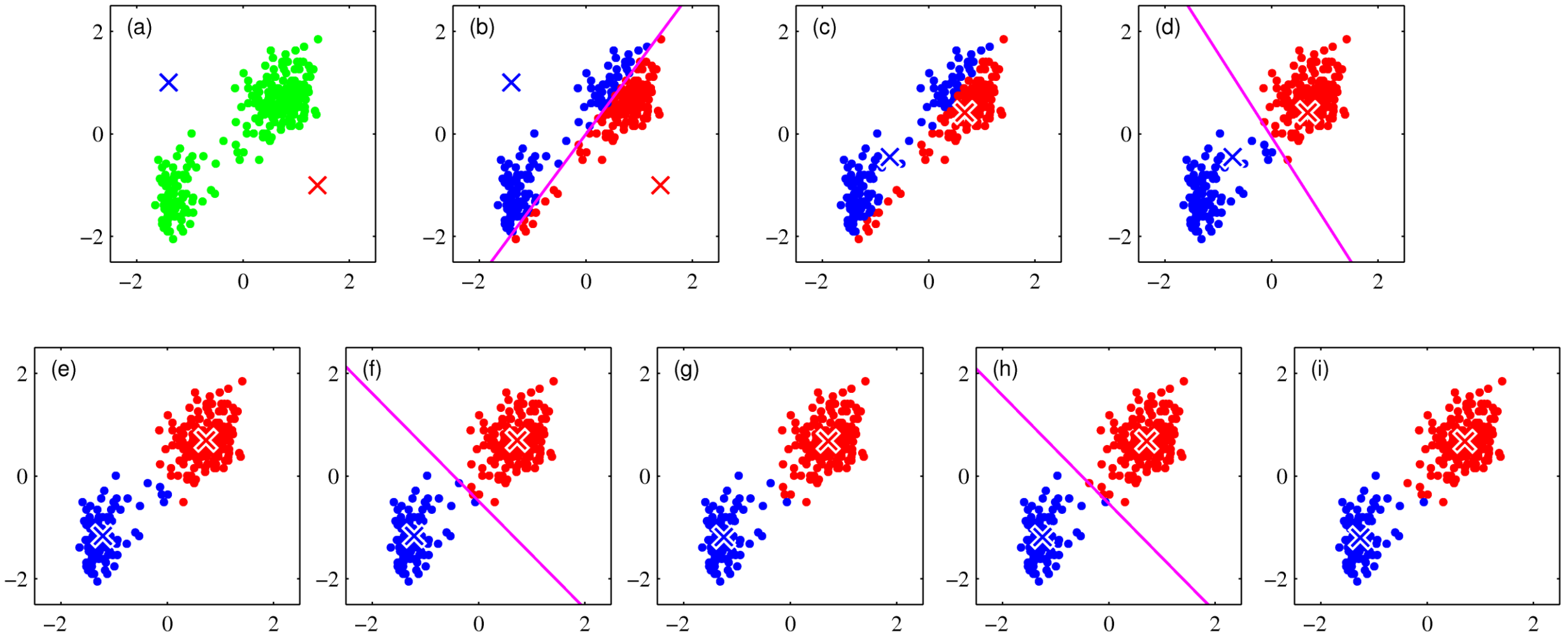
Data Analytics
EEE 4774 & 6777

Module 3

Clustering

Spring 2022

Clustering: K-means



K-means

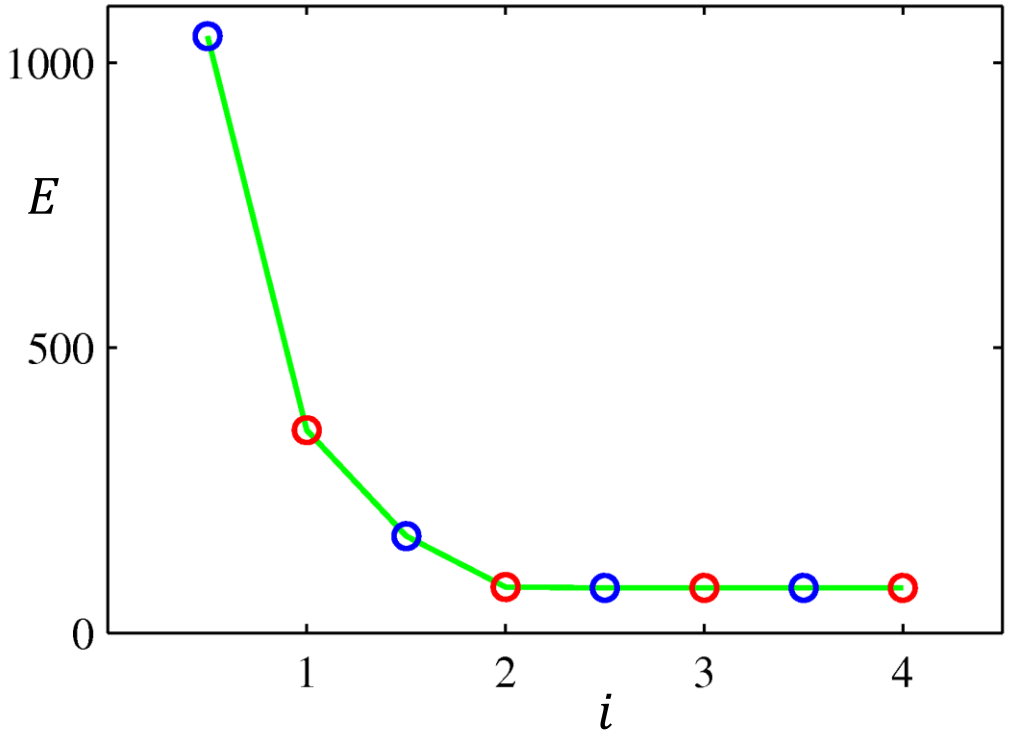
- Unsupervised method for identifying groups: Clustering
- Data $\{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ where $\boldsymbol{x}_n \in \mathbb{R}^D$
- $E(\boldsymbol{c}_n, \boldsymbol{m}_k) = \sum_{n=1}^{N} \sum_{k=1}^{K} c_{nk} \|\boldsymbol{x}_n - \boldsymbol{m}_k\|^2$ where $\boldsymbol{c}_n = [c_{n1} \dots c_{nK}]$ and $c_{nk} \in \{0,1\}$
- Iteratively minimize E over $\boldsymbol{c}_n$ and $\boldsymbol{m}_k$

Initialize $\boldsymbol{m}_k$
for i=1:max_iter
    Minimize E with respect to $\boldsymbol{c}_n$ keeping $\boldsymbol{m}_k$ fixed
    Minimize E with respect to $\boldsymbol{m}_k$ keeping $\boldsymbol{c}_n$ fixed
    if $\frac{\left\|\boldsymbol{c}_n^{(i)} - \boldsymbol{c}_n^{(i-1)}\right\|}{\left\|\boldsymbol{c}_n^{(i-1)}\right\|} < \varepsilon$ and $\frac{\left\|\boldsymbol{m}_k^{(i)} - \boldsymbol{m}_k^{(i-1)}\right\|}{\left\|\boldsymbol{m}_k^{(i-1)}\right\|} < \varepsilon$
        break
    end
end

K-means

$$c_{nk} = \begin{cases} 1 & if \quad k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{m}_j\|^2 \\ 0 & otherwise \end{cases}$$

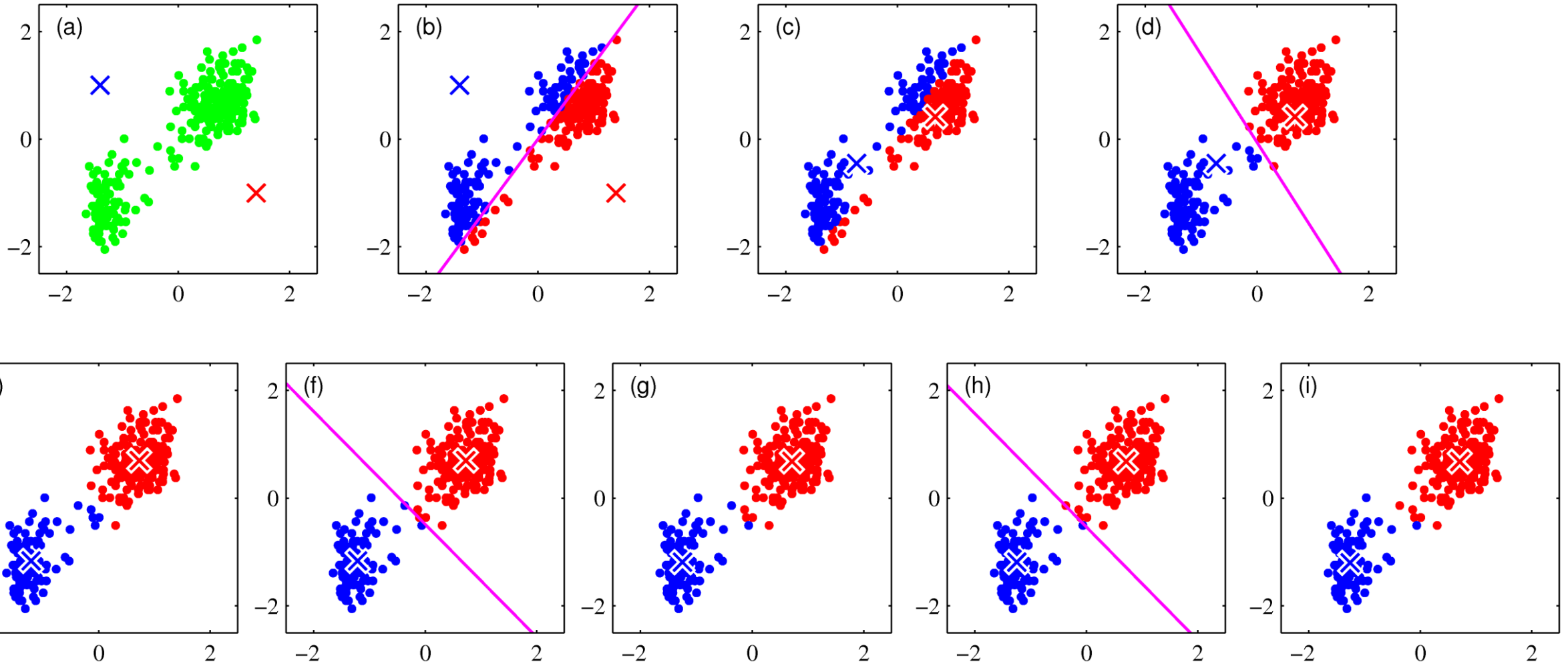
$$\boldsymbol{m}_k = \frac{\sum_n c_{nk}\boldsymbol{x}_n}{\sum_n c_{nk}} = mean\ of\ points\ assigned\ to\ cluster\ k$$



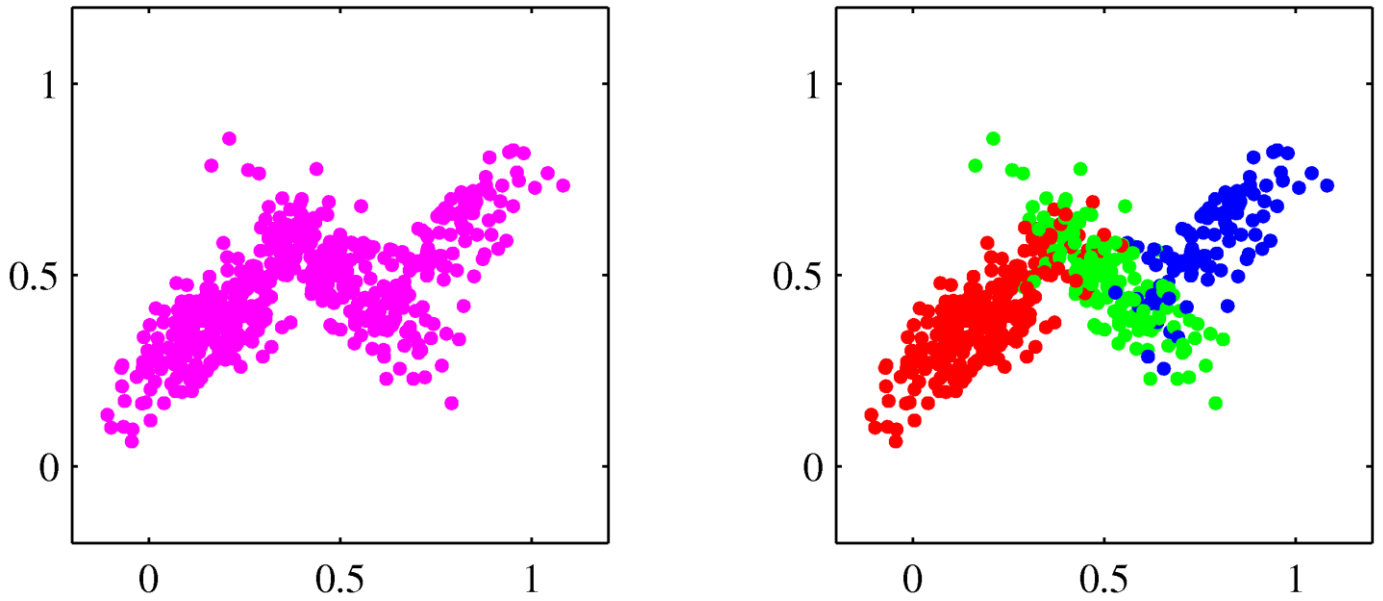
- Since E decreases at each iteration, convergence is guaranteed
- However, it may converge to a local minimum
- K-medoids: generalization of K-means to a general distance measure

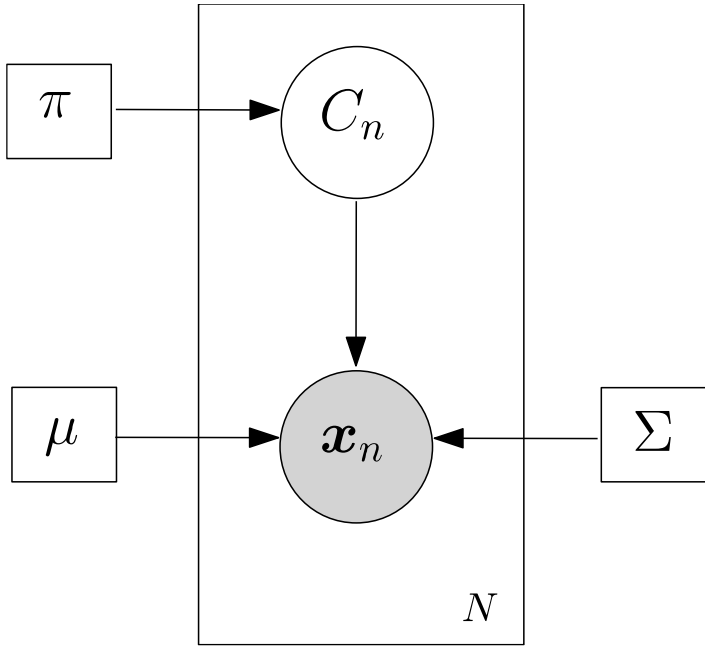
$$E(\boldsymbol{c}_n, \boldsymbol{m}_k) = \sum_{n=1}^{N}\sum_{k=1}^{K} c_{nk}\, V(\boldsymbol{x}_n, \boldsymbol{m}_k)$$

K-means



Gaussian Mixture Model





$$\boldsymbol{C}_n = [C_{nk}]_{k=1,\dots,K} = [0 \cdots 1 \cdots 0] \in [0,1]^K$$

$$p(C_{nk} = 1) = \pi_k, \quad \pi_k \in [0,1], \qquad \sum_{k=1}^{K} \pi_k = 1$$

$$p(\boldsymbol{x}_n) = \sum_{\boldsymbol{C}_n \in [0,1]^K} p(\boldsymbol{x}_n, \boldsymbol{C}_n) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$\log p(\boldsymbol{X}) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \frac{\exp\{-(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)/2\}}{(2\pi)^{d/2} |\boldsymbol{\Sigma}_k|^{1/2}}$$

ML for GMM

$$\max_{\boldsymbol{\mu}_k} \log p(\boldsymbol{X}) \quad \Longrightarrow \quad \frac{\partial}{\partial \boldsymbol{\mu}_k} \log p(\boldsymbol{X}) = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \boldsymbol{\Sigma}_k{}^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k) = 0$$

$$p(C_{nk} = 1|\boldsymbol{x}_n) = \frac{p(C_{nk} = 1)\, p(\boldsymbol{x}_n|C_{nk} = 1)}{\sum_{j=1}^{K} p(C_{nj} = 1)\, p(\boldsymbol{x}_n|C_{nj} = 1)} = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} = \gamma(C_{nk})$$

coupled equations
no closed-form solution!

$$\Longrightarrow \quad \boldsymbol{\mu}_k = \frac{1}{\sum_{n=1}^{N} \gamma(C_{nk})} \sum_{n=1}^{N} \gamma(C_{nk})\, \boldsymbol{x}_n = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(C_{nk})\, \boldsymbol{x}_n$$

Similarly, $$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(C_{nk})\, (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T, \qquad N_k = \sum_{n=1}^{N} \gamma(C_{nk}),$$

and $$\pi_k = \frac{N_k}{N}$$

Iterative Solution: EM for GMM

- Expectation-Maximization for iteratively computing ML in GMM

1. Initialize $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$ and compute the initial value of $\log p(\boldsymbol{X})$

2. **E step:** Compute the posteriors using the current parameter values

$$\gamma(C_{nk}) = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

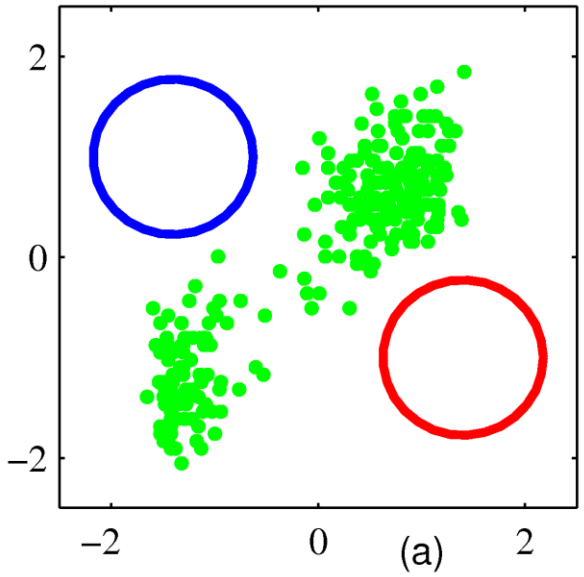
3. **M step:** Re-estimate the parameters using the current posteriors

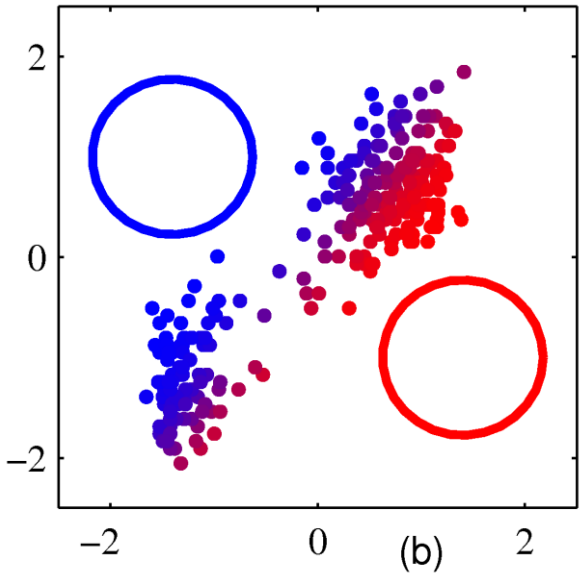
$$\boldsymbol{\mu}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(C_{nk})\, \boldsymbol{x}_n\,, \quad \boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(C_{nk})\, (\boldsymbol{x}_n - \boldsymbol{\mu}_k^{new})(\boldsymbol{x}_n - \boldsymbol{\mu}_k^{new})^T\,, \quad \pi_k^{new} = \frac{N_k}{N}, \quad \text{where} \quad N_k = \sum_{n=1}^{N} \gamma(C_{nk})$$

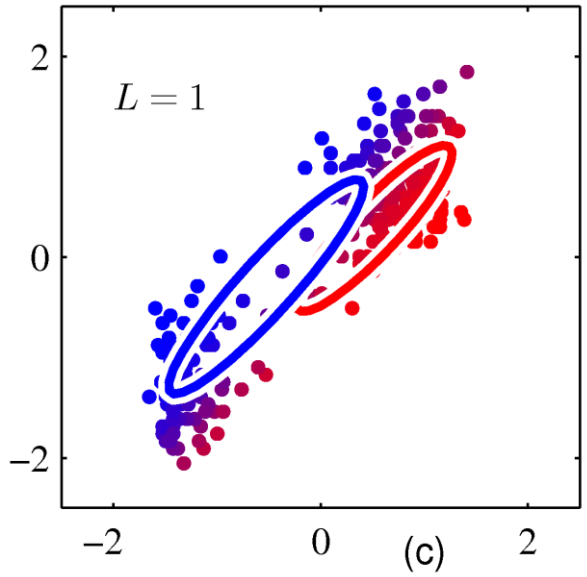
4. Compute the log-likelihood and check for convergence of either the parameters or the log-likelihood.

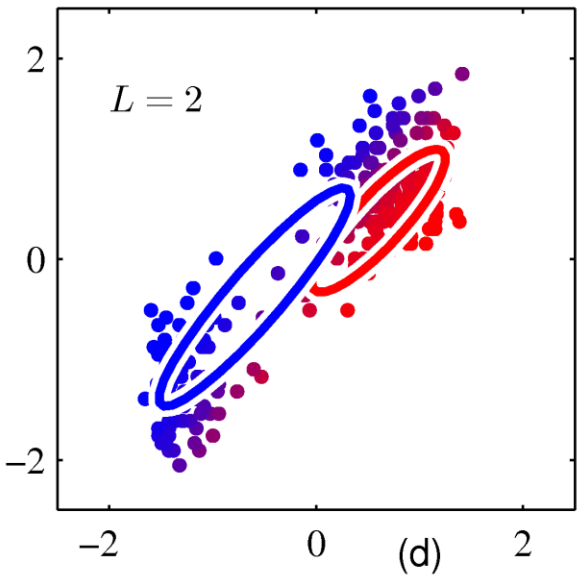
   If no convergence, return to step 2.

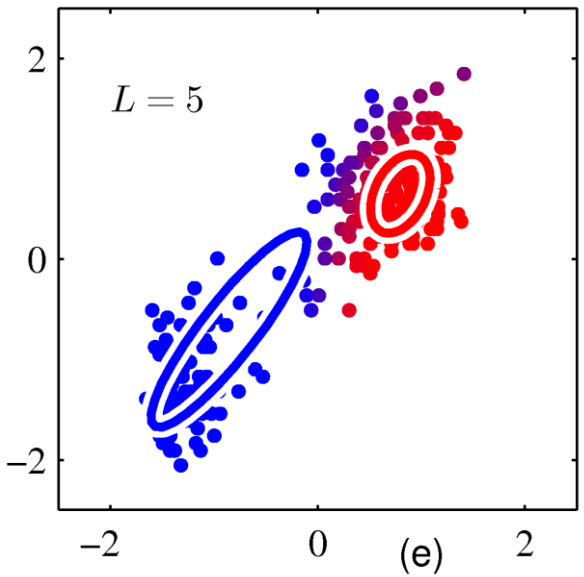
EM for GMM

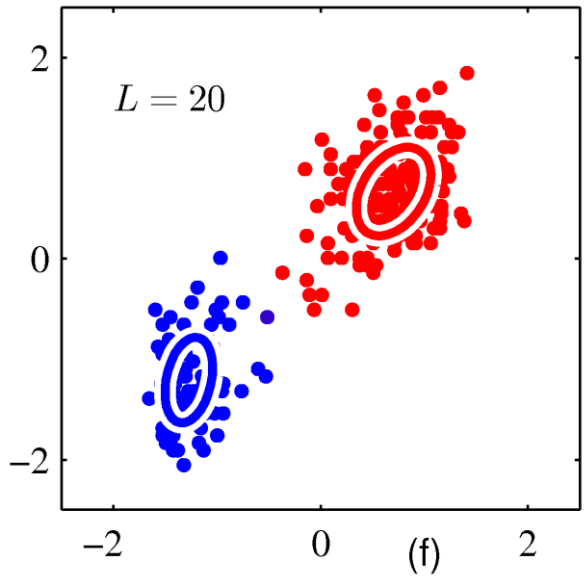












- Many more iterations than K-means, and each iteration much more expensive,
- But provides ***probabilistic modeling*** with ***soft assignments*** and ***covariance***
- Run K-means to initialize EM for GMM
- Converges to a local maximum

Expectation-Maximization (EM) Algorithm

- Objective: find ML for models with latent variables $\boldsymbol{C}$ (e.g., missing values in the dataset), observed data $\boldsymbol{X}$, and parameters $\boldsymbol{\theta}$

$$\log p(\boldsymbol{X}|\boldsymbol{\theta}) = \log \sum_{\boldsymbol{C}} p(\boldsymbol{X}, \boldsymbol{C}|\boldsymbol{\theta})$$

- Assume maximization of the complete-data log-likelihood $\log p(\boldsymbol{X}, \boldsymbol{C}|\boldsymbol{\theta})$ is easy

1. Initialize $\boldsymbol{\theta}^{old}$
2. E step: Evaluate $p(\boldsymbol{C}|\boldsymbol{X}, \boldsymbol{\theta}^{old})$ and

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) = E_{p(\boldsymbol{C}|\boldsymbol{X}, \boldsymbol{\theta}^{old})}[\log p(\boldsymbol{X}, \boldsymbol{C}|\boldsymbol{\theta})] = \sum_{\boldsymbol{C}} p(\boldsymbol{C}|\boldsymbol{X}, \boldsymbol{\theta}^{old}) \log p(\boldsymbol{X}, \boldsymbol{C}|\boldsymbol{\theta})$$

3. M step: $\boldsymbol{\theta}^{new} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old})$ {maximize $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) + \log p(\boldsymbol{\theta})$ for MAP}
4. If no convergence, then $\boldsymbol{\theta}^{old} \leftarrow \boldsymbol{\theta}^{new}$ and return to step 2

GMM by EM vs. K-means

- EM soft assigns data points ***softly*** to a cluster using posterior $p(C_{nk} = 1|\boldsymbol{x}_n)$,

whereas K-means performs ***hard*** assignment

- Consider a GMM with covariance $\epsilon \boldsymbol{I}$ for all clusters, where ϵ is a fixed constant, not a parameter to be re-estimated

$$p(C_{nk} = 1|\boldsymbol{x}_n) = \frac{\pi_k \exp\{-\|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2/2\epsilon\}}{\sum_{j=1}^{K} \pi_j \exp\{-\|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|^2/2\epsilon\}}$$

- As $\epsilon \to 0$, in the denominator the smallest $\|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|^2$ will go to 0 most slowly,

hence posterior for that cluster will go to 1 and the others will go to 0 $\Longrightarrow$ ***Hard assignment to the closest cluster***

- Update for the mean $\boldsymbol{\mu}_k$ also reduces to that of K-means

- K-means does not estimate the covariances of the clusters

Evaluation of Clustering Results

- Several similarity measures for clusters can be used to evaluate the performance of clustering algorithms
- Can be used to determine the optimum number of clusters
- **Internal Evaluation:** based on the clustered data itself
  - typically assigns good score if high similarity within clusters and low similarity between clusters
  - e.g., Silhouette value (works well with K-means), Dunn index, Davies-Bouldin index
- **External Evaluation:** based on data that was not used for clustering, e.g., ground truth
  - measures how close clustering is to the benchmark classes
  - e.g., Rand index, F-measure, Mutual information, Confusion matrix