Machine Learning 10-601

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

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Today:

- Learning from fully labeled data
- Learning from partly observed data
  - EM algorithm
- Learning graph structure
  - Chow-Liu algorithm

Readings:

Required:
- Bishop chapter 9.2,

Strongly recommended:
- 9.3.3, 9.4

Learning of Bayes Nets

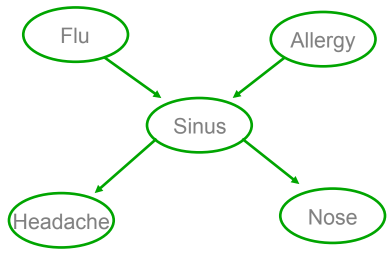
- Four categories of learning problems
  - Graph structure may be known/unknown
  - Variable values may be fully observed / partly unobserved
- Easy case: learn parameters for graph structure is *known*, and data is *fully observed*
- Interesting case: graph *known*, data *partly known*
- Gruesome case: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

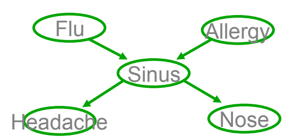


$$\theta_{s|ij} = \frac{\sum_{k=1}^{K} \delta(f_k = i, a_k = j, s_k = 1)}{\sum_{k=1}^{K} \delta(f_k = i, a_k = j)}$$

k^th training example

- 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:

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

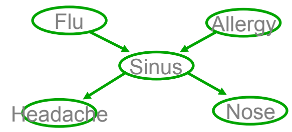
$$P(data|\theta) = \prod_{k=1}^{K} P(f_k)P(a_k)P(s_k|f_k a_k)P(h_k|s_k)P(n_k|s_k)$$

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

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

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

Estimate θ from partly observed data



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

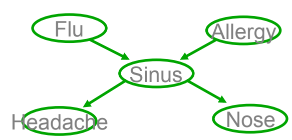
$$\theta \leftarrow \arg\max_{\theta} \log \prod_{k} P(f_k, a_k, s_k, h_k, n_k|\theta)$$

- 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?

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:

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

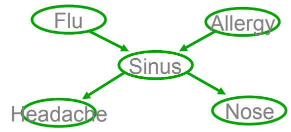
- EM seeks* to estimate:

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

* 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}

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

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

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})

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

Iterate until convergence:

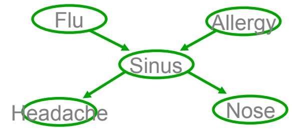
- E Step: Use X and current θ to calculate P(Z|X,θ)
- M Step: Replace current θ by

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

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}



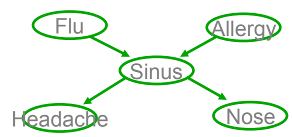
- How? Bayes net inference problem.

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

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

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

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



E step: Calculate P(Z_k|X_k; θ) for each training example, k

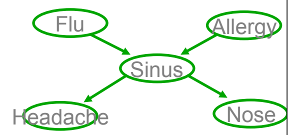
$$P(S_k = 1 | f_k a_k h_k n_k, \theta) = E[s_k] = \frac{P(S_k = 1, f_k a_k h_k n_k | \theta)}{P(S_k = 1, f_k a_k h_k n_k | \theta) + P(S_k = 0, f_k a_k h_k n_k | \theta)}$$

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

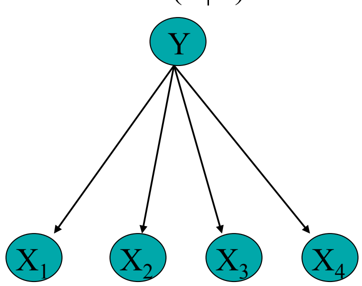
M step:

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

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

Using Unlabeled Data to Help Train Naïve Bayes Classifier

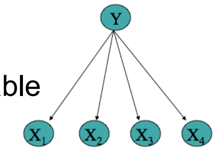
Learn P(Y|X)



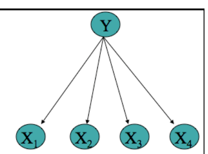
Y	X1	X2	X3	X4
1	0	0	1	1
0	0	1	0	0
0	0	0	1	0
?	0	1	1	0
?	0	1	0	1

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

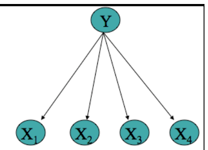
the expected value of each unobserved variable Y

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

M step: Calculate estimates similar to MLE, but replacing each count by its 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 <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: $\hat{P}(X_i = j|Y=m) = \frac{\sum_k \delta((y(k)=m) \wedge (x_i(k)=j))}{\sum_k \delta(y(k)=m)}$

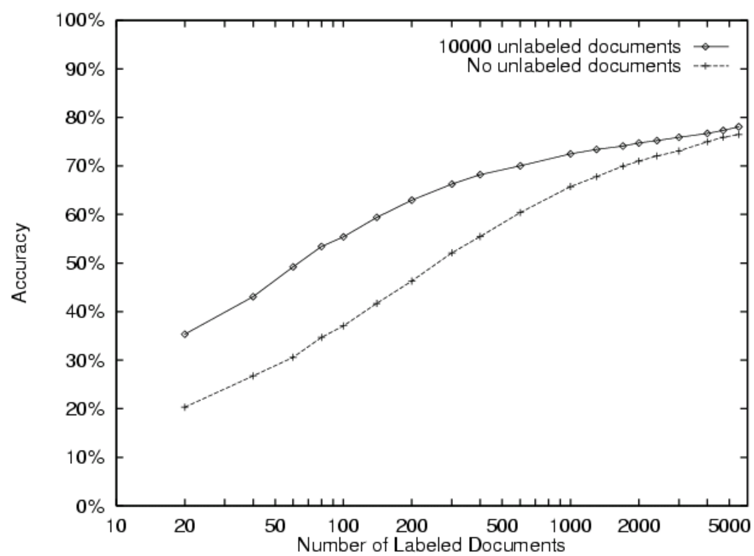
- **Inputs:** Collections $\mathcal{D}^l$ of labeled documents and $\mathcal{D}^u$ of unlabeled documents.
- Build an initial naive Bayes classifier, $\hat{\theta}$, from the labeled documents, $\mathcal{D}^l$, only. Use maximum a posteriori parameter estimation to find $\hat{\theta} = \arg\max_\theta \mathrm{P}(\mathcal{D}|\theta)\mathrm{P}(\theta)$ (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]

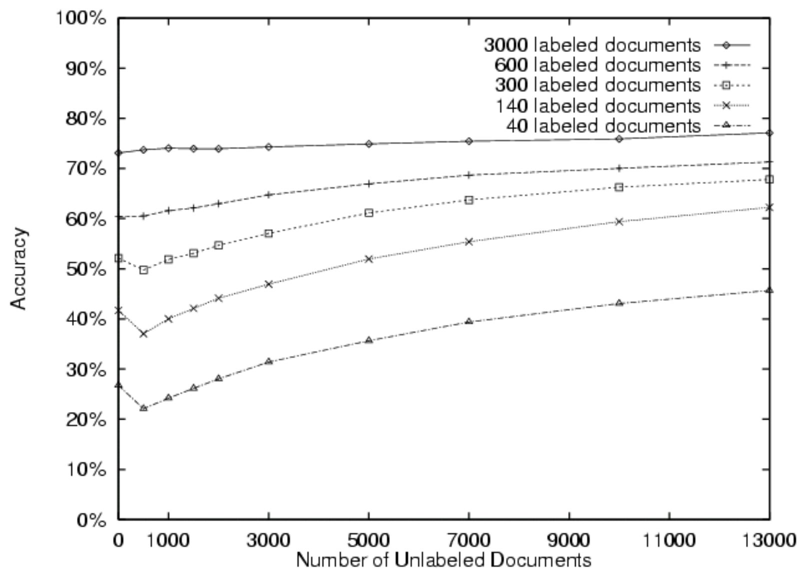
Experimental Evaluation

- 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



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

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

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

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 $N(\mu_i, \Sigma_i)$

EM for Mixture of Gaussian Clustering

Let's simplify to make this easier:

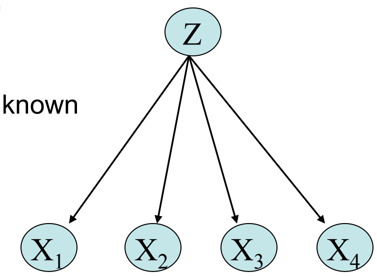
1. assume X=<X_1 ... X_n>, and the X_i are conditionally independent given Z.

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

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

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

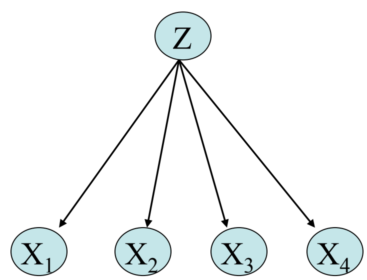
3. Assume σ known, π_1 ... π_K, μ_{1i} ... μ_{Ki} unknown



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 $\theta = \langle \pi, \mu_{ji} \rangle$

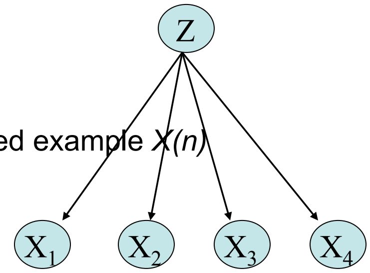
Iterate until convergence:

• 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)*

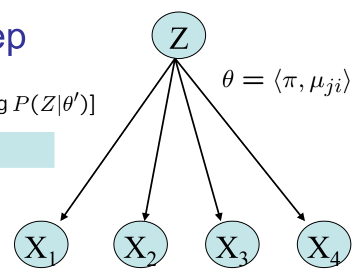
X(n)=<x_1(n), x_2(n), … x_T(n)>.

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

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

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

EM – M Step



First consider update for π

$\theta = \langle \pi, \mu_{ji} \rangle$

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

π' has no influence

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

Count z(n)=1

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

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

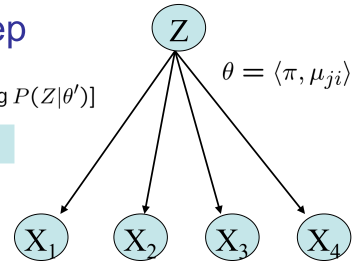
$$= \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\log \pi' + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\log(1-\pi')$$

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

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

EM – M Step

Now consider update for μ_{ji}



$\theta = \langle \pi, \mu_{ji} \rangle$

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

μ_{ji}' has no influence

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

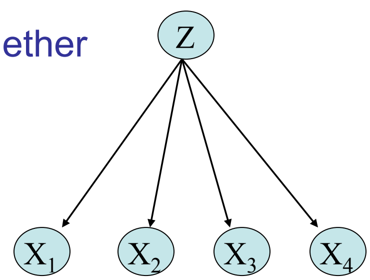
…
…
…

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

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

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

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

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

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

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

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(**X**) is true distribution, T(**X**) is our tree-structured network, where **X** = <X_1, … X_n>
  - 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 $\mathbf{X} \equiv \langle X_1 \dots X_n \rangle$

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

Chow-Liu Algorithm

1. for each pair of vars A,B, use data to estimate P(A,B), P(A), P(B)

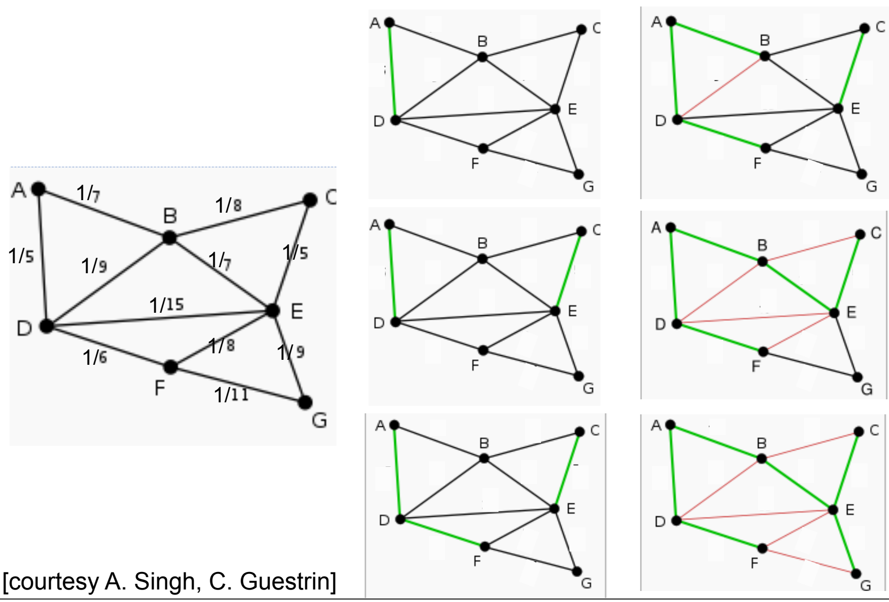
2. for each pair of vars A,B calculate mutual information
$$I(A,B) = \sum_a \sum_b P(a,b) \log \frac{P(a,b)}{P(a)P(b)}$$

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