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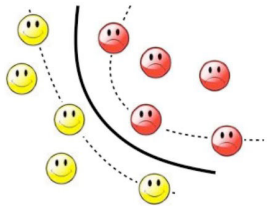

Machine Learning and Data Mining (COMP 5318)

Clustering and Expectation-Maximisation

Nguyen Hoang Tran

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Clustering

C. Bishop, *Pattern Recognition and Machine Learning*,
Chapter 9: Mixture Models and EM
Springer New York, 2006

K.P. Murphy, *Machine Learning: a Probabilistic Perspective*,
Chapters 11 and 25, Massachusetts Institute of Technology, 2006

Types of Learning

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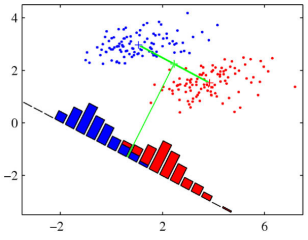
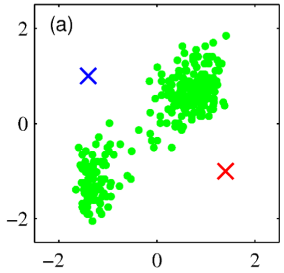
Supervised Learning



Learning input-output from examples

Regression
Classification

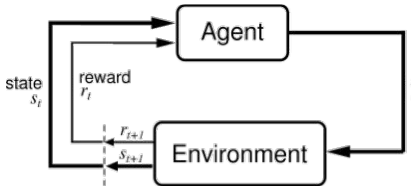
Unsupervised Learning



Learning underlying structure

Clustering
Density Estimation

Reinforcement Learning



Learning policy from state-action-reward sequences.

Learning behaviour

Clustering

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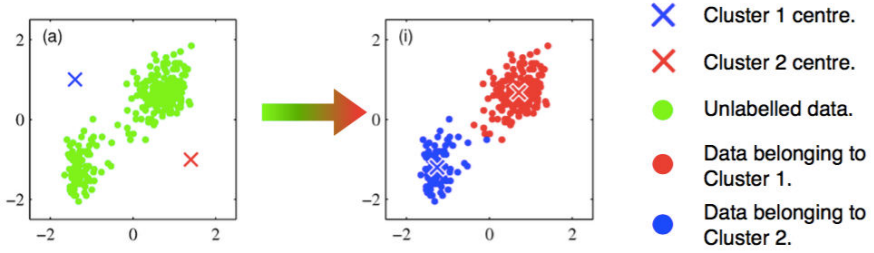
Process of grouping similar objects together



Learn a set of clusters and assign data to a specific cluster.

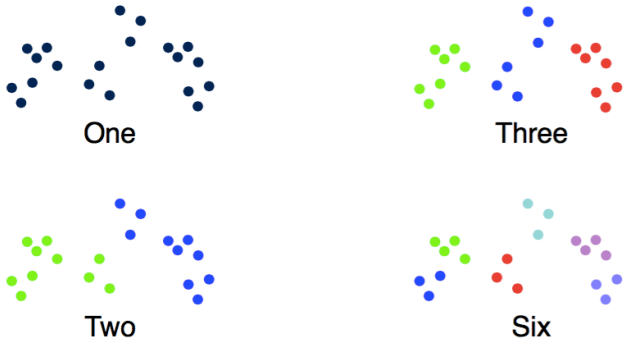
Deterministic: Hard assignment to each cluster (K-means).
Probabilistic: Model assignment as a discrete latent variable. (Mixtures of Gaussians, Dirichlet Process)

Clustering

How many clusters?

Clustering

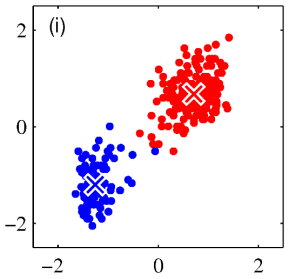
How many clusters?



Presence of ambiguous solutions.

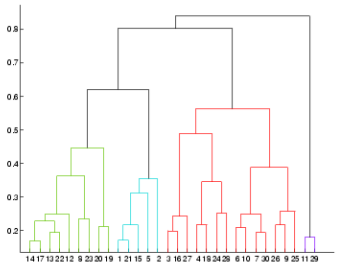
Types of Clustering

Partition Clustering



Partition the objects into disjoint sets. Faster to create.
Sensible to initial conditions.
Model selection for K.

Hierarchical Clustering



Nested tree of partitions.
Slower to create.
Often more useful.
Do not require knowing the number of clusters.

Clustering

Dataset $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ with N Observations

Each data point is D dimension

Goal: Partition dataset into K clusters. (For now, assume K is given)

$\boldsymbol{\mu}_k = (\mu_1, ..., \mu_D)$: Centroid for each cluster $k \in 1, ..., K$

Binary indicator variables

$$r_{nk} = \begin{cases} 1, & \text{if datapoint } n \text{ belongs to cluster } k \\ 0, & \sim \end{cases}$$

If $\mathbf{x}_n$ is assigned to cluster k, then $r_{nk} = 1 \ \wedge \ r_{nj} = 0 \ \forall j \neq k$

K-Means

Objective function:

$$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

Represents the sum of the squares of the distances of each datapoint to its assigned centroid vector.

Goal: Find $\{\boldsymbol{\mu}_k\}$ and $\{r_{nk}\}$ that minimise J.

$$\{r_{nk}, \boldsymbol{\mu}_k\}^\star = \underset{\{r_{nk}, \boldsymbol{\mu}_k\}}{\operatorname{argmin}} \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

K-Means

Iterative solution to minimise J:

1. Data Preprocessing
2. Initialise $\{\boldsymbol{\mu}_k\}$
3. Repeat 4 and 5 until convergence or Max Iterations
4. Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\boldsymbol{\mu}_k\}$
5. Minimise J w.r.t. $\{\boldsymbol{\mu}_k\}$ keeping $\{r_{nk}\}$

K-Means

$$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

Line 4: Optimise w.r.t r_{nk}

Each data point is independent, so we can optimise for each n separately:

$$r_{nk} = \begin{cases} 1 & \text{if } k = \underset{j}{\operatorname{argmin}}\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{Otherwise} \end{cases}$$

Assign each data point to its closest centroid.

K-Means

$$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

Line 5: Optimise w.r.t $\boldsymbol{\mu}_k$

$$\frac{\partial J}{\partial \boldsymbol{\mu}_k} = 0$$

$$2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) = 0$$

$$\sum_{n=1}^{N} r_{nk}\mathbf{x}_n = \sum_{n=1}^{N} r_{nk}\boldsymbol{\mu}_k$$

$$\frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}} = \boldsymbol{\mu}_k$$

Set $\boldsymbol{\mu}_k$ equal to the mean of all data points $\mathbf{x}_n$ assigned to cluster k.

K-means

K-Means Example

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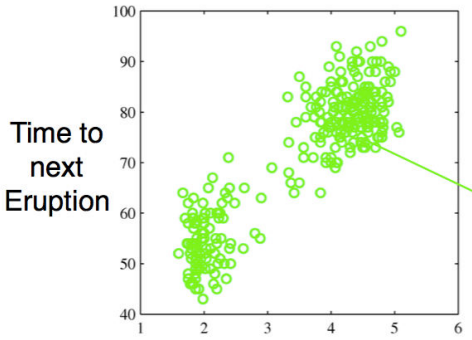
Hydrothermal Geyser: Old Faithful



Singe Eruption

$N = 272$ Observations

K-Means Example

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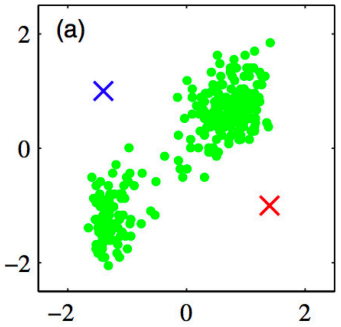
Number of clusters: $K = 2$

1 Data Preprocessing
2 Initialise $\{\mu_k\}$
3 Repeat until convergence or Max Iterations
4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\mu_k\}$ fixed.
5 Minimise J w.r.t. $\{\mu_k\}$ keeping $\{r_{nk}\}$ fixed.



Each dimension has zero mean and unit standard deviation.

Better initialisation: Choose{μk} as average of a random subset.

K-Means Example

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Number of clusters: $K = 2$

1 Data Preprocessing
2 Initialise $\{\mu_k\}$
3 Repeat until convergence or Max Iterations
4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\mu_k\}$ fixed.
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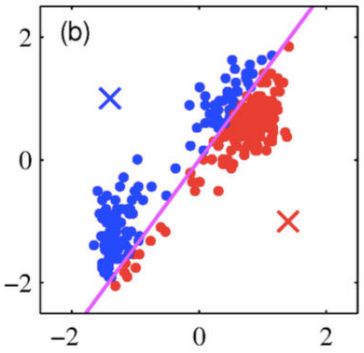

Each data point is assigned to the closest cluster centre.

K-Means Example

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Number of clusters: $K = 2$

1 Data Preprocessing
2 Initialise $\{\mu_k\}$
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4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\mu_k\}$ fixed.
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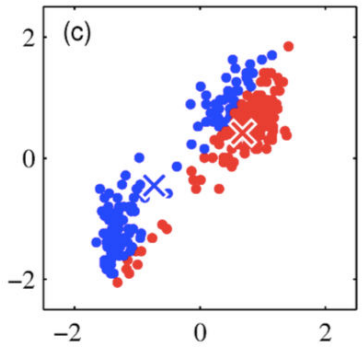
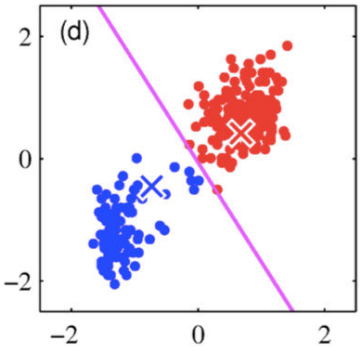


Re-compute each cluster centre to be the mean of the points previously assigned.

K-Means Example

Number of clusters: $K = 2$

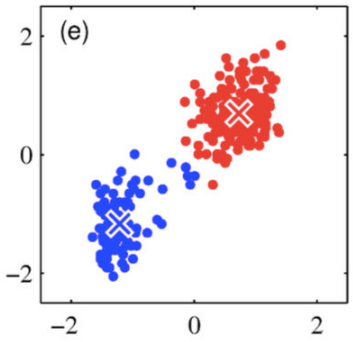


1 Data Preprocessing
2 Initialise $\{\boldsymbol{\mu}_k\}$
3 Repeat until convergence or Max Iterations
4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\boldsymbol{\mu}_k\}$ fixed.
5 Minimise J w.r.t. $\{\boldsymbol{\mu}_k\}$ keeping $\{r_{nk}\}$ fixed.

Each data point is assigned to the closest cluster centre.

K-Means Example

Number of clusters: $K = 2$

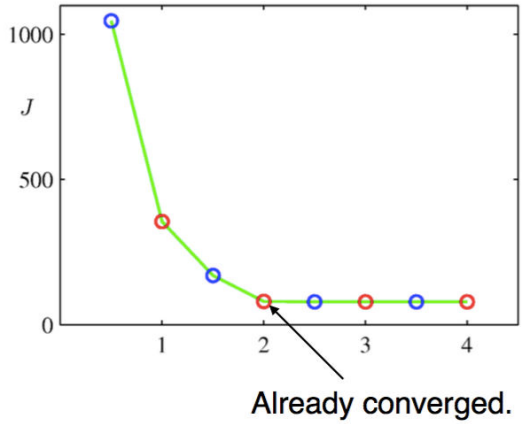


1 Data Preprocessing
2 Initialise $\{\boldsymbol{\mu}_k\}$
3 Repeat until convergence or Max Iterations
4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\boldsymbol{\mu}_k\}$ fixed.
5 Minimise J w.r.t. $\{\boldsymbol{\mu}_k\}$ keeping $\{r_{nk}\}$ fixed.

Re-compute each cluster centre to be the mean of the points previously assigned.

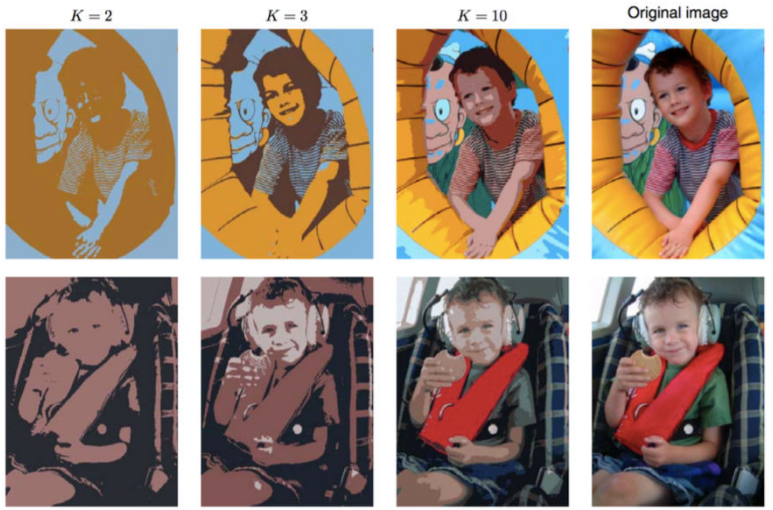
K-Means Example

Plot of the cost function for each iteration.



K-Means Example 2

Image segmentation and compression.



K-Means Limitations

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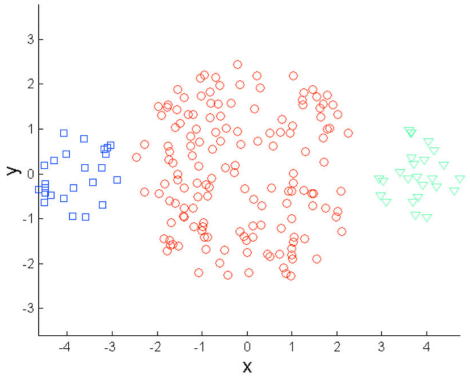
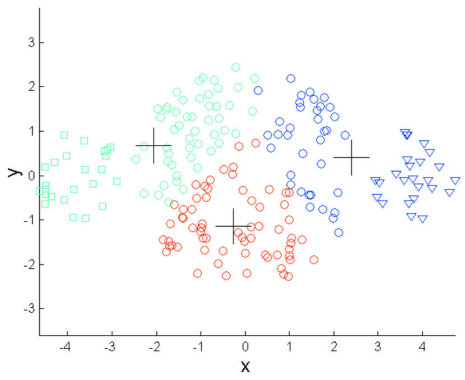
Differing Sizes:



Original Points



K-Means 3 Clusters

K-Means Limitations

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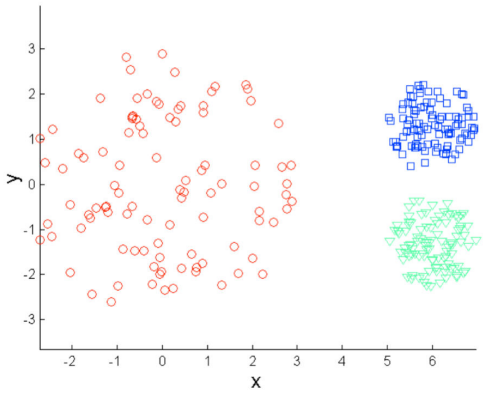
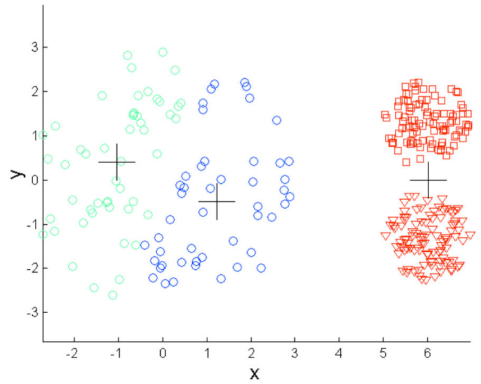
Differing Density:



Original Points



K-Means 3 Clusters

K-Means Limitations

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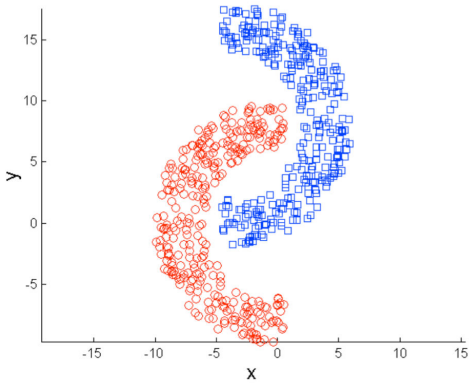
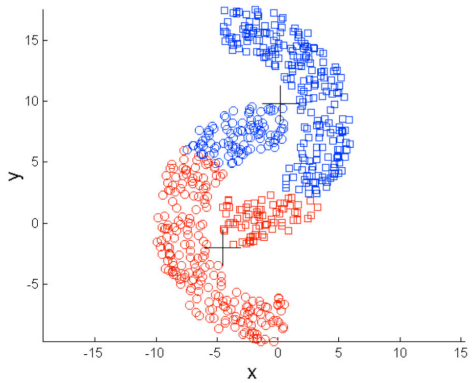
Non-Globular Shapes:



Original Points



K-Means 2 Clusters

Overcome K-Means Limitations

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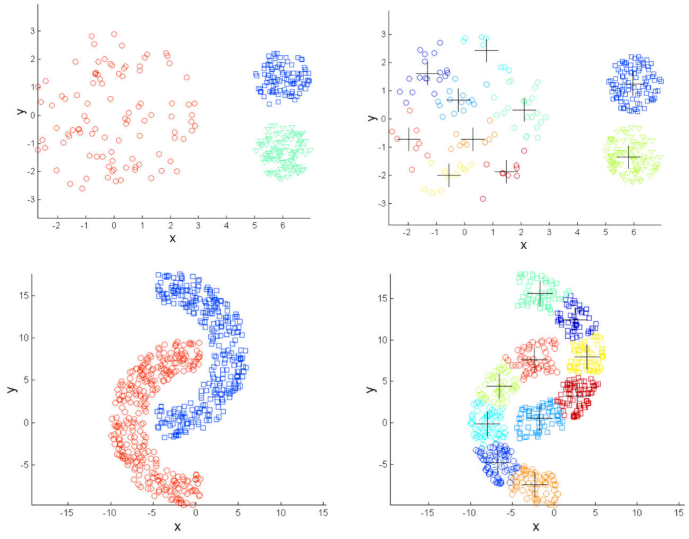
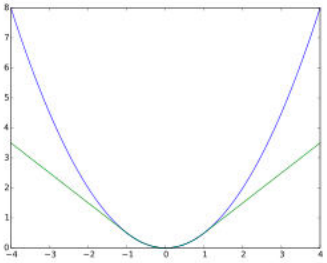
Use large number of clusters.



K-Means Enhancement

Generalise distance function:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$



Robustness to outliers.

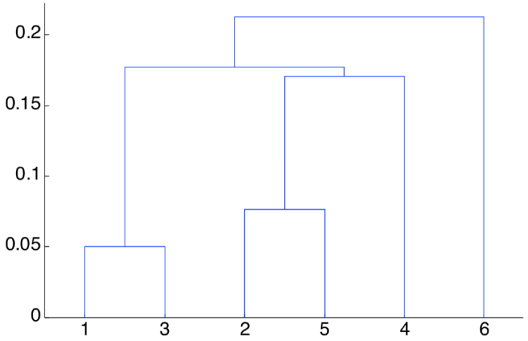
$$\mathcal{V}(\mathbf{x}_n, \mu_k) = \begin{cases} 1/2\|\mathbf{x}_n - \mu_k\|_2^2, & \text{if } \|\mathbf{x}_n - \mu_k\| \leq \delta \\ \delta\|\mathbf{x}_n - \mu_k\|_1 - 1/2\delta^2, & \text{otherwise} \end{cases}$$

Hierarchical Clustering

Hierarchical Clustering

Nested set of clusters organised as a hierarchical tree.

Any number of clusters can be obtained by 'cutting' the dendrogram.



Dendrogram

Uses a similarity matrix.

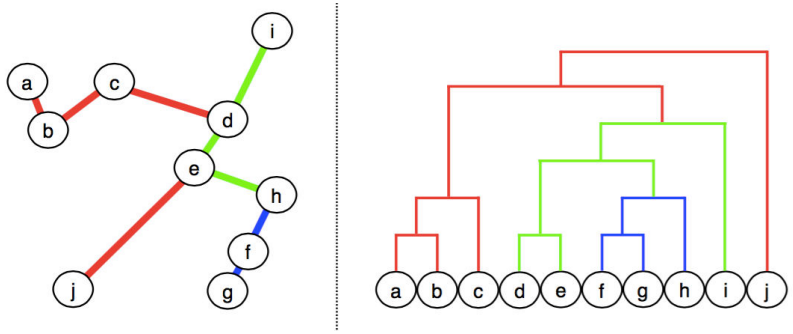
Hierarchical Agglomerative Clustering

Simple clustering algorithm.
Uses a inter cluster similarity measure.

1. Initialise: Every data point is a cluster.
2. Repeat until one cluster remains.
3. Compute distances between all clusters.
4. Merge closest clusters.
5. Update dendrogram.

Hierarchical Agglomerative Clustering

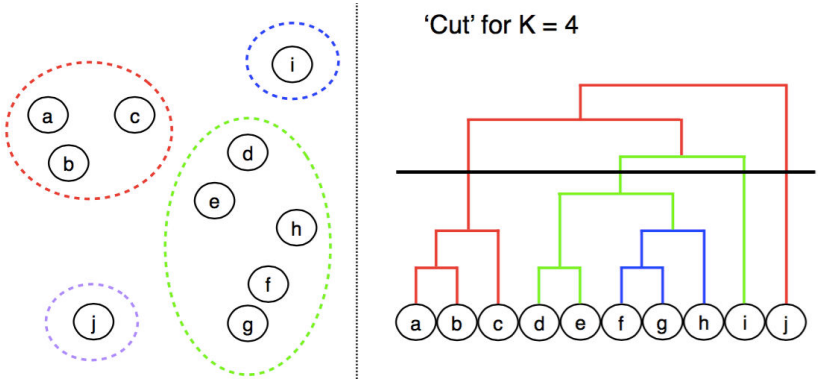
Example:



Dendrogram

Hierarchical Agglomerative Clustering

Example:



Dendrogram

Inter Cluster Similarity

Nearest Neighbour

$$D_{\min}(C_i, C_j) = \min_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|^2$$

Furthest Neighbour

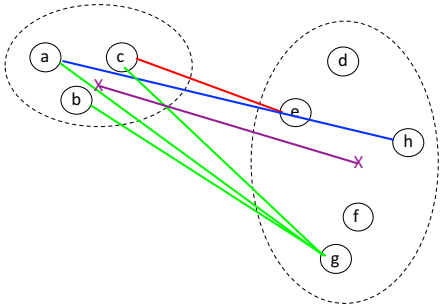
$$D_{\max}(C_i, C_j) = \max_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|^2$$

Group Average

$$D_{\text{avg}}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{\mathbf{x} \in C_i} \sum_{\mathbf{y} \in C_j} \|x - y\|^2$$

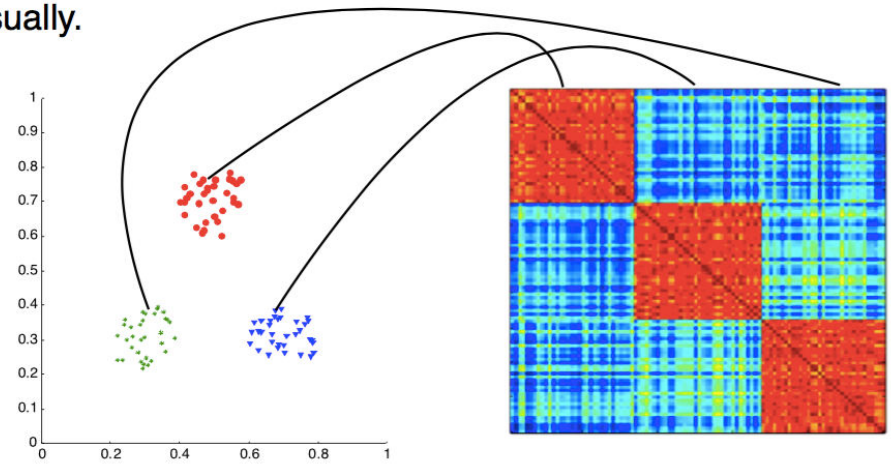
Centroid Distance

$$D_{\text{means}}(C_i, C_j) = \|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|$$



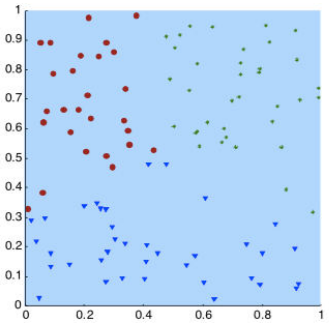
Cluster Validation

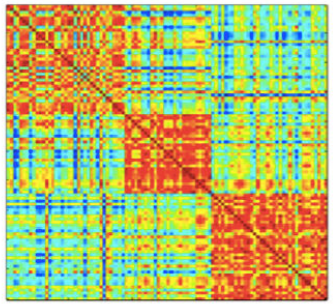
Similarity matrix with respect to cluster labels and inspect visually.



Cluster Validation

Random data clusters are not well defined.





Probabilistic Approach to Clustering

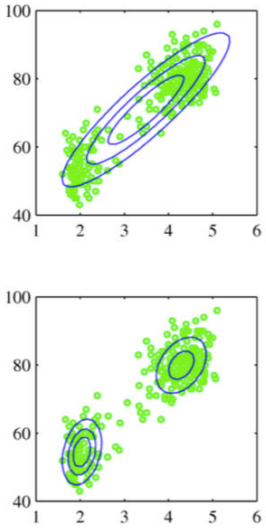
Mixture of Gaussians

Gaussian mixture distribution with K components.

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

$$0 \leq \pi_k \leq 1 \qquad \sum_{k=1}^{K} \pi_k = 1$$

Mixture models provide a probabilistic framework for clustering.



Mixture of Gaussians

Let us introduce a latent random variable

$$\mathbf{z} = \{z_k\}_{k \in 1,\ldots,K} \qquad z_k \in \{0, 1\} \qquad \sum_{k=1}^{K} z_k = 1$$

$\mathbf{z}$ has K possible states.

$$p(z_k = 1) = \pi_k \qquad p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}$$

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$$

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Mixture of Gaussians

Let us apply Bayes theorem and infer the value of the latent variable.

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})}$$

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{p(\mathbf{x})}$$

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

$\gamma(z_k)$ is called *responsibility* that component k takes for explaining $\mathbf{x}$.

π_k is the prior probability of component k.
$\gamma(z_k)$ is the posterior probability after $\mathbf{x}$ is observed.

Expectation Maximisation

EM for Gaussian Mixtures

Expectation Maximisation (EM)

Elegant and powerful method for finding MLE or MAP solutions for models with latent variables.

Intuition: If we knew what cluster each point belonged to (i.e. the z variables), we could partition the data and find the MLE for each cluster separately.

EM for Gaussian Mixtures

Likelihood function:

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

Conditions to be satisfied at maximum likelihood:

$$0 = \frac{\partial \ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \boldsymbol{\mu}_k}$$

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \qquad N_k = \sum_{n=1}^{N} \gamma(z_{nk})$$

N_k is the effective number of points assigned to cluster k.

EM for Gaussian Mixtures

$$0 = \frac{\partial \ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \boldsymbol{\Sigma}_k}$$

$$\Rightarrow \quad \boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

$$0 = \frac{\partial \ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\partial \pi_k}$$

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

EM Algorithm

1 Initialise means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k.

2 E-step

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

3 M-step

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

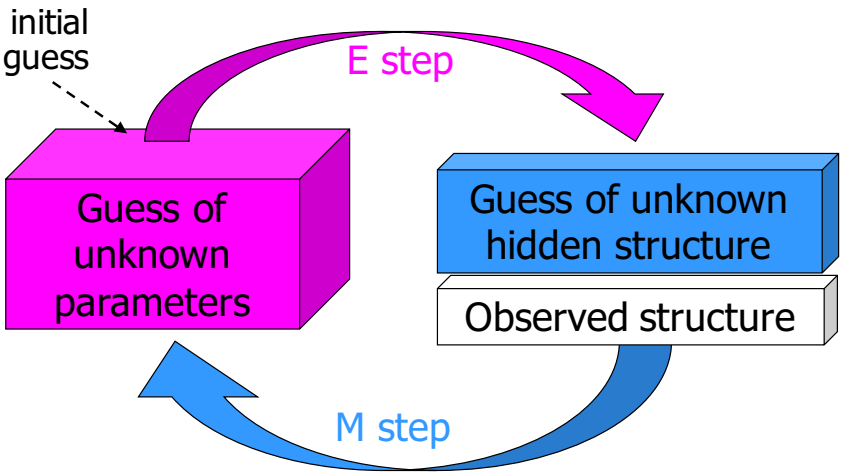
$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\mathrm{T}}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

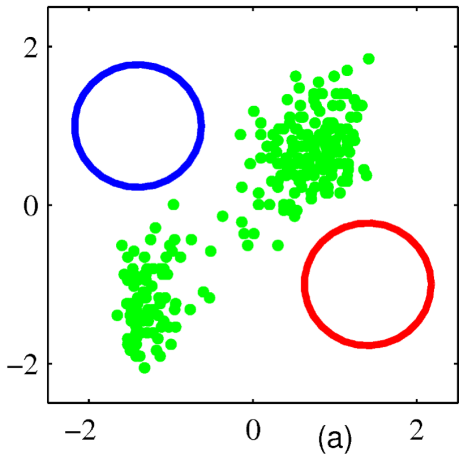
4 Eval Likelihood

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

EM Algorithm



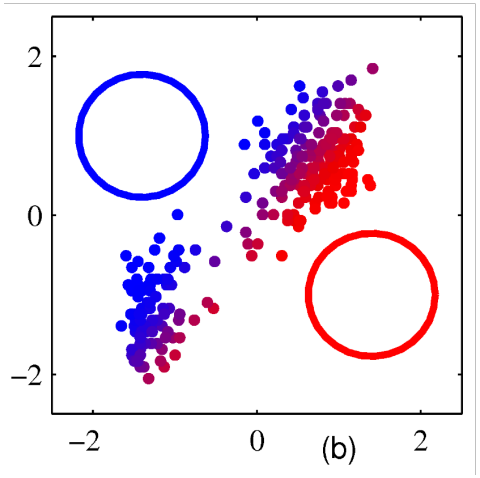
EM Example



Initial values for mean vectors (same as K-means example).

Diagonal covariance matrices (showing one std contour).

EM Example

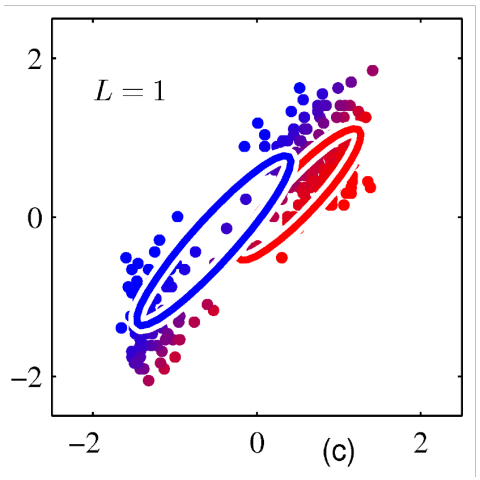


Initial E step.

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

Colour
proportional to responsibilities.

EM Example



M Step:

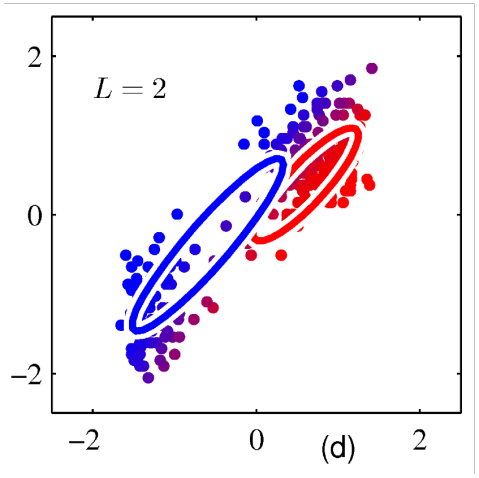
The means move towards the weighted average of dataset with respective ink colour (responsibilities).

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

The covariance matrices adapt to the covariance of the respective ink.

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$$

EM Example



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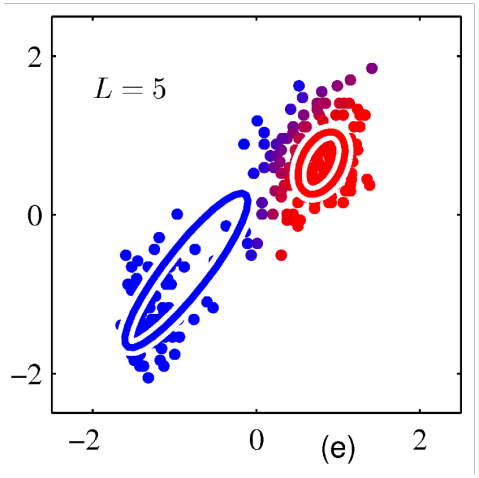
EM Example



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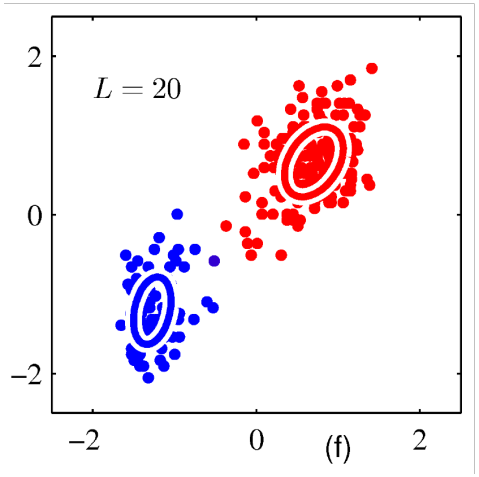
EM Example



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Clustering