

# Clustering

Course of Machine Learning  
Master Degree in Computer Science  
University of Rome "Tor Vergata"  
a.a. 2023-2024

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## Partitional clustering

Given a dataset  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ , with  $\mathbf{x}_i \in \mathbb{R}^d (i = 1, \dots, n)$ .

We wish to derive a set of **clusters** (i.e. a partition of  $\mathbf{X}$  into subsets of "near" elements). Clusters are represented by their **prototypes**  $(\mathbf{m}_1, \dots, \mathbf{m}_k)$ , with  $\mathbf{m}_j \in \mathbb{R}^d, j = 1, \dots, k$ .

Representation of a clustering

1. Cluster prototypes  $(\mathbf{m}_1, \dots, \mathbf{m}_k)$ , with  $\mathbf{m}_j \in \mathbb{R}^d (j = 1, \dots, k)$
2. Element assignment to clusters: for each  $\mathbf{x}_i$ ,  $k$  binary flags  $r_{ij} \in \{0, 1\}, j = 1, \dots, k$ . If  $\mathbf{x}_i$  is assigned the  $t$ -th cluster, then  $r_{it} = 1$  and  $r_{ij} = 0$  for  $j \neq t$

## Clustering types

- Partitional clustering: Given a set of items (points)  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ , we wish to partition  $\mathbf{X}$  by assigning each element to one out of  $k$  clusters  $C_1, \dots, C_k$  in such a way to maximize (or minimize) a given cost  $J$ . The number  $k$  of clusters could be given or should have to be computed.
- Hierarchical clustering: Given a set of items (points)  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ , we wish to derive a set of nested partitions of  $\mathbf{X}$ , from the partition composed by all singletons (one cluster for each node) to the one composed by a single item (the whole set).

## Clustering cost

Sum of squares

Let us define the cost a clustering as follows:

$$J(R, M) = \sum_{i=1}^k \sum_{j=1}^n r_{ij} \|\mathbf{x}_j - \mathbf{m}_i\|^2 = \sum_{i=1}^k \sum_{j=1}^n r_{ij} (\mathbf{x}_j - \mathbf{m}_i)^T (\mathbf{x}_j - \mathbf{m}_i)$$

where

- $R_{ij} = r_{ij}$ , where  $r_{is} = 1$  and  $r_{ij} = 0$  for  $j \neq s$  if  $\mathbf{x}_i$  is assigned to cluster  $C_s$
- $M_i = \mathbf{m}_i, i = 1, \dots, k$  is the prototype (centroid) of cluster  $C_i$ ,

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{j=1}^n r_{ij} \mathbf{x}_j$$

## k-means clustering

Dataset  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ ,  $\mathbf{x}_i \in \mathbb{R}^d$ : we wish to derive  $k$  clusters with prototypes  $\mathbf{m}_1, \dots, \mathbf{m}_k$

Assignment of elements to cluster: for each  $\mathbf{x}_i$ ,  $k$  binary flags  $r_{ij}$  ( $j = 1, \dots, k$ )

- if  $\mathbf{x}_i$  is assigned to cluster  $s$ , then  $r_{is} = 1$ , and  $r_{ij} = 0$  for  $j \neq k$

Cost: sum of the distances of each point from the prototype of the corresponding cluster

$$J(R, M) = \sum_{i=1}^n \sum_{j=1}^k r_{ij} \|\mathbf{x}_i - \mathbf{m}_j\|^2$$

Objective: finding  $r_{ij}$  and  $\mathbf{m}_j$  ( $i = 1, \dots, n$ ,  $j = 1, \dots, k$ ) to minimize  $J(R, M)$

### Algorithm

1. Given a set of prototypes  $\mathbf{m}_{ij}$ , minimize wrt  $r_{ij}$  (assigning elements to clusters).

For each  $\mathbf{x}_i$ , minimize  $\sum_{j=1}^k r_{ij} \|\mathbf{x}_i - \mathbf{m}_j\|^2$ .

The minimum is obtained for  $r_{ik} = 1$  (and  $r_{ij} = 0$  for  $j \neq k$ ), where  $\|\mathbf{x}_i - \mathbf{m}_k\|^2$  is the minimum distance. That is, each point is assigned to the cluster of the nearest prototype.

2. Given a set of assignments  $r_{ij}$ , minimize wrt  $\mathbf{m}_{ij}$  (defining new cluster prototypes)

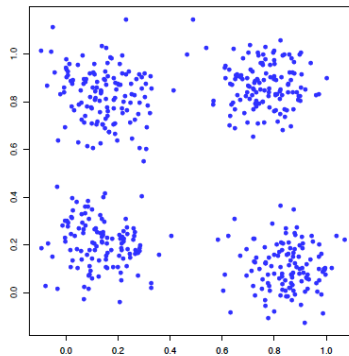
For each  $\mathbf{m}_k$ ,  $J = \sum_{i=1}^n \sum_{j=1}^k r_{ij} \|\mathbf{x}_i - \mathbf{m}_j\|^2$  is a quadratic function of  $\mathbf{m}_k$ . By setting its derivative to zero, the values of  $\mathbf{m}_k$  providing its minimum are obtained

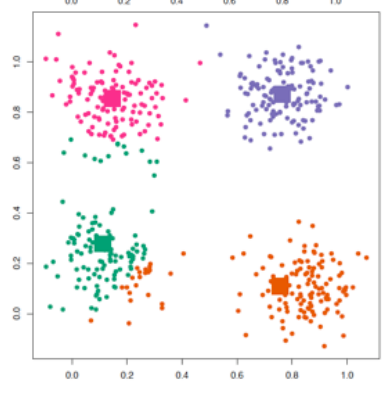
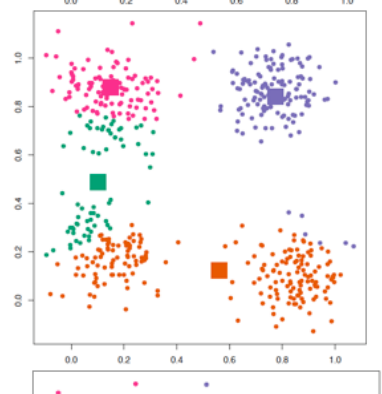
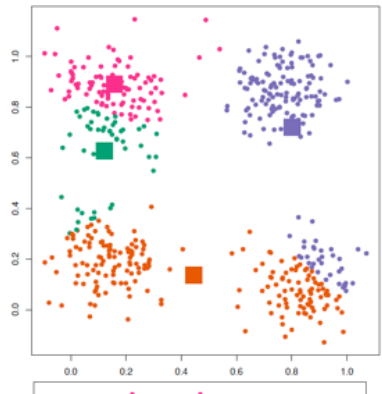
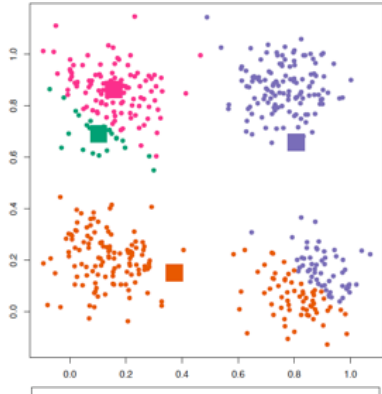
$$\frac{\partial J}{\partial \mathbf{m}_k} = 2 \sum_{i=1}^n r_{ik} (\mathbf{x}_i - \mathbf{m}_k) = 0 \Rightarrow \mathbf{m}_k = \frac{\sum_{i=1}^n r_{ik} \mathbf{x}_i}{\sum_{i=1}^n r_{ik}}$$

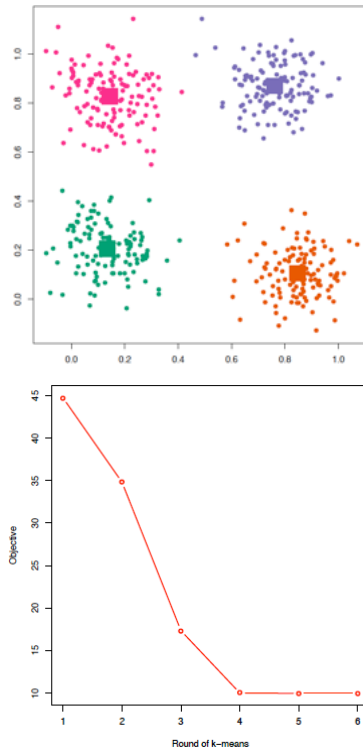
That is, the new prototype is the mean of the elements assigned to the cluster

At each step,  $J$  does not increase. There is a convergence to a local minimum.

### Example of application of k-means







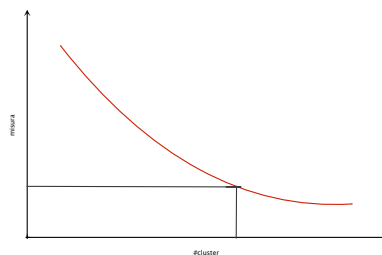
## How to choose $K$

Cross validation

- Apply cross validation for different values of  $K$ , measuring the quality of the clustering obtained
- How to measure the quality of a clustering?
  1. mean distance of elements from the prototypes of their clusters
  2. log-likelihood of the elements wrt the resulting mixture model

Note

Measures improves as  $K$  increases (overfitting). A value such that further increases provide limited improvement should be found



## Hierarchical clustering

Aim

Derivation of a binary tree. Node: cluster; arc: inclusion.

The tree specifies a set of pairwise merge of clusters.

- Aggregation, starting from  $n$  singleton clusters

- Separation, starting from a single cluster of size  $n$

Requirements:  $k$ -means requires:

- a number  $K$  of clusters
- an initial assignment
- a distance function between elements

Hierarchical clustering requires:

- a similarity function between clusters

### Algorithm

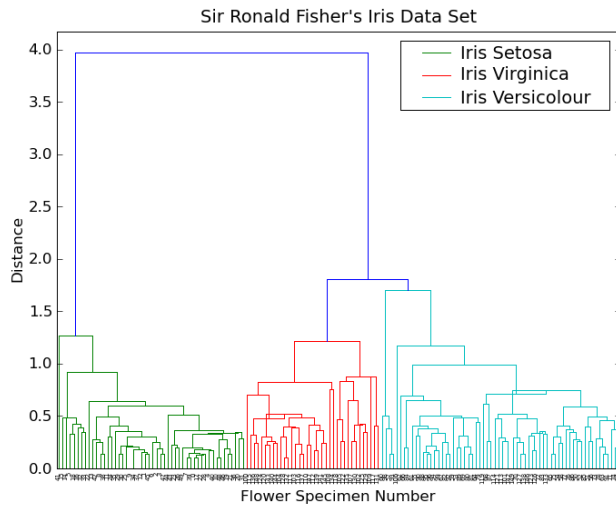
- define  $n$  clusters (singleton)
- repeat
  - compute the matrix of distances between clusters
  - merge the pair of clusters which are “nearest”
- until a single cluster has remained

### Properties

- Each tree prefix is a partition of elements
- The algorithm provides a partial order of clusterings
- The best clustering has to be found
- Monotonicity: similarity between paired clusters decreases

### Dendrogram

- Tree of cluster pairings
- The height of the nodes is inversely proportional to the similarity of the paired clusters



### Cluster similarity

Many measures. Most frequent ones:

- Similarity between nearest nodes (**Single linkage**)

$$d_{SL}(C_1, C_2) = \min_{x_1 \in C_1, x_2 \in C_2} d(x_i, x_j)$$

- Similarity between farthest nodes (**Complete linkage**)

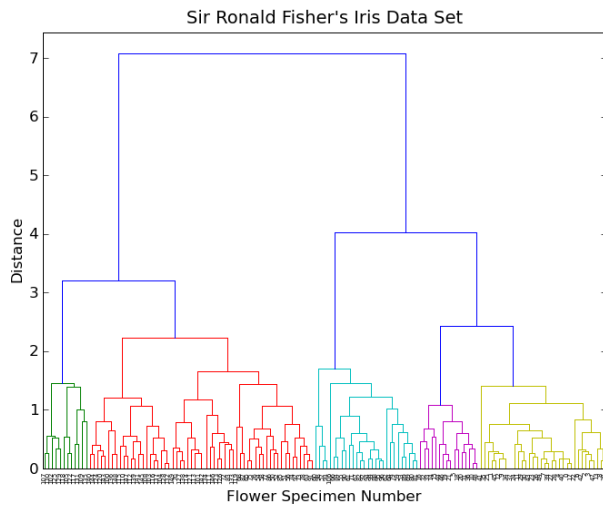
$$d_{CL}(C_1, C_2) = \max_{x_1 \in C_1, x_2 \in C_2} d(x_i, x_j)$$

- Mean similarity (**Group average**)

$$d_{GA}(C_1, C_2) = \frac{1}{|C_1| \cdot |C_2|} \sum_{x_1 \in C_1} \sum_{x_2 \in C_2} d(x_i, x_j)$$

Different measures provide different dendrograms

## Dendrogram with complete linkage



## Mixtures of distributions

Linear combinations of probability distributions

- Same type of distributions  $q(\mathbf{x}|\theta)$
- Differ by parameter values

$$p(\mathbf{x}|\boldsymbol{\pi}, \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k q(\mathbf{x}|\theta_k)$$

where

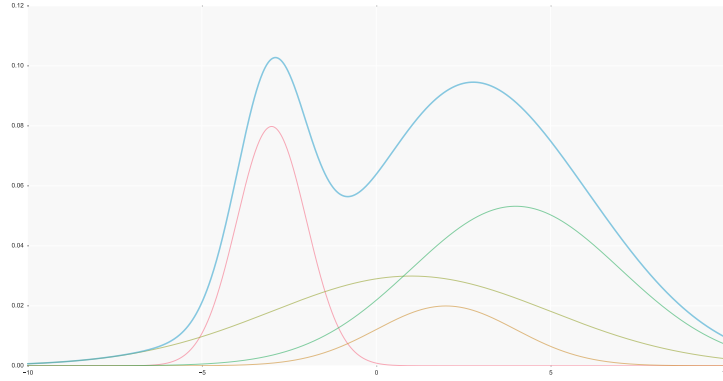
$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K) \quad \boldsymbol{\theta} = (\theta_1, \dots, \theta_K)$$

Mixing coefficients

$$0 \leq \pi_k \leq 1 \quad k = 1, \dots, K \quad \sum_{k=1}^K \pi_k = 1$$

Terms  $\pi_k$  have the properties of probability values

Provide extensive capabilities to model complex distributions. For example, almost all continuous distributions can be modeled by the linear combination of a suitable number of gaussians.



### Mixture parameters estimation

Given a dataset  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ , the parameters  $\boldsymbol{\pi}, \boldsymbol{\theta}$  of a mixture can be estimated by maximum likelihood.

$$L(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X}) = p(\mathbf{X}|\boldsymbol{\theta}, \boldsymbol{\pi}) = \prod_{i=1}^n p(\mathbf{x}_i|\boldsymbol{\theta}, \boldsymbol{\pi}) = \prod_{i=1}^n \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\boldsymbol{\theta}_k)$$

or maximum log-likelihood

$$l(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X}) = \log p(\mathbf{X}|\boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{i=1}^n \log p(\mathbf{x}_i|\boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{i=1}^n \log \left( \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\boldsymbol{\theta}_k) \right)$$

Maximization is however constrained by the conditions  $0 \leq \pi_i \leq 1$  for all  $i$  and  $\sum_{i=1}^K \pi_i = 1$ .

By applying the lagrangian multipliers method, we will maximize

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\pi}, \lambda) = l(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X}) + \lambda \left( 1 - \sum_{i=1}^K \pi_i \right)$$

Let us first consider the derivatives with respect to the weights  $\boldsymbol{\pi}$ , which we set to 0

$$\frac{\partial \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X})}{\partial \pi_j} = \frac{\partial l(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X})}{\partial \pi_j} - \lambda = 0$$

This is equivalent to

$$\begin{aligned} \lambda &= \frac{\partial l(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X})}{\partial \pi_j} = \frac{\partial}{\partial \pi_j} \left[ \sum_{i=1}^n \log \left( \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\boldsymbol{\theta}_k) \right) \right] = \sum_{i=1}^n \frac{\partial}{\partial \pi_j} \left[ \log \left( \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\boldsymbol{\theta}_k) \right) \right] \\ &= \sum_{i=1}^n \frac{q(\mathbf{x}_i|\boldsymbol{\theta}_j)}{\sum_{k=1}^K \pi_k q(\mathbf{x}_i|\boldsymbol{\theta}_k)} = \sum_{i=1}^n \frac{\gamma_j(\mathbf{x}_i)}{\pi_j} = \frac{1}{\pi_j} \sum_{i=1}^n \gamma_j(\mathbf{x}_i) \end{aligned}$$

where,

$$\gamma_k(\mathbf{x}) = \frac{\pi_k q(\mathbf{x}|\boldsymbol{\theta}_k)}{\sum_{j=1}^K \pi_j q(\mathbf{x}|\boldsymbol{\theta}_j)}$$

By setting the derivative wrt  $\lambda$  to 0

$$\frac{\partial \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X})}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left( l(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X}) + \lambda \left( 1 - \sum_{i=1}^K \pi_i \right) \right) = 0$$



we obtain

$$\sum_{i=1}^K \pi_i = 1$$

As a consequence, since, as shown above,

$$\pi_j = \frac{1}{\lambda} \sum_{i=1}^n \gamma_j(\mathbf{x}_i)$$

it results

$$\sum_{j=1}^K \pi_j = \frac{1}{\lambda} \sum_{j=1}^K \sum_{i=1}^n \gamma_j(\mathbf{x}_i) = 1$$

which implies

$$\lambda = \sum_{j=1}^K \sum_{i=1}^n \gamma_j(\mathbf{x}_i) = \sum_{i=1}^n \sum_{j=1}^K \gamma_j(\mathbf{x}_i) = \sum_{i=1}^n \sum_{j=1}^K \frac{\pi_j q(\mathbf{x}_i|\theta_j)}{\sum_{k=1}^K \pi_k q(\mathbf{x}_i|\theta_k)} = \sum_{i=1}^n 1 = n$$

and, finally,

$$\pi_k = \frac{1}{n} \sum_{i=1}^n \gamma_k(\mathbf{x}_i)$$

For what concerns derivatives (or gradients) wrt distribution parameters  $\boldsymbol{\theta}$ , it results

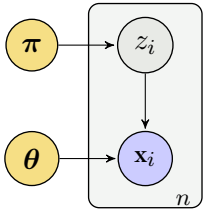
$$\begin{aligned} \frac{\partial \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\pi}|\mathbf{X})}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} \left[ \sum_{i=1}^n \log \left( \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\theta_k) \right) \right] = \sum_{i=1}^n \frac{\partial}{\partial \theta_j} \left[ \log \left( \sum_{k=1}^K \pi_k q(\mathbf{x}_i|\theta_k) \right) \right] \\ &= \sum_{i=1}^n \frac{\pi_j q(\mathbf{x}_i|\theta_j)}{\sum_{k=1}^K \pi_k q(\mathbf{x}_i|\theta_k)} \frac{\partial \log q(\mathbf{x}_i|\theta_j)}{\partial \theta_j} \\ &= \sum_{i=1}^n \gamma_j(\mathbf{x}_i) \frac{\partial \log q(\mathbf{x}_i|\theta_j)}{\partial \theta_j} = 0 \end{aligned}$$

Log likelihood maximization is intractable analytically: its solution cannot be given in closed form.

- $\boldsymbol{\pi}$  and  $\boldsymbol{\theta}$  can be derived from  $\gamma_k(\mathbf{x}_i)$
- Also,  $\gamma_k(\mathbf{x}_i)$  can be derived from  $\boldsymbol{\pi}$  e  $\boldsymbol{\theta}$

Iterative techniques

- Given an estimation for  $\boldsymbol{\pi}$  e  $\boldsymbol{\theta}$ ...
- derive an estimation for  $\gamma_k(\mathbf{x}_i)$ , from which ...
- derive a new estimation for  $\boldsymbol{\pi}$  e  $\boldsymbol{\theta}$ , from which ...
- derive a new estimation for  $\gamma_k(\mathbf{x}_i)$  ...



### Mixtures as generative processes

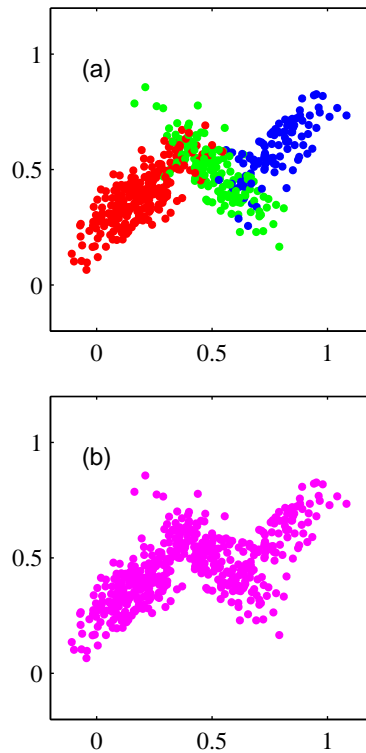
Graphical model representation of a mixture of distributions. Latent variables

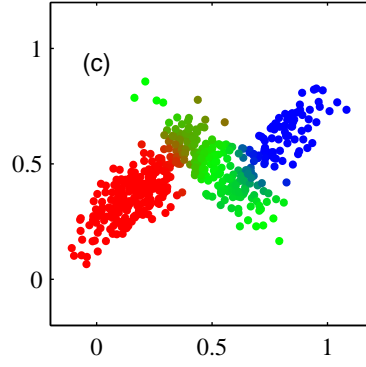
- Terms  $z_i$  are **latent** random variable with domain  $z \in \{1, \dots, K\}$
- While  $\mathbf{x}_i$  is observed, the value of  $z_i$  cannot be observed
- $z_i$  denotes the component distribution  $q(\mathbf{x}|\theta)$  responsible for the generation of  $\mathbf{x}_i$

Generation process

1. Starting from the distribution  $\pi_1, \dots, \pi_K$ , the component distribution to apply to sample the value of  $\mathbf{x}_i$  is sampled: its index is given by  $z_i$ . Hence  $z_i$  is dependent from  $\pi$
2. Let  $z_i = k$ : then,  $\mathbf{x}_i$  is sampled from distribution  $q(\mathbf{x}|\theta_k)$ . That is,  $\mathbf{x}_i$  is dependent from both  $z_i$  and  $\theta$  (through  $\theta_k$ )

Example of generation of dataset from mixture of 3 gaussians





Distributions with latent variables

$$p(\mathbf{x}|z = k, \boldsymbol{\theta}, \boldsymbol{\pi}) = p(\mathbf{x}|z = k, \boldsymbol{\theta}) = q(\mathbf{x}|\theta_k)$$

Marginalizing wrt  $z$ ,

$$\begin{aligned} p(\mathbf{x}|\boldsymbol{\theta}, \boldsymbol{\pi}) &= \sum_{k=1}^K p(\mathbf{x}, z = k|\boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{k=1}^K p(\mathbf{x}|z = k, \boldsymbol{\theta})p(z = k|\boldsymbol{\theta}, \boldsymbol{\pi}) \\ &= \sum_{k=1}^K p(\mathbf{x}|z = k, \boldsymbol{\theta})p(z = k|\boldsymbol{\pi}) = \sum_{k=1}^K q(\mathbf{x}|\theta_k)p(z = k|\boldsymbol{\pi}) \end{aligned}$$

Since, by definition,

$$p(\mathbf{x}|\boldsymbol{\theta}, \boldsymbol{\pi}) = \sum_{k=1}^K \pi_k q(\mathbf{x}|\theta_k)$$

it results

$$\pi_k = p(z = k|\boldsymbol{\pi})$$

Responsibilities

An interpretation for  $\gamma_k(\mathbf{x})$  can be derived as follows

$$\begin{aligned} \gamma_k(\mathbf{x}) &= \frac{\pi_k q(\mathbf{x}|\theta_k)}{\sum_{j=1}^K \pi_j q(\mathbf{x}|\theta_j)} \\ &= \frac{p(z = k)p(\mathbf{x}|z = k)}{\sum_{j=1}^K p(z = j)p(\mathbf{x}|z = j)} = p(z = k|\mathbf{x}) \end{aligned}$$

Mixing coefficients and responsibilities

- A mixing coefficient  $\pi_k = p(z = k)$  can be seen as the prior (wrt to the observation of the point) probability that the next point is generated by sampling the  $k$ -th component distribution
- A responsibility  $\gamma_k(\mathbf{x}) = p(z = k|\mathbf{x})$  can be seen as the posterior (wrt to the observation of the point) probability that a point has been generated by sampling the  $k$ -th component distribution

In the case, of mixtures of gaussian distribution, we have  $q(\mathbf{x}|\boldsymbol{\theta}_k) = \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$ .  
As a consequence,

$$\gamma_k(\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}|\mu_j, \Sigma_j)}$$

and the likelihood is maximized for

$$\pi_j = \frac{1}{n} \sum_{i=1}^n \gamma_j(\mathbf{x}_i)$$

$$\sum_{i=1}^n \gamma_j(\mathbf{x}_i) \frac{\partial \log \mathcal{N}(\mathbf{x}_i|\mu_j, \Sigma_j)}{\partial \theta_j} = 0$$

## Maximum likelihood

Data set

- Let  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$  be the set of values of observed variables and let  $\mathbf{Z} = (z_1, \dots, z_n)$  be the set of values of the latent variables. Then  $(\mathbf{X}, \mathbf{Z})$  is the **complete dataset**: it includes the values of all variables in the model
- $\mathbf{X}$  is the **observed dataset** (incomplete). It only includes “real” data, that is observed data.

Indeed,  $\mathbf{Z}$  is unknown. If values have been assigned to model parameters, the only possible knowledge about  $\mathbf{Z}$  is given by the posterior distribution  $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}, \boldsymbol{\pi})$ .

## Inferring parameters for gaussian mixtures

- If we assume that the complete dataset  $(\mathbf{X}, \mathbf{Z})$  is known (that is the observed points **together with their corresponding components**) a maximum likelihood estimation of  $\boldsymbol{\pi}$  and  $\boldsymbol{\theta}$  would be easy. In particular,
- For the mixing coefficients  $\pi_k$  it would result, as usual

$$\pi_k = \frac{n_k}{n}$$

where  $n_k$  is the number of elements of the set  $C_k$  such that  $z = k$

- For component parameters  $\theta_k = (\mu_k, \Sigma_k)$  the usual estimations for gaussians would provide

$$\boldsymbol{\mu}_k = \frac{1}{n_k} \sum_{\mathbf{x} \in C_k} \mathbf{x}$$

$$\Sigma_k = \frac{1}{n_k} \sum_{\mathbf{x} \in C_k} (\mathbf{x} - \boldsymbol{\mu}_k)(\mathbf{x} - \boldsymbol{\mu}_k)^T$$

## Log likelihood of complete dataset

The above results derive from the maximization, wrt  $\pi_k, \mu_k, \Sigma_k, (k = 1, \dots, K)$  of the log likelihood

$$l(\Sigma, \boldsymbol{\mu}, \boldsymbol{\pi}|\mathbf{X}, \mathbf{Z}) = \log p(\mathbf{X}, \mathbf{Z}|\Sigma, \boldsymbol{\mu}, \boldsymbol{\pi}) = \log \prod_{i=1}^n \prod_{k=1}^K \pi_k^{\zeta_{ik}} \mathcal{N}(\mathbf{x}_i|\mu_k, \Sigma_k)^{\zeta_{ik}}$$

$$= \sum_{i=1}^n \sum_{k=1}^K \zeta_{ik} (\log \pi_k + \log \mathcal{N}(\mathbf{x}_i|\mu_k, \Sigma_k))$$

where,  $\zeta_{ik}$  is the  $k$ -component of the 1-to- $K$  coding of  $z_i$ , that is,  $\zeta_{ik} = 1$  iff  $z_i = k$ , and 0 otherwise

## Dealing with latent variables

Unfortunately, since  $\mathbf{Z}$  is unknown, the log-likelihood of the complete dataset cannot be defined (the sets  $C_k$  are not known).

Our approach will be to consider for maximization, instead of the log-likelihood where each  $z_i$  is specified,

- its expectation wrt to the conditional distribution  $p(\mathbf{Z}|\mathbf{X})$ , that is

$$\begin{aligned} E_{p(\mathbf{Z}|\mathbf{X})}[l(\Sigma, \boldsymbol{\mu}, \boldsymbol{\pi}|\mathbf{X}, \mathbf{Z})] &= \sum_{i=1}^n \sum_{k=1}^K p(z_i = k|\mathbf{x}_i)(\log \pi_k + \log \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_k, \Sigma_k)) \\ &= \sum_{i=1}^n \sum_{k=1}^K \gamma_k(\mathbf{x}_i)(\log \pi_k + \log \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_k, \Sigma_k)) \end{aligned}$$

Observe that this expectation can be derived if  $p(\mathbf{Z}|\mathbf{X})$  (that is the set of all values  $\gamma_k(\mathbf{x}_i)$ ) is known.

## Maximization of expected log-likelihood

The maximization of  $E_{p(\mathbf{Z}|\mathbf{X})}[l(\Sigma, \boldsymbol{\mu}, \boldsymbol{\pi}|\mathbf{X}, \mathbf{Z})]$  wrt to  $\pi_k, \boldsymbol{\mu}_k, \Sigma_k$  results easily into

$$\begin{aligned} \pi_k &= \frac{1}{n} \sum_{i=1}^n \gamma_k(\mathbf{x}_i) \\ \boldsymbol{\mu}_k &= \frac{1}{n_k} \sum_{i=1}^n \gamma_k(\mathbf{x}_i) \mathbf{x}_i \\ \Sigma_k &= \frac{1}{n_k} \sum_{i=1}^n \gamma_k(\mathbf{x}_i) (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \end{aligned}$$

this is named **M-step** (from “Maximization”)

## A new expectation

The computed values for the parameters result into new, different values for  $\gamma_k(\mathbf{x}_i) = p(z_i = k|\mathbf{x}_i)$ , and a different expectation  $E_{p(\mathbf{Z}|\mathbf{X})}[l(\Sigma, \boldsymbol{\mu}, \boldsymbol{\pi}|\mathbf{X}, \mathbf{Z})]$ .

This is named **E-step** (from “Expectation”)

## ML and mixtures of gaussians: iterative approach

1. Assign an initial estimate to  $\boldsymbol{\mu}_j, \Sigma_j, \pi_j, j = 1, \dots, K$
2. Repeat
  - (a) Compute

$$\gamma_j(x_i) = \frac{1}{\gamma_i} \pi_j \mathcal{N}(x_i|\boldsymbol{\mu}_j, \Sigma_j) \quad \text{with} \quad \gamma_i = \sum_{k=1}^K \pi_k \mathcal{N}(x_i|\boldsymbol{\mu}_k, \Sigma_k)$$

- (b) Compute

$$\pi_j = \frac{n_j}{n} \quad \text{with} \quad n_j = \sum_{i=1}^n \gamma_j(x_i)$$

(c) Compute

$$\mu_j = \frac{1}{n_j} \sum_{i=1}^n \gamma_j(x_i) x_i$$

(d) Compute

$$\Sigma_j = \frac{1}{n_j} \sum_{i=1}^n \gamma_j(x_i) (x_i - \mu_j)(x_i - \mu_j)^T$$

3. until some convergence property is verified

The convergence test may refer to the the increase of log-likelihood in the last iteration

This algorithm is indeed the application of a general schema named **Expectation-Maximization**