Statistical Learning (II)
[RN2] Sec 20.3
[RN3] Sec 20.3

CS 486/686

University of Waterloo

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Outline

- Learning from incomplete Data
  - EM algorithm

Incomplete data

- So far…
  - Values of all attributes are known
  - Learning is relatively easy

- But many real-world problems have hidden variables (a.k.a latent variables)
  - Incomplete data
  - Values of some attributes missing

Unsupervised Learning

- Incomplete data → unsupervised learning
- Examples:
  - Categorisation of stars by astronomers
  - Categorisation of species by anthropologists
  - Market segmentation for marketing
  - Pattern identification for fraud detection
  - Research in general!

Maximum Likelihood Learning

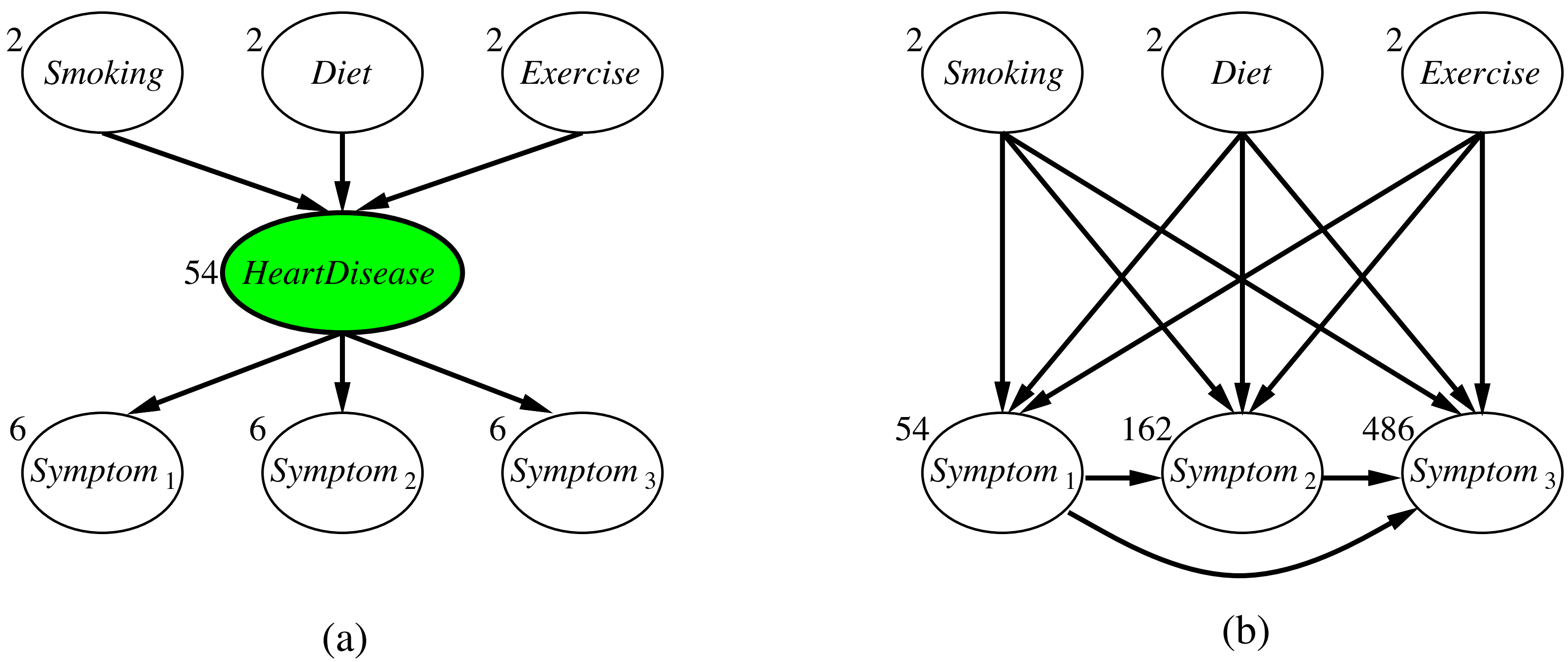
- ML learning of Bayes net parameters:
  - For $\theta_{V=true,pa(V)=\mathbf{v}} = Pr(V=true|par(V) = \mathbf{v})$
  - $\theta_{V=true,pa(V)=\mathbf{v}} = \frac{\#[V=true,pa(V)=\mathbf{v}]}{\#[V=true,pa(V)=\mathbf{v}] + \#[V=false,pa(V)=\mathbf{v}]}$
  - Assumes all attributes have values…

- What if values of some attributes are missing?

"Naive" solutions for incomplete data

- Solution #1: Ignore records with missing values
  - But what if all records are missing values (i.e., when a variable is hidden, none of the records have any value for that variable)
- Solution #2: Ignore hidden variables
  - Model may become significantly more complex!

Heart disease example



- a) simpler (i.e., fewer CPT parameters)
- b) complex (i.e., lots of CPT parameters)

"Direct" maximum likelihood

- Solution 3: maximize likelihood directly
  - Let **Z** be hidden and **E** observable
  - $h_{ML} = \text{argmax}_h P(\mathbf{e}|h)$
    $= \text{argmax}_h \Sigma_Z P(\mathbf{e},\mathbf{Z}|h)$
    $= \text{argmax}_h \Sigma_Z \Pi_i CPT(V_i)$
    $= \text{argmax}_h \log \Sigma_Z \Pi_i CPT(V_i)$
  - Problem: can't push log past sum to linearize product

Expectation-Maximization (EM)

- Solution #4: EM algorithm
  - Intuition: if we knew the missing values, computing h_{ML} would be trival

- Guess h_{ML}
- Iterate
  - Expectation: based on h_{ML}, compute expectation of the missing values
  - Maximization: based on expected missing values, compute new estimate of h_{ML}

Expectation-Maximization (EM)

- More formally:
  - Approximate maximum likelihood
  - Iteratively compute:
    $$h_{i+1} = \underbrace{\text{argmax}_h \underbrace{\Sigma_Z P(\mathbf{Z}|h_i,\mathbf{e}) \log P(\mathbf{e},\mathbf{Z}|h)}_{\text{Expectation}}}_{\text{Maximization}}$$

Expectation-Maximization (EM)

- Derivation
  - $\log P(\mathbf{e}|h) = \log [P(\mathbf{e},\mathbf{Z}|h) / P(\mathbf{Z}|\mathbf{e},h)]$
    $= \log P(\mathbf{e},\mathbf{Z}|h) - \log P(\mathbf{Z}|\mathbf{e},h)$
    $= \Sigma_Z P(\mathbf{Z}|\mathbf{e},h) \log P(\mathbf{e},\mathbf{Z}|h)$
    $\quad - \Sigma_Z P(\mathbf{Z}|\mathbf{e},h) \log P(\mathbf{Z}|\mathbf{e},h)$
    $\geq \Sigma_Z P(\mathbf{Z}|\mathbf{e},h) \log P(\mathbf{e},\mathbf{Z}|h)$

- EM finds a local maximum of $\Sigma_Z P(Z|e,h) \log P(\mathbf{e},\mathbf{Z}|h)$ which is a lower bound of $\log P(\mathbf{e}|h)$

Expectation-Maximization (EM)

- Log inside sum can linearize product
  - $h_{i+1} = \text{argmax}_h \sum_Z P(\mathbf{Z}|h_i,\mathbf{e}) \log P(\mathbf{e},\mathbf{Z}|h)$
    $= \text{argmax}_h \sum_Z P(\mathbf{Z}|h_i,\mathbf{e}) \log \prod_j CPT_j$
    $= \text{argmax}_h \sum_Z P(\mathbf{Z}|h_i,\mathbf{e}) \sum_j \log CPT_j$
- Monotonic improvement of likelihood
  - $P(\mathbf{e}|h_{i+1}) \geq P(\mathbf{e}|h_i)$

Expectation-Maximization (EM)

- Objective: $\max_h \Sigma_Z P(Z|e,h) \log P(\mathbf{e},\mathbf{Z}|h)$
- Iterative approach
  $h_{i+1} = \mathrm{argmax}_h \ \Sigma_Z P(\mathbf{Z}|\mathbf{e},h_i) \log P(\mathbf{e},\mathbf{Z}|h)$
- Convergence guaranteed
  $h_\infty = \mathrm{argmax}_h \ \Sigma_Z P(\mathbf{Z}|\mathbf{e},h) \log P(\mathbf{e},\mathbf{Z}|h)$
- Monotonic improvement of likelihood
  $P(\mathbf{e}|h_{i+1}) \geq P(\mathbf{e}|h_i)$

Optimization Step

- For one data point e:
  $h_{i+1} = \mathrm{argmax}_h \Sigma_Z P(\mathbf{Z}|h_i,\mathbf{e}) \log P(\mathbf{e},\mathbf{Z}|h)$
- For multiple data points:
  $h_{i+1} = \mathrm{argmax}_h \Sigma_{\mathbf{e}} n_{\mathbf{e}} \Sigma_Z P(\mathbf{Z}|h_i,\mathbf{e}) \log P(\mathbf{e},\mathbf{Z}|h)$
  Where $n_{\mathbf{e}}$ is frequency of **e** in dataset
- Compare to ML for complete data
  $h^* = \mathrm{argmax}_h \Sigma_{\mathbf{d}} n_{\mathbf{d}} \log P(\mathbf{d}|h)$

Optimization Solution

- Since $\mathbf{d} \equiv \langle z,e \rangle$
- Let $n_d = n_e P(\mathbf{z}|h_i,\mathbf{e})$ ← **expected frequency**

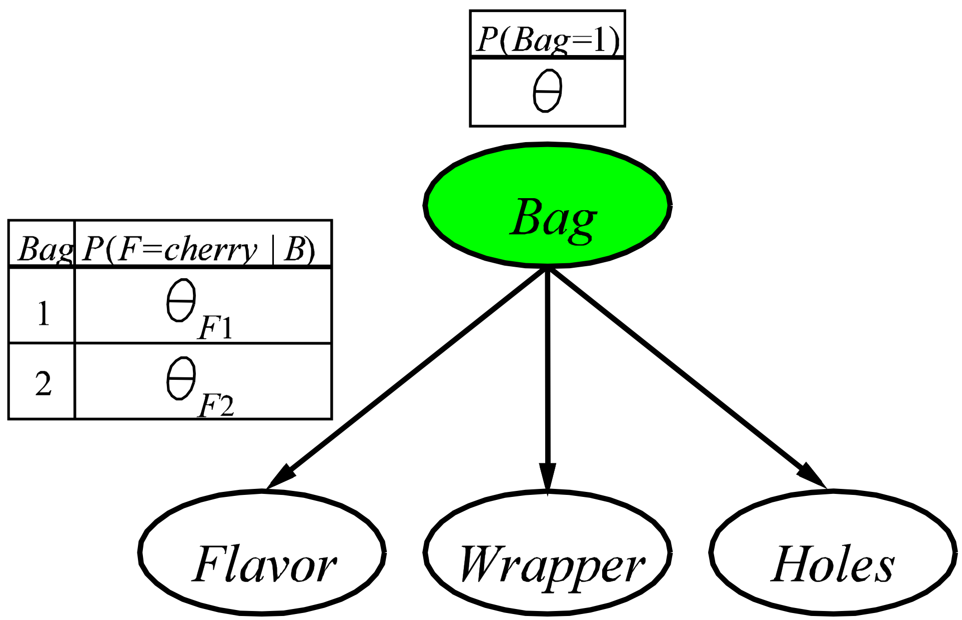
- Similar to the complete data case, the optimal parameters are obtained by setting the derivative to 0, which yields relative expected frequencies
  - E.g. $\theta_{V,pa(V)} = P(V|pa(V)) = n_{V,pa(V)} / n_{pa(V)}$

Candy Example

- Suppose you buy two bags of candies of unknown type (e.g. flavour ratios)
- You plan to eat sufficiently many candies of each bag to learn their type
- Ignoring your plan, your roommate mixes both bags…
- How can you learn the type of each bag despite being mixed?

Candy Example

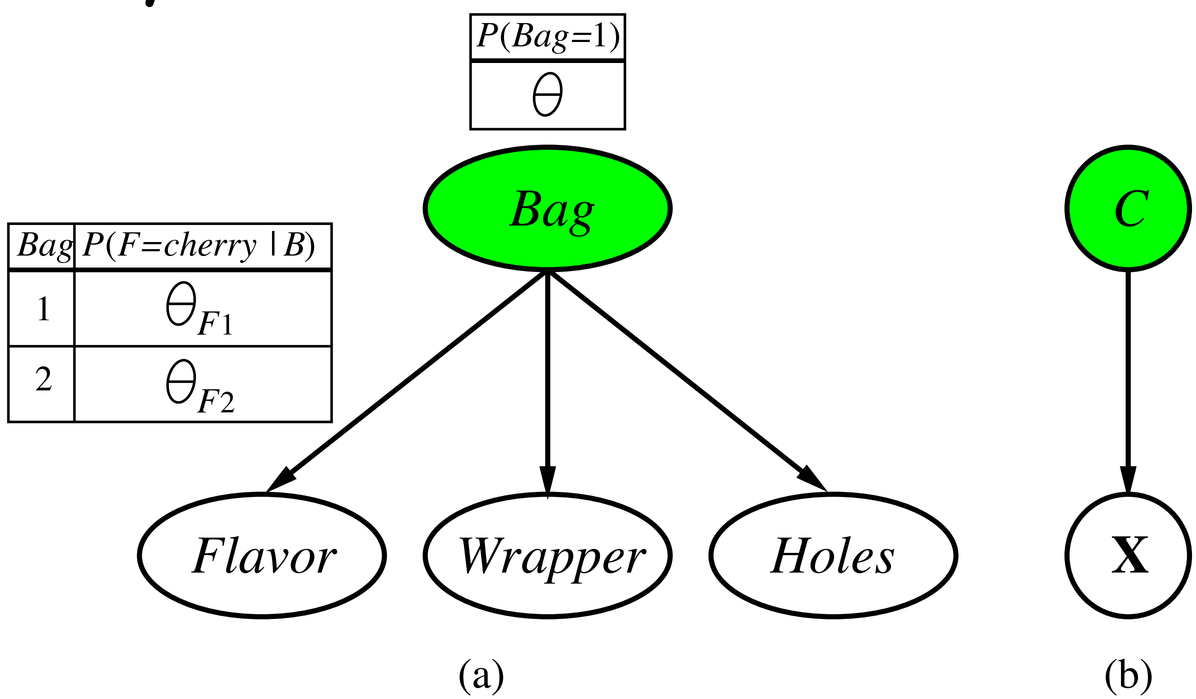
- "Bag" variable is hidden



(a)

Unsupervised Clustering

- "Class" variable is hidden
- Naïve Bayes model



Candy Example

- Unknown Parameters:
  - θ_i = P(Bag=i)
  - θ_{Fi} = P(Flavour=cherry|Bag=i)
  - θ_{Wi} = P(Wrapper=red|Bag=i)
  - θ_{Hi} = P(Hole=yes|Bag=i)
- When eating a candy:
  - F, W and H are observable
  - B is hidden

Candy Example

- Let true parameters be:
  - $\theta=0.5$, $\theta_{F1}=\theta_{W1}=\theta_{H1}=0.8$, $\theta_{F2}=\theta_{W2}=\theta_{H2}=0.3$
- After eating 1000 candies:

	W=red		W=green	
	H=1	H=0	H=1	H=0
F=cherry	273	93	104	90
F=lime	79	100	94	167

Candy Example

- EM algorithm
- Guess h_0:
  - θ=0.6, θ_{F1}=θ_{W1}=θ_{H1}=0.6, θ_{F2}=θ_{W2}=θ_{H2}=0.4
- Alternate:
  - Expectation: expected # of candies in each bag
  - Maximization: new parameter estimates

Candy Example

- Expectation: expected # of candies in each bag
  - $\#[Bag=i] = \Sigma_j P(B=i|f_j,w_j,h_j)$
  - Compute $P(B=i|f_j,w_j,h_j)$ by variable elimination (or any other inference alg.)

- Example:
  - #[Bag=1] = 612
  - #[Bag=2] = 388

Candy Example

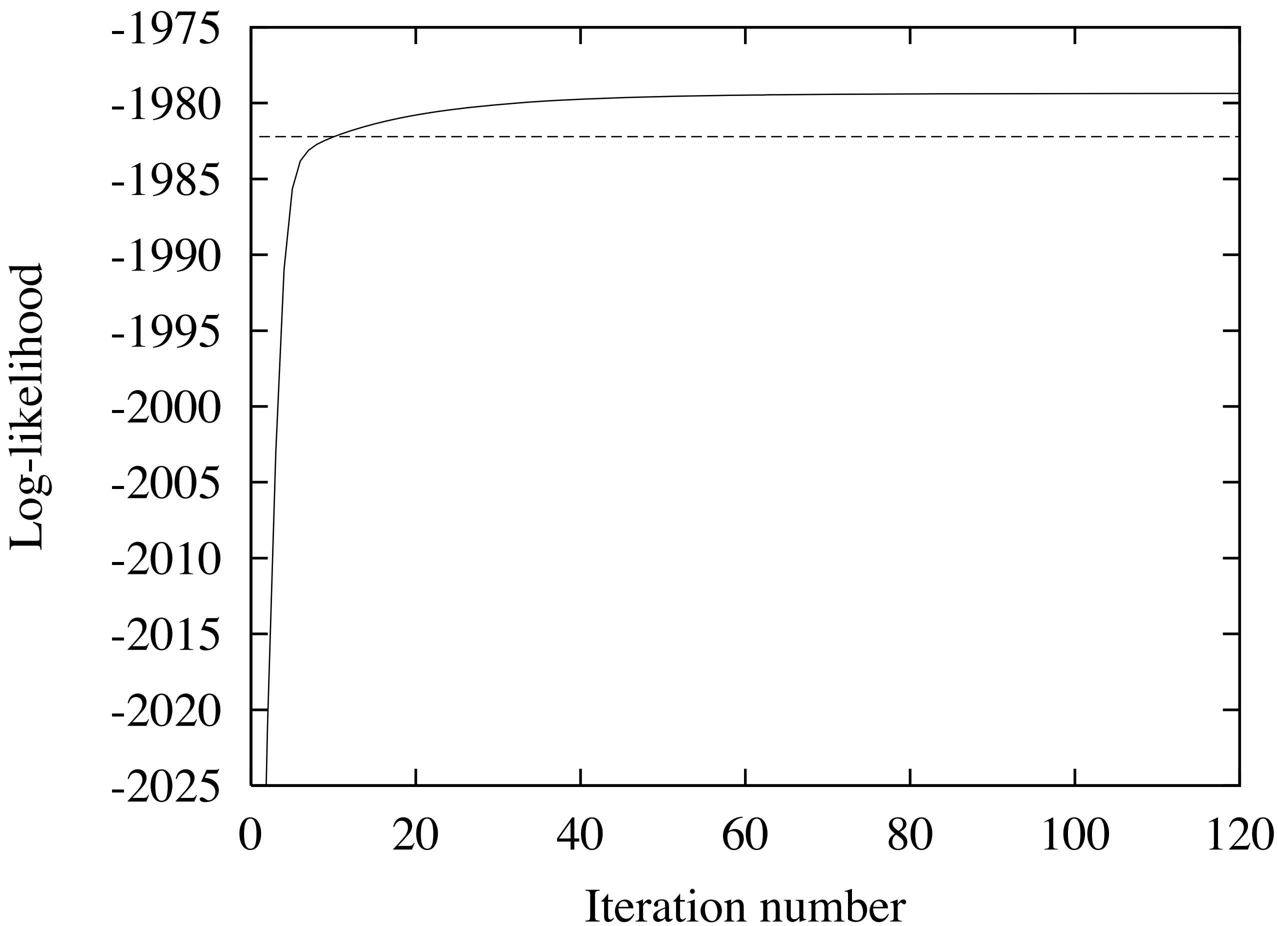
- Maximization: relative frequency of each bag
  - $\theta_1 = 612/1000 = 0.612$
  - $\theta_2 = 388/1000 = 0.388$

Candy Example

- Expectation: expected # of cherry candies in each bag
  - $\#[B=i,F=cherry] = \Sigma_j P(B=i|f_j=cherry,w_j,h_j)$
  - Compute $P(B=i|f_j=cherry,w_j,h_j)$ by variable elimination (or any other inference alg.)

- Maximization:
  - $\theta_{F1} = \#[B=1,F=cherry] / \#[B=1] = 0.668$
  - $\theta_{F2} = \#[B=2,F=cherry] / \#[B=2] = 0.389$

Candy Example



Bayesian networks

- EM algorithm for general Bayes nets
- Expectation:
  - $\#[V_i=v_{ij},Pa(V_i)=pa_{ik}]$ = expected frequency
- Maximization:
  - $\theta_{v_{ij},pa_{ik}} = \#[V_i=v_{ij},Pa(V_i)=pa_{ik}] \,/\, \#[Pa(V_i)=pa_{ik}]$