# K-Means Clustering and Gaussian Mixture Model

Il-Chul Moon Dept. of Industrial and Systems Engineering KAIST

icmoon@kaist.ac.kr

## Weekly Objectives

- Understand the clustering task and the K-means algorithm
  - Know what the unsupervised learning is
  - Understand the K-means iterative process
  - Know the limitation of the K-means algorithm
- Understand the Gaussian mixture model
  - Know the multinomial distribution and the multivariate Gaussian distribution
  - Know why mixture models are useful
  - Understand how the parameter updates are derived from the Gaussian mixture model
- Understand the EM algorithm
  - Know the fundamentals of the EM algorithm
  - Know how to derive the EM updates of a model

#### **EM ALGORITHM**

### Inference with Latent Variables

- Difference between classification and clustering
- Let's say
  - {X,Z}: complete set of variables
  - X: observed variables
  - Z: hidden (latent) variables
  - $\theta$ : parameters for distributions
  - $P(X|\theta) = \sum_{Z} P(X, Z|\theta) \rightarrow \ln P(X|\theta) = \ln \{\sum_{Z} P(X, Z|\theta)\}$ 
    - Any problem here?
    - The locations of summation and log make this complicated
    - Eventually, we want to exchange the locations of the two operators
- What we want to know is
  - The values of Z and  $\theta$ 
    - Optimizing  $P(X|\theta) = \sum_{Z} P(X, Z|\theta)$
  - The interacting terms for the optimization

## Probability Decomposition

- $l(\theta) = \ln P(X|\theta) = \ln \{\sum_{Z} P(X, Z|\theta)\} = \ln \{\sum_{Z} q(Z) \frac{P(X, Z|\theta)}{q(Z)}\}$ 
  - Use the Jensen's inequality

• 
$$\ln\{\sum_{Z} q(Z) \frac{P(X, Z|\theta)}{q(Z)}\} \ge \sum_{Z} q(Z) \ln \frac{P(X, Z|\theta)}{q(Z)}$$

- =  $\sum_{Z} q(Z) \ln P(X, Z|\theta) q(Z) \ln q(Z)$ 
  - Recall the second term?

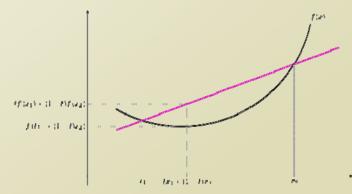
• 
$$H(X) = -\sum_{X} P(X = x) \log_b P(X = x)$$

• = 
$$E_{q(Z)} \ln P(X, Z|\theta) + H(q)$$

• 
$$Q(\theta, q) = E_{q(Z)} \ln P(X, Z|\theta) + H(q)$$

- This hold for any distribution of q
- This is only the lower bound of  $l(\theta)$ 
  - Need to make it tight!
  - How to?

#### Jensen's Inequality



When  $\varphi(x)$  is concave

$$\varphi(\frac{\sum a_i x_i}{\sum a_j}) \ge \frac{\sum a_i \varphi(x_i)}{\sum a_j}$$

When  $\varphi(x)$  is convex

$$\varphi(\frac{\sum a_i x_i}{\sum a_j}) \le \frac{\sum a_i \varphi(x_i)}{\sum a_j}$$