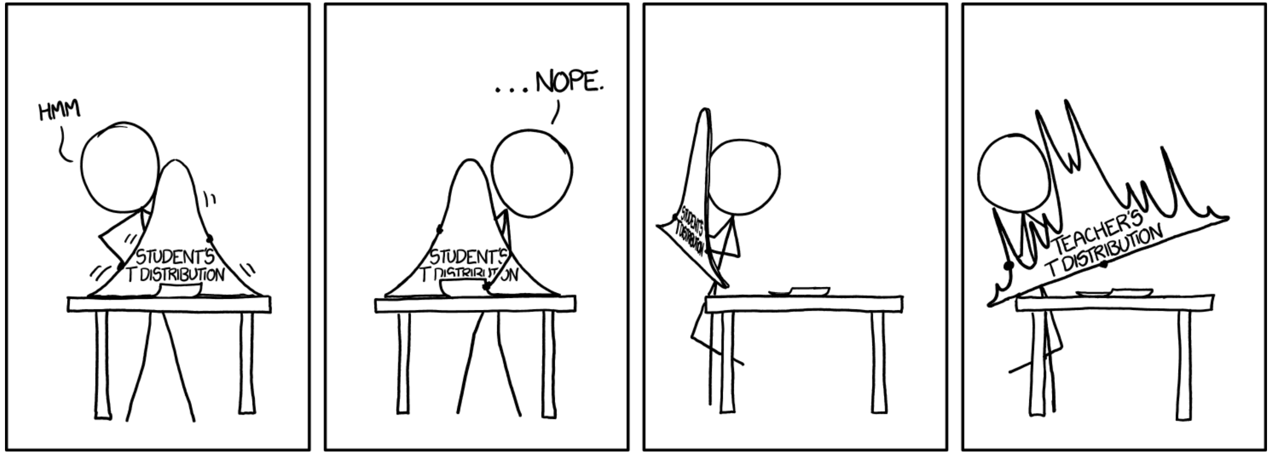
Model-based clustering

Gaussian mixture models

June 15th, 2023

Previously...

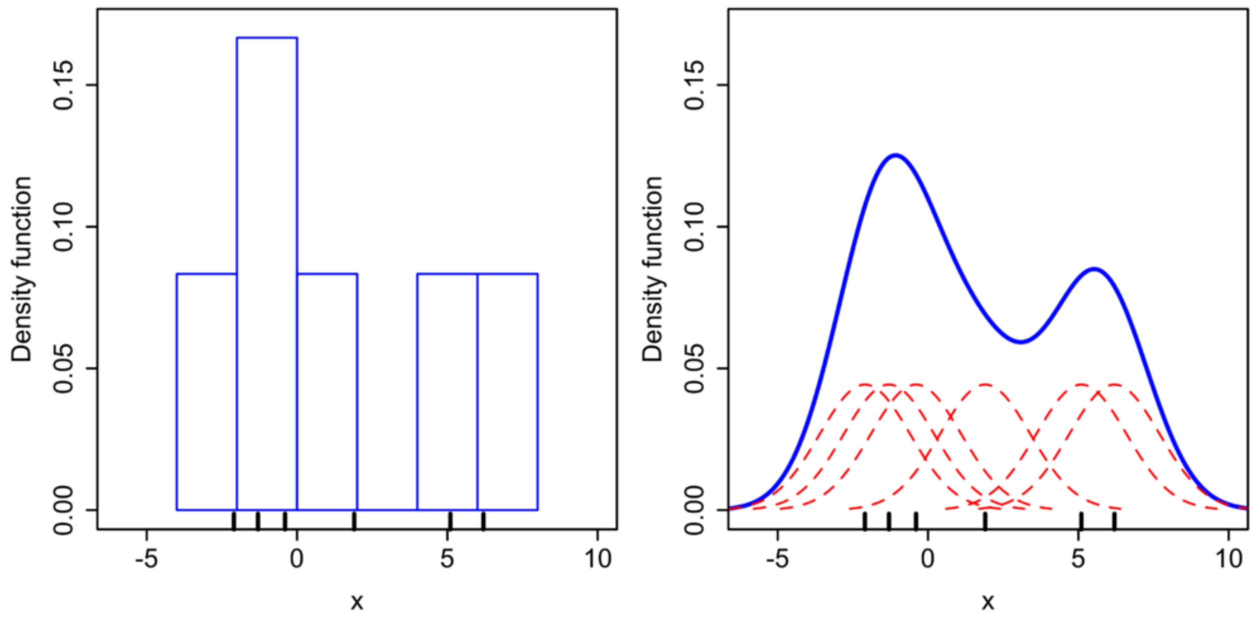
- We explored the use of **K-means** and **hierarchical clustering** for clustering
- These methods yield **hard** assignments, strictly assigning observations to only one cluster
- What about **soft** assignments? Allow for some **uncertainty** in the clustering results
- Welcome to the wonderful world of **mixture models**



Previously in kernel density estimation...

$$\text{Kernel density estimate: } \hat{f}(x) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{h}K_h(x - x_i)$$

- We have to use **every observation** when estimating the density for new points



- Instead we can make **assumptions** to "simplify" the problem

Mixture models

We assume the distribution $f(x)$ is a **mixture** of K **component** distributions:

$$f(x) = \sum_{k=1}^{K} \pi_k f_k(x)$$

- $\pi_k =$ **mixing proportions (or weights)**, where $\pi_k > 0$, and $\sum_k \pi_k = 1$

This is a **data generating process**, meaning to generate a new point:

1. **pick a distribution / component** among our K options, by introducing a new variable:
    - $z \sim \text{Multinomial}(\pi_1, \pi_2, \ldots, \pi_k)$, i.e. categorical variable saying which group the new point is from
2. **generate an observation with that distribution / component**, i.e. $x|z \sim f_z$

So what do we use for each f_k?

Gaussian mixture models (GMMs)

Assume a **parametric mixture model**, with **parameters** θ_k for the kth component

$$f(x) = \sum_{k=1}^{K} \pi_k f_k(x; \theta_k)$$

Assume each component is Gaussian / Normal where for 1D case:

$$f_k(x; \theta_k) = N(x; \mu_k, \sigma_k^2) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\Big(-\frac{(x - \mu_k)^2}{2\sigma_k^2} \Big)$$

We need to estimate each $\pi_1, \ldots, \pi_k$, $\mu_1, \ldots, \mu_k$, $\sigma_1, \ldots, \sigma_k$!

Let's pretend we only have one component...

If we have n observations from a single Normal distribution, we estimate the distribution parameters using the **likelihood function**, the probability / density of observing the data given the parameters

$$\mathcal{L}(\mu, \sigma | x_1, \ldots, x_n) = f(x_1, \ldots, x_n | \mu, \sigma) = \prod_i^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp \ - \frac{(x_i - \mu)^2}{2\sigma^2}$$

We can compute the **maximum likelihood estimates (MLEs)** for μ and σ

You already know these values!

- $\hat{\mu}_{MLE} = \frac{1}{n} \sum_i^n x_i$, sample mean
- $\hat{\sigma}_{MLE} = \sqrt{\frac{1}{n} \sum_i^n (x_i - \mu)^2}$, sample standard deviation (plug in $\hat{\mu}_{MLE}$)

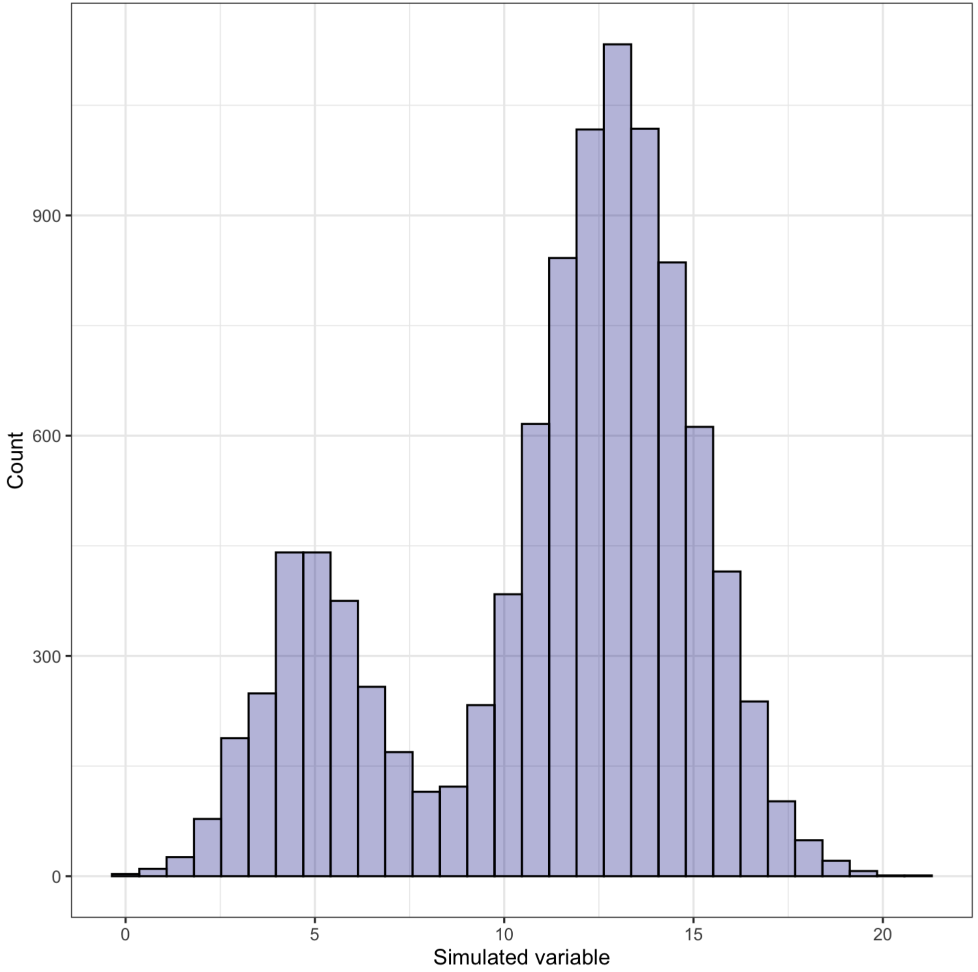
The problem with more than one component...

- **We don't know which component an observation belongs to**
- **IF WE DID KNOW**, then we could compute each component's MLEs as before
- But we don't know because z is a **latent variable**! So what about its distribution given the data?

$$P(z_i = k|x_i) = \frac{P(x_i|z_i = k)P(z_i = k)}{P(x_i)}$$

$$= \frac{\pi_k N\left(\mu_k, \sigma_k^2\right)}{\sum_{k=1}^{K} \pi_k N\left(\mu_k, \sigma_k\right)}$$

- **But we do NOT know these parameters!**
- This leads to a very useful algorithm in statistics...



Expectation-maximization (EM) algorithm

We alternate between the following:

- *pretending* to know the probability each observation belongs to each group, to estimate the parameters of the components
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Where have you seen this before? K-means algorithm!

1. Start with initial guesses about $\pi_1, \ldots, \pi_k$, $\mu_1, \ldots, \mu_k$, $\sigma_1, \ldots, \sigma_k$
2. Repeat until nothing changes:

- **Expectation** step: calculate $\hat{z}_{ik}$ = expected membership of observation i in cluster k
- **Maximization** step: update parameter estimates with **weighted** MLE using $\hat{z}_{ik}$

How does this relate back to clustering?

From the EM algorithm: $\hat{z}_{ik}$ is a **soft membership** of observation i in cluster k

- you can assign observation i to a cluster with the largest $\hat{z}_{ik}$
- measure cluster assignment **uncertainty** $= 1 - \text{max}_k \hat{z}_{ik}$

Our parameters determine the type of clusters

In 1D we only have two options:

1. each cluster **is assumed to have equal variance** (spread): $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2$
2. each cluster **is allowed to have a different variance**

But that is only 1D... what happens in multiple dimensions?

Multivariate GMMs

$$f(x) = \sum_{k=1}^{K} \pi_k f_k(x; \theta_k)$$
$$\text{where } f_k(x; \theta_k) \sim N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Each component is a **multivariate normal distribution**:

- $\boldsymbol{\mu}_k$ is a *vector* of means in p dimensions
- $\boldsymbol{\Sigma}_k$ is the $p \times p$ **covariance** matrix - describes the joint variability between pairs of variables

$$\sum = \begin{bmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,p} \\ \sigma_{2,1} & \sigma_2^2 & \cdots & \sigma_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p,1} & \sigma_{p,2}^2 & \cdots & \sigma_p^2 \end{bmatrix}$$

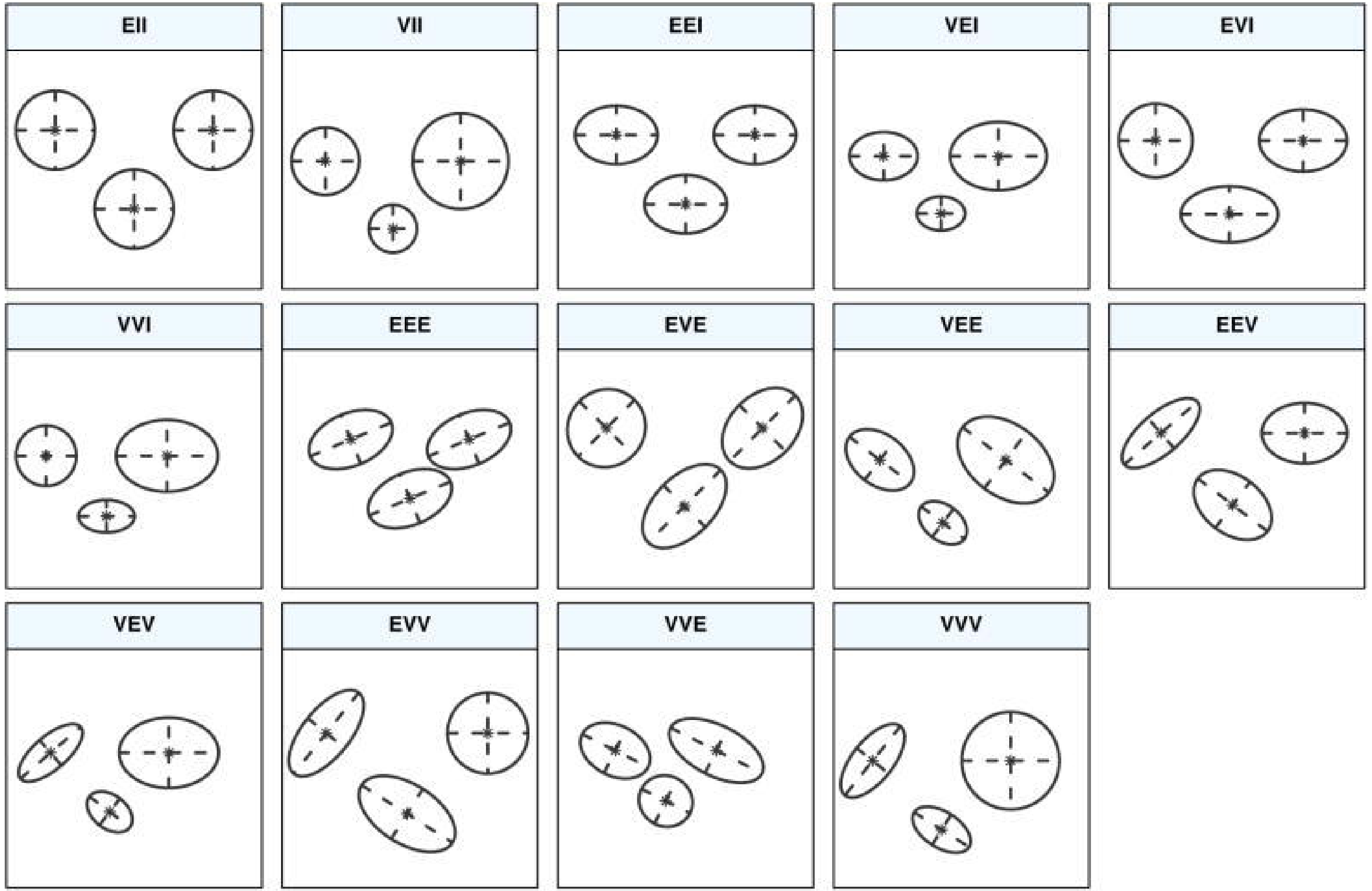
Covariance constraints

$$\sum = \begin{bmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,p} \\ \sigma_{2,1} & \sigma_2^2 & \cdots & \sigma_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p,1} & \sigma_{p,2}^2 & \cdots & \sigma_p^2 \end{bmatrix}$$

As we increase the number of dimensions, model fitting and estimation becomes increasingly difficult

We can use **constraints** on multiple aspects of the k covariance matrices:

- **volume**: size of the clusters, i.e., number of observations,
- **shape**: direction of variance, i.e. which variables display more variance
- **orientation**: aligned with axes (low covariance) versus tilted (due to relationships between variables)



- Control volume, shape, orientation
- **E** means equal and **V** means variable (*VVV* is the most flexible, but has the most parameters)
- Two II is **spherical**, one I is **diagonal**, and the remaining are **general**

So many options! How do we know what to do?

Bayesian information criterion (BIC)

This is a statistical model

$$f(x) = \sum_{k=1}^{K} \pi_k f_k(x; \theta_k)$$

$$\text{where } f_k(x; \theta_k) \sim N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Meaning we can use a **model selection** procedure for determining which best characterizes the data

Specifically - we will use a **penalized likelihood** measure

$$BIC = 2 \log \mathcal{L} - m \log n$$

- $\log \mathcal{L}$ is the log-likelihood of the considered model
- with m parameters (*VVV* has the most parameters) and n observations
- **penalizes** large models with **many clusters without constraints**
- **we can use BIC to choose the covariance constraints AND number of clusters K!**

The above BIC is really the -BIC of what you typically see, this sign flip is just for ease

Mixture model for NBA players... New dataset!

Created dataset of NBA player statistics per 100 possessions using `ballr`

```r
library(tidyverse)
nba_pos_stats <-
  read_csv("https://shorturl.at/mFGY2")
# Find rows for players indicating a full season worth of stats
tot_players <- nba_pos_stats %>% filter(tm == "TOT")
# Stack this dataset with players that played on just one team
nba_player_stats <- nba_pos_stats %>%
  filter(!(player %in% tot_players$player)) %>%
  bind_rows(tot_players)
# Filter to only players with at least 125 minutes played
nba_filtered_stats <- nba_player_stats %>% filter(mp >= 125)
head(nba_filtered_stats)
```

```
## # A tibble: 6 × 31
##   player      pos     age tm        g    gs    mp    fg   fga fgper…¹  x3p  x3pa
##   <chr>       <chr> <dbl> <chr> <dbl> <dbl> <dbl> <dbl> <dbl>   <dbl> <dbl> <dbl>
## 1 Precious …  C        22 TOR      73    28  1725   7.7  17.5   0.439   1.6   4.5
## 2 Steven Ad…  C        28 MEM      76    75  1999   5     9.2   0.547   0     0
## 3 Bam Adeba…  C        24 MIA      56    56  1825  11.1  20     0.557   0     0.2
## 4 Santi Ald…  PF       21 MEM      32     0   360   7    17.5   0.402   0.8   6.4
## 5 LaMarcus …  C        36 BRK      47    12  1050  11.6  21.1   0.55    0.6   2.1
## 6 Grayson A…  SG       26 MIL      66    61  1805   6.8  15.1   0.448   4.2  10.4
```

Gaussian Mixture Models with `mclust`

Use the `Mclust` function to search over 1 to 9 clusters (K = `G`) and the different covariance constraints (i.e. models)

```
library(mclust)
nba_mclust <- Mclust(dplyr::select(nba_filtered_stats, x3pa, trb))
```

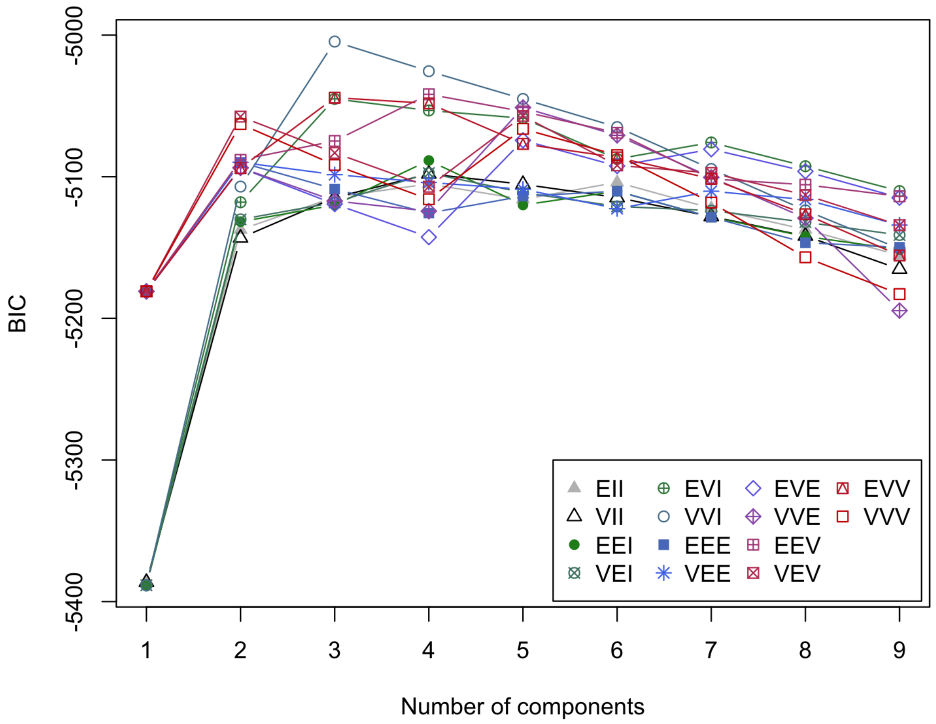
We can use the `summary()` function to display the selection and resulting table of assignments:

```
summary(nba_mclust)
```

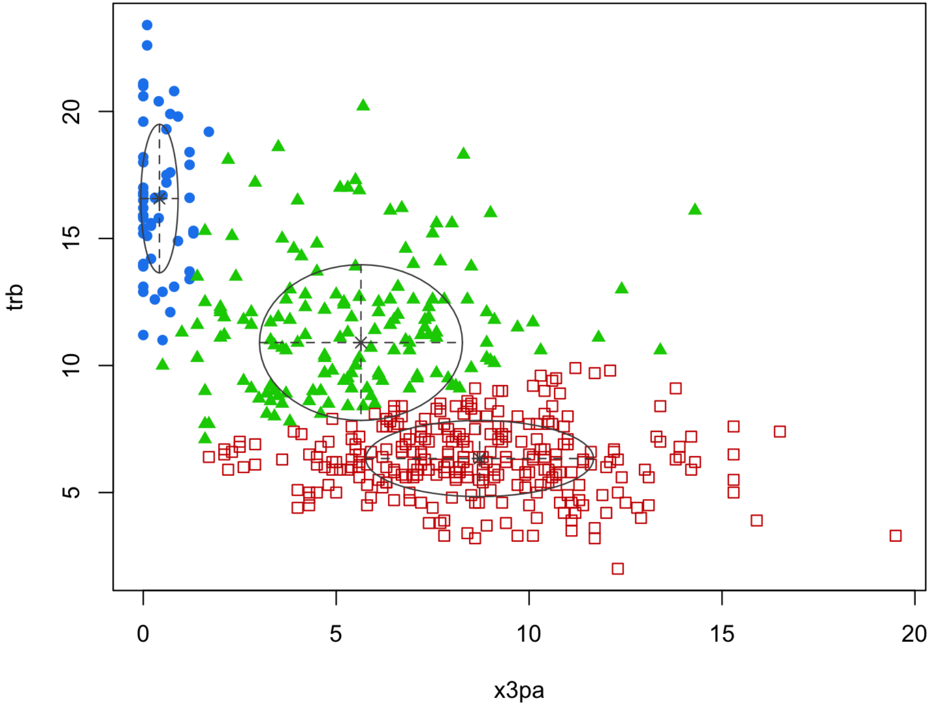
```
## ----------------------------------------------------
## Gaussian finite mixture model fitted by EM algorithm
## ----------------------------------------------------
##
## Mclust VVI (diagonal, varying volume and shape) model with 3 components:
##
##  log-likelihood   n df       BIC       ICL
##        -2459.03 483 14 -5004.581 -5141.138
##
## Clustering table:
##   1   2   3
##  52 276 155
```

Display the BIC for each model and number of clusters

```r
plot(nba_mclust, what = 'BIC',
     legendArgs = list(x = "bottomright",
                       ncol = 4))
```




```r
plot(nba_mclust, what = 'classification')
```



How do the cluster assignments compare to the positions?

We can again compare the clustering assignments with player positions:

```
table("Clusters" = nba_mclust$classification, "Positions" = nba_filtered_stats$pos)
```

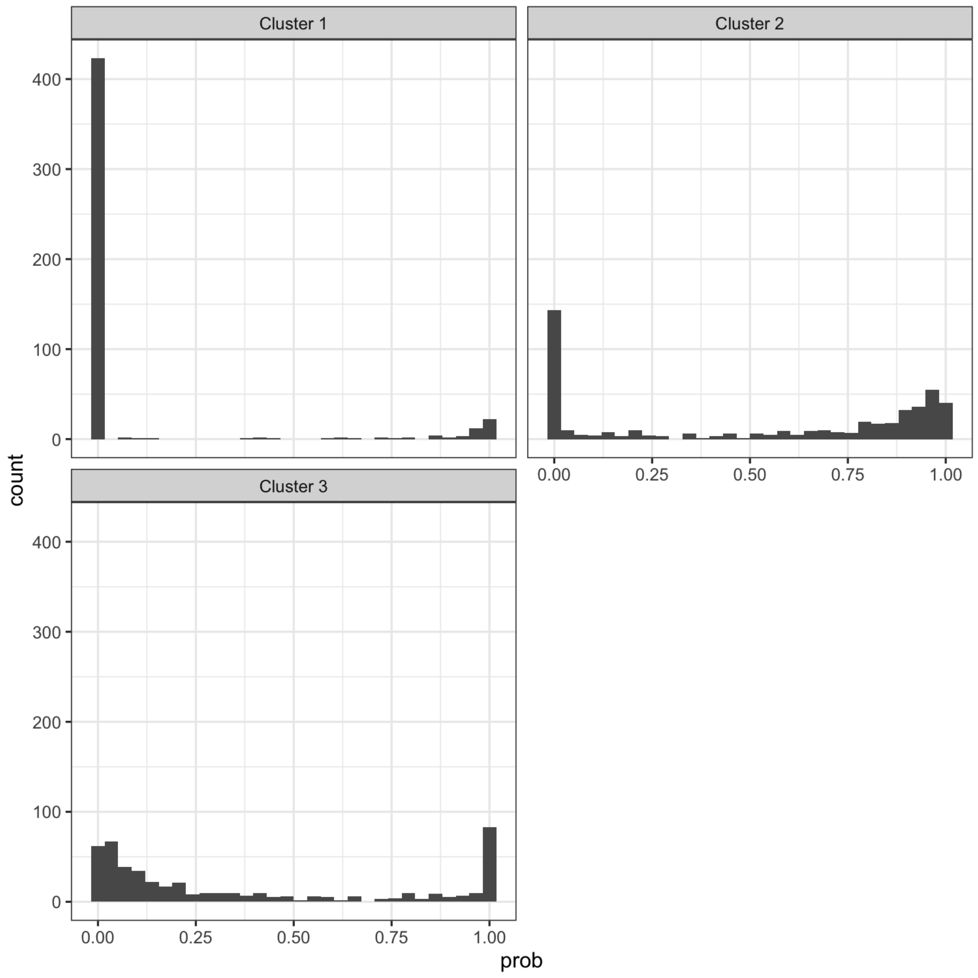
```
##          Positions
## Clusters  C C-PF PF PF-SF PG PG-SG SF SF-SG SG SG-PG SG-SF
##        1 43    0  9     0  0     0  0     0  0     0     0
##        2  3    0 28     0 84     0 54     5 96     3     3
##        3 39    2 56     1  8     1 38     0  9     0     1
```

What about the cluster probabilities?

```r
nba_player_probs <- nba_mclust$z
colnames(nba_player_probs) <-
  paste0('Cluster ', 1:3)

nba_player_probs <- nba_player_probs %>%
  as_tibble() %>%
  mutate(player =
           nba_filtered_stats$player) %>%
  pivot_longer(contains("Cluster"),
               names_to = "cluster",
               values_to = "prob")

nba_player_probs %>%
  ggplot(aes(prob)) +
  geom_histogram() +
  theme_bw() +
  facet_wrap(~ cluster, nrow = 2)
```



Which players have the highest uncertainty?

```
nba_filtered_stats %>%
  mutate(cluster =
           nba_mclust$classification,
         uncertainty =
           nba_mclust$uncertainty) %>%
  group_by(cluster) %>%
  arrange(desc(uncertainty)) %>%
  slice(1:5) %>%
  ggplot(aes(y = uncertainty,
             x = reorder(player,
                         uncertainty))) +
  geom_point() +
  coord_flip() +
  theme_bw() +
  facet_wrap(~ cluster,
             scales = 'free_y', nrow = 3)
```