Expectation Maximisation (EM)

CS 486/686: Introduction to Artificial Intelligence
University of Waterloo

Incomplete Data

- So far we have seen problems where
  - Values of all attributes are known
  - Learning is relatively easy
- Many real-world problems have hidden variables
  - Incomplete data
  - Missing attribute values

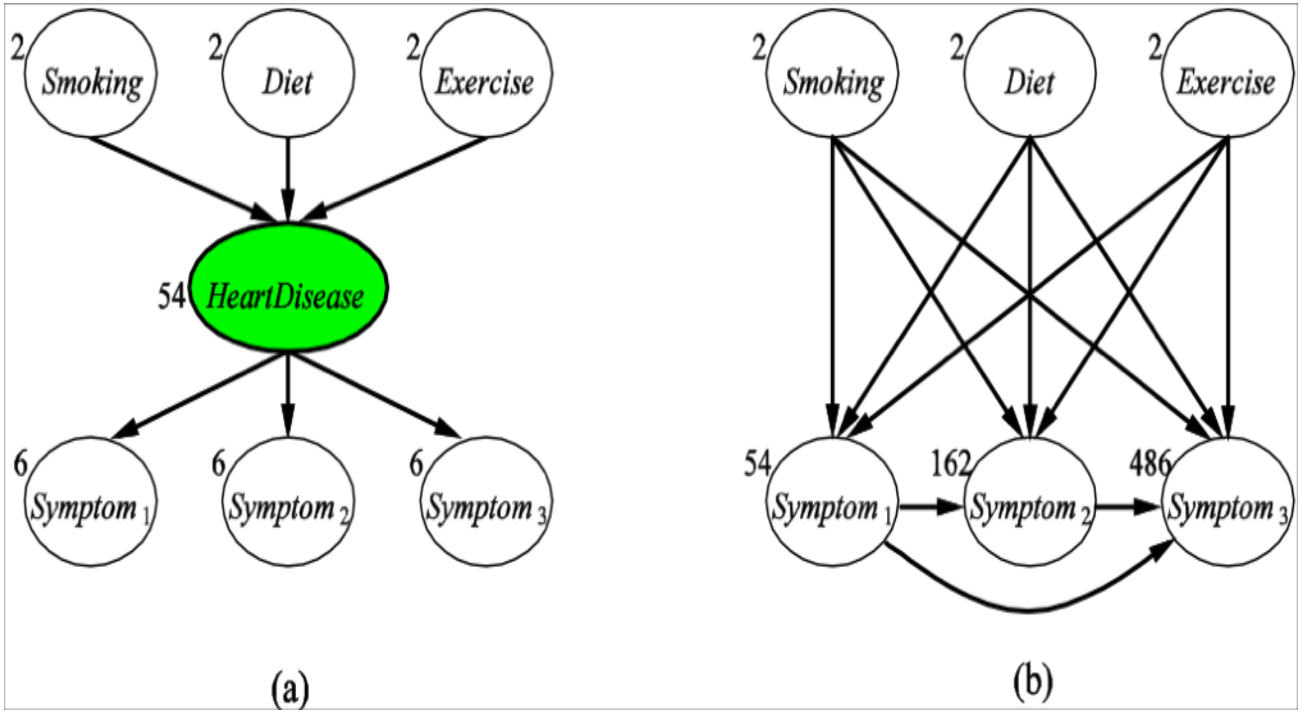
Bayes Nets: Maximum Likelihood Learning

- Review: ML Learning of Bayes nets parameters
  - $\Theta_{V=true,\ Par(V)=x} = P(V=true|Par(V)=x)$
  - $\Theta_{V=true,\ Par(V)=x} = (\#Insts\ V=true)/(Total\ \#V=x)$
  - Assumes all attributes have values
    - What if some values are missing?

Naïve Solutions

- Ignore examples with missing attribute values
  - What if all examples have missing attribute values?
- Ignore hidden variables
  - Model might become much more complex

Hidden Variables
Heart disease example



a) Uses a Hidden Variable, simpler (fewer CPT parameters)
b) No Hidden Variable, complex (many CPT parameters)

“Direct” ML

Maximize likelihood directly where E are the evidence variables and Z are the hidden variables

$$\begin{aligned} h_{ML} &= \arg\max_h P(E|h) \\ &= \arg\max_h \sum_Z P(E, Z|h) \\ &= \arg\max_h \sum_Z \prod_i \mathrm{CPT}(V_i) \\ &= \arg\max_h \log \sum_z \prod_i \mathrm{CPT}(V_i) \end{aligned}$$

Expectation-Maximization (EM)

- If we knew the missing values computing h_{ML} is trivial
- Guess h_{ML}
- Iterate
  - **Expectation**: based on h_{ML} compute expectation of (missing) values
  - **Maximization**: based on expected (missing) values compute new h_{ML}

Expectation-Maximization (EM)

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

EM Derivation

$$\begin{aligned}
\log P(\mathbf{e}|h) &= \log \left[\frac{P(\mathbf{e}, \mathbf{Z}|h)}{P(\mathbf{Z}|\mathbf{e}, h)} \right] \\
&= \log P(\mathbf{e}, \mathbf{Z}|h) - \log P(\mathbf{Z}|\mathbf{e}, h) \\
&= \sum_{Z} P(\mathbf{Z}|\mathbf{e}, h) \log P(\mathbf{e}, \mathbf{Z}|h) - \sum_{Z} P(\mathbf{Z}|\mathbf{e}, h) \log P(\mathbf{Z}|\mathbf{e}, h) \\
&\geq \sum_{Z} P(\mathbf{Z}|\mathbf{e}, h) \log P(\mathbf{e}, \mathbf{Z}|h)
\end{aligned}$$

EM finds a local maxima of $\sum_{Z} P(\mathbf{Z}|\mathbf{e}, h) \log P(\mathbf{e}, \mathbf{Z}|h)$

which is a lower bound of $\log P(\mathbf{e}|h)$

EM

Log inside can linearize the product

$$
\begin{aligned}
h_{i+1} &= \arg\max_h \sum_Z P(\mathbf{Z}|h, \mathbf{e}) \log P(\mathbf{e}, \mathbf{Z}|h) \\
&= \arg\max_h \sum_Z P(\mathbf{Z}|h, \mathbf{e}) \log \prod_j \mathrm{CPT}_j \\
&= \arg\max_h \sum_Z P(\mathbf{Z}|h, \mathbf{e}) \sum_j \log \mathrm{CPT}_j
\end{aligned}
$$

Monotonic improvement of likelihood

$$P(\mathbf{e}|h_{i+1}) \geq P(\mathbf{e}|h_i)$$

Example

- Assume we have two coins, A and B
- The probability of getting heads with A is θ_A
- The probability of getting heads with B is θ_B
- We want to find θ_A and θ_B by performing a number of trials

Example from S. Zafeiriohu, Advanced Statistical Machine Learning, Imperial College

Example

Coin A and **Coin B**

- **H T T T H H T H T H**
- **H H H H T H H H H H**
- **H T H H H H H T H H**
- **H T H T T T H H T T**
- **T H H H T H H H T H**

Coin A	Coin B
	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	**9 H, 11 T**

Example

Coin A	Coin B
	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	**9 H, 11 T**

$$\theta_A = \frac{24}{24+6} = 0.8$$

$$\theta_B = \frac{9}{9+11} = 0.45$$

Example

Now assume we do not know which coin was used in which trial (hidden variable)

- **H T T T H H T H T H**
- **H H H H T H H H H H**
- **H T H H H H H T H H**
- **H T H T T T H H T T**
- **T H H H T H H H T H**

Example

Initialization:

$$\theta_A^0 = 0.60$$

$$\theta_B^0 = 0.50$$

E Step: Compute the Expected counts of Heads and Tails

Trial 1: H T T T H H T H T H

$$P(A|\text{Trial } 1) = \frac{P(\text{Trial } 1|A)P(A)}{\sum_{i\in\{A,B\}} P(\text{Trial } 1|i)P(i)} = 0.45$$

$$P(B|\text{Trial } 1) = \frac{P(\text{Trial } 1|B)P(B)}{\sum_{i\in\{A,B\}} P(\text{Trial } 1|i)P(i)} = 0.55$$

Coin A	Coin B
2.2 H, 2.2 T	2.8 H, 2.8 T

Example

- **H T T T H H T H T H**
  (0.55 A, 0.45 B)
- **H H H H T H H H H H**
  (0.80 A, 0.20 B)
- **H T H H H H H T H H**
  (0.73 A, 0.27 A)
- **H T H T T T H H T T**
  (0.35 A, 0.65 B)
- **T H H H T H H H T H**
  (0.65 A, 0.35 B)

Coin A	Coin B
2.2H, 2.2T	2.8H, 2.8T
7.2H, 0.8T	1.8H, 0.2T
5.9H, 1.5T	2.1H, 0.5T
1.4H, 2.1T	2.6H, 3.9T
4.5H, 1.9T	2.5H, 1.1T
21.3H, 8.6T	**11.7H, 8.4T**

Example

M Step: Compute parameters based on expected counts

Coin A	Coin B
2.2H, 2.2T	2.8H, 2.8T
7.2H, 0.8T	1.8H, 0.2T
5.9H, 1.5T	2.1H, 0.5T
1.4H, 2.1T	2.6H, 3.9T
4.5H, 1.9T	2.5H, 1.1T
21.3H, 8.6T	**11.7H, 8.4T**

$$\theta_A^1 = \frac{21.3}{21.3 + 8.6} = 0.71$$

$$\theta_B^1 = \frac{11.7}{11.7 + 8.4} = 0.58$$

Repeat

$$\theta_A^{10} = 0.80$$

$$\theta_B^{10} = 0.52$$

EM: k-means Algorithm

Input

- Set of examples, E
- Input features X_1, …,X_n
- val(e,X)=value of feature j for example e
- k classes

Output

- Function class:E->{1,…,k} where class(e)=i means example e belongs to class i
- Function pval where pval(i,X_j) is the predicted value of feature X_j for each example in class i

k-means Algorithm

- Sum-of-squares error for class i and pval is

$$\sum_{e \in E} \sum_{j=1}^{n} (\mathrm{pval}(\mathrm{class}(e), X_j) - \mathrm{val}(e, X_j))^2$$

- Goal: Final class and pval that minimizes sum-of-squares error.

Minimizing the error

$$\sum_{e \in E} \sum_{j=1}^{n} (\mathrm{pval}(\mathrm{class}(e), X_j) - \mathrm{val}(e, X_j))^2$$

- Given class, the pval that minimizes sum-of-square error is the mean value for that class
- Given pval, each example can be assigned to the class that minimizes the error for that example

k-means Algorithm

- Randomly assign the examples to classes
- Repeat the following two steps until E step does not change the assignment of any example
  - **M**: For each class i and feature Xj

$$\mathrm{pval}(i, X_j) = \frac{\sum_{e:\mathrm{class}(e)=i} \mathrm{val}(e, X_j)}{|\{e : \mathrm{class}(e) = i\}|}$$

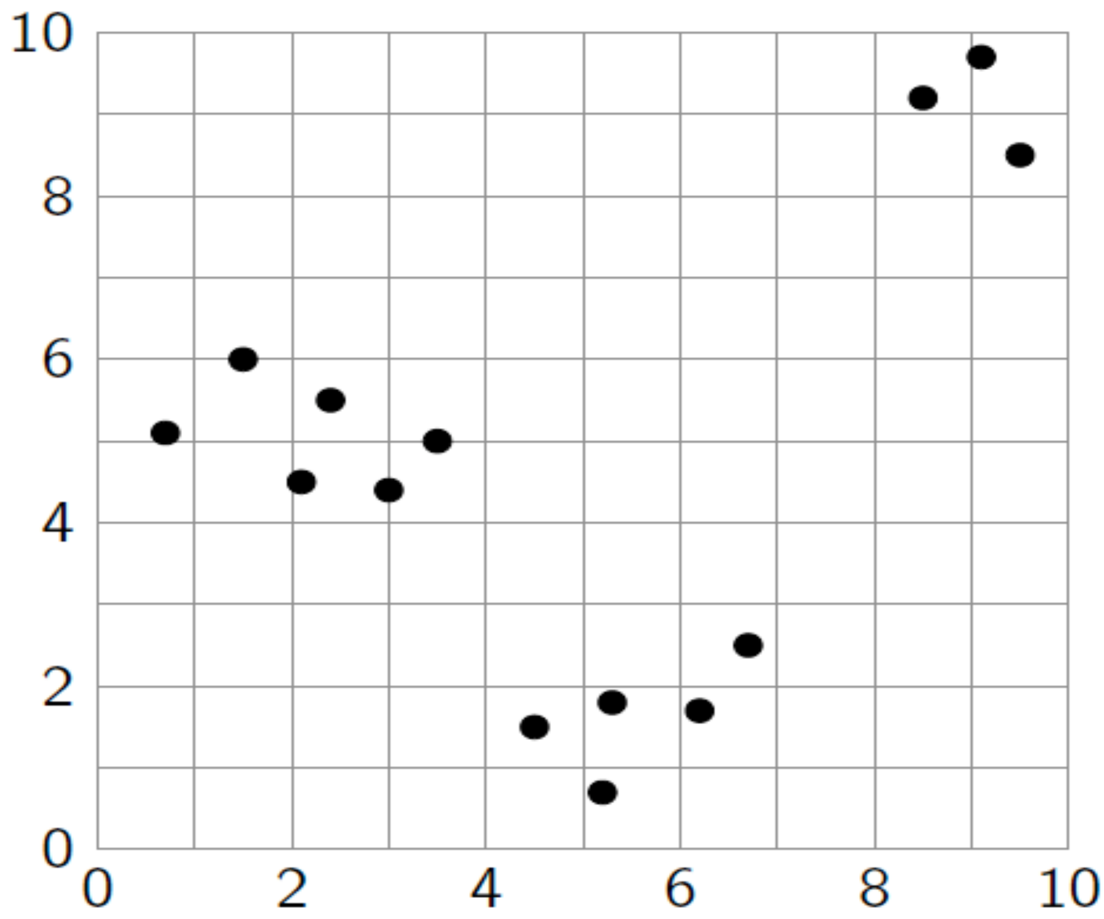
  - **E**: For each example e, assign e to the class that minimizes

$$\sum_{j=1}^{n} (\mathrm{pval}(\mathrm{class}(e), X_j) - \mathrm{val}(e, X_j))^2$$

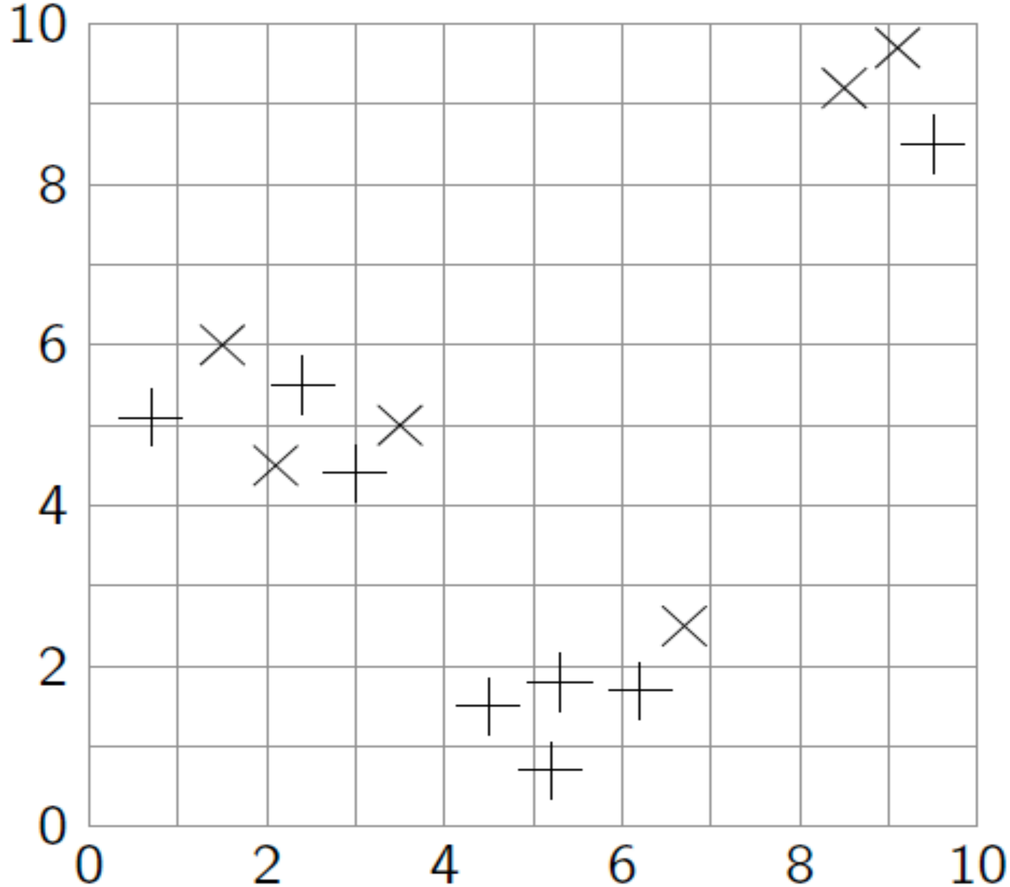
k-means Example

- Data set: (X,Y) pairs
  - (0.7,5.1) (1.5,6), (2.1, 4.5), (2.4, 5.5), (3, 4.4), (3.5, 5), (4.5, 1.5), (5.2, 0.7), (5.3, 1.8), (6.2, 1.7), (6.7, 2.5), (8.5, 9.2), (9.1, 9.7), (9.5, 8.5)

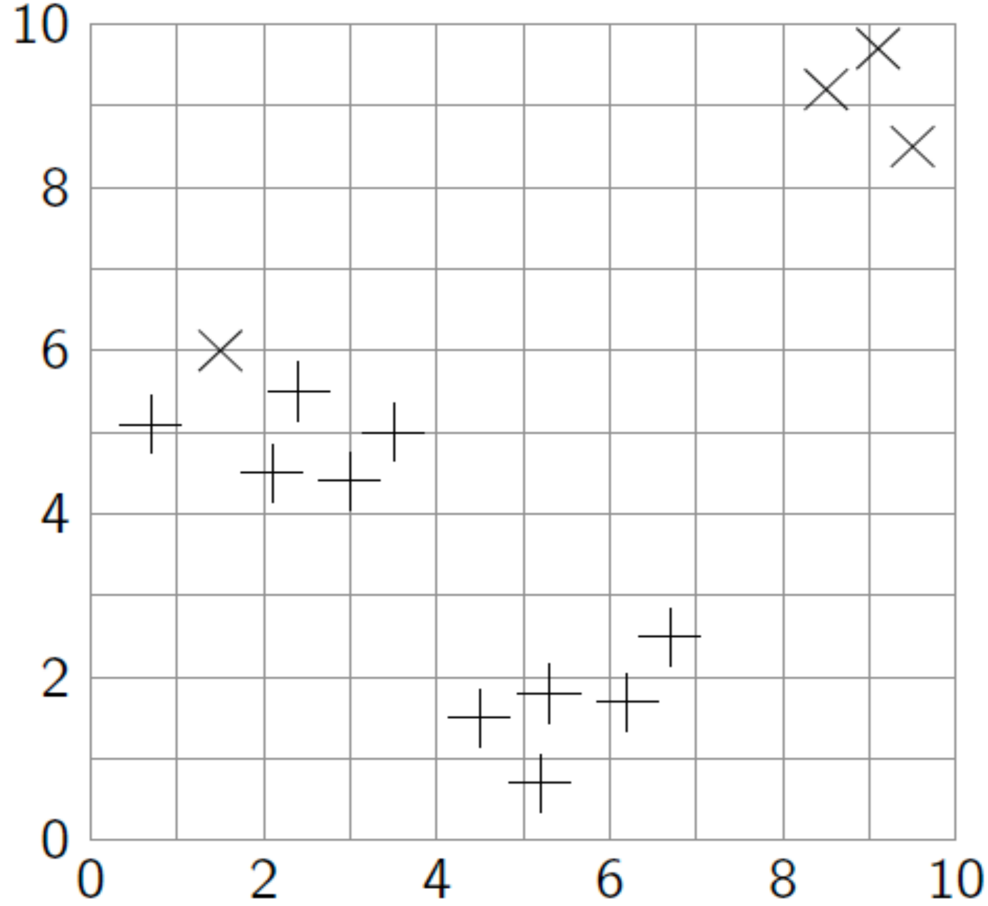
Example Data



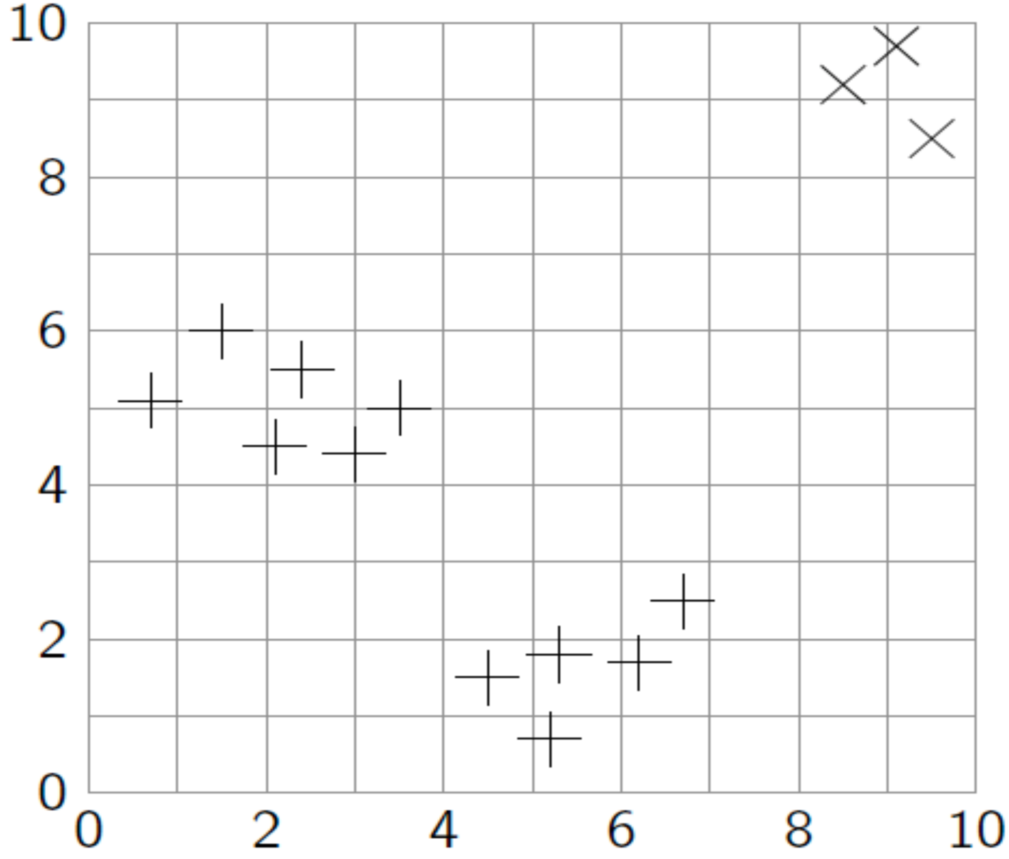
Random Assignment to Classes



Assign Each Example to Closest Mean



Reassign each example



Properties of k-means

- An assignment is stable if both M step and E step do not change the assignment
  - Algorithm will eventually converge to a stable local minimum
  - No guarantee that it will converge to a global minimum
- Increasing k can always decrease error until k is the number of different examples