CS247: ADVANCED DATA MINING

3: K-Means and Mixture Model

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Announcement

- PTE: if you are still interested in this class, please send email (reply your original request) to me before 5PM today.
- Quiz: You will have 24 hours to complete your quiz (i.e., 10am next day)

Methods to Learn

	Vector Data	Text Data	Graph & Network	Recommender Systems
Classification	**Naïve Bayes; Logistic Regression**; NN		Label Propagation	
Clustering	**K-means; kernel k-means; Mixture Models**	PLSA; LDA	Spectral Clustering	Matrix Factorization
Prediction	NN			Collaborative Filtering; Factorization machine; Hybrid CF; Recommendation with graph regularization
Ranking			PageRank	
Similarity Search			P-PageRank	
Representation Learning		Word embedding	Network embedding	Deep collaborative learning

Clustering

- Clustering 
- K-means
- Kernel K-means
- Mixture Model and EM algorithm
- Summary

What is Cluster Analysis?

- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation, …*)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes (i.e., *learning by observations* vs. learning by examples: supervised)
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

Applications of Cluster Analysis

- Data reduction
  - Summarization: Preprocessing for regression, PCA, classification, and association analysis
  - Compression: Image processing: vector quantization
- Prediction based on groups
  - Cluster & find characteristics/patterns for each group
- Finding K-nearest Neighbors
  - Localizing search to one or a small number of clusters
- Outlier detection: Outliers are often viewed as those “far away” from any cluster

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Recall K-Means

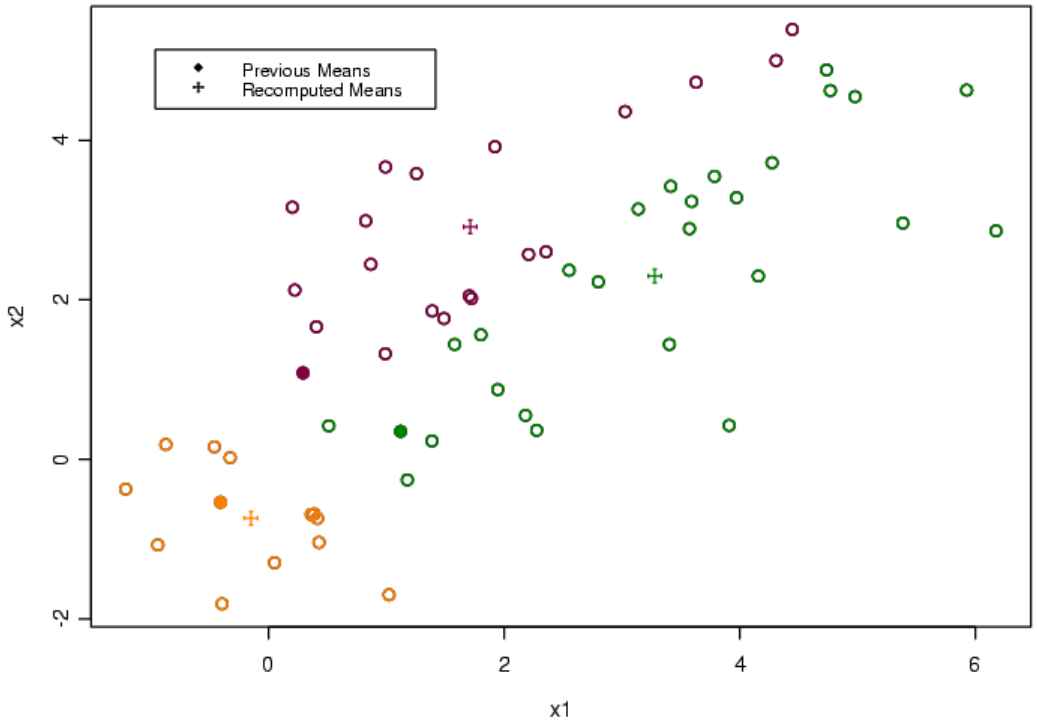
- Objective function
  - $J = \sum_{j=1}^{k} \sum_{C(i)=j} ||x_i - c_j||^2$
  - Total within-cluster variance
- Re-arrange the objective function
  - $J = \sum_{j=1}^{k} \sum_{i} w_{ij} ||x_i - c_j||^2$
    - $w_{ij} \in \{0,1\}$
    - $w_{ij} = 1, if\ x_i\ belongs\ to\ cluster\ j; w_{ij} = 0, otherwise$
  - Looking for:
    - The best assignment w_{ij}
    - The best center c_j

Solution of K-Means

- Iterations

$$J = \sum_{j=1}^{k} \sum_{i} w_{ij} ||x_i - c_j||^2$$

  - Step 1: Fix centers c_j, find assignment w_{ij} that minimizes J
    - => $w_{ij} = 1, if\ ||x_i - c_j||^2$ is the smallest
  - Step 2: Fix assignment w_{ij}, find centers that minimize J
    - => first derivative of J = 0
    - => $\frac{\partial J}{\partial c_j} = -2 \sum_i w_{ij}(x_i - c_j) = 0$
    - => $c_j = \frac{\sum_i w_{ij} x_i}{\sum_i w_{ij}}$
      - Note $\sum_i w_{ij}$ is the total number of objects in cluster j


Previous Means
Recomputed Means
x2
x1
-2
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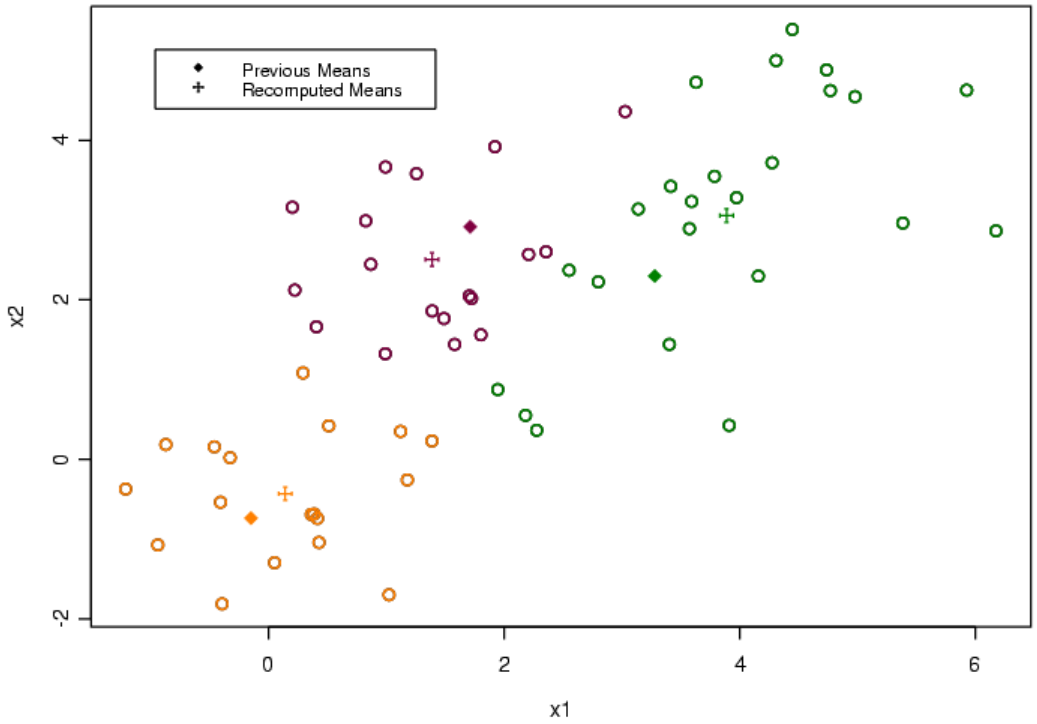
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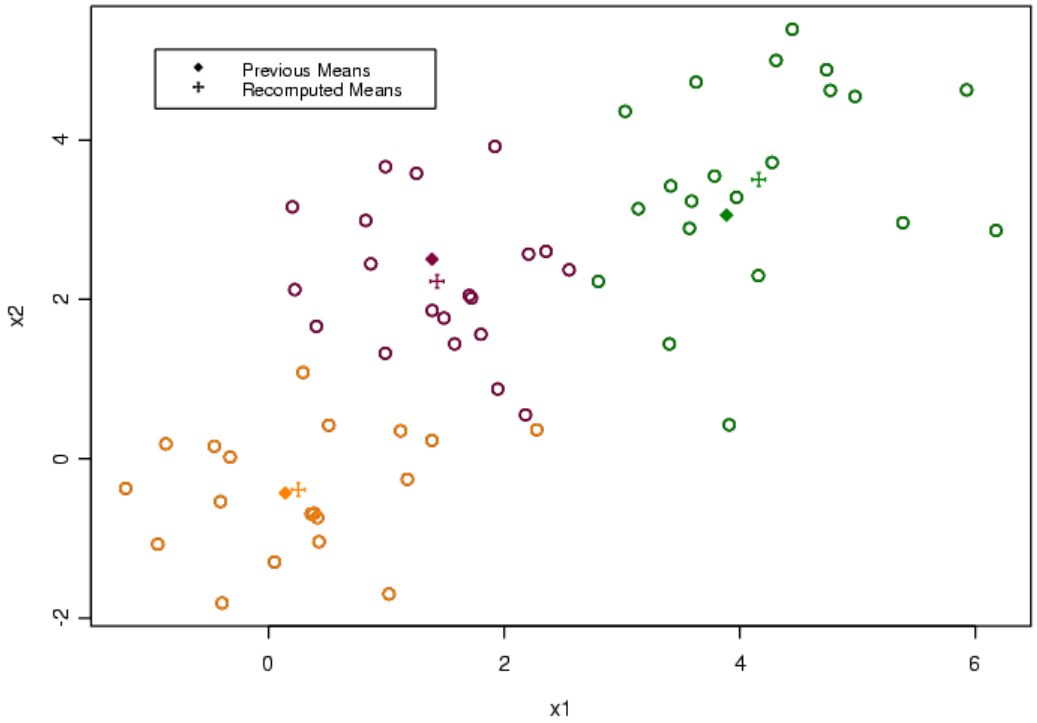
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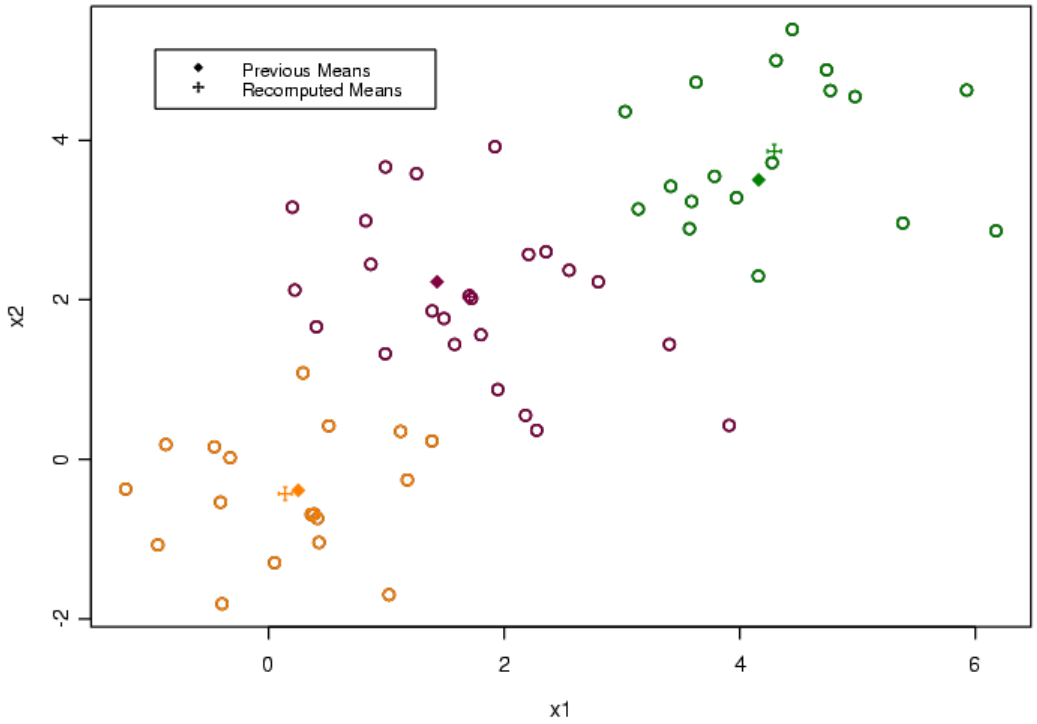
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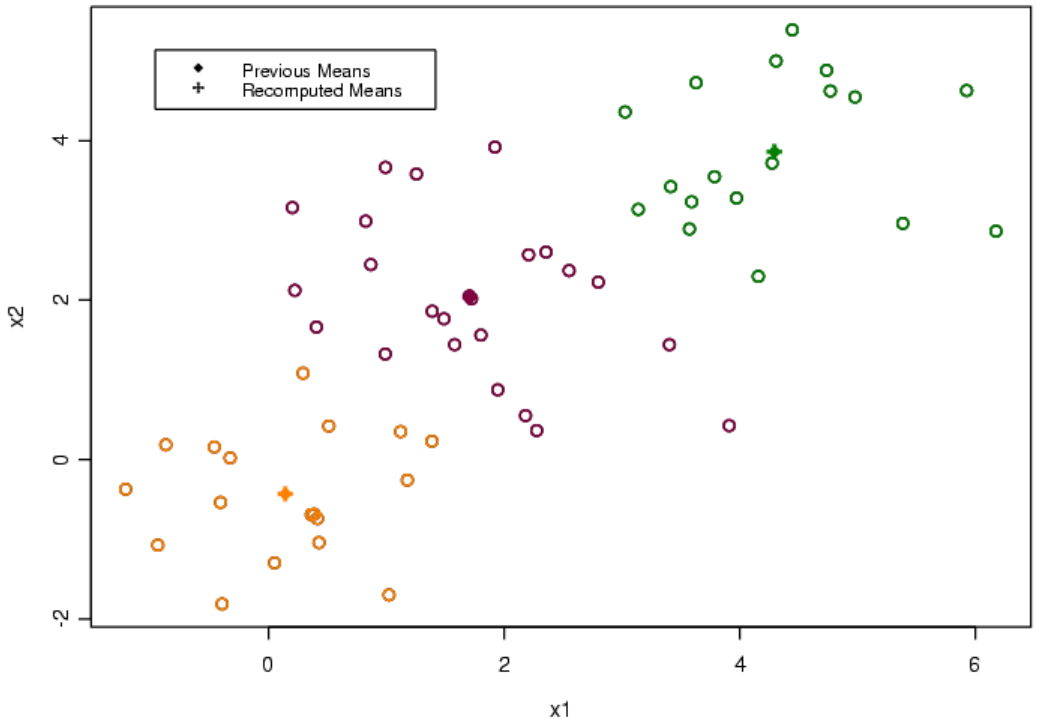
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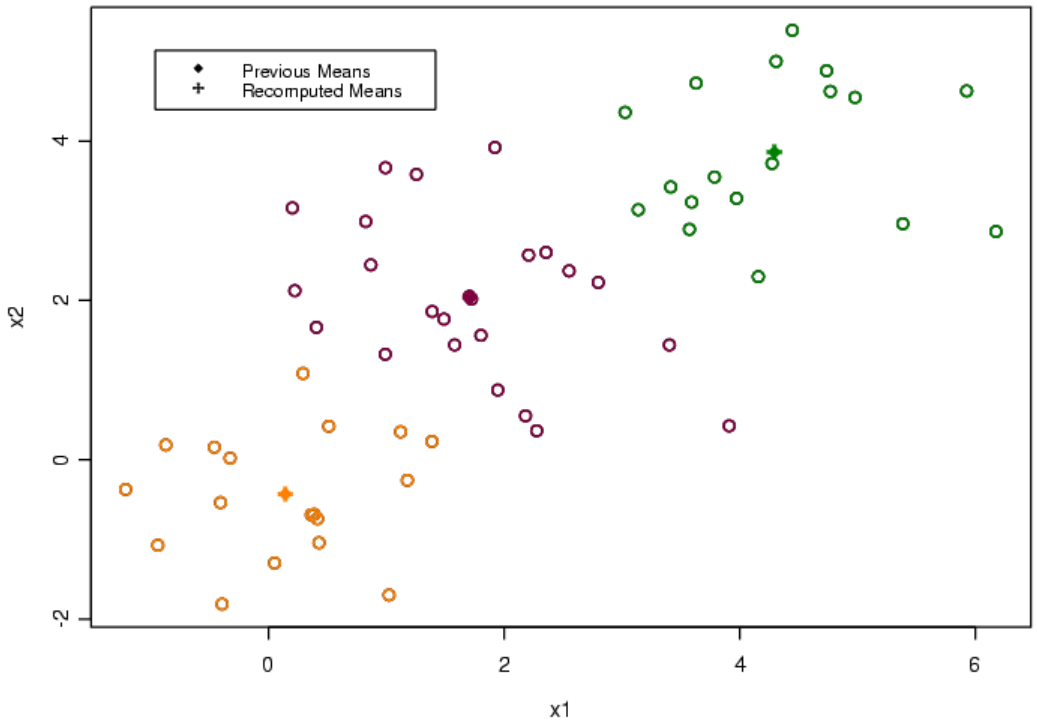
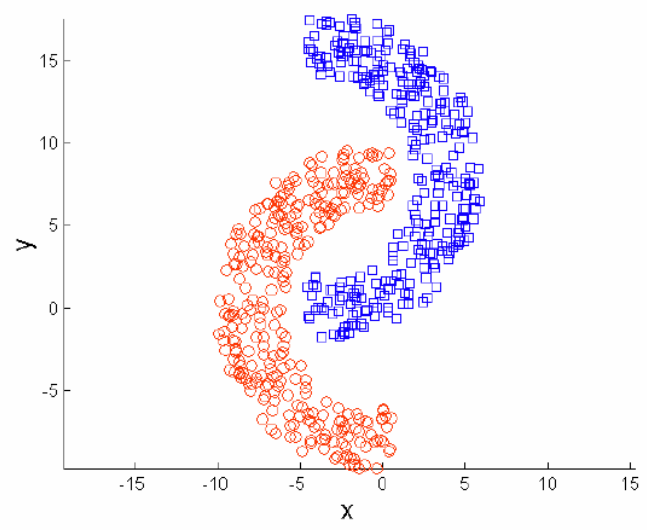


Converges! Why?

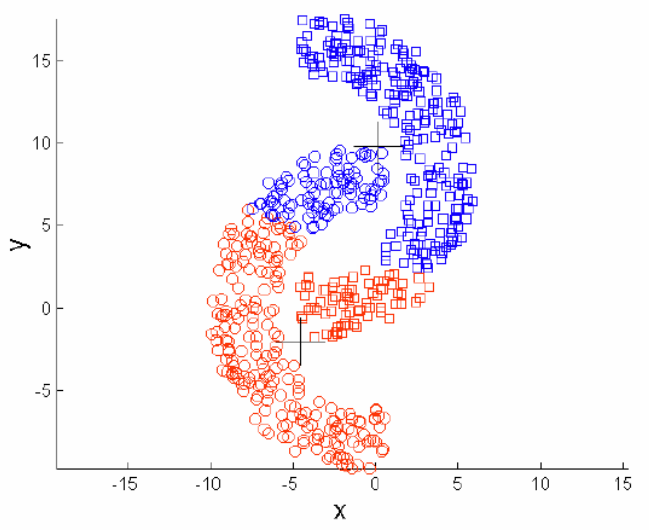
Limitations of K-Means

- K-means has problems when clusters are of
  - Non-Spherical Shapes
  - Different Sizes and density

Limitations of K-Means: Non-Spherical Shapes

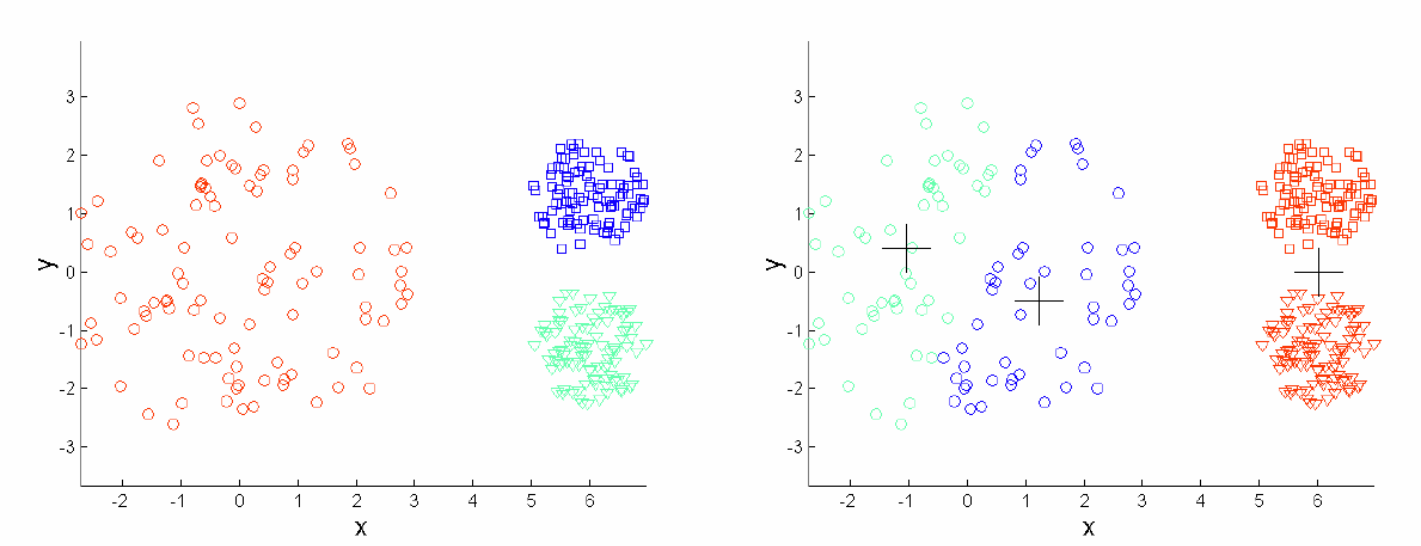


Original Points



K-means (2 Clusters)

Limitations of K-Means: Different Sizes and Variances

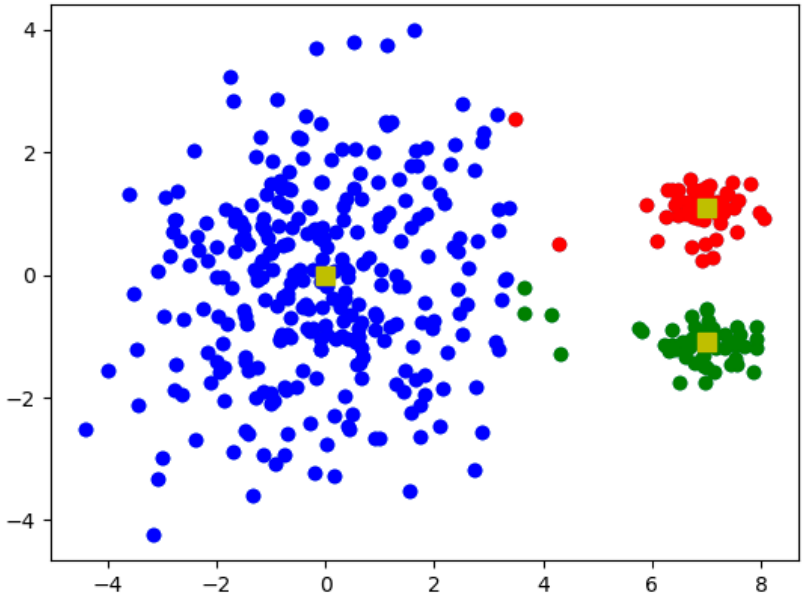


Original Points

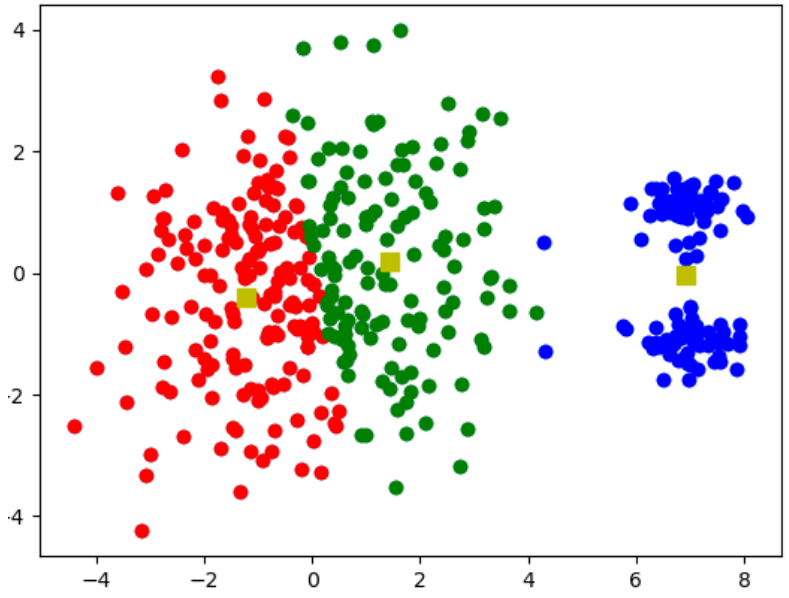
K-means (3 Clusters)

Example

- Consider the cost of K-means in two cases



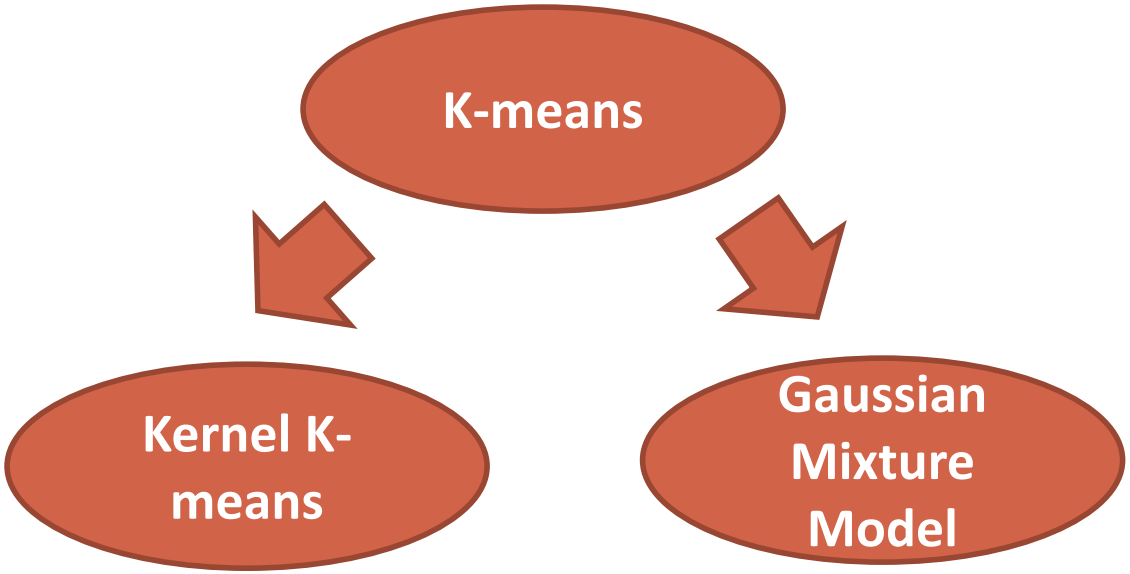
Cost: J = 1560.86



Cost: J = 1147.42

Recall: $J = \sum_{j=1}^{k} \sum_{C(i)=j} ||x_i - c_j||^2$

Connections of K-means to Other Methods



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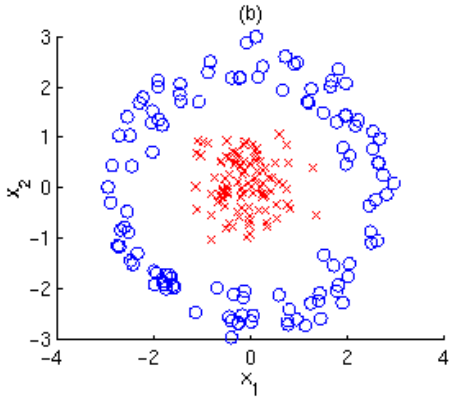
Kernel K-Means

- How to cluster the following data?



- A non-linear map: ϕ: $R^n \rightarrow F$
  - Map a data point into a higher/infinite dimensional space
  - $x \rightarrow \phi(x)$
- Dot product matrix K_{ij}
  - $K_{ij} =< \phi(x_i), \phi(x_j) >$

Typical Kernel Functions

- Recall kernel SVM:

$$\text{Polynomial kernel of degree } h: \quad K(\boldsymbol{X_i}, \boldsymbol{X_j}) = (\boldsymbol{X_i} \cdot \boldsymbol{X_j} + 1)^h$$

$$\text{Gaussian radial basis function kernel}: \quad K(\boldsymbol{X_i}, \boldsymbol{X_j}) = e^{-\|\boldsymbol{X_i} - \boldsymbol{X_j}\|^2 / 2\sigma^2}$$

$$\text{Sigmoid kernel}: \quad K(\boldsymbol{X_i}, \boldsymbol{X_j}) = \tanh(\kappa \boldsymbol{X_i} \cdot \boldsymbol{X_j} - \delta)$$

Solution of Kernel K-Means

- Objective function under new feature space:
  - $J = \sum_{j=1}^{k} \sum_i w_{ij} ||\phi(x_i) - c_j||^2$
- Algorithm
  - By fixing assignment w_{ij}
    - $c_j = \sum_i w_{ij}\, \phi(x_i) / \sum_i w_{ij}$
  - In the assignment step, assign the data points to the closest center
    - $d(x_i, c_j) = \left\| \phi(x_i) - \frac{\sum_{i'} w_{i'j} \phi(x_{i'})}{\sum_{i'} w_{i'j}} \right\|^2 = \phi(x_i) \cdot \phi(x_i) - 2 \frac{\sum_{i'} w_{i'j} \phi(x_i) \cdot \phi(x_{i'})}{\sum_{i'} w_{i'j}} + \frac{\sum_{i'} \sum_l w_{i'j} w_{lj} \phi(x_{i'}) \cdot \phi(x_l)}{(\sum_{i'} w_{i'j})\text{^}2}$

Do not really need to know $\phi(x)$, *but only* K_{ij}

Advantages and Disadvantages of Kernel K-Means

- **Advantages**
  - Algorithm is able to identify the non-linear structures.
- **Disadvantages**
  - Number of cluster centers need to be predefined.
  - Algorithm is complex in nature and time complexity is large.
- **References**
  - Kernel k-means and Spectral Clustering by Max Welling.
  - Kernel k-means, Spectral Clustering and Normalized Cut by Inderjit S. Dhillon, Yuqiang Guan and Brian Kulis.
  - An Introduction to kernel methods by Colin Campbell.

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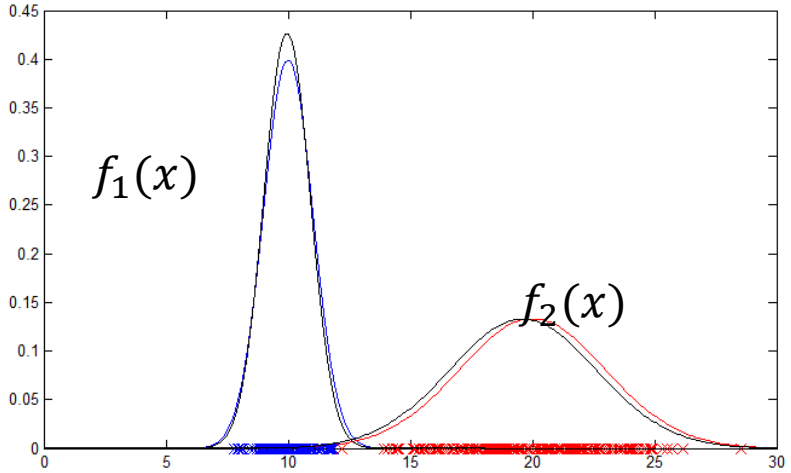
Hard Clustering vs. Soft Clustering

- Hard Clustering
  - Every object *i* is assigned to one cluster *j*, e.g., k-means
    - $w_{ij} = \{0,1\}\ and\ \sum_j w_{ij} = 1$
- Soft Clustering
  - Every object *i* is assigned with a probability to different clusters
    - $w_{ij} \in [0,1]\ and\ \sum_j w_{ij} = 1$

Mixture Model-Based Clustering

- A set *C* of *k* probabilistic clusters $C_1, \ldots, C_k$
  - probability density functions: $f_1, \ldots, f_k$,
  - Cluster prior probabilities: $w_1, \ldots, w_k, \sum_j w_j = 1$
- Joint Probability of an object *i and its* cluster C_j is:
  - $p(x_i, z_i = j) = w_j f_j(x_i)$
  - z_i: hidden random variable
- Probability of *i* is:
  - $p(x_i) = \sum_j w_j f_j(x_i)$



Maximum Likelihood Estimation

- Since objects are assumed to be generated independently, for a data set D = {x_1, …, x_n}, we have,

$$p(D) = \prod_i p(x_i) = \prod_i \sum_j w_j f_j(x_i)$$

$$\Rightarrow logp(D) = \sum_i logp(x_i) = \sum_i log \sum_j w_j f_j(x_i)$$

- Task: Find *k* probabilistic clusters s.t. *p*(*D*) is maximized

The EM (Expectation Maximization) Algorithm

- **The (EM) algorithm:** A framework to approach maximum likelihood or maximum a posteriori estimates of parameters in statistical models.
  - **E-step** assigns objects to clusters according to the current soft clustering or parameters of probabilistic clusters
    - $w_{ij}^{(t+1)} = p(z_i = j|\Theta^{(t)}, x_i) \propto p(x_i|z_i = j, \Theta^{(t)})p(z_i = j|\Theta^{(t)})$

      $f_j(x_i)$ w_j
  - **M-step** finds the new clustering or parameters that maximize the expected likelihood, with respect to conditional distribution $p(z_i = j|\Theta^{(t)}, x_i)$
    - $\Theta^{(t+1)} = argmax_\Theta \sum_i \sum_j w_{ij}^{(t+1)} \log p(x_i, z_i = j|\Theta)$

Gaussian Mixture Model

- Generative model
  - For each object:
    - Pick its cluster, i.e., a distribution component: $Z \sim Categorical(w_1, \ldots, w_k)$
    - Sample a value from the selected distribution: $X|Z \sim N(\mu_Z, \sigma_Z^2)$
- Overall likelihood function
  - $L(D; \Theta) = \prod_i \sum_j w_j p(x_i|\mu_j, \sigma_j^2)$

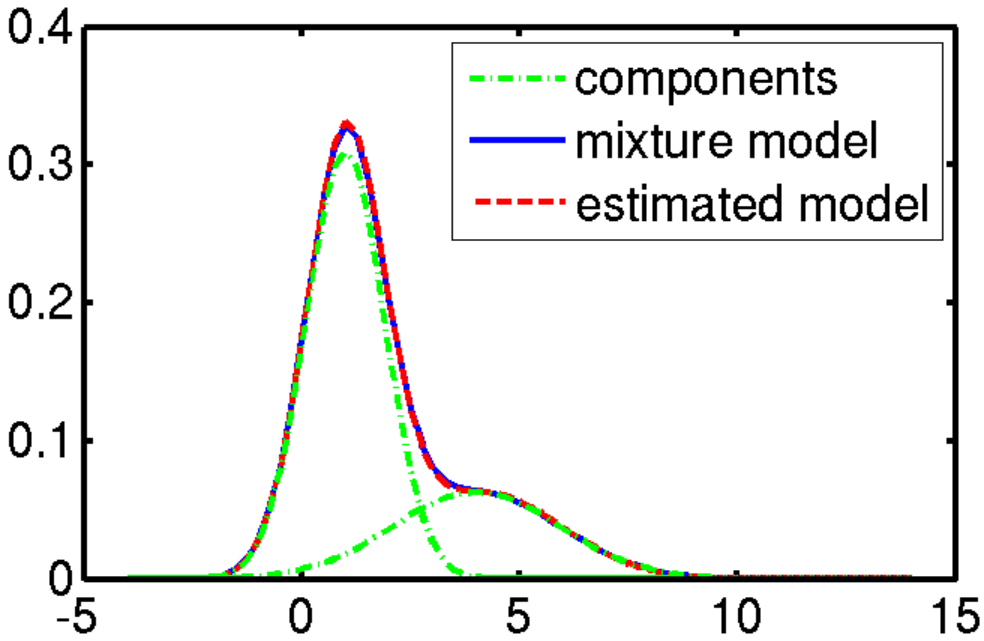
  s.t. $\sum_j w_j = 1 \; and \; w_j \geq 0$
  - Q: What is Θ here?

Apply EM algorithm: 1-d

- An iterative algorithm (at iteration t+1)
  - E(expectation)-step
    - Evaluate the weight w_{ij} when μ_j, σ_j, w_j are given
    - $w_{ij}^{(t+1)} = \frac{w_j^{(t)} p(x_i|\mu_j^{(t)},(\sigma_j^2)^{(t)})}{\sum_k w_k^{(t)} p(x_i|\mu_k^{(t)},(\sigma_k^2)^{(t)})}$, where $p(x_i|\mu_j^{(t)},(\sigma_j^2)^{(t)}) = f_j^{(t)}(x_i)$
  - M(maximization)-step
    - Find μ_j, σ_j, w_j that maximize the weighted log likelihood, where w_{ij}'s are the weights: $\sum_{ij} w_{ij}^{(t+1)} log w_j p(x_i|\mu_j, \sigma_j^2)$
    - It is equivalent to Gaussian distribution parameter estimation when each point has a weight belonging to each distribution
      - $\mu_j^{(t+1)} = \frac{\sum_i w_{ij}^{(t+1)} x_i}{\sum_i w_{ij}^{(t+1)}}; (\sigma_j^2)^{(t+1)} = \frac{\sum_i w_{ij}^{(t+1)} \left(x_i - \mu_j^{(t+1)}\right)^2}{\sum_i w_{ij}^{(t+1)}}; w_j^{(t+1)} = \sum_i w_{ij}^{(t+1)} / n$

Example: 1-D GMM

- Blue curve: ground truth distribution
- Sample data points from blue curve
- Red curve: estimated distribution



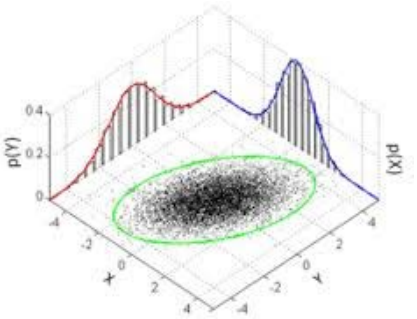
https://www.mathworks.com/matlabcentral/fileexchange/24867-gaussian_mixture_model-m

2-d Gaussian

- Bivariate Gaussian distribution
  - Two dimensional random variable: $\mathrm{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N(\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \Sigma = \begin{pmatrix} \sigma_1^2 & \sigma(X_1, X_2) \\ \sigma(X_1, X_2) & \sigma_2^2 \end{pmatrix})$$

  - $\mu_1 \; and \; \mu_2$ are means of $X_1 and \; X_2$
  - $\sigma_1 \; and \; \sigma_2 \; are$ standard deviations of $X_1 and \; X_2$
  - $\sigma(X_1, X_2) \; is \; the \; covariance \; between \; X_1 and \; X_2,$ $i.e., \sigma(X_1, X_2) = E(X_1 - \mu_1)(X_2 - \mu_2)$

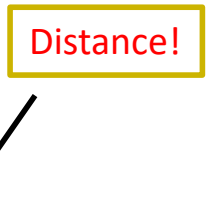


Apply EM algorithm: 2-d

- An iterative algorithm (at iteration t+1)
  - E(expectation)-step
    - Evaluate the weight w_{ij} when $\boldsymbol{\mu}_j, \Sigma_j, w_j$ are given
    - $w_{ij}^{(t+1)} = \frac{w_j^{(t)} p(\boldsymbol{x}_i | \boldsymbol{\mu}_j^{(t)}, \Sigma_j^{(t)})}{\sum_j w_j^{(t)} p(\boldsymbol{x}_i | \boldsymbol{\mu}_j^{(t)}, \Sigma_j^{(t)})}$
  - M(maximization)-step
    - Find $\boldsymbol{\mu}_j, \Sigma_j, w_j$ that maximize the weighted likelihood, where w_{ij}'s are weights: $\sum_{ij} w_{ij}^{(t+1)} log w_j p(\boldsymbol{x}_i | \boldsymbol{\mu}_j, \Sigma_j)$
    - It is equivalent to Gaussian distribution parameter estimation when each point has a weight belonging to each distribution
      - $\boldsymbol{\mu}_j^{(t+1)} = \frac{\sum_i w_{ij}^{(t+1)} \boldsymbol{x}_i}{\sum_i w_{ij}^{(t+1)}}; (\sigma_{j,1}^2)^{t+1} = \frac{\sum_i w_{ij}^{(t+1)} \left\| x_{i,1} - \mu_{j,1}^{(t+1)} \right\|^2}{\sum_i w_{ij}^{t+1}}; (\sigma_{j,2}^2)^{(t+1)} = \frac{\sum_i w_{ij}^{(t+1)} \left\| x_{i,2} - \mu_{j,2}^{(t+1)} \right\|^2}{\sum_i w_{ij}^{t+1}};$
      - $(\sigma(X_1, X_2)_j)^{(t+1)} = \frac{\sum_i w_{ij}^{(t+1)} (x_{i,1} - \mu_{j,1}^{(t+1)})(x_{i,2} - \mu_{j,2}^{(t+1)})}{\sum_i w_{ij}^{(t+1)}}; w_j^{(t+1)} \propto \sum_i w_{ij}^{(t+1)}$

K-Means: A Special Case of Gaussian Mixture Model

- When each Gaussian component with covariance matrix $\sigma^2 I$, and with the same size w_j
  - Soft K-means
  - $w_{ij} \propto p(x_i|\mu_j, \sigma^2) w_j \propto \exp\left\{-\frac{(x_i-\mu_j)^2}{2\sigma^2}\right\} w_j$



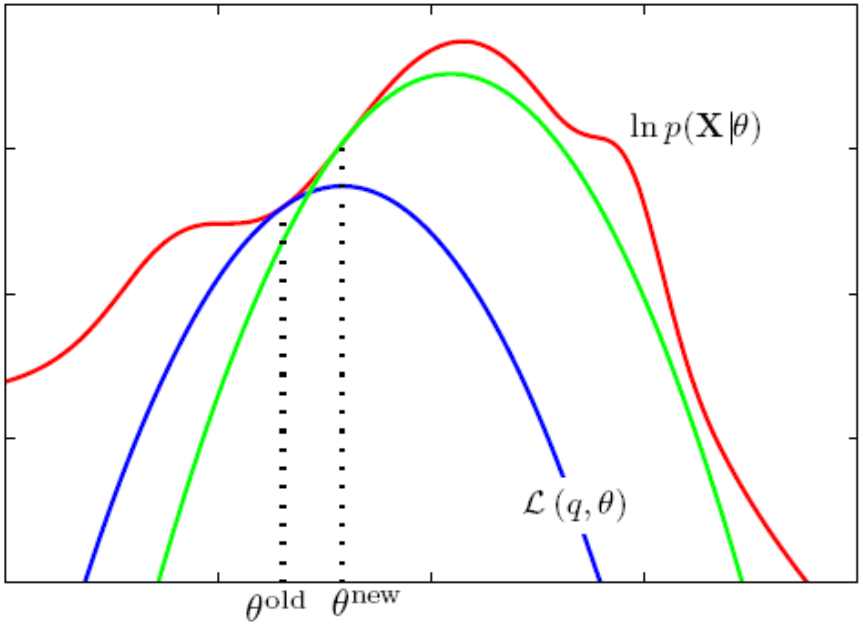
- When $\sigma^2 \to 0$
  - Soft assignment becomes hard assignment
  - $w_{ij} \to 1, if\ x_i$ is closest to μ_j (why?)

Mapping Soft Clustering to Hard Clustering

- For evaluation purpose
  - $j^* = \text{argmax}_j w_{ij}$
  - $w_{ij^*} = 1; w_{ij} = 0 \; for \; all \; other \; j \neq j^*$
- Example:
  - $K = 3; the \; output \; of \; GMM \; for \; object \; i \; is$
    - $w_{i1} = 0.7, w_{i2} = 0.2, w_{i3} = 0.1$
    - $\Rightarrow mapping \; result: \; assign \; i \; to \; cluster \; 1$

Why EM Works?

- E-Step: computing a **tight** lower bound L of the original objective function l at θ_{old}
- M-Step: find θ_{new} to maximize the lower bound
- $l(\theta_{new}) \geq L(\theta_{new}) \geq L(\theta_{old}) = l(\theta_{old})$



How to Find Tight Lower Bound?

- $$\begin{aligned} \ell(\theta) &= \log \sum_h p(d,h;\theta) \\ &= \log \sum_h \frac{q(h)}{q(h)} p(d,h;\theta) \\ &= \log \sum_h q(h) \frac{p(d,h;\theta)}{q(h)} \end{aligned}$$

$q(h)$: the key to tight lower bound we want to get

- Jensen's inequality
  - $$\log \sum_h q(h) \frac{p(d,h;\theta)}{q(h)} \geq \sum_h q(h) \log \frac{p(d,h;\theta)}{q(h)}$$

the tight lower bound

  - When "=" holds to get a tight lower bound?
    - $q(h) = p(h|d,\theta)$ (why?)

In GMM Case

$$L(D;\theta) = \sum_i \log \sum_j w_j p(x_i|\mu_j, \sigma_j^2)$$

$$\geq \sum_i \sum_j w_{ij} \left(\log w_j p\left(x_i \middle| \mu_j, \sigma_j^2\right) - log w_{ij}\right)$$

$\log L(x_i, z_i = j|\theta)$

Does not involve θ, can be dropped

Advantages and Disadvantages of GMM

- Strength
  - Mixture models are more general than partitioning: different densities and sizes of clusters
  - Clusters can be characterized by a small number of parameters
  - The results may satisfy the statistical assumptions of the generative models
- Weakness
  - Converge to local optimal (overcome: run multi-times w. random initialization)
  - Computationally expensive if the number of distributions is large
  - Hard to estimate the number of clusters
  - Can only deal with spherical clusters

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Summary

- Revisit k-means
  - Objective function, Limitations
- Kernel k-means
  - Distance in higher-dimensional space
- Mixture models
  - Gaussian mixture model; multinomial mixture model; EM algorithm; Connection to k-means