Incomplete Data Analysis

V. Inácio de Carvalho & M. de Carvalho

University of Edinburgh

PRR Plano de Recuperação e Resiliência

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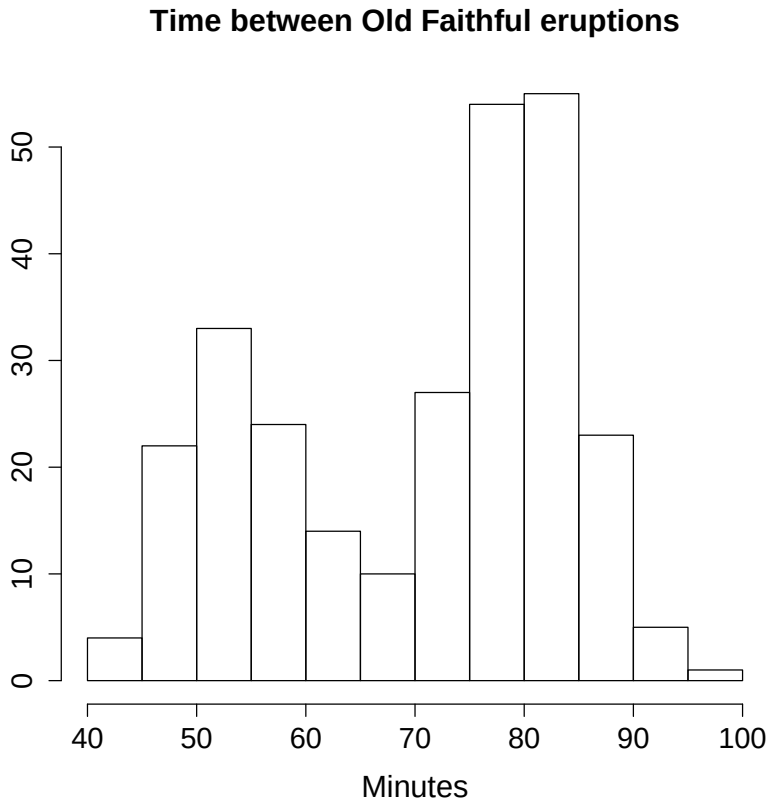
FACULDADE DE CIÊNCIAS
UNIVERSIDADE DO PORTO

EM algorithm

Mixture models

↪ Let us consider the popular old faithful data. The data consists of 272 waiting times between eruptions for the Old Faithful geyser in Yellowstone National park, Wyoming, USA.



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Mixture models

↪ For this dataset we posit as a model a mixture model with two normal components, i.e.,

$$y_1, \ldots, y_n \overset{\text{iid}}{\sim} f(y; \theta),$$

where

$$f(y; \boldsymbol{\theta}) = p\phi(y; \mu_1, \sigma_1^2) + (1-p)\phi(y; \mu_2, \sigma_2^2), \qquad \boldsymbol{\theta} = (p, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

↪ The observed data likelihood is

$$L(\boldsymbol{\theta}; y) = \prod_{i=1}^{n} \{p\phi(y_i; \mu_1, \sigma_1^2) + (1-p)\phi(y_i; \mu_2, \sigma_2^2)\},$$

with corresponding log likelihood given by

$$\log L(\boldsymbol{\theta}; y) = \sum_{i=1}^{n} \log \left\{ p\phi(y_i; \mu_1, \sigma_1^2) + (1-p)\phi(y_i; \mu_2, \sigma_2^2) \right\}.$$

↪ This log likelihood is difficult to maximise due to the sum inside the logarithm.

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Mixture models

- **Idea**: If we knew the group each observation belongs to, we could simply fit a normal distribution to each group.

- We define an augmented complete dataset where $\mathbf{y}_{\text{obs}} = (y_1, \ldots, y_n)$ and $\mathbf{y}_{\text{mis}} = z = (z_1, \ldots, z_n)$ is a vector of unobserved/latent group data indicator, such that

$$z_i = \begin{cases} 1, & \text{if } y_i \text{ belongs to the first component (short waiting times),} \\ 0 & \text{if } y_i \text{ belongs to the second component (long waiting times).} \end{cases}$$

- Note that $\Pr(Z_i = 1) = p$ or, equivalently stated, $Z_i \overset{\text{iid}}{\sim} \text{Bernoulli}(p)$.

- Then, the complete data likelihood is

$$L(\theta \mid y, z) = \prod_{i=1}^{n} \left\{ [p\phi(y_i; \mu_1, \sigma_1^2)]^{z_i} [(1-p)\phi(y_i; \mu_2, \sigma_2^2)]^{1-z_i} \right\}.$$

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Mixture models

↪ Therefore,

$$\log L(\theta \mid y, z) = \sum_{i=1}^{n} z_i \left\{ \log p + \log \phi(y_i; \mu_1, \sigma_1^2) \right\} + \sum_{i=1}^{n} (1 - z_i) \left\{ \log(1-p) + \log \phi(y_i; \mu_2, \sigma_2^2) \right\}.$$

↪ For the E-step we would need to compute

$$\begin{aligned} Q(\theta \mid \theta^{(t)}) &= E_Z[\log L(\theta \mid y, z) \mid y, \theta^{(t)}] \\ &= \sum_{i=1}^{n} E[Z_i \mid y, \theta^{(t)}] \left\{ \log p + \log \phi(y_i; \mu_1, \sigma_1^2) \right\} \\ &+ \sum_{i=1}^{n} \left(1 - E[Z_i \mid y, \theta^{(t)}]\right) \left\{ \log(1-p) + \log \phi(y_i; \mu_2, \sigma_2^2) \right\}. \end{aligned}$$

↪ Now,

$$\begin{aligned} E[Z_i \mid y, \theta^{(t)}] &= E[Z_i \mid y_i, \theta^{(t)}] \\ &= 1 \times \Pr(Z_i = 1 \mid y_i, \theta^{(t)}) + 0 \times \Pr(Z_i = 0 \mid y_i, \theta^{(t)}) \\ &= \frac{p^{(t)} \phi\left(y_i; \mu_1^{(t)}, (\sigma_1^{(t)})^2\right)}{p^{(t)} \phi\left(y_i; \mu_1^{(t)}, (\sigma_1^{(t)})^2\right) + (1 - p^{(t)}) \phi\left(y_i; \mu_2^{(t)}, (\sigma_2^{(t)})^2\right)} \\ &= \widetilde{p}_i^{(t)} \end{aligned}$$

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Mixture models

↪ Thus,

$$Q(\theta \mid \theta^{(t)}) = \sum_{i=1}^{n} \widetilde{p}_i^{(t)} \left\{ \log p + \log \phi(y_i; \mu_1, \sigma_1^2) \right\} + \sum_{i=1}^{n} \left(1 - \widetilde{p}_i^{(t)}\right) \left\{ \log(1-p) + \log \phi(y_i; \mu_2, \sigma_2^2) \right\}.$$

↪ For the M-step,

$$\frac{\partial}{\partial p} Q(\theta \mid \theta^{(t)}) = 0 \Rightarrow p^{(t+1)} = \frac{\sum_{i=1}^{n} \widetilde{p}_i^{(t)}}{n}$$

$$\frac{\partial}{\partial \mu_1} Q(\theta \mid \theta^{(t)}) = 0 \Rightarrow \mu_1^{(t+1)} = \frac{\sum_{i=1}^{n} \widetilde{p}_i^{(t)} y_i}{\sum_{i=1}^{n} \widetilde{p}_i^{(t)}}$$

$$\frac{\partial}{\partial \sigma_1^2} Q(\theta \mid \theta^{(t)}) = 0 \Rightarrow (\sigma_1^{(t+1)})^2 = \frac{\sum_{i=1}^{n} \widetilde{p}_i^{(t)} (y_i - \mu_1^{(t+1)})^2}{\sum_{i=1}^{n} \widetilde{p}_i^{(t)}}$$

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Mixture models

↪ Continuing the M-step:

$$\frac{\partial}{\partial \mu_2} Q(\theta \mid \theta^{(t)}) = 0 \Rightarrow \mu_2^{(t+1)} = \frac{\sum_{i=1}^{n}(1-\widetilde{p}_i^{(t)})y_i}{\sum_{i=1}^{n}(1-\widetilde{p}_i^{(t)})}$$

$$\frac{\partial}{\partial \sigma_2^2} Q(\theta \mid \theta^{(t)}) = 0 \Rightarrow (\sigma_2^{(t+1)})^2 = \frac{\sum_{i=1}^{n}(1-\widetilde{p}_i^{(t)})(y_i-\mu_2^{(t+1)})^2}{\sum_{i=1}^{n}(1-\widetilde{p}_i^{(t)})},$$

which can be solved iteratively.

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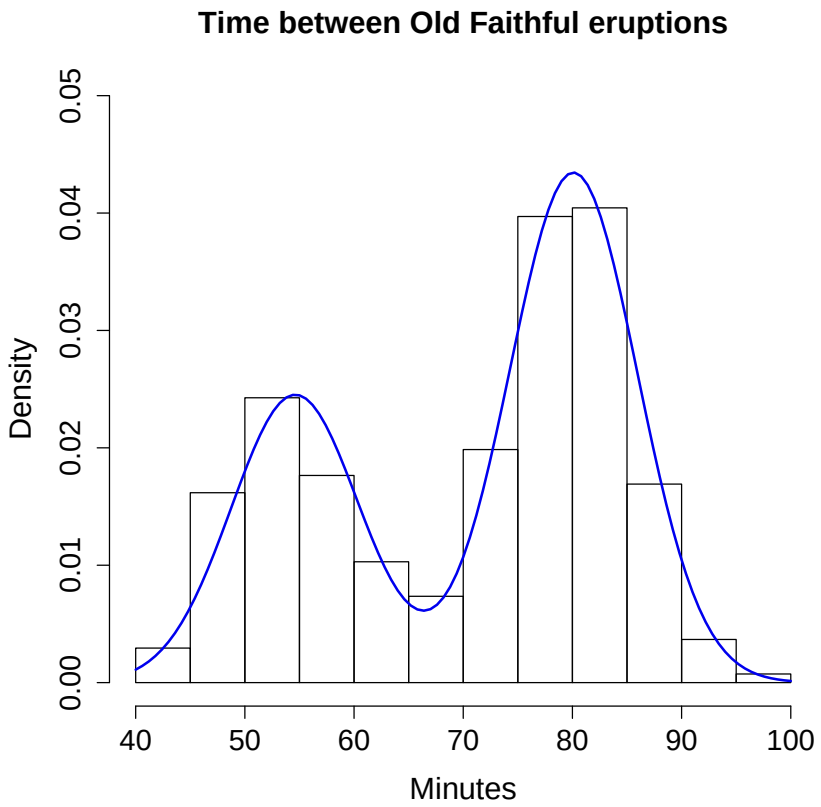
Mixture models

↪ The plot below depicts the fit of two-component Gaussian mixture model to the observed data.



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Mixture models

↪ More generally, we may have a K-component mixture model

$$f(y) = \sum_{k=1}^{K} p_k f(y; \theta_k), \qquad \sum_{k=1}^{K} p_k = 1.$$

↪ In the particular case of normal components, we have

$$f(y) = \sum_{k=1}^{K} p_k \phi(y; \mu_k, \sigma_k^2).$$

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Mixture models and identifiability issues

- ↪ Due to identifiability issues, such as the so-called label switching problem, it makes difference whether there is interest in making inferences about the mixture component-specific parameters and clustering.

- ↪ The label switching problem (also known as label ambiguity) refers to the fact that there is nothing in the likelihood to distinguish mixture component k from mixture component k'.

- ↪ Permuting the K labels in any of $K!$ ways results in the same model for the data.

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Mixture models and identifiability issues

- As a concrete example, in the $K = 2$ case, consider

$$p_1 = 0.3, \quad \mu_1 = 1, \quad p_2 = 0.7, \quad \mu_2 = 1.5, \quad \sigma_1^2 = \sigma_2^2 = 1, \qquad \text{(Scenario A)}.$$

- Then, the model is equivalent to one with

$$p_1 = 0.7, \quad \mu_1 = 1.5, \quad p_2 = 0.3, \quad \mu_2 = 1, \quad \sigma_1^2 = \sigma_2^2 = 1, \qquad \text{(Scenario B)}.$$

- If one is only interested in density estimation, then everything is fine, because as illustrated in the example

$$\begin{aligned} f_{\text{A}}(y) &= 0.3\phi(y \mid 1, 1) + 0.7\phi(y \mid 1.5, 1) \\ &= 0.7\phi(y \mid 1.5, 1) + 0.3\phi(y \mid 1, 1) = f_{\text{B}}(y). \end{aligned}$$

- Of course, if we are 'only' interested in estimating the density, the label switching poses no problem.

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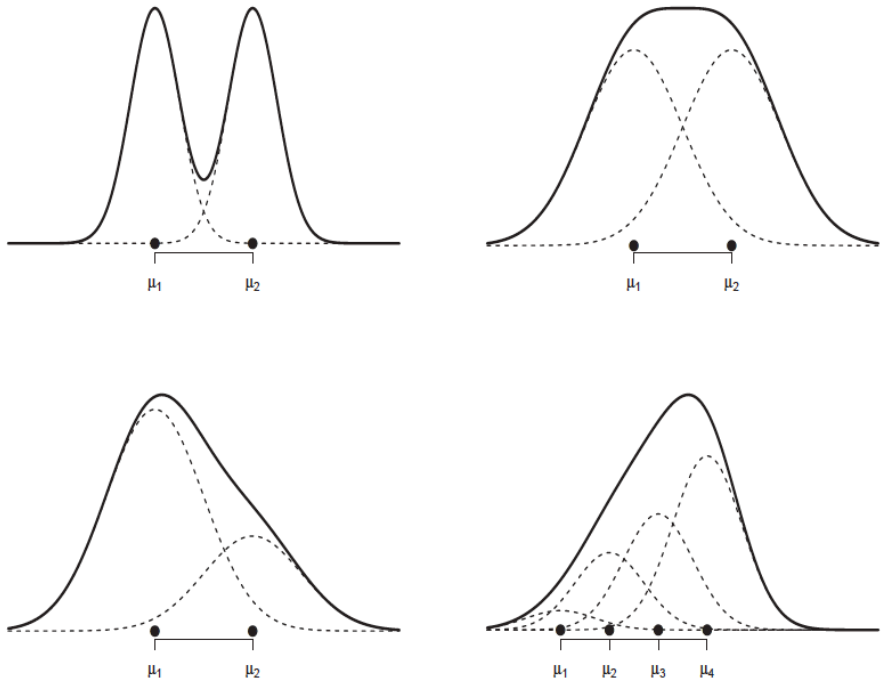
Mixture models

↪ It is worth noting that multimodality is not the sole motivation for the use of mixture models. For instance, skewed data can also be handled by mixtures.



source: Komarek, A., 2006, PhD thesis

EM algorithm

- ↪ The following paper, available on Learn, is an interesting reading (I think!). It advocates the use of direct (numerical) maximisation of the likelihood, in several well-known problems, where the EM algorithm is the 'gold standard' solution.
- ↪ We will explore the first example mentioned in the paper (mixture of Poisson distributions), from the EM perspective, in Workshop 4.

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Numerical Maximisation of Likelihood: A Neglected Alternative to EM?

Iain L. MacDonald

Actuarial Science, University of Cape Town, 7701 Rondebosch, South Africa
Email: iain.macdonald@uct.ac.za