

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

Gaussian Mixture Model

- Let's assume that the data points are drawn from a mixture distribution of multiple multivariate Gaussian distributions

- $P(x) = \sum_{k=1}^K P(z_k)P(x|z) = \sum_{k=1}^K \pi_k N(x|\mu_k, \Sigma_k)$
- How to model such mixture?
 - Mixing coefficient, or Selection variable: z_k
 - The selection is stochastic which follows the multinomial distribution
 - $z_k \in \{0,1\}, \sum_k z_k = 1, P(z_k = 1) = \pi_k, \sum_{k=1}^K \pi_k = 1, 0 \leq \pi_k \leq 1$
 - $P(Z) = \prod_{k=1}^K \pi_k^{z_k}$
 - Mixture component
 - $P(X|z_k = 1) = N(x|\mu_k, \Sigma_k) \rightarrow P(X|Z) = \prod_{k=1}^K N(x|\mu_k, \Sigma_k)^{z_k}$
- This is the marginalized probability. How about conditional?

$$\begin{aligned} \gamma(z_{nk}) &\equiv p(z_k = 1|x_n) = \frac{P(z_k=1)P(x|z_k = 1)}{\sum_{j=1}^K P(z_j=1)P(x|z_j = 1)} \\ &= \frac{\pi_k N(x|\mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j N(x|\mu_j, \Sigma_j)} \end{aligned}$$

- Log likelihood of the entire dataset is
 - $\ln P(X|\pi, \mu, \Sigma) = \sum_{n=1}^N \ln \{ \sum_{k=1}^K \pi_k N(x|\mu_k, \Sigma_k) \}$

