# CS 2750 Machine Learning
# Lecture 14

## Learning with hidden variables and missing values

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## Hidden variables

**Modeling assumption:**

Variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$ are related through hidden variables

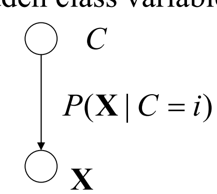
**Why to add hidden variables?**

- **More flexibility in describing the distribution** $P(\mathbf{X})$
- **Smaller parameterization of** $P(\mathbf{X})$
  - **New independences can be introduced via hidden variables**

**Example:**

- Latent variable models
  - hidden classes (categories)

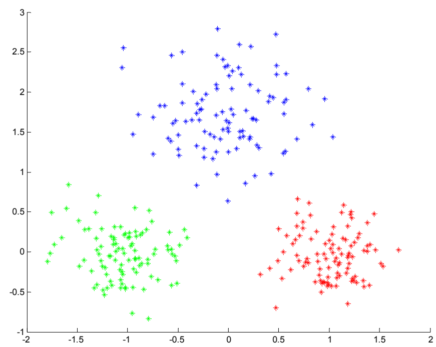
Hidden class variable



## Hidden variable model. Example.

- We want to represent the probability model of a population in a two dimensional space $\mathbf{X} = \{X_1, X_2\}$

**Observed data**





## Hidden variable model

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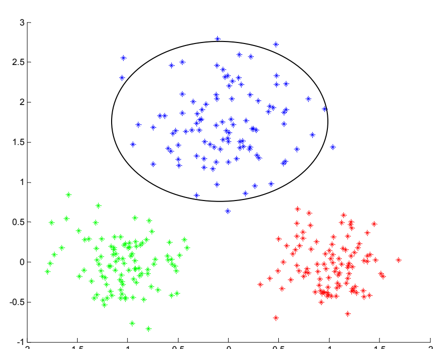
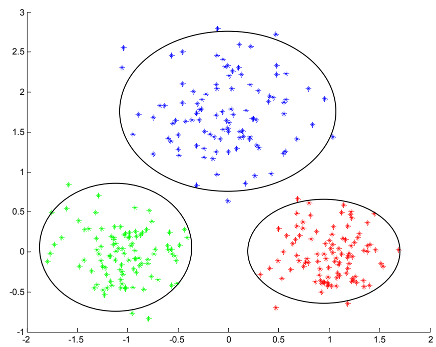
**Observed data**



## Hidden variable model

- We want to represent a model of a population in a two dimensional space $\mathbf{X} = \{X_1, X_2\}$

**Observed data**

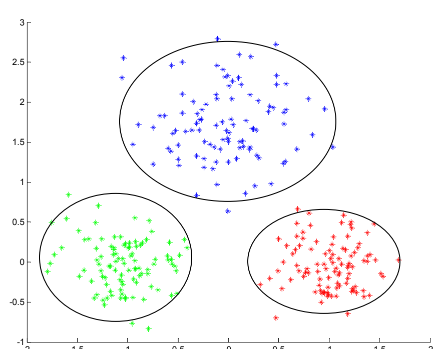




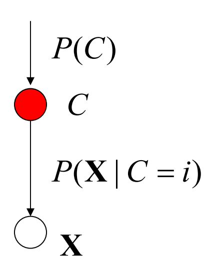
## Hidden variable model

- We want to represent the probability model of a population in a two dimensional space $\mathbf{X} = \{X_1, X_2\}$

**Observed data**



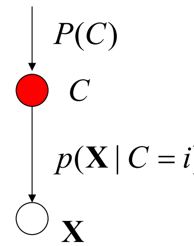
**Model** : 3 Gaussians with a hidden class variable



## Mixture of Gaussians

Probability of the occurrence of a data point $\boldsymbol{x}$ is modeled as

$$p(\mathbf{x}) = \sum_{i=1}^{k} p(C = i)\, p(\mathbf{x} \mid C = i)$$




where

$p(C = i)$

= probability of a data point coming from class $C=i$

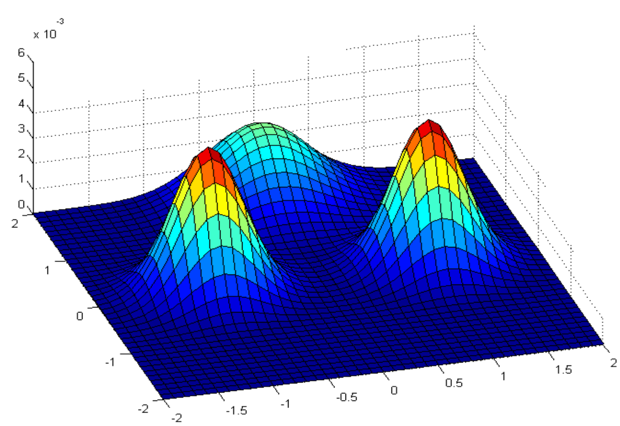
$p(\mathbf{x} \mid C = i) \approx N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

= class-conditional density (modeled as Gaussian) for class i



## Mixture of Gaussians

- Density function for the Mixture of Gaussians model

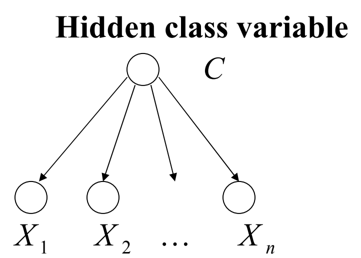


## Naïve Bayes with a hidden class variable

**Introduction of a hidden variable can reduce the number of parameters defining** $P(\mathbf{X})$

**Example:**

- Naïve Bayes model with a hidden class variable




Attributes are independent given the class

- **Useful in customer profiles**
  - Class value = type of customers



## Missing values

A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$

- **Data** $D = \{D_1, D_2, .., D_N\}$
- **But some values are missing**

$D_i = (x_1^i, x_3^i, \ldots x_n^i)$

Missing value of $x_2^i$

$D_{i+1} = (x_3^i, \ldots x_n^i)$

Missing values of $x_1^i, x_2^i$

Etc.

- **Example: medical records**
- **We still want to estimate parameters of** $P(\mathbf{X})$

## Density estimation

**Goal: Find the set of parameters** $\hat{\Theta}$

**Estimation criteria:**

- **ML** $\max_{\Theta} p(D \mid \Theta, \xi)$
- **Bayesian** $p(\Theta \mid D, \xi)$

**Optimization methods for ML:** gradient-ascent, conjugate gradient, Newton-Rhapson, etc.

- **Problem:** the methods often do not take advantage of the structure of the belief network

**Expectation-maximization (EM) method**

- An alternative optimization method
- Suitable when there are missing or hidden values
- **Takes advantage of the structure of the belief network**



## General EM

**The key idea of a method:**

**Compute the parameter estimates** iteratively by performing the following two steps:

**Two steps of the EM:**

1. **Expectation step**. Complete all hidden and missing variables with expectations for the current set of parameters $\Theta'$
2. **Maximization step**. Compute the new estimates of $\Theta$ for the completed data

**Stop when no improvement possible**

# EM

Let $H$ – be a set of all variables with hidden or missing values

**Derivation**

$$P(H, D \mid \Theta, \xi) = P(H \mid D, \Theta, \xi) P(D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log P(H \mid D, \Theta, \xi) + \log P(D \mid \Theta, \xi)$$

$$\underline{\log P(D \mid \Theta, \xi)} = \log P(H, D \mid \Theta, \xi) - \log P(H \mid D, \Theta, \xi)$$

**Log-likelihood of data**

**Average both sides** with $P(H \mid D, \Theta', \xi)$ for $\Theta'$

$$E_{H|D,\Theta'} \log P(D \mid \Theta, \xi) = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) - E_{H|D,\Theta'} \log P(H \mid D, \Theta, \xi)$$

$$\underbrace{\log P(D \mid \Theta, \xi)}_{\text{Log-likelihood of data}} = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$



# EM algorithm

**Algorithm** (general formulation)

Initialize parameters $\Theta$

Repeat

Set $\Theta' = \Theta$

1. **Expectation step**

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

2. **Maximization step**

$$\Theta = \arg \max_{\Theta} Q(\Theta \mid \Theta')$$

until no or small improvement in $\Theta$ $(\Theta = \Theta')$

**Questions:** Why this leads to the ML estimate ?

What is the advantage of the algorithm?

## EM algorithm

- Why is the EM algorithm correct?
- **Claim: maximizing Q improves the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

**Difference in log-likelihoods (current and next step)**

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

**Subexpression** $H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') \geq 0$

**Kullback-Leibler (KL) divergence** (distance between 2 distributions)

$$KL(P \mid R) = \sum_i P_i \log \frac{P_i}{R_i} \geq 0$$ Is always positive !!!

$$H(\Theta \mid \Theta') = -E_{H|D,\Theta'} \log P(H \mid D, \Theta, \xi) = -\sum_{\{H\}} p(H \mid D, \Theta') \log P(H \mid D, \Theta, \xi)$$

$$H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') = \sum_i P(H \mid D, \Theta') \log \frac{P(H \mid D, \Theta', \xi)}{P(H \mid D, \Theta, \xi)} \geq 0$$



## EM algorithm

**Difference in log-likelihoods**

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

$$l(\Theta) - l(\Theta') \geq Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta')$$

**Thus**

by **maximizing Q we maximize the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

EM is a first-order optimization procedure

- **Climbs the gradient**
- **Automatic learning rate**

No need to adjust the learning rate !!!!

## EM advantages

**Key advantages:**

- For Bayesian belief networks

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

  - **Q decomposes along variables** (has a nice form)

$$\log P(H,D \mid \Theta,\xi) = \log \prod_{l=1}^{N} P(H^{(l)}, D^{(l)} \mid \Theta, \xi) = \log \prod_{l=1}^{N} \prod_{i=1}^{n} \theta_{ijk}(l)$$

$$Q(\Theta,\Theta') = \sum_{l=1}^{N} \sum_{\{H\}} P(H^{(l)} \mid D^{(l)}, \Theta') \sum_{i=1}^{n} \log \theta_{ijk}(l)$$

$$= \sum_{l=1}^{N} \sum_{i=1}^{n} \sum_{\{H_i = X_i \cup pa(X_i)\}} P(H_i^{(l)} \mid D^{(l)}, \Theta') \log \theta_{ijk}(l)$$

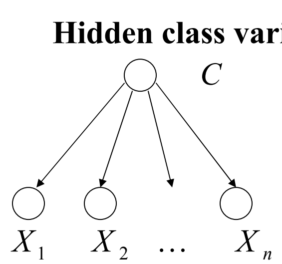
  - **The maximization of Q can be carried in the closed form**
    - No need to compute Q before maximizing
    - We directly optimize using quantities corresponding to expected counts



## Naïve Bayes with a hidden class and missing values

**Assume:**

- $P(\mathbf{X})$ is modeled using a Naïve Bayes model with hidden class variable
- Missing entries (values) for attributes in the dataset D




Attributes are independent given the class

## EM for the Naïve Bayes

- **We can use EM to learn the parameters**

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

- **Parameters:**

  $\pi_j$ prior on class j

  $\theta_{ijk}$ probability of an attribute i having value k given class j

- **Indicator variables:**

  $\delta_j^l$ for example $l$, the class is $j$ ; if true (=1) else false (=0)

  $\delta_{ijk}^l$ for example $l$, the class is $j$ and the value of attrib $i$ is $k$

  because the class is hidden and some attributes are missing, the values (0,1) of indicator variables are not known; they are hidden

***H*** – a collection of all indicator variables



## EM for the Naïve Bayes model

- We can use EM to do the learning of parameters

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log \prod_{l=1}^{N} \prod_{j} \pi_j^{\delta_j^l} \prod_{i} \prod_{k} \theta_{ijk}^{\delta_{ijk}^l}$$

$$= \sum_{l=1}^{N} \sum_{j} (\delta_j^l \log \pi_j + \sum_{i} \sum_{k} \delta_{ijk}^l \log \theta_{ijk})$$

$$E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) = \sum_{l=1}^{N} \sum_{j} (E_{H|D,\Theta'}(\delta_j^l) \log \pi_j + \sum_{i} \sum_{k} E_{H|D,\Theta'}(\delta_{ijk}^l) \log \theta_{ijk})$$

$$E_{H|D,\Theta'}(\delta_j^l) = p(C_l = j \mid D_l, \Theta')$$

$$E_{H|D,\Theta'}(\delta_{ijk}^l) = p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

Substitutes 0,1 with expected value

# EM for Naïve Bayes model

- Computing derivatives of $\boldsymbol{Q}$ for parameters and setting it to 0 we get:

$$\pi_j = \frac{\tilde{N}_j}{N} \qquad \theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}}$$

$$\tilde{N}_j = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_j^l) = \sum_{l=1}^{N} p(C_l = j \mid D_l, \Theta')$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_{ijk}^l) = \sum_{l=1}^{N} p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

- **Important:**
  - **Use expected counts instead of counts !!!**
  - Re-estimate the parameters using expected counts



# EM for BBNs

- The same result applies to learning of parameters of any Bayesian belief network with discrete-valued variables

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}} \longleftarrow \text{ Parameter value maximizing } \boldsymbol{Q}$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} p(x_i^l = k, pa_i^l = j \mid D^l, \Theta')$$

**may require inference**

- **Again:**
  - Use expected counts instead of counts