# Mixtures

Course of Machine Learning
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Linear combinations of probability distributions $q(x|\theta)$

- Same type of distributions
- Differ by parameter values

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

where

$$\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K) \qquad \boldsymbol{\theta} = (\theta_1, \ldots, \theta_K) \qquad \boldsymbol{\psi} = (\boldsymbol{\theta}, \boldsymbol{\pi})$$

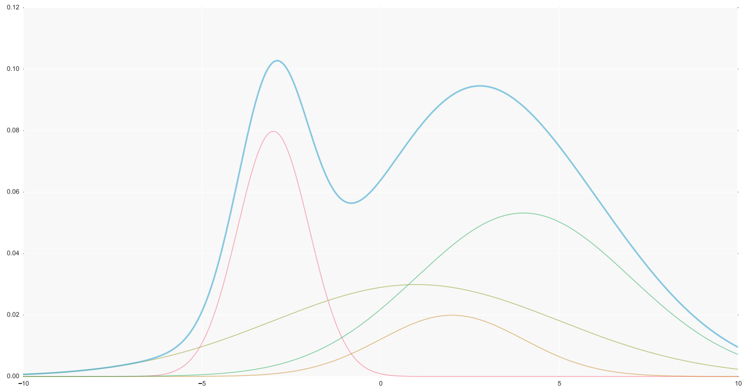
Mixing coefficients

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

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.



Given a dataset $\mathbf{X} = (x_1, \ldots, x_n)$, the parameters $\boldsymbol{\pi}, \boldsymbol{\theta}$ of a mixture can be estimated by maximum likelihood.

$$L(\boldsymbol{\psi}|\mathbf{X}) = p(\mathbf{X}|\boldsymbol{\psi}) = \prod_{i=1}^{n} p(x_i|\boldsymbol{\psi}) = \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k q(x|\theta_k)$$

or maximum log-likelihood

$$l(\boldsymbol{\psi}|\mathbf{X}) = \log p(\mathbf{X}|\boldsymbol{\psi}) = \sum_{i=1}^{n} \log p(x_i|\boldsymbol{\psi}) = \sum_{i=1}^{n} \log \left( \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) \right)$$

# Mixture parameters estimation

Let us derive the set of derivatives for $j = 1, \ldots, K$ and set them to 0

$$\frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{n} \log\left(\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)\right)\right] = 0$$

$$\frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \pi_j} = \frac{\partial}{\partial \pi_j}\left[\sum_{i=1}^{n} \log\left(\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)\right)\right] = 0$$

which itself results, for $k = 1, \ldots, K$, into

$$\pi_k = \frac{1}{n}\sum_{i=1}^{n} \gamma_k(x_i) \qquad\qquad \sum_{i=1}^{n} \gamma_k(x_i)\frac{\partial \log q(x_i|\theta_k)}{\partial \theta_k} = 0$$

where

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

# Mixture parameters estimation

The constraint $\sum_{i=1}^{K} \pi_i = 0$ can be taken into account by introducing a Lagrange multiplier $\lambda$ and considering the Lagrangian

$$L(\boldsymbol{\psi}, \lambda) = l(\boldsymbol{\psi}|\mathbf{X}) + \lambda(1 - \sum_{i=1}^{K} \pi_i)$$

Setting the derivative wrt $\pi_j$ to 0 turns out to be equivalent to

$$\lambda = \frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \pi_j} = \frac{\partial}{\partial \pi_j} \left[ \sum_{i=1}^{n} \log \left( \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) \right) \right] = \sum_{i=1}^{n} \frac{\partial}{\partial \pi_j} \left[ \log \left( \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) \right) \right]$$

$$= \sum_{i=1}^{n} \frac{1}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \frac{\partial}{\partial \pi_j} \left( \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) \right)$$

$$= \sum_{i=1}^{n} \frac{1}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \sum_{k=1}^{K} \frac{\partial}{\partial \pi_j} \left( \pi_k q(x_i|\theta_k) \right)$$

$$= \sum_{i=1}^{n} \frac{q(x_i|\theta_j)}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} = \sum_{i=1}^{n} \frac{\gamma_j(x_i)}{\pi_j} = \frac{1}{\pi_j} \sum_{i=1}^{n} \gamma_j(x_i)$$

# Mixture parameters estimation

Setting the derivative wrt $\lambda$ to 0

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

is equivalent to

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

Moreover, since, as shown above,

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

it results

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

and

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

# Mixture parameters estimation

Finally,

$$
\begin{aligned}
\frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{n} \log\left(\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)\right)\right] = \sum_{i=1}^{n} \frac{\partial}{\partial \theta_j}\left[\log\left(\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)\right)\right] \\
&= \sum_{i=1}^{n} \frac{1}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \frac{\partial}{\partial \theta_j}\left(\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)\right) \\
&= \sum_{i=1}^{n} \frac{1}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \sum_{k=1}^{K} \frac{\partial}{\partial \theta_j}\left(\pi_k q(x_i|\theta_k)\right) \\
&= \sum_{i=1}^{n} \frac{\pi_j}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \frac{\partial}{\partial \theta_j} q(x_i|\theta_j) \\
&= \sum_{i=1}^{n} \frac{\pi_j q(x_i|\theta_j)}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \frac{1}{q(x_i|\theta_j)} \frac{\partial}{\partial \theta_j} q(x_i|\theta_j) \\
&= \sum_{i=1}^{n} \frac{\pi_j q(x_i|\theta_j)}{\sum_{k=1}^{K} \pi_k q(x_i|\theta_k)} \frac{\partial \log q(x_i|\theta_j)}{\partial \theta_j} = \sum_{i=1}^{n} \gamma_j(x_i) \frac{\partial \log q(x_i|\theta_j)}{\partial \theta_j} = 0
\end{aligned}
$$

# Mixture parameters estimation

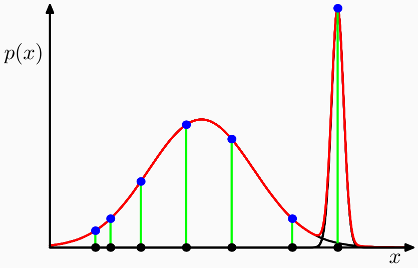
Log likelihood maximization is intractable analytically: its solution cannot be given in closed form.

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

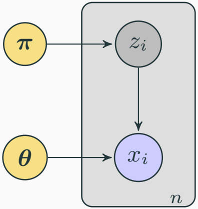
## Iterative techniques

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

- Identifiability: for each solution (assignment of parameters to component distributions), there exist $K! - 1$ equivalent solutions
- Singularity: risk of severe overfitting. A mixture collapses to a single point.



Graphical model representation of a mixture of distributions.




### Latent variables

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

## Generation process

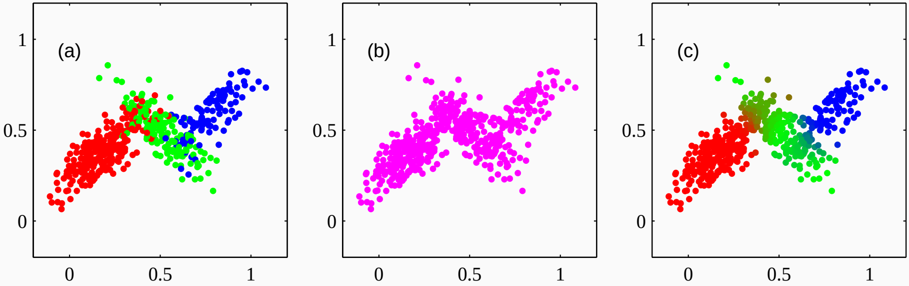
1. Starting from the distribution $\pi_1, \ldots, \pi_K$, the component distribution to apply to sample the value of $x_i$ is sampled: its index is given by $z_i$: hence $z_i$ is dependent from $\boldsymbol{\pi}$
2. Let $z_i = k$: then, $x_i$ is sampled from distribution $q(x|\theta_k)$. That is, $x_i$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

## Latent variables coding

Indeed, $z_i$ can be seen as components of a single latent $K$-dimensional variable $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_K)$

1-to-$K$ coding: $K$ possible values $\zeta_i \in \{0, 1\}$, $\sum_{i=1}^{K} \zeta_i$.

Example of generation of dataset from mixture of 3 gaussians



# Mixtures as generative processes

## Distributions with latent variables

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

Marginalizing wrt $z$,

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

Since, by definition,

$$p(x|\boldsymbol{\psi}) = \sum_{k=1}^{K} \pi_k q(x_i|\theta_k)$$

it results

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

### Responsibilities

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

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

### 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 $\gamma_k(x) = p(z=k|x)$ 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

# Expectation maximization for gaussian mixtures

## Data set

- Let $\mathbf{X} = (x_1, \ldots, x_n)$ be the set of values of observed variables and let $\mathbf{Z} = (z_1, \ldots, z_n)$ 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 $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\psi})$.

Let $\boldsymbol{\psi}$ be the values assigned to model parameters, then the evidence of both dataset can be defined as follows.

## Observed dataset

$$p(\mathbf{X}|\boldsymbol{\psi}) = \prod_{i=1}^{n} p(x_i|\boldsymbol{\psi}) = \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k q(x_i|\theta_k)$$

## Complete dataset

$$\begin{aligned} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\psi}) &= \prod_{i=1}^{n} p(x_i, z_i|\boldsymbol{\psi}) = \prod_{i=1}^{n} p(z_i|\boldsymbol{\psi}) p(x_i|z_i, \boldsymbol{\psi}) \\ &= \prod_{i=1}^{n} \prod_{k=1}^{K} (p(z_{ik}|\boldsymbol{\pi}) p(x_i|z_{ik}, \boldsymbol{\theta}))^{z_{ik}} = \prod_{i=1}^{n} \prod_{k=1}^{K} \pi_k^{z_{ik}} q(x_i|\theta_k)^{z_{ik}} \end{aligned}$$

where $z_i = (z_{i1}, \ldots, z_{ik})$

Log likelihood of observed dataset

$$l(\boldsymbol{\psi}|\mathbf{X}) = \log p(\mathbf{X}|\boldsymbol{\psi}) = \log \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) = \sum_{i=1}^{n} \log \left( \sum_{k=1}^{K} \pi_k q(x_i|\theta_k) \right)$$

Log likelihood of complete dataset

$$\begin{aligned} l(\boldsymbol{\psi}|\mathbf{X}, \mathbf{Z}) = \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\psi}) = \log \prod_{i=1}^{n} \prod_{k=1}^{K} \pi_k^{z_{ik}} q(x_i|\theta_k)^{z_{ik}} \\ = \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} (\log \pi_k + \log q(x_i|\theta_k)) \end{aligned}$$

# Maximization of log-likelihood of observed dataset

Usually hard to compute, the equations

$$\frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \theta_k} = 0$$
$$\frac{\partial l(\boldsymbol{\psi}|\mathbf{X})}{\partial \pi_k} = 0$$

do not have a closed form solution.

## Complete dataset

To maximize wrt $\pi_k$ the constraint $\sum_{j=1}^{K} \pi_j = 1$ must be taken into account

$$0 = \frac{\partial}{\partial \pi_k} \left( l(\boldsymbol{\psi}|\mathbf{X}, \mathbf{Z}) + \lambda(1 - \sum_{j=1}^{K} \pi_i) \right) \qquad k = 1, \ldots, K$$

$$0 = \frac{\partial}{\partial \lambda} \left( l(\boldsymbol{\psi}|\mathbf{X}, \mathbf{Z}) + \lambda(1 - \sum_{j=1}^{K} \pi_i) \right)$$

which is verified for

$$\lambda = n$$

$$\pi_k = \frac{1}{n} \sum_{i=1}^{n} z_{ik} \qquad k = 1, \ldots, K$$

**Complete dataset**

To maximize wrt $\theta_k$

$$0 = \frac{\partial l(\boldsymbol{\psi}|\mathbf{X},\mathbf{Z})}{\partial \theta_k} = \sum_{i=1}^{n} z_{ik} \frac{1}{q(x_i|\theta_k)} \frac{\partial q(x_i|\theta_k)}{\partial \theta_k}$$

In most cases, this has a closed form solution.

# Mixtures of gaussians

$$q(x|\theta) = \mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right)$$

$$p(x) = \sum_{j=1}^{K} \pi_j \mathcal{N}(x|\mu_j, \Sigma_j)$$

- Latent variable $z = (z_1, \ldots, z_K)$
- Joint distribution $p(x, z) = p(x|z)p(z)$
- Latent variable distribution $p(z = k) = p(z_k = 1) = \pi_k$; in general, $p(z) = \prod_{j=1}^{K} \pi_j^{z_j}$
- Conditional distribution $p(x|z) = \prod_{j=1}^{K} \mathcal{N}(x|\mu_j, \Sigma_j)$
- Marginal distribution $p(x) = \sum_z p(z)p(x|z) = \sum_{j=1}^{K} \pi_j \mathcal{N}(x|\mu_j, \Sigma_j)$

- Dataset $X = (x_1, \dots, x_n)$, $x_i \in \mathbb{R}^d$; latent variables values $z = (z_1, \dots, z_n)$, $z_i \in \mathbb{R}^K$
- Log-likelihood

$$\log p(X|\pi, \mu, \Sigma) = \sum_{i=1}^{n} \log \left( \sum_{j=1}^{K} \pi_j \mathcal{N}(x_i|\mu_j, \Sigma_j) \right)$$

- To maximize:

$$0 = \frac{\partial \log p(X|\pi, \mu, \Sigma)}{\partial \mu_j} = -\sum_{i=1}^{n} \frac{\pi_j \mathcal{N}(x_i|\mu_j, \Sigma_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)} \Sigma_j (x_i - \mu_j)$$

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

which results into

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

where $n_j = \sum_{i=1}^{n} \gamma_j(x_i)$ depends from the elements assigned to the $j$-th component

$$0 = \frac{\partial \log p(X|\pi, \mu, \Sigma)}{\partial \Sigma_j} \Rightarrow \Sigma_j = \frac{1}{n_j} \sum_{i=1}^{n} \gamma_j(x_i)(x_i - \mu_j)(x_i - \mu_j)^T$$

To maximize $\log p(X|\pi, \mu, \Sigma)$ wrt $\pi_j$, with the constraint $\sum_{i=1}^{K} \pi_i = 1$, introduce a Lagrange multiplier

$$\log p(X|\pi, \mu, \Sigma) + \lambda(\sum_{i=1}^{K} \pi_i - 1)$$

hence $\pi_j = n_j/n$

- $\pi_j$ is a function of $\gamma_j(x_i), i = 1, \ldots, n$
- $\mu_j$ is a function of $\gamma_j(x_i), i = 1, \ldots, n$
- $\Sigma_j$ is a function of $\gamma_j(x_i), i = 1, \ldots, n$ e di $\mu_j$
- $\gamma_j(x_i) = p(z_i = j|x_i)$ is a function of $\pi_k, \mu_k, \Sigma_k, k = 1, \ldots, K$

Solution not in closed form: apply an iterative technique

# 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
   $$\gamma_j(x_i) = \frac{1}{\gamma_i} \pi_j \mathcal{N}(x_i | \mu_j, \Sigma_j) \qquad \text{con} \qquad \gamma_i = \sum_{k=1}^{K} \pi_k \mathcal{N}(x_i | \mu_j, \Sigma_j)$$
   2.2 Compute
   $$\pi_j = \frac{n_j}{n} \qquad \text{con} \qquad n_j = \sum_{i=1}^{n} \gamma_j(x_i)$$
   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

At each step, the algorithm performs two operations:

- Compute all $\gamma_j(x_i)$, that is the probabilities that an element $x_i$ belong to a component; this is equivalent to computing the posterior probability distributions of all latent variables $z_i$. The posterior probability is computed from the current parameter values.
- Maximize the log-likelihood wrt to the parameters, assuming the posterior probability of latent variables computed in the previous phase

# Example of application of the algorithm