Preliminaries (Task 1)

Reading in data

- Datasets which are part of R packages can be loaded easily through the the `data` command. For instance, the data set `galaxies` in R package **MASS** can be loaded via

  ```
  library(MASS)
  data(galaxies)
  ```

  or

  ```
  data(galaxies, package="MASS")
  ```

- Data in text files (usually, with .txt or .dat ending):

  ```
  test <- read.table("testdata.dat", header=TRUE)
  ```

  The option `header=TRUE` tells R that the first row just contains the column names (but no data).

- Similarly, for data in .csv files (**c**omma–**s**eparated–**v**alue) format, use e.g.

  ```
  energy.use <- read.csv("energy.csv", header=TRUE)
  ```

  It is possible to read in data directly from a web address:

  ```
  energy.use <-read.csv("http://www.maths.dur.ac.uk/~dma0je/PG/Mix/energy.csv", header=TRUE)
  ```

- Excel (.xls) files can be saved as .csv files in Excel, and so easily read into R using `read.csv`.

Data description

The energy data were retrieved from the Worldbank data base,

`http://data.worldbank.org/indicator/EG.USE.PCAP.KG.OE`

Below is the description of the data, taken word by word from the original source file:

Indicator: Energy use (kg of oil equivalent per capita)
Description: Energy use refers to use of primary energy before transformation to other end-use fuels, which is equal to indigenous production plus imports and stock changes, minus exports and fuels supplied to ships and aircraft engaged in international transport.
Source: International Energy Agency.
Catalog Source: World Development Indicators

Basic programming (Task 2)

if/then

This command performs an *action* if the *condition* is met. One can specify an alternative *action2* if an alternative *condition2* is met, and a further alternative *action3* if not any condition was met.

```
if (condition){
      action
} else if (condition2){
      action2
} else {
      action3
}
```

Both the parts commencing with `else` and `else if` are optional and can be omitted. For instance, the command

```
if (log(10)<pi){
      pi
} else {
      log(10)
}
```

gives the value of `pi`.

for

A `for` loop repeats an *action* for all elements of a *set*. Formally,

```
for (i in set ){
      action
}
```

For instance,

```
for (i in 1:10){
      cat('This is loop', i, '\n')
}
```

will produce 10 rows of text which report the number of the loop (The string '\ n' is borrowed from the C language and means to start a new line).

while

A `while` loop works similar as `for`, but instead of working though a *set*, it checks in every iteration whether a *condition* is met:

```
while (condition){
      action
}
```

apply

This function allows to carry out some operation onto all rows or columns of a matrix. For instance, if `W` is a $n \times p$ matrix, then

$$\texttt{apply}(\texttt{W}, 1, \texttt{sum})$$

would give a $n \times 1$ vector which contains the sums over each row, and

$$\texttt{apply}(\texttt{W}, 2, \texttt{mean})$$

would give the column means. Useful variants are `tapply` (carries out operations on the elements of `W` grouped by a factor, the name of which is given as second argument), and `lapply` (for operations on each element of a list `W`; here the second argument is not needed).

Functions

Functions allow to prepare some code which can be used later with different function arguments. For instance,

```
testlog <- function(x){
    if (x>0){
       log(x)
    } else {
       cat("log not defined for non-positive argument.")
    }
}
```

will give the logarithm of `x` if `x` is positive, and an error message otherwise.
Functions can also have more than one argument, which are then separated by commas. Default values can be given behind a `=` symbol, for instance

```
max1<- function(a,b=1){
   result<- max(a,b)
   return(result)
}
```

```
max1(0.5)
[1] 1
max1(0.5,0)
[1] 0.5
```

Finite Gaussian Mixtures (Tasks 3-5)

Finite Gaussian mixtures

Assume we are given K univariate normal distributions $N(\mu_k, \sigma^2)$, $k = 1, \ldots, K$. A finite Gaussian mixture is a distribution which draws with probability π_k from the $k-$th normal distribution. Formally, the density of a finite Gaussian mixture is given by

$$f(y|\theta) = \sum_{k=1}^{K} \pi_k \phi_{\mu_k, \sigma^2}(y) \tag{1}$$

where $K < \infty$ is the number of mixture components, $\theta = (\pi_1, \ldots, \pi_{K-1}, \mu_1, \ldots, \mu_K, \sigma)^T$ is the vector of parameters, and $\phi_{\mu_k,\sigma^2}(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}\left(\frac{y-\mu_k}{\sigma}\right)^2\right\}$ is the probability density function of a normal distribution with mean μ_k and variance σ^2, evaluated at y. Note that $\pi_K = 1 - \sum_{k=1}^{K-1} \pi_k$.

Estimation of Gaussian mixtures

Given some data $y_i, i = 1, \ldots, n$, we wish to obtain an estimator, $\hat{\theta}$, of θ. This is done by the **EM algorithm** (**E**xpectation - **M**aximization). Based on a vector of starting values, say θ_0, the EM algorithm iterates between....

E-step Update membership probabilities $w_{ik} = P(\text{obs. } i \text{ belongs to comp. } k)$ via

$$w_{ik} = \frac{\pi_k \exp\left\{-\frac{1}{2}\left(\frac{y_i-\mu_k}{\sigma}\right)^2\right\}}{\sum_{\ell=1}^{K} \pi_\ell \exp\left\{-\frac{1}{2}\left(\frac{y_i-\mu_\ell}{\sigma}\right)^2\right\}} \tag{2}$$

M-Step Update parameter estimates via

$$\hat{\pi}_k = \frac{1}{n}\sum_{i=1}^{n} w_{ik} \tag{3}$$

$$\hat{\mu}_k = \frac{\sum_{i=1}^{n} w_{ik} y_i}{\sum_{i=1}^{n} w_{ik}} \tag{4}$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K} w_{ik}(y_i - \mu_k)^2 \tag{5}$$

...until convergence is reached.

Note: If one decided to fit a mixture $N(\mu_k, \sigma_k^2)$ with *unequal* component st. dev.'s σ_k, then the resulting estimator of σ_k^2 would be

$$\hat{\sigma}_k^2 = \frac{\sum_{i=1}^{n} w_{ik}(y_i - \mu_k)^2}{\sum_{i=1}^{n} w_{ik}}.$$

We will not do this in this course as this can lead to technical difficulties for $\hat{\sigma}_k \longrightarrow 0$, known in the literature as 'likelihood spikes'. These need some ad–hoc adjustments, such as enforcing minimum values of $\hat{\sigma}_k$.

Derivation of EM algorithm for Gaussian mixtures

Complete Likelihood. Given some data $y_i, i = 1, \ldots, n$, we wish to obtain an estimator, $\hat{\theta}$, of θ. Let G be the random vector which draws a class $k \in \{1, \ldots, K\}$. We know that $P(G = k) = \pi_k$. Denoting $f_{ik} \equiv P(y_i|G = k) = \phi_{\mu_k,\sigma^2}(y_i)$, then we also know that

$$P(y_i, G = k) = P(y_i|G = k)P(G = k) = f_{ik}\pi_k \tag{6}$$

The key idea is now as follows. Assume that, for an observation y_i, *the value of G is known*, i.e. we know to which of the K components the $i-$th observation belongs. We can express this knowledge through an indicator variable,

$$G_{ik} = \begin{cases} 1 & \text{if observation} \quad i \quad \text{belongs to component} \quad k \\ 0 & \text{otherwise.} \end{cases}$$

This gives "complete" data $(y_i, G_{i1}, \ldots G_{iK})$, $i = 1, \ldots, n$, with probability

$$P(y_i, G_{i1}, \ldots, G_{iK}) = \prod_{k=1}^{K} (f_{ik}\pi_k)^{G_{ik}}$$

(this follows from (6) since only one of the G_{ik}'s is true). The corresponding likelihood function, called *complete likelihood*, is

$$L^*(\theta|y_1, \ldots, y_n) = \prod_{i=1}^{n}\prod_{k=1}^{K} (\pi_k f_{ik})^{G_{ik}}. \tag{7}$$

One obtains the log-likelihood

$$\ell^* = \log L^* = \sum_{i=1}^{n}\sum_{k=1}^{K} G_{ik}\log\pi_k + G_{ik}\log f_{ik} \tag{8}$$

E-step. As the G_{ik} are in fact unknown, we replace them by their conditional expectations

$$w_{ik} \equiv E(G_{ik}|y_i) = P(G_{ik} = 1|y_i) = P(G = k|y_i)$$

Using Bayes' theorem, one has

$$w_{ik} = P(G = k|y_i) = \frac{P(G = k)P(y_i|G = k)}{\sum_\ell P(G = \ell)P(y_i|G = \ell)} = \frac{\pi_k f_{ik}}{\sum_\ell \pi_\ell f_{i\ell}} \tag{9}$$

which is equivalent to the expression provided in (2).

M-step. Setting $\partial\ell^*/\partial\mu_k = 0$ for $k = 1, \ldots, K$, $\partial\ell^*/\partial\sigma = 0$, one obtains exactly the estimates which are given for μ_k and σ in (4) and (5), respectively. For the π_k, one needs to apply a Lagrange multiplier since $\sum_{k=1}^{K}\pi_k = 1$. Setting

$$\partial\left(\ell^* - \lambda(\sum_{k=1}^{K}\pi_k - 1)\right)/\partial\pi_k = 0, \qquad k = 1, \ldots, K$$

one obtains the updated formula for π_k given in (3).

Convergence was proven in Dempster et al. (1977), Wu (1983).

Simulation from Gaussian mixtures

Given a set of parameters θ, data are simulated from a Gaussian mixture in two steps: Firstly we draw a $k \in \{1, \ldots, K\}$, then we simulate from a Gaussian:

- Draw a value x from a uniform distribution on $[0, 1]$ (using `runif`). If

$$x \in \left] \sum_{j=1}^{k-1} \pi_j, \sum_{j=1}^{k} \pi_j \right],$$

  we decide for component k.

- Draw a value y from a normal distribution with mean μ_k and variance σ^2 (using `rnorm`).

Likelihood and Disparity

We wish to compute the likelihood $L(\hat{\theta}|y_1, \ldots, y_n)$ (this is *not* the complete likelihood used in EM) of the fitted model. One has

$$L(\hat{\theta}|y_1, \ldots, y_n) = \prod_{i=1}^{n} f(y_i|\hat{\theta}) = \prod_{i=1}^{n} \left(\sum_{k=1}^{K} \hat{\pi}_k \phi_{\hat{\mu}_k, \hat{\sigma}^2}(y_i) \right) \tag{10}$$

so that the log-likelihood is given by

$$\ell(\hat{\theta}|y_1, \ldots, y_n) = \sum_{i=1}^{n} \log f(y_i|\hat{\theta}) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \hat{\pi}_k \phi_{\hat{\mu}_k, \hat{\sigma}^2}(y_i) \right) \tag{11}$$

An alternative quantity which is often more convenient to use and interpret (for instance, in conjunction with likelihood ratio tests, see below), is the *disparity*

$$D(\hat{\theta}|y_1, \ldots, y_n) = -2 \log L(\hat{\theta}|y_1, \ldots, y_n) = -2\ell(\hat{\theta}|y_1, \ldots, y_n).$$

For the computation of either of these, we will need to compute all entries of the $n \times K$ matrix, say F, which is defined by the values of

$$\hat{\pi}_k \phi_{\hat{\mu}_k, \hat{\sigma}^2}(y_i), \qquad 1 \leq i \leq n, 1 \leq k \leq K$$

Note that, with `y` $=(y_1, \ldots y_n)$, the command

$$\texttt{pi}[\texttt{k}] * \texttt{dnorm}(\texttt{y}, \texttt{mu}[\texttt{k}], \texttt{sigma})$$

provides immediately the $k-$th column of F.

Likelihood ratio test for K

We wish to test

$$H_0 : K = K_0 \quad vs. \quad H_1 : K = K_0 + 1.$$

Denote by $\hat{\theta}_K$ the estimate of θ when K mixture components are used.
Wilk's likelihood ratio statistics:

$$\begin{aligned} W &= -2 \log \frac{L(\hat{\theta}_{K_0} | y_1, \ldots, y_n)}{L(\hat{\theta}_{K_0+1} | y_1, \ldots, y_n)} = \\ &= D(\hat{\theta}_{K_0} | y_1, \ldots, y_n) - D(\hat{\theta}_{K_0+1} | y_1, \ldots, y_n) \end{aligned}$$

The actual test is implemented through the bootstrap:

(i) Compute W as above. Call this value W_0.

(ii) From the model with K_0 components, simulate, say, 99 data sets of size n.

(iii) For each of these 99 data sets, recalculate $\hat{\theta}_{K_0}$ and $\hat{\theta}_{K_0+1}$, and compute the corresponding values of W.

(iv) Find the position P of W_0 within all the other values of W. The $p-$value is given by $1 - P/100$.

Multivariate extension (Task 6)

The multivariate Gaussian mixture model

In the case of multivariate distributions, there are no substantial changes to the methodology. Given data $\boldsymbol{y}_i \in \mathbb{R}^d$, assume, for instance, that we are modelling a mixture of multivariate Gaussian distributions $N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ with means $\boldsymbol{\mu}_k = (\mu_{1k}, \ldots, \mu_{dk})^T \in \mathbb{R}^d$ and component-dependent variance matrices $\boldsymbol{\Sigma}_k \in \mathbb{R}^{d \times d}$ (more restrictive configurations are possible). Then, using

$$f_{ik} = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}_k|^{1/2}} \exp \left\{ -\frac{1}{2} (\boldsymbol{y}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{y}_i - \boldsymbol{\mu}_k) \right\}$$

it is clear that the EM step continues to take the shape (9), and that (3) is unchanged too. For the estimates of $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$ one obtains

$$\begin{aligned} \hat{\boldsymbol{\mu}}_k &= \frac{\sum_{i=1}^n w_{ik} \boldsymbol{y}_i}{\sum_{i=1}^n w_{ik}} \\ \hat{\boldsymbol{\Sigma}}_k &= \frac{1}{\sum_{i=1}^n w_{ik}} \sum_{i=1}^n w_{ik} (\boldsymbol{y}_i - \hat{\boldsymbol{\mu}}_k)(\boldsymbol{y}_i - \hat{\boldsymbol{\mu}}_k)^T \end{aligned}$$

Simulation from multivariate mixtures as well as bootstrapped LR tests can be carried out similarly as before.