Mixture models: introduction

Mixtures are complicated distributions build from simpler ones. In this respect, these distributions can be viewed as a weighted combination of densities. Let Y be a random variable (or a d-dimensional random vector in the multivariate case) and y be any observed values of this random variable. Then Y obeys a finite mixture distribution if its density can be written as:

$$f(y) = \lambda_1 f_1(y) + ... + \lambda_k f_k(y) = \sum_{j=1}^{k} \lambda_j f_j(y),$$

provided that $\lambda_j > 0$ and $\sum_{j=1}^{k} \lambda_j = 1$. The weights λ_j are called the *mixing proportions* and $f_j(y)$ are called the *component densities*. Further, a k-component parametric finite mixture model has the form:

$$f(y \mid \boldsymbol{\Psi}) = \sum_{j=1}^{k} \lambda_j f_j(y \mid \boldsymbol{\theta}_j) \ .$$

Gaussian Mixture models

We are concerned with the particular case of univariate gaussian mixture models. The simplest case of a two-component model, parametrized by μ_j and σ_j^2, for $j = 1, 2$, decomposes as follows:

$$\begin{aligned} f(y \mid \boldsymbol{\Psi}) &= \sum_{j=1}^{2} \lambda_j f_j(y \mid \boldsymbol{\theta}_j) \\ &= \lambda_1 N_1(y \mid \boldsymbol{\theta_1}) + \lambda_2 N_2(y \mid \boldsymbol{\theta_2}) \\ &= \lambda_1 \frac{1}{\sqrt{2\pi\sigma_1^2}} \exp\left(- \frac{(y-\mu_1)^2}{2\sigma_1^2} \right) + \lambda_2 \frac{1}{\sqrt{2\pi\sigma_2^2}} \exp\left(- \frac{(y-\mu_2)^2}{2\sigma_2^2} \right) . \end{aligned}$$

The mixture parameter vector is $\boldsymbol{\Psi} = (\lambda_1, \lambda_2, \mu_1, \mu_2, \sigma_1^2, \sigma_2^2)$; the number of components is $k = 2$; the component density parameters are $\boldsymbol{\theta_1} = (\mu_1, \sigma_1^2)$ and $\boldsymbol{\theta_2} = (\mu_2, \sigma_2^2)$; the mixing proportions are λ_1 and $\lambda_2 = (1 - \lambda_1)$.

'faithful' dataset

faithful: A data frame with 272 observations on 2 variables.

eruptions: (numeric) Eruption time in mins

waiting: (numeric) Waiting time to next eruption (in mins)

```
> data(faithful)
> head(faithful)
  eruptions waiting
1     3.600      79
2     1.800      54
3     3.333      74
4     2.283      62
5     4.533      85
6     2.883      55
```

By looking at the distribution of the variable 'waiting' using kernel density estimator, we clearly see that this distribution is bimodal. We will therefore model the distribution using a Gaussian Mixture model with $k = 2$ components.

Choice of prior structure

Several kind of prior structures for $\boldsymbol{\theta}$ have proved to be appropriate for normal mixtures. We first mention the *independence prior* (IP) having the form:

$$p(\boldsymbol{\theta}) = \prod_{j=1}^{k} p(\mu_j)\ p(\sigma_j^2)\ ,$$

where μ_j is modeled using the conjugate normal distribution prior $\mathrm{N}(m_0,\, v_0)$ and σ_j^2 the conjugate inverse gamma prior $\mathrm{IG}(sh_0,\, ra_0)$. Such prior structure reflects the belief that a priori no particular reason justifies to introduce any kind of dependence whatsoever. Another common type of prior structure is the *conditionnally conjugate prior* (CCP) which has been used for example in Diebolt and Robert (1994), and takes the form:

$$p(\boldsymbol{\theta}) = \prod_{j=1}^{k} p(\mu_j \mid \sigma_j^2)\ p(\sigma_j^2)\ ,$$

where $\mu_j \mid \sigma_j^2$ comes from a normal distribution $\mathrm{N}(m_0,\, p_0^{-1}\sigma_j^2)$ and σ_j^2 comes from an inverse gamma distribution $\mathrm{IG}(sh_0,\, ra_0)$. This prior assumes that there is a dependance between μ_j and σ_j^2 within a given subpopulation j. Such a prior for $\boldsymbol{\theta}$ has also been studied in Raftery (1996). To remain weakly informative, hyperparameter values are chosen so that their influence on the posterior is limited.

Gibbs Sampler - Conditionally Conjugate Priors (1/3)

Under the conditionally conjugate priors, a possible implementation of a Gibbs sampler could be as follows :

1. Specify a number of simulations T.

2. At iteration $t = 0$, start with some preliminary parameter estimation and classification.

3. At iteration $t \geq 1$, compute the ratio $\hat{w}_{ij}$

$$\hat{w}_{ij}^{(t)} = P(Z_{ij} = 1 \mid y_i) = \frac{\lambda_j f_j(y_i \mid \boldsymbol{\theta}_j)}{\sum_{j'=1}^{k} \lambda_{j'} f_{j'}(y_i \mid \boldsymbol{\theta}_{j'})}$$

Gibbs Sampler -Conditionally Conjugate Priors (2/3)

4. Sample the indicator variable Z from a multinomial distribution

$$z_i^{(t)} \sim M(1, \hat{w}_{i1}, ..., \hat{w}_{ik})$$

5. (a) Sample the mixing proportions from the full conditional Dirichlet distribution

$$\hat{\boldsymbol{\lambda}}^{(t)} \mid \mathbf{z} \sim D(\delta_1 + n_1, ..., \delta_k + n_k)$$

Gibbs Sampler - Conditionally Conjugate Priors (3/3)

(b) Sample jointly the variance and the mean of the component j

from their respective full conditional distributions

$$\hat{\sigma}_j^{2(t)} \mid \mathbf{y}, \mathbf{z}, \boldsymbol{\lambda}, \mu_j \sim IG\Big(\; sh_0 + \frac{n_j + 1}{2} \; , \; ra_0 + \frac{s_j + p_0(\mu_j - m_0)^2}{2} \Big)$$

and

$$\hat{\mu}_j^{(t)} \mid \mathbf{y}, \mathbf{z}, \boldsymbol{\lambda}, \sigma_j^2 \sim N\Big(\; \frac{m_0 p_0 + y_j}{p_0 + n_j} \; , \; \frac{\sigma_j^2}{p_0 + n_j} \Big)$$

6. Return to step 3 and loop through step 5 untill the specified number of simulations T is achieved.

R code and Results summary

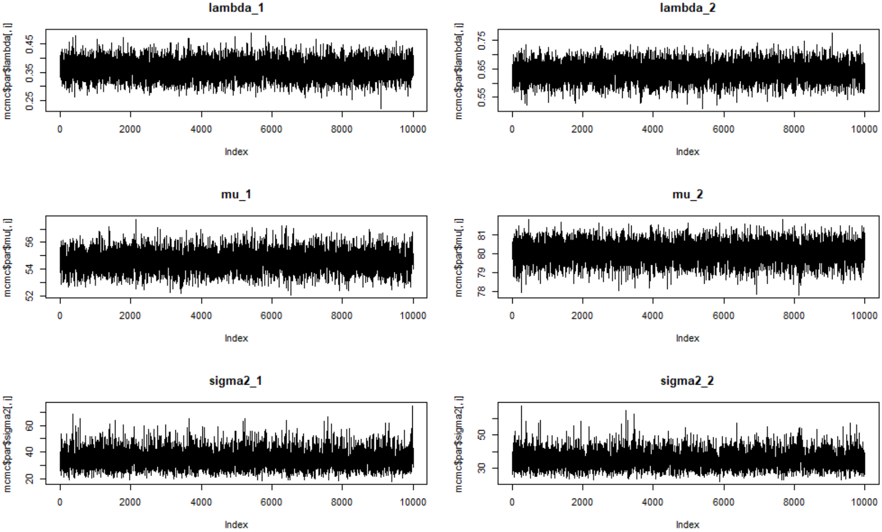
The R code to perform Bayesian Gaussian Mixture Modelling using Gibbs sampling with independent prior is accessible here:

`https://github.com/JRigh/Short-Analyses-in-R-and-Python/blob/main/Mixture%20Models/R/Bayesian%20Mixture%20Modelling`
`GMMb_CCP.R`

Bay IP	*mean*	*sd*	2.5 %	97.5 %
λ_j	0.3611	0.0314	0.2995	0.4239
	0.6389	0.0314	0.5761	0.7005
μ_j	54.599	0.7069	53.2200	56.0176
	80.057	0.5123	79.0065	81.0385
σ_j	5.8468	0.5438	4.8715	7.0086
	5.898	0.4173	5.1719	6.7854

Visualizing GMM

Traceplots (Convergence of the chains)



Main observations

- The GMM distinctly separates the waiting times into two clusters, corresponding to shorter (around 55 minutes) and longer (around 80 minutes) eruption intervals.
- The mixing proportions typically show a near 36-64 split, indicating that long eruptions are more frequent than short ones.
- The standard deviation within each cluster suggests that the longer eruptions exhibit more variability in waiting times compared to the shorter eruptions.
- Despite clear separation, there is moderate overlap between the two clusters in the 65-75 minute range, indicating some ambiguity in classifying waiting times within this interval.

References

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Raftery, A.E. (1996). Hypothesis testing and model selection. In Markov Chain Monte Carlo in Practice(W.R. Gilks, D.J. Spiegelhalter and S. Richardson, eds.), *London: Chapman and Hall*, pp. 163–188.

Walsh, D., course notes. (2016). available for download ath this address :
`http://www.massey.ac.nz/~dcwalsh/161304/CourseMaterials/LectureN`

Walsh, D., R Code to implement Gibbs sampling for component univariate normal mixture. available for download at this address :
`http://www.massey.ac.nz/~dcwalsh/161304/Code/MCMC.R`

The R Project for Statistical Computing:
https://www.r-project.org/