

Finite Mixture Models

Example data: Banknote

STAT 32950-24620

Spring 2023 (5/4)

1 / 20

Finite Mixture Models

A random vector X with probability density (or mass) function $f(x), x \in \mathbb{R}^p$ is a k -mixture distribution if

$$f(x) = p_1 f_1(x) + \cdots + p_k f_k(x)$$

where

$$p_1 + \cdots + p_k = 1,$$

k — number of mixtures

p_i — membership probability

2 / 20

Finite Mixture identifiability

In

$$f(x) = p_1 f_1(x) + \cdots + p_k f_k(x)$$

$f_i(x), x \in \mathbb{R}^p$ are probability density (or mass) functions,
 $\int_{\mathbb{R}^p} f_i(x) dx = 1.$

Identifiability:

$$f_i \neq f_j \text{ when } i \neq j, \quad p_i > 0, \quad i, j = 1, \dots, k.$$

3 / 20

Finite mixture model Example

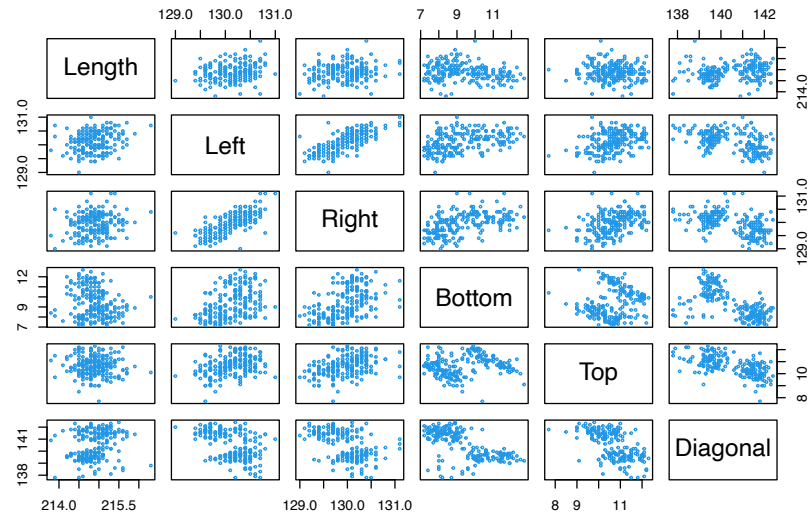
Example: Banknote data

```
# {mclust}:  
library(mclust)  
#Normal Mixture for Cluster, Classify, density est.  
data(banknote)  
str(banknote)  
  
## 'data.frame':    200 obs. of  7 variables:  
## $ Status : Factor w/ 2 levels "counterfeit",...: 2 2 2  
## $ Length : num  215 215 215 215 215 ...  
## $ Left : num  131 130 130 130 130 ...  
## $ Right : num  131 130 130 130 130 ...  
## $ Bottom : num  9 8.1 8.7 7.5 10.4 9 7.9 7.2 8.2 9.2 ...  
## $ Top : num  9.7 9.5 9.6 10.4 7.7 10.1 9.6 10.7 11 ...  
## $ Diagonal: num  141 142 142 142 142 ...
```

4 / 20

Visual check of data

```
pairs(banknote[2:7],cex=.4,col=4)
```



5 / 20

Mixture model example setup

- Using the measurements only (variable 2 to 7)
- Treat the data as “unsupervised”
- Cluster analysis using finite Gaussian mixture model
- EM algorithm for parameter estimation
- Number of clusters $k = 2, \dots, 9$ is selected by BIC

$$BIC = -2\ln(L) + k^* \ln(n)$$

where L is the maximum likelihood of the model given the data,
 k^* is the number of parameters in the model.
 (not to be confused with the number of mixtures k)

6 / 20

EM algorithm estimation and model fit

```
mbank=Mclust(banknote[,2:7]) #BIC choose k from 2 to 9
summary(mbank)

## -----
## Gaussian finite mixture model fitted by EM algorithm
## -----
##
## Mclust VVE (ellipsoidal, equal orientation) model with 3
##
## log-likelihood   n df   BIC   ICL
##          -663.4 200 53 -1608 -1608
##
## Clustering table:
##  1  2  3
## 18 98 84
```

7 / 20

Number of clusters selected

The chosen number of clusters is

$$k = 3$$

BIC is used to selection k .

Under various covariance structure assumptions

In terms of

- Shape (e.g. ellipsoidal)
- Volume (equal or unequal among clusters)
- Orientation (equal or unequal)

8 / 20

BIC of selected mixture model

For the selected model of $k = 3$ mixtures,

Number of observations $n = 200$

Number of parameters $k^* = 53$

Log-likelihood $\log(L) = -663.4$

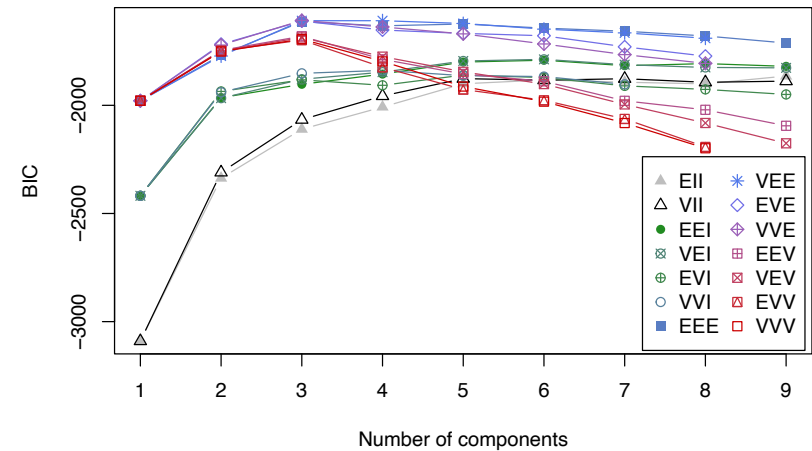
$$\Rightarrow BIC = -2\ln(L) + k * \ln(n) = 1607.6 \approx 1608$$

Note: in `mclust` -BIC is used (but called BIC)

```
plot(mbank, what=c("BIC"))
```

9 / 20

BIC plot for model selection



10 / 20

Best candidates of model assumptions by BIC

```
summary(mclustBIC(banknote[,2:7]))
```

Best BIC values:

VVE,3 VEE,4 VEE,3

BIC -1608 -1608.768 -1608.79

BIC diff 0 -1.194 -1.22

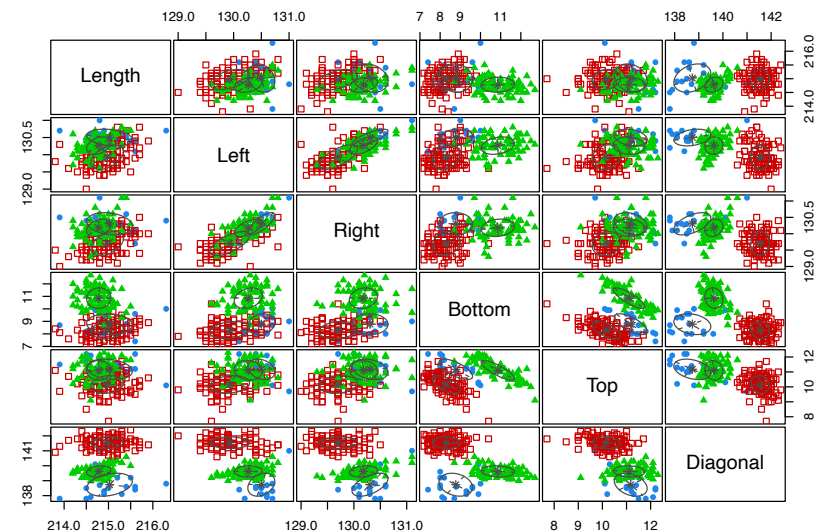
Model types:

- “EEE” = ellipsoidal, equal volume, shape, and orientation
- “EVE” = ellipsoidal, equal volume and orientation
- “VEE” = ellipsoidal, equal shape and orientation
- “VVE” = ellipsoidal, equal orientation

##?mclustModelNames # for model name definitions

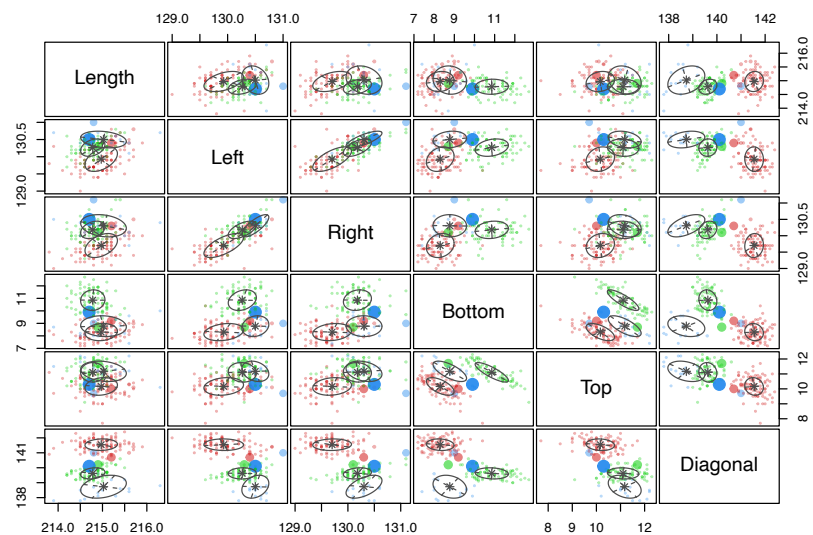
11 / 20

```
plot(mbank, what=c("classification")) # => k=3 selected
```



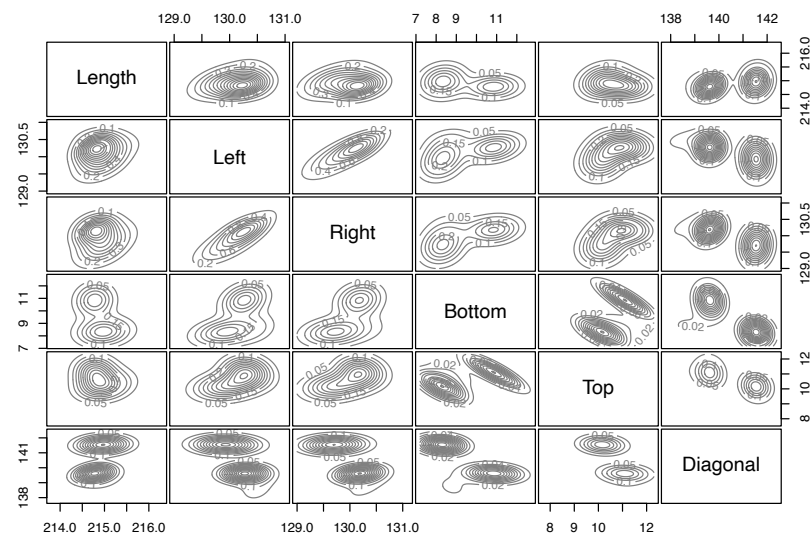
12 / 20

```
plot(mbank, what=c("uncertainty"))
```



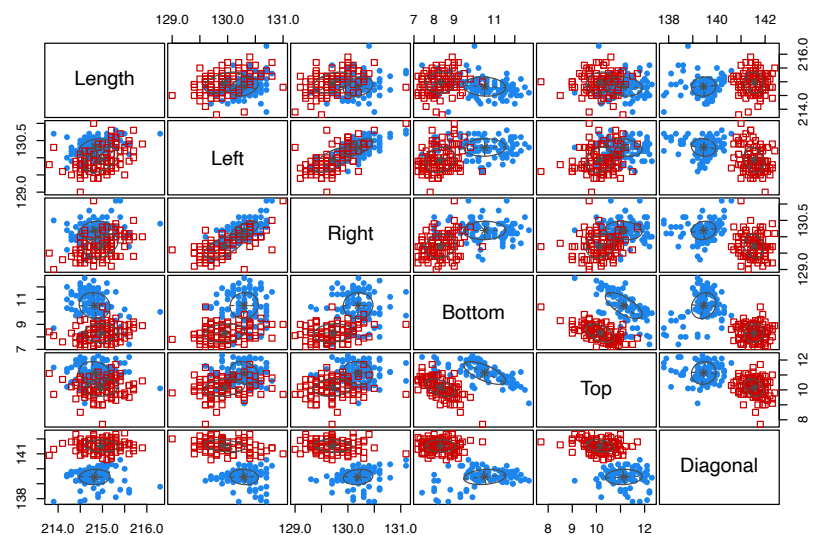
13 / 20

```
plot(mbank, what=c("density")) # 3 clusters
```



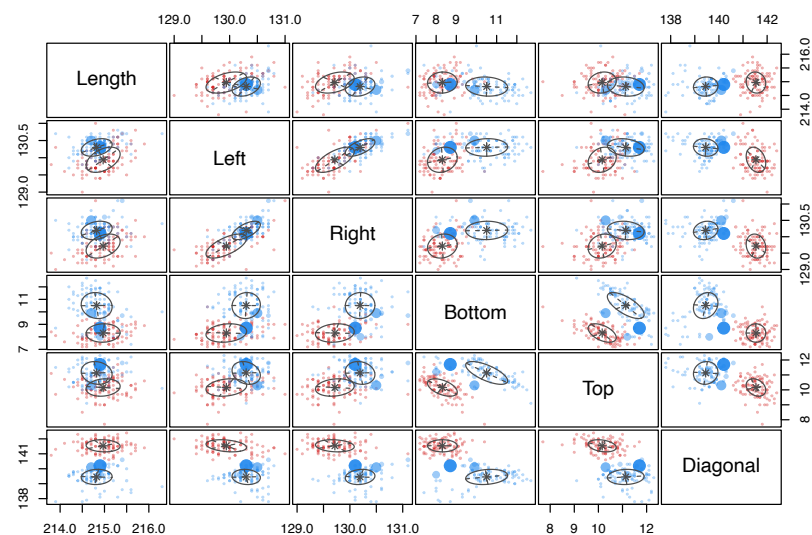
14 / 20

```
bank2=Mclust(banknote[,2:7],G=2) # force k=2
plot(bank2, what = c("classification"))
```



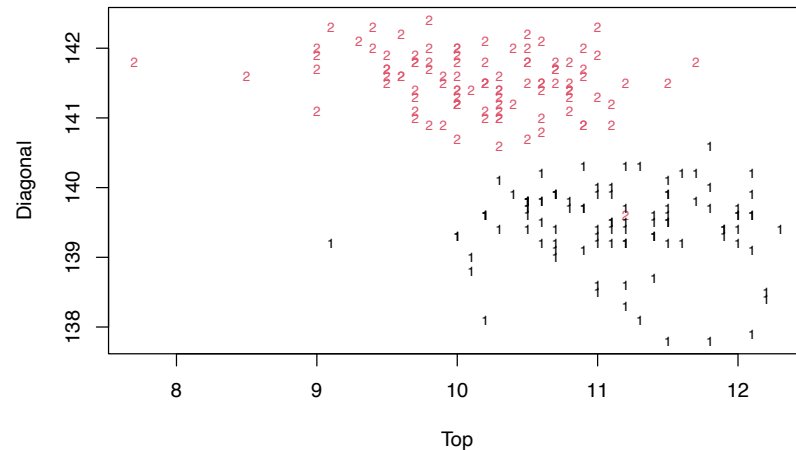
15 / 20

```
plot(bank2, what = c("uncertainty"))
```



16 / 20

```
par(mfrow=c(1,1))
plot(banknote[,6:7],type="n")
text(banknote[,6:7],label=as.numeric(banknote[,1]),
     col=as.numeric(banknote[,1]),cex=.7,lwd=2)
```



17 / 20

Fix number of mixtures $k = 2$

```
summary(Mclust(banknote[,2:7], G=2))
```

```
## -----
## Gaussian finite mixture model fitted by EM algorithm
## -----
##
## Mclust EVE (ellipsoidal, equal volume and orientation) r
##
## log-likelihood    n df    BIC    ICL
##               -755.4 200 39 -1717 -1717
##
## Clustering table:
##    1  2
## 101  99
```

18 / 20

Model assumptions for $k = 2$ mixtures

```
summary(mclustBIC(banknote[,2:7],G=2))
```

```
## Best BIC values:
##           EVE,2      VVE,2      EEV,2
## BIC        -1717 -1721.311 -1745.84
## BIC diff      0      -3.867  -28.39
```

- “EVE” = ellipsoidal, equal volume and orientation
- “VEE” = ellipsoidal, equal shape and orientation
- “EEV” = ellipsoidal, equal volume and equal shape

19 / 20

Estimated mixture proportions (for $k = 2, 3$)

For $k = 2$

```
Mclust(banknote[,2:7], G=2)$parameters$pro
```

```
## [1] 0.5049 0.4951
```

For $k = 3$

```
Mclust(banknote[,2:7])$parameters$pro
```

```
## [1] 0.08988 0.49005 0.42006
```

```
#summary(Mclust(banknote[,2:7]), parameters=T)
```

20 / 20