parameters for graph structure is *known*, and data is *fully observed*
- Interesting case: graph *known*, data *partly known*
- Gruesome case: graph structure *unknown*, data *partly unobserved*

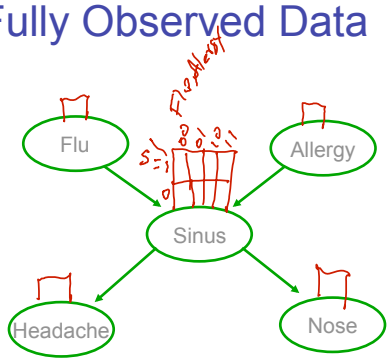
Learning CPTs from Fully Observed Data

- Example: Consider learning the parameter

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

- MLE (Max Likelihood Estimate) is





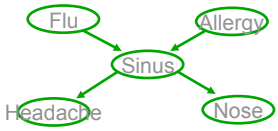
- Remember why?

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

- Maximum likelihood estimate

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

- Our case:



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

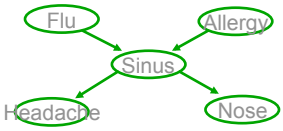
$$P(data|\theta) = \prod_{k=1}^{K} P(f_k)P(a_k)P(s_k|f_k a_k)P(h_k|s_k)P(n_k|s_k)$$

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

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

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

Estimate θ from partly observed data



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

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

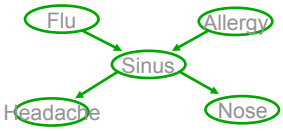
- Let X be all *observed* variable values (over all examples)
- Let Z be all *unobserved* variable values
- Can't calculate MLE:

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

- WHAT TO DO?

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

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:

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

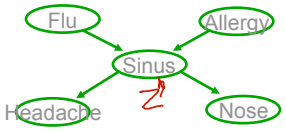
- EM seeks* to estimate:

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

* 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}

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

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

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

E step provides this!

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})

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

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

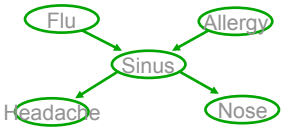
value of each var∈Z for each train example

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.

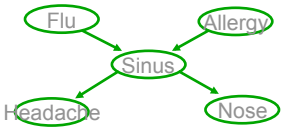
$$P(S_k = 1 | f_k a_k h_k n_k, \theta) =$$

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

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

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

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

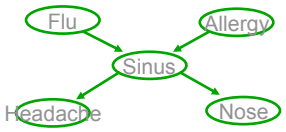


- How? Bayes net inference problem.

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

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

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

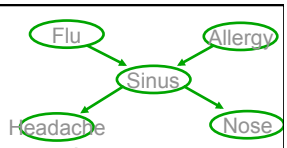
$$P(S_k = 1|f_k a_k h_k n_k, \theta) = E[s_k] = \frac{P(S_k = 1, f_k a_k h_k n_k|\theta)}{P(S_k = 1, f_k a_k h_k n_k|\theta) + P(S_k = 0, f_k a_k h_k n_k|\theta)}$$

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

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

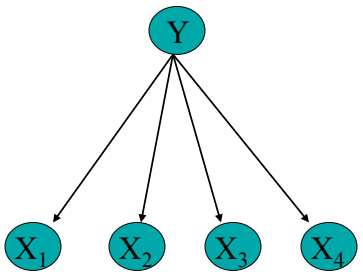
M step:

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

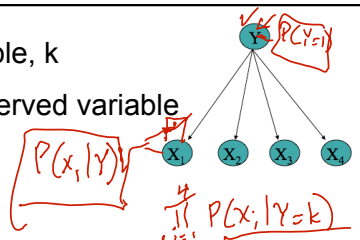
Learn P(Y|X)



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



$P(X_1|Y)$

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

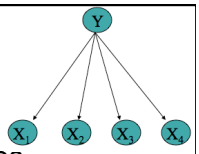
$E[Y]$

$P(Y|X_1 \cdots X_4, \theta)$

$= P_\theta(Y=k|X_1 \cdots X_4)$

$= \frac{P_\theta(X_1 \cdots X_4|Y=k)\, P_\theta(Y=k)}{\sum_j P_\theta(X_1 \cdots X_4|Y=j)\, P_\theta(Y=j)}$

EM and estimating θ



Given observed set X, unobserved set Y of boolean values

E step: Calculate for each training example, k

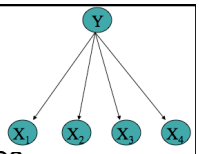
the expected value of each unobserved variable Y

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

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

let's use y(k) to indicate value of Y on kth example

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

- **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]

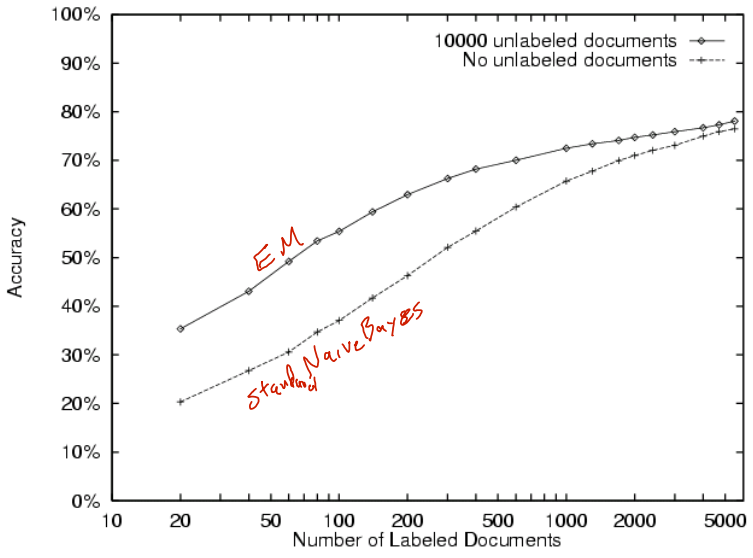
Experimental Evaluation

- 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

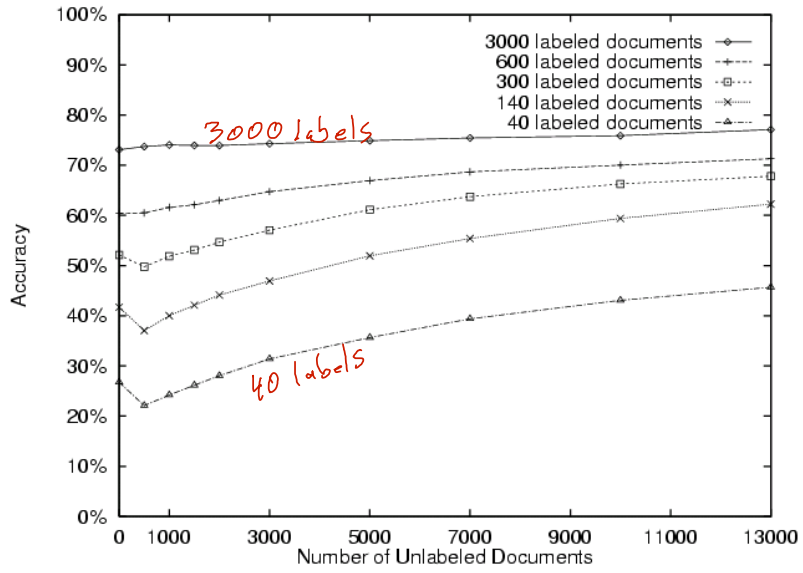
Table 3. Lists of the words most predictive of the course class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common course-related words appear. The symbol *D* indicates an arbitrary digit.

Iteration 0		Iteration 1	Iteration 2
intelligence	word w ranked by P(w|Y=course) / P(w|Y ≠ course)	*DD*	*D*
DD		*D*	*DD*
artificial		lecture	lecture
understanding		cc	cc
*DD*w		*D**	*DD:DD*
dist		*DD:DD*	due
identical		handout	*D**
rus		due	homework
arrange		problem	assignment
games		set	handout
dartmouth		tay	set
natural		*DD*am	hw
cognitive	Using one labeled example per class	yurttas	exam
logic		homework	problem
proving		kfoury	*DD*am
prolog		sec	postscript
knowledge		postscript	solution
human		exam	quiz
representation		solution	chapter
field		assaf	ascii

20 Newsgroups



20 Newsgroups



Usupervised clustering

Just extreme case for EM with zero labeled examples…