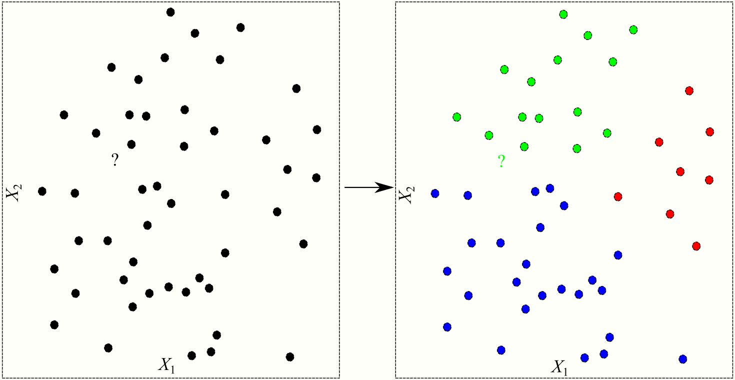
Fundamentals of Probabilistic Data Mining

Chapter III - Model-based clustering

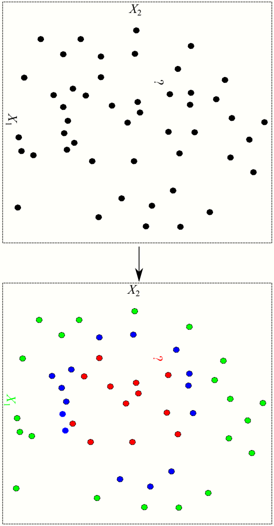


Clustering with 3 clusters

Mixture models

Clustering

- Data: points $(x_j)_{j=1,\ldots,n}$ in $\mathbb{R}^d$.
- Aim: find (maybe predict?) K clusters (K fixed here).
- Distance-based approaches: close points tend to be in the same cluster. No explicit assumption required. Clusters cannot be nested.
- Model-based approaches: let z_j be the cluster of x_j. If $z_i = z_j = k$ then x_i and z_j should have the same (conditional) distribution p_k.



Z is an unknown / latent variable, useful for clustering. (e.g. $z = 0 \to$ blue)

Mixture models

- Added value: to incorporate probabilistic constraints (clusters with different means, or same means but different covariances...)
- Example (latter case): $p(x|z=k) = \mathcal{N}(0, \sigma_k I)$, or $p(x|z=k) = \mathcal{N}(0, \sigma_k \Sigma)$, etc.

Definition 1 (McLachalan & Peel, 2000).

Let $\{p_\theta\}_{\theta \in \Theta}$ be a parametric family of distributions. $x \to p(x)$ is a mixture of distributions iff there exists $K, \pi_1, \ldots, \pi_K, \theta_1, \ldots, \theta_K$, such that

$$p = \sum_{k=1}^{K} \pi_k p_{\theta_k}.$$

- Mixtures: convex combinations of distributions.
- Defines new parametric families of distributions. Parameter $\lambda = (\pi_1, \ldots, \pi_K, \theta_1, \ldots, \theta_K)$ (for given K).

Mixtures and clustering

- Equivalence of mixture representation and existence of some hidden state variable Z with

$$\forall K \in \{1, \dots, K\},\ \pi_k = P(Z = k),\ \forall x\, p_{\theta_k}(x) = p(x|Z = k)$$

$$p(x) = \sum_{k=1}^{K} P(Z = k)p(x|Z = k) = \sum_{k=1}^{K} \pi_k p_{\theta_k}(x)$$

- Clustering: Z interpreted as the cluster of X (find Z).
- More generally: representation of heterogeneous sources (find λ).
- Potential use of mixtures in various settings (density estimation, ...).
- Cluster: essentially a conditional distribution – referred to as emission distribution – plus a prior on Z (see generative models for classification).

Remark

- Possible extensions to $p(.|z=k)$ being in different parametric families.
- Examples: mixtures of Weibull and Gamma distributions, mixtures of PDFs with respect to the same reference measures, mixtures of arbitrary measures, ...

$$\text{for } x \geq 0,\ p(x) =$$
$$0.2\frac{a}{b}\left(\frac{x}{b}\right)^{a-1}\exp\left[\left(-\frac{x}{b}\right)^{a}\right] + 0.8\frac{c^k}{(k-1)!}x^{k-1}\exp(-cx).$$

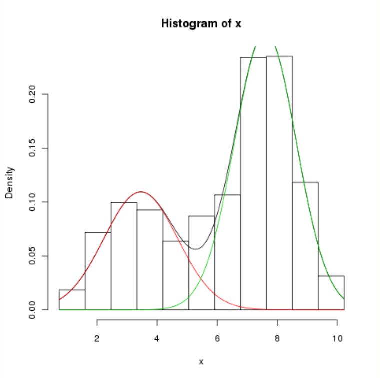
Interpretation: example (I)

- X: weight of some rodent.
- Proportion of females 1/3, males 2/3.
- Females generally lighter than males, the heaviest females potentially heavier than the lightest males.
- Gaussian (conditional) distribution of X for each gender. Dependence of means on gender.
- Unknown genders in population – both genders are mixed ("mixture").

Interpretation: example (II)

$$\pi_1 = 1/3;\ \pi_2 = 2/3;\ \mu_1 = 3;\ \mu_2 = 7;\ \sigma = 2$$

- If some rodent weighs 3g, its probability to be a female ($Z = 1$) is no longer 1/3 (compute it)



Histogram and mixture density function

Interpretation: example (III)

$$\pi_1 = 1/3;\ \pi_2 = 2/3;\ \mu_1 = 3;\ \mu_2 = 7;\ \sigma = 2$$

$$\begin{aligned} p_X(3) =& \frac{1}{3} \times \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{1}{8}(3-3)^2\right) \\ &+ \frac{2}{3} \times \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{1}{8}(7-3)^2\right) \end{aligned}$$

Hence,

$$P(Z=1|X=3) = \frac{p_X(3|Z=1)P(Z=1)}{p_X(3)}$$

$$= \frac{\frac{1}{3}\exp(-0)}{\frac{1}{3}\exp(-0) + \frac{2}{3}\exp(-2)}$$

$$\approx 0.79 > \frac{1}{3} = P(Z=1)$$

Identifiability issues

- Generally in statistics, a parametric family of models $\{p_\lambda\}_{\lambda \in \Lambda}$ has identifiable parameter iff $\forall (\lambda, \lambda') \in \Lambda^2,\ p_\lambda = p_{\lambda'} \Rightarrow \lambda = \lambda'$.
- Ensures uniqueness of parameter (interpretation, necessary condition for unique estimation, ...).
- Identifiability cannot be achieved for mixtures with variable and even fixed K, since for every $\lambda = (\pi_1, \ldots, \pi_K, \theta_1, \ldots, \theta_K)$, for every permutation $\kappa \in \mathcal{S}_K$ of the labels (values of the categorical value Z), if we set $\lambda' = (\pi_{\kappa(1)}, \ldots, \pi_{\kappa(K)}, \theta_{\kappa(1)}, \ldots, \theta_{\kappa(K)})$, we have

$$p_\lambda = \sum_{k=1}^{K} \pi_k p_{\theta_k} = \sum_{k=1}^{K} \pi_{\kappa(k)} p_{\theta_{\kappa(k)}} = p_{\lambda'}.$$

Identifiability for mixtures

- For mixture models: identifiability required up to a permutation of the labels (equivalence classes), requiring that

$$\sum_{k=1}^{K} \pi_k p_{\theta_k} = \sum_{k=1}^{K'} \pi'_k p'_{\theta_k}$$
$$\Rightarrow K = K' \text{ and } \exists \kappa \in \mathcal{S}_K \, \forall k,\ \pi_k = \pi'_{\kappa(k)} \text{ and } \theta_k = \theta'_{\kappa(k)}.$$

- Necessary condition: $\forall k,\ \pi_k > 0$.
- Additional sufficient condition for mixture identifiability: $\{p_\theta\}_{\theta \in \Theta}$ linearly independent PDFs.

Exercise 1

Show that the mixtures of uniform distributions $\{\mathcal{U}(a,b) | (a,b) \in \mathbb{R}^2, a < b\}$ are not identifiable.

Identifiability for mixtures (II)

Show that the mixtures of uniform distributions $\{\mathcal{U}(a,b) | (a,b) \in \mathbb{R}^2, a < b\}$ are not identifiable.
We consider

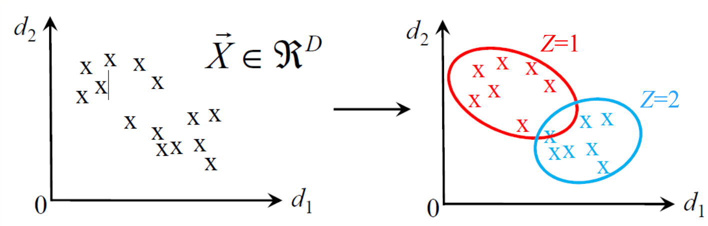
$$\frac{1}{2}\mathcal{U}(0,1) + \frac{1}{2}\mathcal{U}(1,2) = \mathcal{U}(0,2) = \frac{1}{4}\mathcal{U}(0,\frac{1}{2}) + \frac{3}{4}\mathcal{U}(\frac{1}{2},2).$$

Indeed,

$$\forall x \in [0,2],\ x \notin \{\frac{1}{2},1\} \Rightarrow \frac{1}{2}\mathbb{1}_{[0,1]}(x) + \frac{1}{2}\mathbb{1}_{[1,2]}(x) = \frac{1}{2}$$
$$= \mathbb{1}_{[0,2]}(x) = \frac{1}{4}\mathbb{1}_{[0,\frac{1}{2}]}(x) + \frac{3}{4}\mathbb{1}_{[\frac{1}{2},2]}(x).$$

Clustering with mixtures in three steps

1. $(Z_i, X_i)_{i=1,\dots,n}$ assumed independent (“independent mixture model”).
2. Parameter estimation (maximum likelihood) $\equiv$ learning from an unlabelled sample of size $n \ \rightarrow \hat{\lambda}_n$.
3. $\forall (i,k)$ compute $P_{\hat{\lambda}_n}(Z_i = k | X_i = x_i)$ (see previous slide)
4. MAP: $\forall i,\ \hat{Z}_i = \arg\max_k P_{\hat{\lambda}_n}(Z_i = k | X_i = x_i)$



Clustering with bivariate mixtures

Learning stage

$$\hat{\lambda}_n = \arg\max_{\lambda \in \mathcal{C}} \sum_{i=1}^{n} \ln\left[\sum_{k=1}^{K} \pi_k p_{\theta_k}(x_i)\right] = \arg\max_{\lambda \in \mathcal{C}} \ell_{x_1,\dots,x_n}(\lambda)$$

with $\mathcal{C} = \{(\pi_1, \dots, \pi_K, \theta_1, \dots, \theta_K) | \sum_k \pi_k = 1 \text{ and } \forall k\, \pi_k \geq 0\}$.

Likelihood equations:

$$\left.\begin{array}{l} \frac{\partial \ell_{x_1,\dots,x_n}}{\partial \pi_k}(\lambda) = \sum_{i=1}^{n} \frac{p_{\theta_k}(x_j)}{\sum_{l=1}^{K} \pi_l p_{\theta_l}(x_j)} = 0 \\ \nabla_{\theta_k} \ell_{x_1,\dots,x_n}(\lambda) = \sum_{i=1}^{n} \frac{\pi_k \nabla_{\theta_k} p_{\theta_k}(x_j)}{\sum_{l=1}^{K} \pi_l p_{\theta_l}(x_j)} = 0 \\ \text{and constraints...} \end{array}\right\}$$

- Non linear equations
- No closed form solution
- Newton method may work but what properties to expect from it?

EM algorithm: basic idea

Learning stage

Difficulty $\equiv$ non-linearity, from

$$\hat{\lambda}_n = \arg\max_{\lambda \in \mathcal{C}} \sum_{i=1}^{n} \underbrace{\ln \left[\sum_{k=1}^{K} \pi_k p_{\theta_k}(x_i) \right]}_{\text{Comes from } z \text{ being hidden}}$$

If known states $(Z_1, \ldots, Z_n)$: maximize

$$\sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}_{\{z_i=k\}} \ln \left[\pi_k p_{\theta_k}(x_i)\right] = \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}_{\{z_i=k\}} \ln(\pi_k) + \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}_{\{z_i=k\}} \ln p_{\theta_k}(x_i).$$

with same complexity as MLE estimation on K independent i.i.d. samples within family $\{p_\theta\}_{\theta \in \Theta}$.

EM algorithm: principle

$$\hat{\lambda} = \arg\max_{\lambda} \ln\left[p_\lambda(\boldsymbol{x})\right] = \arg\max_{\lambda} \ln\left[\sum_{\boldsymbol{z}} p_\lambda(\boldsymbol{x}, \boldsymbol{z})\right]$$

where:

- $\boldsymbol{x}$ observed, $\boldsymbol{z}$ hidden with finite values (arbitrary random vectors, extension to continuous $\boldsymbol{z}$ with integrals).
- $p_\lambda(\boldsymbol{x}, \boldsymbol{z})$ easy to maximize, $p_\lambda(\boldsymbol{x})$ difficult to maximize.

Example: $\boldsymbol{x} = (x_1, \ldots, x_n), \boldsymbol{z} = (z_1, \ldots, z_n)$

- Try to maximize $\ln p_\lambda(\boldsymbol{x}, \boldsymbol{z})$ rather than $\ln p_\lambda(\boldsymbol{x})$.
- Since $\boldsymbol{z}$ is hidden, consider $E[\ln p_\lambda(\boldsymbol{X}, \boldsymbol{Z}) | \boldsymbol{X} = \boldsymbol{x}]$.
- Expectation under which p_λ if λ and $\hat{\lambda}$ are unknown?
- $\arg\max_{\lambda} E_\lambda[\ln p_\lambda(\boldsymbol{X}, \boldsymbol{Z}) | \boldsymbol{X} = \boldsymbol{x}]$ seems too complicated: proceed iteratively.

EM algorithm: formulation

We need an initial value $\lambda^{(0)}$.

$$\lambda^{(m+1)} = \arg\max_{\lambda} E_{\lambda^{(m)}} \left[\ln p_{\lambda}(\boldsymbol{X}, \boldsymbol{Z}) | \boldsymbol{X} = \boldsymbol{x}\right] = \arg\max_{\lambda} Q(\lambda, \lambda^{(m)})$$

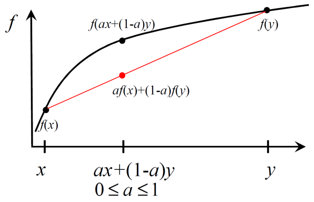
where

$$Q(\lambda, \lambda^{(m)}) = \sum_{\boldsymbol{z}} \ln p_{\lambda}(\boldsymbol{x}, \boldsymbol{z}) p_{\lambda^{(m)}}(\boldsymbol{z}|\boldsymbol{x}).$$

- E = Expectation (compute $E_{\lambda^{(m)}} \left[\ln p_{\lambda}(\boldsymbol{X}, \boldsymbol{Z}) | \boldsymbol{X} = \boldsymbol{x}\right]$ or at least any relevant quantity for the maximisation)
- M = maximisation (update parameter $\lambda \to \lambda^{(m+1)}$ using $\lambda^{(m)}$).

EM algorithm: main property

Theorem 1 (Dempster *et al.*, 1977).
$(\ln p_{\lambda^{(m)}}(x))_{m \geq 0}$ *is a non-decreasing sequence.*



Some concave function f

Remark 1.

- $(\ln p_{\lambda^{(m)}}(x))_{m \geq 0}$ *may not converge.*
- $(\lambda^{(m)})_{m \geq 0}$ *may not converge, or may converge to a saddle point, a local maximum, ...)*

Application of EM to clustering

Exercise 2

- Compute the so-called completed likelihood

$$\ell_{\boldsymbol{x},\boldsymbol{z}}(\lambda) = \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}_{\{z_i=k\}} \ln\left[\pi_k p_{\theta_k}(x_i)\right]$$

  and its maximizer $\hat{\lambda}_{\boldsymbol{x},\boldsymbol{z}}$ if $X \in \mathbb{R}^d$ has conditional multivariate Gaussian distribution with parameter $\theta = (\mu, \Sigma)$.
- We give

$$\nabla\mu\left[(x-\mu)^T\Sigma^{-1}(x-\mu)\right] = -2\Sigma^{-1}(x-\mu),$$
$$\nabla_\Sigma\left[(x-\mu)^T\Sigma^{-1}(x-\mu)\right] = -\Sigma^{-2}(x-\mu)(x-\mu)^T$$

and $\nabla_\Sigma\left[\ln(\text{det}(\Sigma))\right] = \Sigma^{-1}$.

EM algorithm: reestimation formulas

Exercise 3

- Read and answer the preparatory questions for next lab session (Independent mixture models).
- Give the reestimation formulas of the EM algorithm for independent mixtures with multivariate Gaussian emission distributions.

References

References

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