

Expectation Maximization [KF Chapter 19]

CS 786

University of Waterloo

Lecture 17: June 28, 2012

Incomplete data

- Complete data
 - 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!

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3

Maximum Likelihood Learning

- ML learning of Bayes net parameters:
 - For $\theta_{V=\text{true}, \text{pa}(V)=\mathbf{v}} = \Pr(V=\text{true} | \text{pa}(V) = \mathbf{v})$
 - $\theta_{V=\text{true}, \text{pa}(V)=\mathbf{v}} = \frac{\#[V=\text{true}, \text{pa}(V)=\mathbf{v}]}{\#[V=\text{true}, \text{pa}(V)=\mathbf{v}] + \#[V=\text{false}, \text{pa}(V)=\mathbf{v}]}$
 - Assumes all attributes have values...
- What if values of some attributes are missing?

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4

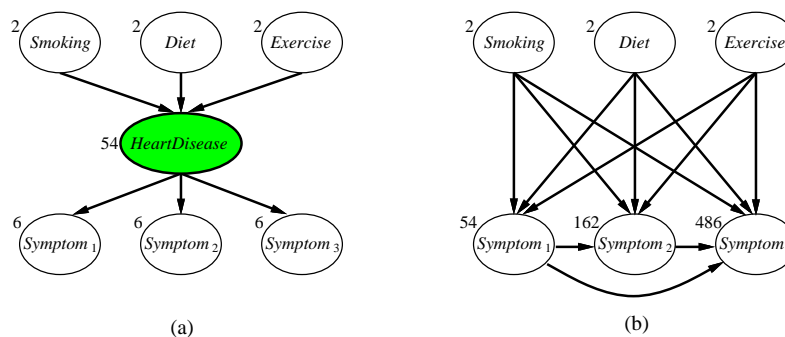
"Naive" solutions for incomplete data

- 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!

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Heart disease example



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

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6

"Direct" maximum likelihood

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

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7

Expectation-Maximization (EM)

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

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8

Expectation-Maximization (EM)

- More formally:

- Approximate maximum likelihood

- Iteratively compute:

$$h_{i+1} = \operatorname{argmax}_h \underbrace{\sum_Z P(Z|h_i, \mathbf{e}) \log P(\mathbf{e}, Z|h)}_{\text{Expectation}}$$

Maximization

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9

Expectation-Maximization (EM)

- Derivation

$$\begin{aligned} -\log P(\mathbf{e}|h) &= \log [P(\mathbf{e}, Z|h) / P(Z|\mathbf{e}, h)] \\ &= \log P(\mathbf{e}, Z|h) - \log P(Z|\mathbf{e}, h) \\ &= \sum_Z P(Z|\mathbf{e}, h) \log P(\mathbf{e}, Z|h) \\ &\quad - \sum_Z P(Z|\mathbf{e}, h) \log P(Z|\mathbf{e}, h) \\ &\geq \sum_Z P(Z|\mathbf{e}, h) \log P(\mathbf{e}, Z|h) \end{aligned}$$

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

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10

Expectation-Maximization (EM)

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

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11

Optimization Step

- For one data point e :
 $h_{i+1} = \operatorname{argmax}_h \sum_Z P(Z|h_i,e) \log P(e,Z|h)$
- For multiple data points:
 $h_{i+1} = \operatorname{argmax}_h \sum_e n_e \sum_Z P(Z|h_i,e) \log P(e,Z|h)$
Where n_e is frequency of e in dataset
- Compare to ML for complete data
 $h^* = \operatorname{argmax}_h \sum_d n_d \log P(d|h)$

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12

Optimization Solution

- Since $\mathbf{d} \equiv \langle \mathbf{z}, \mathbf{e} \rangle$
- 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. $\theta_{V, \text{pa}(V)} = P(V | \text{pa}(V)) = n_{V, \text{pa}(V)} / n_{\text{pa}(V)}$

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13

Candy Example

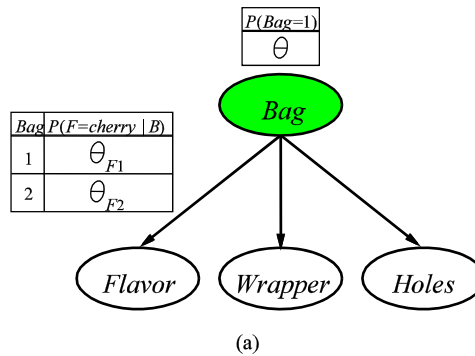
- Suppose you buy two bags of candies of unknown type (e.g. flavour ratios)
- You plan to eat sufficiently many candies of each bag to learn their type
- Ignoring your plan, your roommate mixes both bags...
- How can you learn the type of each bag despite being mixed?

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14

Candy Example

- "Bag" variable is hidden

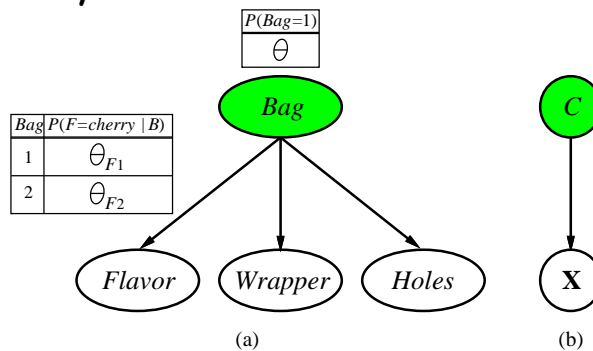


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15

Unsupervised Clustering

- "Class" variable is hidden
- Naïve Bayes model



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16

Candy Example

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

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17

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

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18

Candy Example

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

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19

Candy Example

- Expectation: expected # of candies in each bag
 - $\#[\text{Bag}=i] = \sum_j P(B=i | f_j, w_j, h_j)$
 - Compute $P(B=i | f_j, w_j, h_j)$ by variable elimination (or any other inference alg.)
- Example:
 - $\#[\text{Bag}=1] = 612$
 - $\#[\text{Bag}=2] = 388$

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20

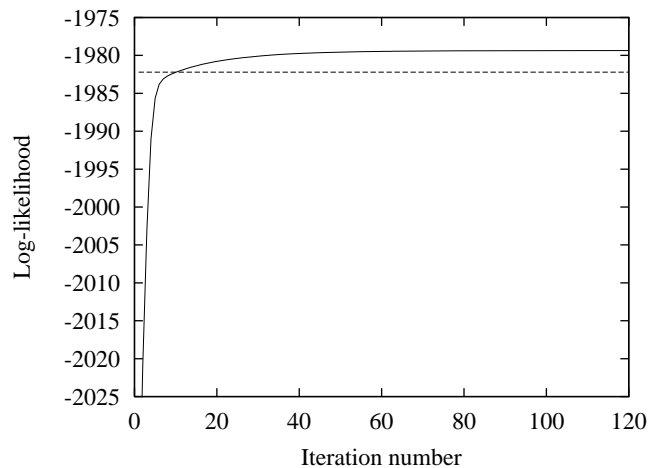
Candy Example

- 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
 - $\#[B=i, F=\text{cherry}] = \sum_j P(B=i | f_j=\text{cherry}, w_j, h_j)$
 - Compute $P(B=i | f_j=\text{cherry}, w_j, h_j)$ by variable elimination (or any other inference alg.)
- Maximization:
 - $\theta_{F1} = \#[B=1, F=\text{cherry}] / \#[B=1] = 0.668$
 - $\theta_{F2} = \#[B=2, F=\text{cherry}] / \#[B=2] = 0.389$

Candy Example



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23

Bayesian networks

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

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24