

# MACHINE LEARNING

## Clustering

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Corso di Laurea Magistrale in Informatica

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## PARTITIONAL CLUSTERING

### Problem

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).

## 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  $j \neq s$

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

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

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

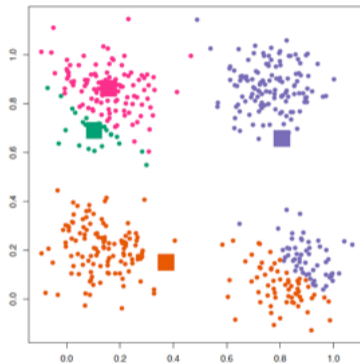
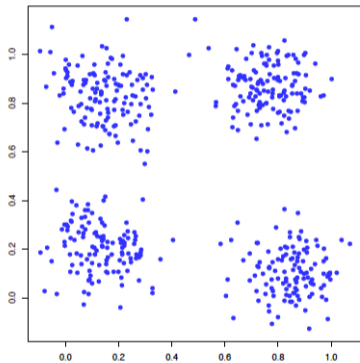
## ALGORITHM

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

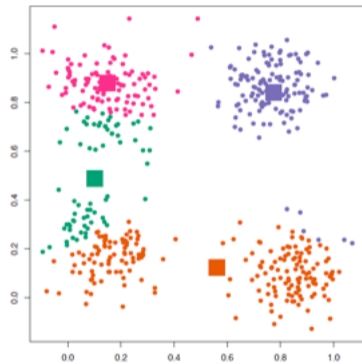
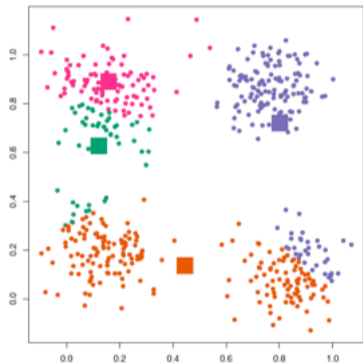
$$\frac{\partial J}{\partial \mathbf{m}_k} = 2 \sum_{i=1}^n r_{ik} (\mathbf{x}_i - \mathbf{m}_k) = 0 \implies \mathbf{m}_k = \frac{\sum_{i=1}^n r_{ik} \mathbf{x}_i}{\sum_{i=1}^n r_{ik}}$$

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.

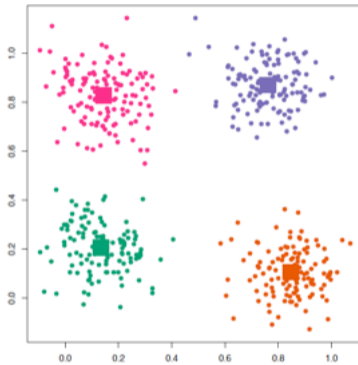
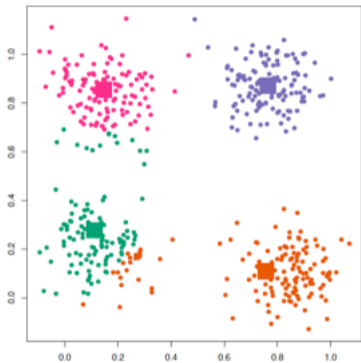
## EXAMPLE OF APPLICATION OF K-MEANS



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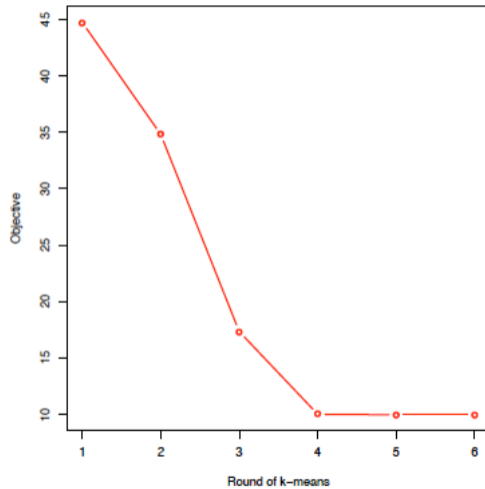


## EXAMPLE OF APPLICATION OF K-MEANS





## EXAMPLE OF APPLICATION OF K-MEANS



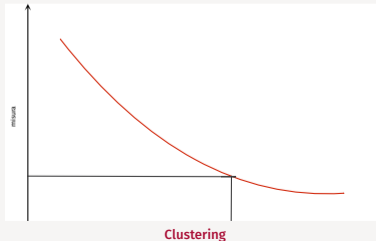
# HOW TO CHOOSE $K$

## 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

# HIERARCHICAL CLUSTERING BY AGGREGATION

## 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

# HIERARCHICAL CLUSTERING BY AGGREGATION

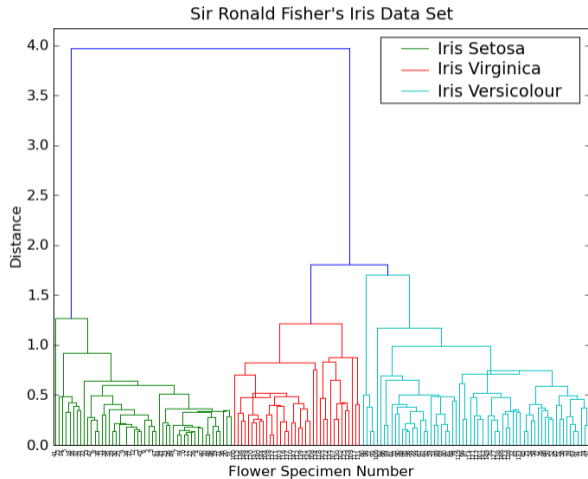
## Properties

- 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

# DENDROGRAM



## CLUSTER SIMILARITY

Many measures. Most frequent ones:

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

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

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

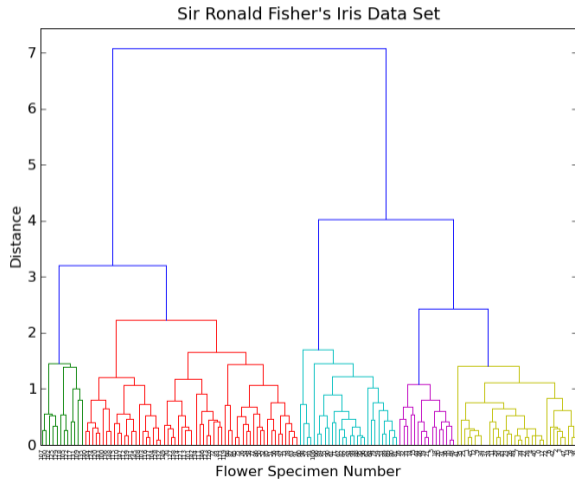
$$d_{CL}(C_1, C_2) = \max_{x_1 \in C_1, x_2 \in C_2} d(x_1, x_2)$$

- Mean similarity (**Group average**)

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

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

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

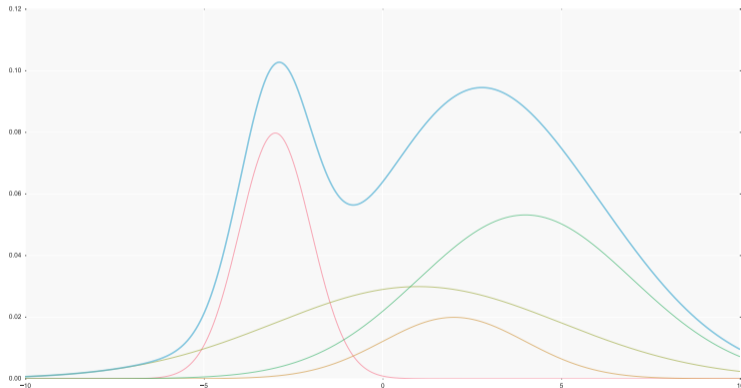
### Mixing coefficients

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

Terms  $\pi_k$  have the properties of probability values

## MIXTURES OF DISTRIBUTIONS

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

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

## MIXTURE PARAMETERS ESTIMATION

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

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

where,

$$\gamma_k(\mathbf{x}) = \frac{\pi_k q(\mathbf{x} | \theta_k)}{\sum_{j=1}^K \pi_j q(\mathbf{x} | \theta_j)}$$

## MIXTURE PARAMETERS ESTIMATION

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

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

## MIXTURE PARAMETERS ESTIMATION

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,

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

## MIXTURE PARAMETERS ESTIMATION

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

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

## MIXTURE PARAMETERS ESTIMATION

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

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

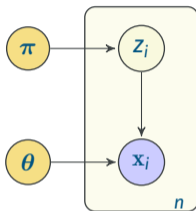
### Iterative techniques

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

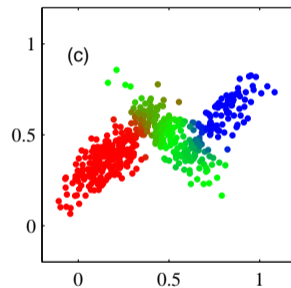
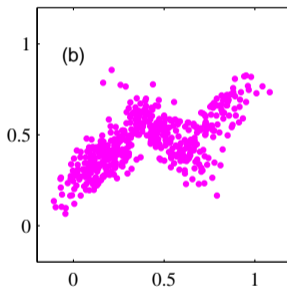
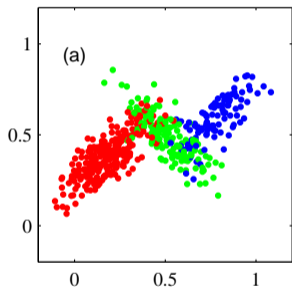
## MIXTURES AS GENERATIVE PROCESSES

### Generation process

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

# MIXTURES AS GENERATIVE PROCESSES

Example of generation of dataset from mixture of 3 gaussians



# MIXTURES AS GENERATIVE PROCESSES

## Distributions with latent variables

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

Marginalizing wrt  $z$ ,

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

Since, by definition,

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

it results

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

## MIXTURES AS GENERATIVE PROCESSES

### 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

## MIXTURES AS GENERATIVE PROCESSES

In the case, of mixtures of gaussian distribution, we have  $q(\mathbf{x}|\theta_k) = \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$ .  
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  $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_n)$  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  $p(\mathbf{Z}|\mathbf{X}, \theta, \pi)$ .

## 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  $\theta_k = (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$  the usual estimations for gaussians would provide

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



## 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

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

where,  $\zeta_{ik}$  is the  $k$ -component of the 1-to- $K$  coding of  $\mathbf{z}_i$ , that is,  $\zeta_{ik} = 1$  iff  $\mathbf{z}_i = k$ , 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  $\mathbf{z}_i$  is specified,

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

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

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

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

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

$$\Sigma_k = \frac{1}{n_k} \sum_{i=1}^n \gamma_j(\mathbf{x}_i) (\mathbf{x}_i - \boldsymbol{\mu}_k) (\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

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  $E_{p(z|\mathbf{x})}[l(\boldsymbol{\Sigma}, \boldsymbol{\mu}, \boldsymbol{\pi} | \mathbf{X}, \mathbf{Z})]$ . This is named **E-step** (from “Expectation”)

## ML AND MIXTURES OF GAUSSIANS: ITERATIVE APPROACH

1. Assign an initial estimate to  $\mu_j, \Sigma_j, \pi_j, j = 1, \dots, K$
2. Repeat
  - 2.1 Compute

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

- 2.2 Compute

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

- 2.3 Compute

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

- 2.4 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

## EXPECTATION MAXIMIZATION ALGORITHM

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