Mixtures

Course of Machine Learning
Master Degree in Computer Science
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Mixtures of distributions

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

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

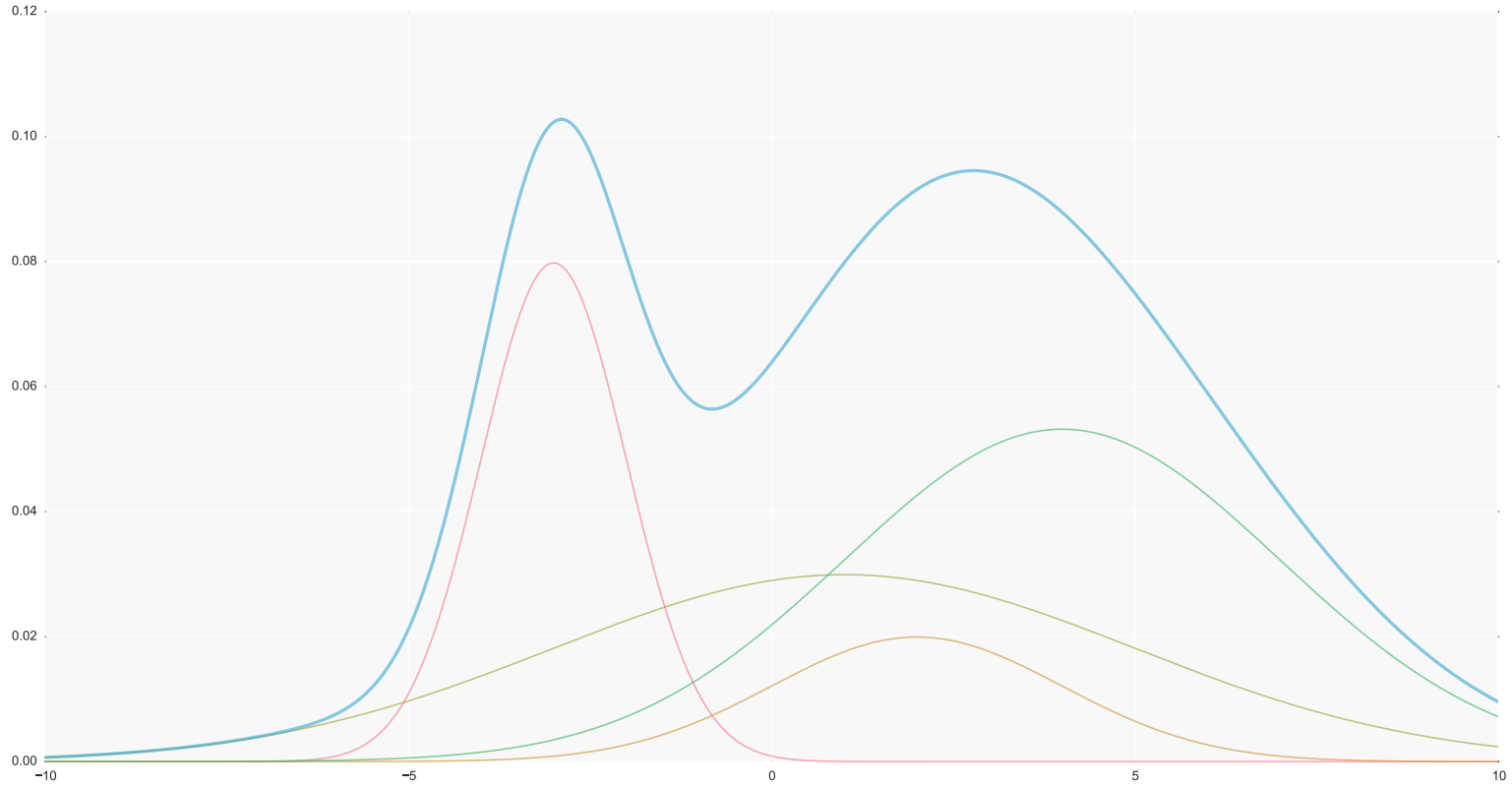
Mixing coefficients

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

Terms π_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 $\mathbf{X} = (x_1, \ldots, x_n)$, 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

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

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 λ 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 π_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 λ 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,

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

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

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

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

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

$$= \sum_{i=1}^{n}\frac{\pi_j q(x_i|\theta_j)}{\sum_{k=1}^{K}\pi_k q(x_i|\theta_k)}\frac{\partial \log q(x_i|\theta_j)}{\partial \theta_j} = \sum_{i=1}^{n}\gamma_j(x_i)\frac{\partial \log q(x_i|\theta_j)}{\partial \theta_j} = 0$$

Mixture parameters estimation

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

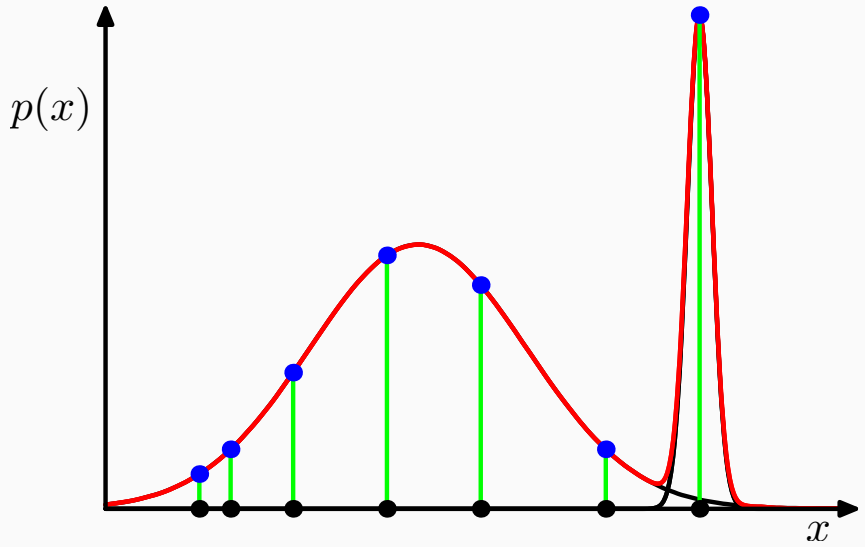
- $\boldsymbol{\pi}$ and $\boldsymbol{\theta}$ can be derived from $\gamma_k(x_i)$
- Also, $\gamma_k(x_i)$ can be derived from $\boldsymbol{\pi}$ e $\boldsymbol{\theta}$

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 $\gamma_k(x_i)$ ...

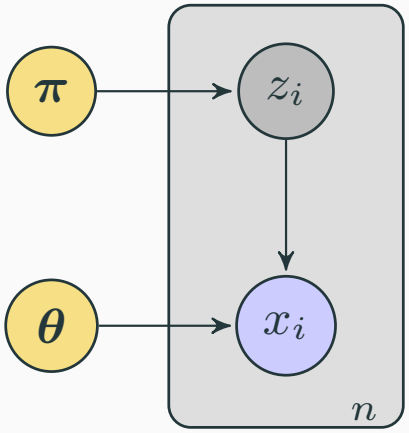
Issues in ML for mixtures

- 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.



Mixtures as generative processes

Graphical model representation of a mixture of distributions.



Latent variables

- Terms z_i are latent random variable with domain $z \in \{1, \ldots, K\}$
- 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

Mixtures as generative processes

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 $\boldsymbol{\theta}$

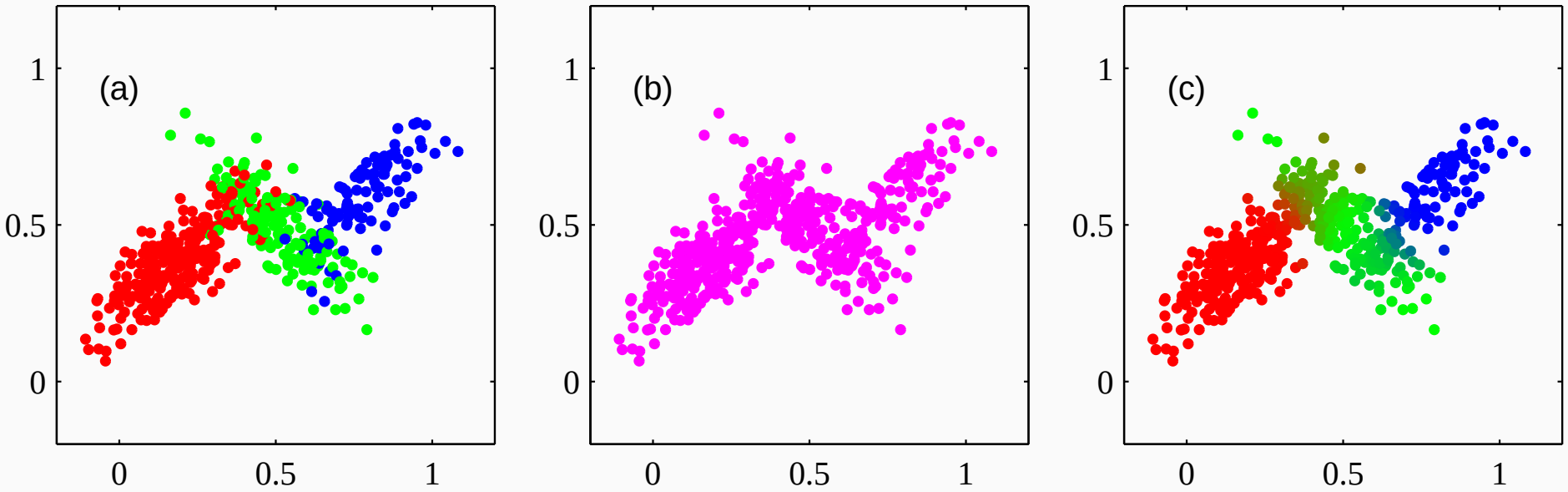
Latent variables coding

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 $\zeta_i \in \{0, 1\}$, $\sum_{i=1}^{K} \zeta_i$.

Mixtures as generative processes

Example of generation of dataset from mixture of 3 gaussians



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

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

Mixtures as generative processes

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 $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\psi})$.

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 π_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

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

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

Log likelihood of complete dataset

The above results derive from the maximimization, wrt π_k, μ_k, Σ_k, $(k = 1, \ldots, K)$ of the log likelihood

$$l(\boldsymbol{\psi}|\mathbf{X}, \mathbf{Z}) = \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\psi}) = \log \prod_{i=1}^{n} \prod_{k=1}^{K} \pi_k^{z_{ik}} \mathcal{N}(x_i|\mu_k, \Sigma_k)^{z_{ik}}$$

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

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

- the expectation of the log-likelihood with respect to probabilities $p(z|x_i)$ is specified

$$E_{p(\mathbf{Z}|\mathbf{X})}[l(\boldsymbol{\psi}|\mathbf{X},\mathbf{Z})] = \sum_{i=1}^{n}\sum_{k=1}^{K} p(z_i = k|\mathbf{x}_i)(\log \pi_k + \log q(\mathbf{x}_i|\theta_k))$$
$$= \sum_{i=1}^{n}\sum_{k=1}^{K} \gamma_k(\mathbf{x}_i)(\log \pi_k + \log q(\mathbf{x}_i|\theta_k))$$

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 $E_{p(\mathbf{Z}|\mathbf{X})}[l(\boldsymbol{\psi}|\mathbf{X}, \mathbf{Z})]$ wrt to π_k, μ_k, Σ_k results easily into

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

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

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

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

A new expectation

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

$$p(z_i = k|x_i) = \frac{p(z_i = k)p(x_i|z_i = k)}{\sum_{j=1}^{K} p(z_i = j)p(x_i|z_i = j)} = \frac{\pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_i|\mu_j, \Sigma_j)}$$

this is named E-step (from “Expectation”)

ML and mixtures of gaussians: iterative approach

1. Assign an initial estimate to $\mu_j, \Sigma_j, \pi_j, j = 1, \ldots, K$
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

Expectation maximization algorithm

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