Homework Model-Based Statistical Learning

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Your report must be a pdf, a jupyter notebook, or a R markdown.

In this Notebook, we will implement the EM algorithm and the KMeans algorithm, compare them and adapt to higher dimensional cases.

I - Introduction

Tasks

1 - Implementing the EM

- Implement (from scratch) the EM for a GMM on the variables 2 and 4 of the wine data set. Cluster the data and compare your results with k-means.
- An R file called `useful_functions.R` (**renamed `utils.R`**) can be useful for EM. Apart from that, try not to use packages to implement EM.
- To assess the quality of the clustering, you may use the function classError and/or adjustedRandIndex from the Mclust package.

2 - Model selection

- Try to find a relevant number of clusters using the three methods seen in class: AIC, BIC, and (cross-)validated likelihood.

3 - Towards higher dimensional spaces

- Try to model more than just two variables of the same data set. Do you find the same clusters, the same number of clusters.

Imports

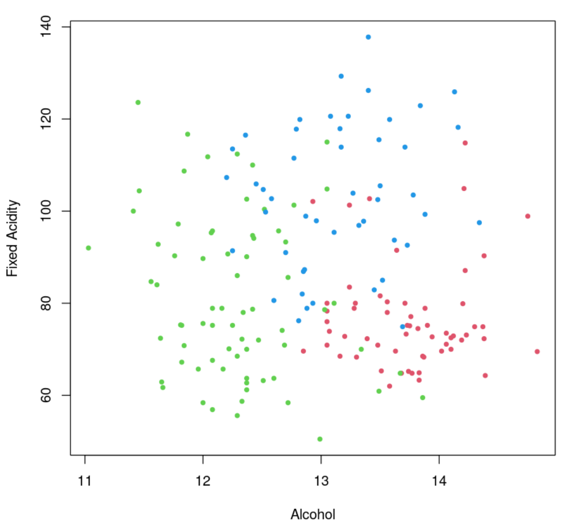
In [ ]:
```
library(pgmm)
library(mvtnorm)
library(mclust)
library(ggplot2)
```

Load & explore slightly the data

In [ ]:
```
# Import data
data(wine)


X <- as.matrix(wine[, c(2, 4)])
y <- wine[, 1]

cat("X has", nrow(X), "rows and", ncol(X), "cols:", paste(colnames(X), collapse = " and "))
```

```
X has 178 rows and 2 cols: Alcohol and Fixed Acidity
```

In [ ]:
```
# Basic visualization
plot(X, col = y + 1, pch = 20)
```



Train/test split

In order to evaluate the algorithm, we need to train it on some data and measure its performances on other, unseen, data.

In [ ]:
```
# We use the indices to randomize the dataset
randomized_indexes <- sample(1:nrow(X))
randomized_X <- X[randomized_indexes, ]
randomized_y <- y[randomized_indexes]


n <- dim(X)[1]
training_split <- round(0.7 * n, 0)

X_train <- randomized_X[1:training_split, ]
X_test <- randomized_X[(training_split + 1):n, ]
y_train <- randomized_y[1:training_split]
y_test <- randomized_y[(training_split + 1):n]
```

II - Declare functions

The following functions will be used through the whole document. They are clustered under different sections.

Utility functions

In [ ]:
```
euclidian_distance <- function(x, centroid) {
  # Compute the euclidian distance between a point and a centroid.

  # Declare intermediary functions for computing the euclidian distance
  dist <- function(a, b) (a - b)^2
  norm <- function(a) sqrt(sum(mapply(dist, a, centroid)))

  # Compute the distances
  distances <- t(apply(x, 1, norm))

  return(distances)
}

find_closest_centroids <- function(x, centroids, clusters) {
  # For each datapoint, compute the closest centroid

  # Initialize variables
  n <- dim(x)[1]
  distances <- c()

  # Compute euclidian distances
  for (cluster in 1:clusters) {
    cluster_dist <- euclidian_distance(x, centroids[cluster, ])
    distances <- append(distances, cluster_dist)
  }
  distances <- array(distances, dim = c(n, clusters))

  # Find closest centroid
  closest <- (distances == apply(distances, 1, min))

  return(list("distances" = distances, "closest" = closest))
}

find_clusters <- function(likelihoods) {
  # Given a 2D-array of likelihood values (likelihood of a point belonging to
  # a cluster), return the most likely cluster.

  clustering <- apply((likelihoods == apply(likelihoods, 1, max)), 1, which)

  return(clustering)
}

generate_centroid <- function(x) {
  # Generate random centroids from a multivariate normal distribution,
  # based on data mean and covariance

  # Variable initialization
  centroid <- c()

  # Randomly draws a value for each dimension of the dataset
  centroid <- rmvnorm(1, colMeans(x), cov(x))
  colnames(centroid) <- NULL

  return(centroid)
}

log_likelihood <- function(n, clusters, x, prop, mu, sigma) {
  # Compute the gamma values of a dataset as part of an EM algorithm.

  # Variable initialization
```

```
  lgn <- matrix(nrow = n, ncol = clusters)

  # Computes the gammas per clusters
  for (cluster in 1:clusters) {
    log_proba <- matrix(dmvnorm(x, mu[cluster, ], sigma[[cluster]], log = TRUE))
    lgn[, cluster] <- log(prop[cluster]) + log_proba
  }

  return(lgn)
}

log_sum_exp <- function(x) {
  # Compute the log-sum-exponential of a vector/list of variables.

  max(x) + log(sum(exp(x - max(x))))
}

most_matching_distribution <- function(clusters, x, prop, mu, sigma) {
  # Given a set of test points, find the best matching distributions.

  # Computes the likelihood of belonging to a distribution
  likelihoods <- log_likelihood(dim(x)[1], clusters, x, prop, mu, sigma)
  clustering <- find_clusters(likelihoods)

  return(list("likelihoods" = likelihoods, "clustering" = clustering))
}
```

KMeans

In [ ]:
```
k_means <- function(x, clusters, max_iterations = 200, debug = T) {
  # Implementation of a K-Means algorithm.

  if (debug) {
    cat("Performing KM-Means with", clusters, "cluster(s).")
  }

  # Set variables for the dimension of data
  n <- dim(x)[1]
  K <- dim(x)[2]

  # Initialize variables
  centroids <- t(lapply(1:clusters, function(i) generate_centroid(x)))
  centroids <- matrix(unlist(centroids), ncol = K, byrow = TRUE)
  history_centroids <- c(centroids)

  # KM loop
  for (loop in 1:max_iterations) {

    # Compute the current closest centroids for each datapoint
    closest_centroids <- find_closest_centroids(x, centroids, clusters)

    # Update the closest centroids
    centroids <- c()
    for (cluster in 1:clusters) {
      # Check if ==2, to prevent colMeans crashes
      if (length(x[closest_centroids$closest[, cluster], ]) == 2) {
        column_means <- x[closest_centroids$closest[, cluster], ]
      } else {
        column_means <- colMeans(x[closest_centroids$closest[, cluster], ])
      }
      centroids <- rbind(centroids, column_means)
    }

    # Erase the matrix's columns and rows names coming from the dataset
    colnames(centroids) <- NULL
    rownames(centroids) <- NULL

    # Record the loop's update
    history_centroids <- append(history_centroids, centroids)
  }

  ret <- list(
    "centroids" = centroids,
    "distances" = closest_centroids$distances,
    "closest_centroids" = apply(closest_centroids$closest, 1, which),
    "centroids_history" = history_centroids
  )
  return(ret)
}
```

EM algorithm

In [ ]:
```
expectation_maximization <- function(x, clusters, max_iterations = 200,
                                     km_init = F, debug = T) {
  # Implementation of an EM algorithm in high dimension.
```

```r
if (debug) {
  if (km_init) {
    cat("Performing EM with", clusters, "cluster(s), KM initialization.")
  } else {
    cat("Performing EM with", clusters, "cluster(s), random initialization.")
  }
}

# Set variables for dimensions of the input dataset
n <- dim(x)[1]
K <- dim(x)[2]

# Initialize EM parameters. Use KMeans depending on parameter
prop <- rep(1 / clusters, clusters)
if (km_init) {
  mu <- k_means(x, clusters, max_iterations, debug = F)$centroids
} else {
  mu <- rmvnorm(clusters, colMeans(x), cov(x))
}
sigma <- lapply(1:clusters, function(i) cov(x))

# Initialize variables
record_log_lik <- c()
record_prop <- c()
record_mu <- c()
record_sigma <- c()
previous_log_lik <- -Inf
counter <- 0
loop_counter <- 0

# Start EM loop
for (loop in 1:max_iterations) {

  # E-Step (with log-exp trick)
  loop_counter <- loop_counter + 1

  # Compute log-likelihood
  log_lik <- log_likelihood(n, clusters, x, prop, mu, sigma)
  sum_log_lik <- sum(apply(log_lik, 1, log_sum_exp))

  # Implement early stopping after 5 rounds without improvement
  if (round(sum_log_lik, 4) <= round(previous_log_lik, 4)) {
    counter <- counter + 1
    if (counter >= 5) {
      if (debug) {
        cat("\nEarly stopping at loop:", loop)
      }
      break
    }
  } else {
    counter <- 0
    previous_log_lik <- sum_log_lik
  }

  # Record the current log_lik to plot later
  record_log_lik <- append(record_log_lik, sum_log_lik)

  # Compute the gamma values per datapoints and clusters with the log-exp trick
  gam <- exp(log_lik - apply(log_lik, 1, log_sum_exp))

  # M-Step
  # Update the parameters
  for (cluster in 1:clusters) {

    # Compute the sum of gammas and updates the cluster's probabilities
    nk <- sum(gam[, cluster])
    prop[cluster] <- nk / n

    # Update the mean parameters
    mean_compute <- function(i) gam[i, cluster] * x[i, ]
    mu[cluster, ] <- Reduce("+", lapply(1:n, mean_compute)) / nk

    # Update the covariance matrix parameters
    m <- mu[cluster, ]
    sigma_compute <- function(i) gam[i, cluster] * (x[i, ] - m) %*% t(x[i, ] - m)
    sigma[[cluster]] <- Reduce("+", lapply(1:n, sigma_compute)) / nk
  }

  # Record parameter values
  record_prop <- append(record_prop, prop)
  record_mu <- append(record_mu, mu)
  record_sigma <- append(record_sigma, sigma)
}

# Compute the log-likelihood results on the given dataset
log_lik_results <- most_matching_distribution(clusters, x, prop, mu, sigma)
log_lik_sum <- sum(apply(log_lik_results$likelihoods, 1, log_sum_exp))
```

```
  if (debug) {
    cat("\nFinal log-likelihood: ", log_lik_sum)
  }

  # Formatting the record variables
  record_prop <- array(record_prop, c(loop_counter, clusters))
  record_mu <- array(record_mu, c(clusters, K, loop_counter))
  record_sigma <- array(record_sigma, c(clusters, K, K, loop_counter))

  ret <- list(
    "n" = n,
    "n_clusters" = clusters,
    "prop" = prop,
    "means" = mu,
    "sigma" = sigma,
    "clustering" = log_lik_results$clustering,
    "ll_of_points" = log_lik_results$likelihoods,
    "ll_sum" = log_lik_sum,
    "prop_history" = record_prop,
    "means_history" = record_mu,
    "sigma_history" = record_sigma,
    "ll_history" = record_log_lik
  )
  return(ret)
}
```

Akaike Information Criterion

In [ ]:
```
akaike_ic <- function(ll, clusters, K) {
  # Computation of the the Akaike Information Criterion.
  # It is given by:
  # AIC = log-likelihood - eta(M)
  # That is :
  # - the final log-likelihood of a model
  # - minus the number of free scalar parameters in the model
  #   (nb of proportions - 1 for because there is one less degree of freedom)
  # - plus nb of means
  # - plus nb of sigmas
  akaike <- ll - (clusters - 1) + clusters * K + clusters * ((K * (K + 1)) / 2)
  return(akaike)
}

compute_aic <- function(x, max_cluster = max_clusters, print_steps = TRUE) {
  # Compute the AIC of an EM algorithm.

  # Initialize variable
  akaike_results <- c()

  # Loop through nb of clusters to compute the AIC
  for (cluster in min_clusters:max_cluster) {
    EM <- expectation_maximization(x, clusters = cluster, debug = F)
    akaike <- akaike_ic(EM$ll_sum, cluster, dim(x)[2])
    akaike_results <- append(akaike_results, akaike)
    if (print_steps) {
      print(paste("Total LL with ", cluster, " clusters: ", round(akaike, 3)))
    }
  }

  # Print the result
  print(paste(
    "The best AIC result is achieved with ",
    which.max(akaike_results) + 2,
    " clusters."
  ))
}
```

Bayesian Information Criterion

In [ ]:
```
bayesian_ic <- function(ll, clusters, n, K) {
  # Computation of the Bayesian Information Criterion.
  # It is given by:
  # BIC = LL - 1/2*eta(M)*log(n)
  # That is:
  # - the final log-likelihood of a model
  # - minus half the number of free scalar parameters in the model
  #   (nb of proportions-1 as there is 1 less degree of freedom)
  # - plus nb of means + nb of sigmas
  # - times the log of the number of samples

  ll - ((clusters - 1) / 2 + clusters * K + clusters * ((K * (K + 1)) / 2)) * log(n)
}

compute_bic <- function(x, max_cluster = max_clusters, print_steps = TRUE) {
  # Computes the BIC of an EM algorithm.

  # Initialize variable
```

```
  bayesian_results <- c()

  # Loop through nb of clusters to compute the BIC
  for (cluster in min_clusters:max_cluster) {
    EM <- expectation_maximization(x, clusters = cluster, debug = F)
    bayesian <- bayesian_ic(EM$ll_sum, cluster, dim(x)[1], dim(x)[2])
    bayesian_results <- append(bayesian_results, bayesian)
    if (print_steps) {
      print(paste("Total LL with ", cluster, " clusters: ", round(bayesian, 3)))
    }
  }

  # Prints the result
  print(paste(
    "The best BIC result is achieved with ",
    which.max(bayesian_results) + 2,
    " clusters."
  ))
}
```

(Cross-)Validated Likelihood

In [ ]:
```
double_cross_validation <- function(x_train, x_test, folds = 10, max_cl = max_clusters) {
  # Perform double cross-validation, using log-likelihood as the selection criterion.

  # Initialize variables
  n_train <- dim(x_train)[1]
  fold_allocation <- ceiling(seq_along(c(1:n_train)) / (n_train / 10))
  fold_indexes <- split(c(1:n_train), fold_allocation)
  mean_cluster_criteria <- c()

  # Iterate over cluster range
  for (cluster in min_clusters:max_cl) {

    lls <- c()
    best_model <- NULL

    # Iterate over the k-folds
    for (k_fold in fold_indexes) {

      # Set train and val datasets
      x_train_train <- x_train[-k_fold, ]
      x_train_val <- x_train[k_fold, ]

      # Compute EM on current training set
      EM <- expectation_maximization(x_train_train, cluster, debug = F)

      # Compute the LL's on the current validation set
      dists <- most_matching_distribution(
        EM$n_clusters, x_train_val, EM$prop, EM$means, EM$sigma
      )

      # Store the resulting LL
      sum_of_lls <- sum(apply(dists$likelihoods, 1, log_sum_exp))
      lls <- append(lls, sum_of_lls)

      # Update the best model if current is better
      if (is.null(best_model) || sum_of_lls == min(lls)) {
        best_model <- EM
      }
    }

    # Use best model on validation to compute likelihood on test set
    dists <- most_matching_distribution(
      best_model$n_clusters,
      x_test,
      best_model$prop,
      best_model$means,
      best_model$sigma
    )

    # Store log-likelihood
    lls <- append(lls, sum(apply(dists$likelihoods, 1, log_sum_exp)))

    # Store the mean LLs achieved with the current number of clusters
    print(paste(
      "Mean LL achieved with ", cluster, " clusters: ",
      round(mean(lls), 4)
    ))
    mean_cluster_criteria <- append(mean_cluster_criteria, mean(lls))
  }

  # Extract best performing number of clusters
  best_cluster <- which.max(mean_cluster_criteria)
  print(paste(
    "The best result is achieved with ",
    best_cluster + 2,
```

```
  " clusters (using double CV)."
  ))

  return(mean_cluster_criteria)
}
```

Plots

In [ ]:
```
plot_data <- function(x, clustering, mean_clusters,
                      t = "K-Means", xl = "Alcohol", yl = "Fixed Acidity") {
  # Make a scatter plot with ellipses for clusters

  # Formats the input data as a dataframe
  df <- data.frame(x)
  mean_clusters <- data.frame(mean_clusters)
  names(mean_clusters) <- names(df)

  # Formats the clustering labels as factors for coloring
  colors <- as.factor(clustering)

  # Declares the plot
  p <- ggplot(df, aes_string(names(df)[1], names(df)[2], color = colors)) +
    geom_point() +
    stat_ellipse(geom = "polygon", aes(fill = colors), alpha = 0.05) +
    guides(fill = "none") +
    labs(
      color = "Wine Type",
      title = paste("Clustering obtained via", t),
      x = xl, y = yl
    ) +
    geom_point(data = mean_clusters, color = "black")

  return(p)
}
```

Compare algorithms

In this section we compare the following algorithms:

- KMeans
- EM with random initialization
- EM with KMeans initialization

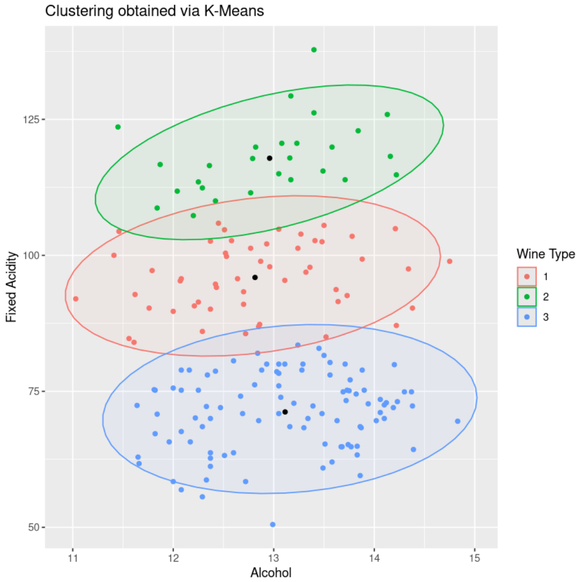
One choice of parameters is the number of clusters, but in this case we can *cheat* as we know that there are 3 clusters in the wine dataset. For this reason, we already set that choice right.

In [ ]:
```
n_clusters <- 3
min_clusters <- length(unique(y))
max_clusters <- 10
```

KMeans with 3 clusters

In [ ]:
```
results_km <- k_means(X, n_clusters)

plot_data(X, results_km$closest_centroids, results_km$centroids)
```

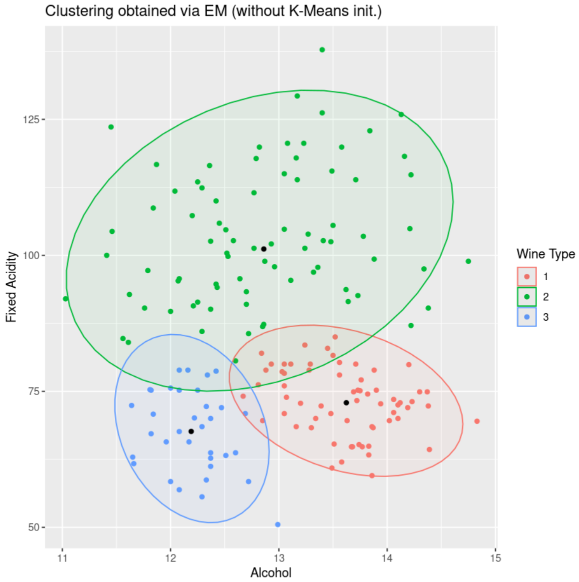
```
Performing KM-Means with 3 cluster(s).
```



EM (random initialization) with 3 clusters

In [ ]:
```
results_em_without_km <- expectation_maximization(X, n_clusters)

plot_data(X, results_em_without_km$clustering, results_em_without_km$means,
  t = "EM (without K-Means init.)"
)
```

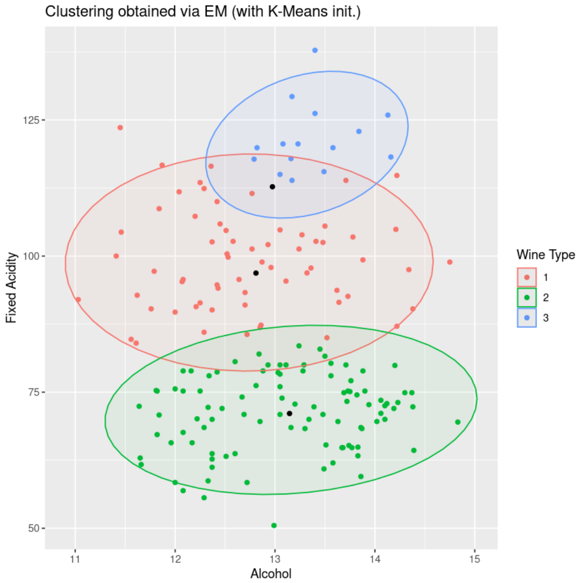
```
Performing EM with 3 cluster(s), random initialization.
Early stopping at loop: 63
Final log-likelihood:  -949.7947
```



EM (KMeans initialization) with 3 clusters

In [ ]:
```
results_em_with_km <- expectation_maximization(X, n_clusters, km_init = T)

plot_data(X, results_em_with_km$clustering, results_em_with_km$means,
  t = "EM (with K-Means init.)"
)
```

```
Performing EM with 3 cluster(s), KM initialization.
Final log-likelihood:  -963.3112
```



Analysis

It seems that KMeans and EM with KMeans exhibit somewhat similar behaviors. One could say that the KMeans initialization influences the EM algorithm. As a result, the clusters look similar.

We cannot precisely say which algorithm performs better, but with respect to the shape of the clusters, it seems that the winner is EM with random initialization. However, we are now clustering the whole dataset. We need to perform a train-test split and see of each algorithm performs.

Split the data

We now split the data into train and test sets before applying each algorithm respectively.

Train on train set

In [ ]:
```
results_train_km <- k_means(X_train, n_clusters)
```

```
Performing KM-Means with 3 cluster(s).
```

In [ ]:
```
results_train_em_without_km <- expectation_maximization(X_train, n_clusters)
```

```
Performing EM with 3 cluster(s), random initialization.
Early stopping at loop: 125
Final log-likelihood:  -663.5038
```

In [ ]:
```
results_train_em_with_km <- expectation_maximization(X_train, n_clusters, km_init = T)
```

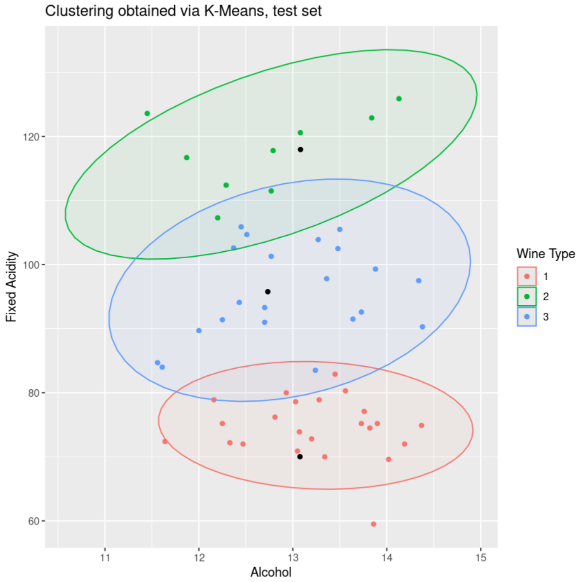
```
Performing EM with 3 cluster(s), KM initialization.
Early stopping at loop: 155
Final log-likelihood:  -672.493
```

Evaluate on test set

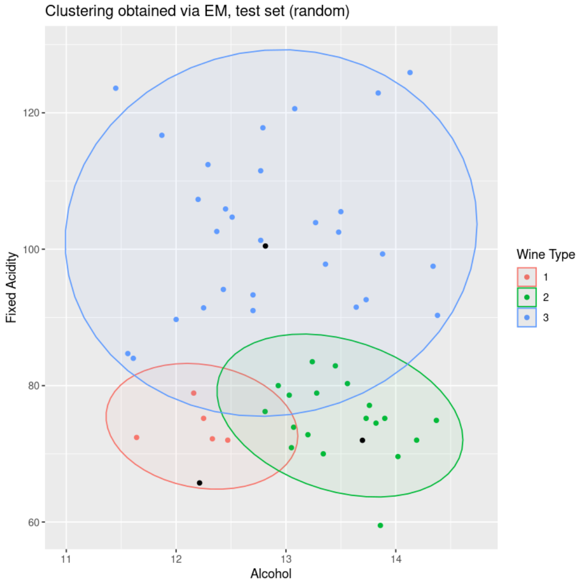
In [ ]:
```
# KM on test set
results_test_km <- find_closest_centroids(
  X_test,
  results_train_km$centroids,
  n_clusters
)
results_test_km$closest <- apply(results_test_km$closest, 1, which)

# EM (random) on test set
results_test_em_without_km <- most_matching_distribution(
  n_clusters,
  X_test,
  results_train_em_without_km$prop,
  results_train_em_without_km$means,
  results_train_em_without_km$sigma
)

# EM (KMeans) on test set
results_test_em_with_km <- most_matching_distribution(
  n_clusters,
  X_test,
  results_train_em_with_km$prop,
  results_train_em_with_km$means,
  results_train_em_with_km$sigma
)
```

Plot clustering on test set

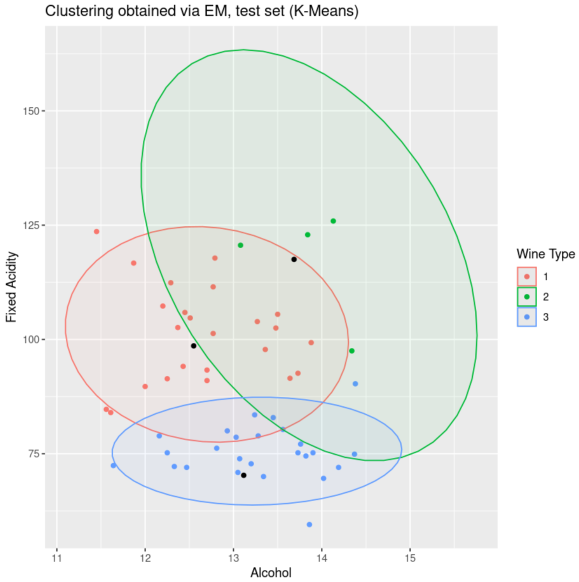
In [ ]:
```
plot_data(X_test, results_test_km$closest, results_train_km$centroids,
  t = "K-Means, test set"
)

plot_data(X_test, results_test_em_without_km$clustering,
  results_train_em_without_km$means,
  t = "EM, test set (random)"
)
plot_data(X_test, results_test_em_with_km$clustering,
  results_train_em_with_km$means,
  t = "EM, test set (K-Means)"
)
```



Clustering obtained via EM, test set (random)



Clustering obtained via EM, test set (K-Means)



Analysis

When splitting the data, we see that KMeans and the random EM still cluster very differently. The Kmeans EM however oscillates (depending on runs) between clusters that are sometimes similar to KMeans, sometimes to the random EM.

Evaluate performance

Using class error on the whole dataset

We now evaluate the performance of each algorithm on the whole dataset. As suggested, we will use the `classError` function from the `mclust` library. It provides the missclasified samples indices, as well as the classification error rate. Both of these values should be as small as possible.

KMeans

In [ ]:
```
classError(results_km$closest_centroid, y)
```

$misclassified 14 · 20 · 22 · 40 · 42 · 44 · 46 · 47 · 57 · 61 · 63 · 64 · 65 · 66 · 67 · 68 · 69 · 71 · 72 · 73 · 74 · 75 · 76 · 77 · 78 · 79 · 81 · 82 · 83 · 85 · 86 · 87 · 88 · 89 · 90 · 91 · 92 · 93 · 96 · 97 · 98 · 99 · 100 · 101 · 102 · 103 · 104 · 105 · 106 · 107 · 109 · 117 · 121 · 123 · 124 · 125 · 130 · 131 · 132 · 133 · 134 · 135 · 136 · 137 · 138 · 140 · 141 · 142 · 143 · 144 · 147 · 148 · 149 · 151 · 153 · 155 · 158 · 159 · 160 · 162 · 163 · 164 · 165 · 166 · 167 · 176

$errorRate 0.48314606741573

EM (random)

In [ ]:
```
classError(results_em_without_km$clustering, y)
```

$misclassified	14 · 20 · 22 · 40 · 42 · 44 · 46 · 47 · 57 · 60 · 62 · 63 · 67 · 69 · 70 · 72 · 73 · 77 · 78 · 80 · 84 · 86 · 94 · 95 · 100 · 108 · 110 · 111 · 112 · 113 · 114 · 115 · 116 · 118 · 119 · 120 · 121 · 122 · 123 · 124 · 125 · 126 · 127 · 128 · 129 · 130 · 132 · 133 · 140 · 141 · 143 · 162 · 167
$errorRate	0.297752808988764

EM (KMeans)

In [ ]:
```
classError(results_em_with_km$clustering, y)
```

$misclassified	14 · 20 · 22 · 40 · 42 · 44 · 46 · 47 · 57 · 61 · 63 · 64 · 65 · 66 · 67 · 68 · 69 · 71 · 72 · 73 · 74 · 75 · 76 · 77 · 79 · 81 · 82 · 83 · 85 · 86 · 87 · 88 · 89 · 90 · 91 · 92 · 93 · 96 · 97 · 98 · 99 · 101 · 102 · 103 · 104 · 105 · 106 · 107 · 109 · 117 · 124 · 131 · 132 · 133 · 134 · 135 · 136 · 137 · 138 · 140 · 141 · 142 · 143 · 144 · 145 · 147 · 148 · 149 · 151 · 153 · 155 · 158 · 159 · 160 · 161 · 162 · 163 · 164 · 165 · 166 · 167 · 171 · 172 · 174 · 176
$errorRate	0.47752808988764

Using class error on the test dataset

We do the same on the test dataset

KMeans

In [ ]:
```
classError(results_test_km$closest, y_test)
```

$misclassified	2 · 4 · 5 · 7 · 9 · 10 · 15 · 19 · 20 · 23 · 27 · 28 · 33 · 36 · 38 · 39 · 41 · 42 · 43 · 45 · 46 · 47 · 50 · 53
$errorRate	0.452830188679245

EM (random)

In [ ]:
```
classError(results_test_em_without_km$clustering, y_test)
```

$misclassified	2 · 4 · 5 · 7 · 15 · 19 · 20 · 23 · 28 · 33 · 36 · 38 · 39 · 43 · 45 · 46 · 50 · 53
$errorRate	0.339622641509434

EM (KMeans)

In [ ]:
```
classError(results_test_em_with_km$clustering, y_test)
```

$misclassified	2 · 4 · 5 · 7 · 9 · 10 · 15 · 19 · 20 · 23 · 27 · 28 · 33 · 36 · 38 · 39 · 41 · 42 · 45 · 46 · 50 · 53
$errorRate	0.415094339622642

Using adjusted rand index on the whole dataset

Now we follow the instruction suggestion to use the adjusted rand index, from the `mclust` library.

KMeans

In [ ]:
```
adjustedRandIndex(results_km$closest_centroid, y)
```

0.156047787516888

EM (random)

In [ ]:
```
adjustedRandIndex(results_em_without_km$clustering, y)
```

0.328568707810203

EM (KMeans)

In [ ]:
```
adjustedRandIndex(results_em_with_km$clustering, y)
```

0.159839732360137

Using adjusted rand index on the test dataset

We do the same on the test dataset

KMeans

In [ ]:
```
adjustedRandIndex(results_test_km$closest, y_test)
```

0.102067698534263

EM (random)

```
In [ ]: adjustedRandIndex(results_test_em_without_km$clustering, y_test)
```

0.260701694365518

EM (KMeans)

```
In [ ]: adjustedRandIndex(results_test_em_with_km$clustering, y_test)
```

0.189653713017949

Analysis

On a given run, we observed the following quantities, summarized in a table. Subsequent runs may produce different quantities.

dataset	algorithm	init.	class error	adjusted rand index
full	KMeans	NA	0.49	0.15
full	EM	random	0.43	0.33
full	EM	KMeans	0.48	0.16
test	KMeans	NA	0.47	0.12
test	EM	random	**0.30**	**0.38**
test	EM	KMeans	0.45	0.13

We notice that EM (both versions) tens to perform better than KMeans. We also note that in this case, random EM perform the best. This seems to generalize over runs, but due to the random nature of the algorithm, these results change from runs to others.

One should note that KMeans EM performing better than KMeans means that performing KMeans, then continuing the iterations with EM steps moves toward a better solution. This means that even after the total number of iterations made KMeans move towards a better solution, EM still manages to move further and end up in a better setting.

Select the best model for EM

```
In [ ]: compute_aic(X)
```

```
[1] "Total LL with  3  clusters:  -950.387"
[1] "Total LL with  4  clusters:  -930.402"
[1] "Total LL with  5  clusters:  -923.578"
[1] "Total LL with  6  clusters:  -911.728"
[1] "Total LL with  7  clusters:  -903.84"
[1] "Total LL with  8  clusters:  -892.903"
[1] "Total LL with  9  clusters:  -883.47"
[1] "Total LL with  10  clusters:  -869.86"
[1] "The best AIC result is achieved with  10  clusters."
```

```
In [ ]: compute_bic(X)
```

```
[1] "Total LL with  3  clusters:  -1032.703"
[1] "Total LL with  4  clusters:  -1055.674"
[1] "Total LL with  5  clusters:  -1084.248"
[1] "Total LL with  6  clusters:  -1100.712"
[1] "Total LL with  7  clusters:  -1128.479"
[1] "Total LL with  8  clusters:  -1146.172"
[1] "Total LL with  9  clusters:  -1176.752"
[1] "Total LL with  10  clusters:  -1190.521"
[1] "The best BIC result is achieved with  3  clusters."
```

```
In [ ]: cv_ll <- double_cross_validation(X_train, X_test)
```

```
[1] "Mean LL achieved with  3  clusters:  -89.9281"
[1] "Mean LL achieved with  4  clusters:  -90.6216"
[1] "Mean LL achieved with  5  clusters:  -90.598"
[1] "Mean LL achieved with  6  clusters:  -91.3853"
[1] "Mean LL achieved with  7  clusters:  -93.2293"
[1] "Mean LL achieved with  8  clusters:  -98.0685"
[1] "Mean LL achieved with  9  clusters:  -101.1479"
[1] "Mean LL achieved with  10  clusters:  -101.1171"
[1] "The best result is achieved with  3  clusters (using double CV)."
```

Analysis

We notice that the AIC consistently favors a greater number of clusters. We use such criteria to prevent always favoring more complex models and over-fitting. It seems that in this case, the AIC does meet this purpose.

We see that the BIC and double CV prefer the 3-clusters parameters, which is what we would hope.

High dimension

Custom selected variables

We now increase the number of dimensions to the problem. For instance, instead of choosing features 2 and 4, we may pick features 2 to 4.

BIC

We compute the BIC on the whole (HD) dataset.

In [ ]:
```
X_hd <- as.matrix(wine[, c(2:4)])
compute_bic(X_hd)
```

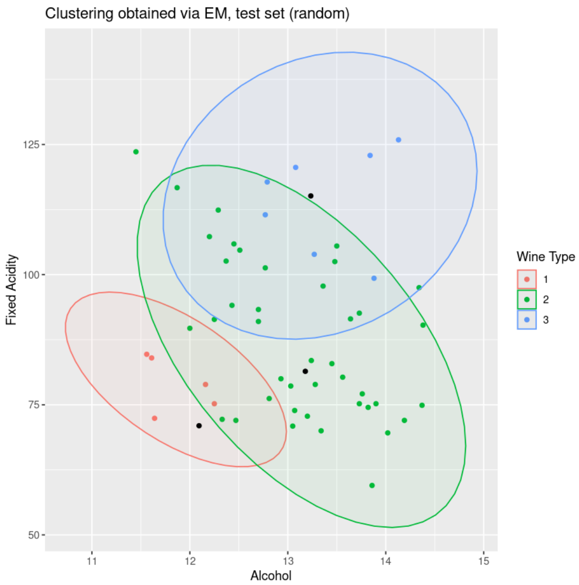
```
[1] "Total LL with  3  clusters:  -1463.336"
[1] "Total LL with  4  clusters:  -1495.003"
[1] "Total LL with  5  clusters:  -1537.936"
[1] "Total LL with  6  clusters:  -1575.815"
[1] "Total LL with  7  clusters:  -1611.598"
[1] "Total LL with  8  clusters:  -1691.438"
[1] "Total LL with  9  clusters:  -1681.928"
[1] "Total LL with  10  clusters:  -1758.377"
[1] "The best BIC result is achieved with  3  clusters."
```

In [ ]:
```
# randomized_indexes same as in low-dim case
randomized_X_hd <- X_hd[randomized_indexes, ]
randomized_y_hd <- y[randomized_indexes]
X_hd_train <- randomized_X_hd[1:training_split, ]
X_hd_test <- randomized_X_hd[(training_split + 1):n, ]
y_hd_train <- randomized_y_hd[1:training_split]
y_hd_test <- randomized_y_hd[(training_split + 1):n]

results_em_hd_train <- expectation_maximization(X_hd_train, 3)

test_results_em_hd <- most_matching_distribution(
  3,
  X_hd_test,
  results_em_hd_train$prop,
  results_em_hd_train$means,
  results_em_hd_train$sigma
)
```

```
Performing EM with 3 cluster(s), random initialization.
Early stopping at loop: 69
Final log-likelihood:  -931.0217
```

Now we plot the obtained results.

In [ ]:
```
plot_data(X_hd_test[, c(1, 3)], test_results_em_hd$clustering,
  results_em_hd_train$means[, c(1, 3)],
  t = "EM, test set (random)"
)
```



We compute the misclassification stats.

In [ ]:
```
classError(test_results_em_hd$clustering, y_hd_test)
```

$misclassified 1 · 2 · 4 · 5 · 7 · 10 · 12 · 15 · 16 · 19 · 20 · 23 · 24 · 25 · 28 · 30 · 34 · 35 · 36 · 38 · 40 · 42 · 45 · 50 · 51 · 53

$errorRate 0.490566037735849

As before, we also compute the adjusted rand index.

In [ ]:
```
adjustedRandIndex(test_results_em_hd$clustering, y_hd_test)
```

0.0411240202194397

Analysis

We are reassured by the fact that even in this tri-dimensional case, the BIC criterion still indicates that 3 clusters is the best possible setting. This is coherent with what we know to be the case and it makes for a nice rationale in our analysis.

Select features at random

In the previous case, we selected features by hand. This is nice because it lets us choose which features we want to use, but we may not know which features to use. It is also interesting to see how random selection of features behaves with EM and BIC. So this is what we will do.

We select a few permutations for several number of number of features. Namely, we extract:

- 5 permutations for the case of 10 features
- 5 permutations for the case of 5 features
- 20 permutations for the case of 4 features
- 20 permutations for the case of 3 features

This brings us to to a total of 50 tries. We will apply EM in each case and see how AIC/BIC behaves for each number of features.

In [ ]:
```r
# Extract the features from the original dataset
wine_features <- subset(wine, select = -c(Type))

# Produce 5 10-element permutations by random sampling
ten_perms <- c()
for (p in 1:5) {
  ten_perms <- rbind(ten_perms, sample(colnames(wine_features), 10))
}

# Produce 5 5-element permutations by random sampling
five_perms <- c()
for (p in 1:5) {
  five_perms <- rbind(five_perms, sample(colnames(wine_features), 5))
}

# Produce the set of 4-element permutations
four_perms <- NULL
for (p in 1:nrow(five_perms)) {
  all <- expand.grid(
    p1 = five_perms[p, ],
    p2 = five_perms[p, ],
    p3 = five_perms[p, ],
    p4 = five_perms[p, ],
    stringsAsFactors = FALSE
  )
  perms <- all[apply(all, 1, function(x) {
    length(unique(x)) == 4
  }), ]
  if (is.null(four_perms)) {
    four_perms <- perms
  } else {
    four_perms <- rbind(four_perms, perms)
  }
}
four_perms <- as.matrix(four_perms)

# Produce the set of 3-element permutations
three_perms <- NULL
for (p in 1:nrow(four_perms)) {
  all <- expand.grid(
    p1 = four_perms[p, ],
    p2 = four_perms[p, ],
    p3 = four_perms[p, ],
    stringsAsFactors = FALSE
  )
  perms <- all[apply(all, 1, function(x) {
    length(unique(x)) == 3
  }), ]
  if (is.null(three_perms)) {
    three_perms <- perms
  } else {
    three_perms <- rbind(three_perms, perms)
  }
}
three_perms <- as.matrix(three_perms)
```

Select model on 10-features models

AIC & BIC

In [ ]:
```r
for (perm in 1:nrow(ten_perms)) {
  cat("\nSelected features: ", paste(ten_perms[perm,], collapse=", "), "\n")
  compute_aic(as.matrix(wine_features[ten_perms[perm,]]), print_steps=FALSE)
  compute_bic(as.matrix(wine_features[ten_perms[perm,]]), print_steps=FALSE)
}
```

```
Selected features:  Uronic Acids, Proline, pH, Alcohol, Chloride, 2-3-Butanediol, Magnesium, Calcium, Total Phenol
s, Glycerol
[1] "The best AIC result is achieved with  7  clusters."
[1] "The best BIC result is achieved with  7  clusters."

Selected features:  Glycerol, Calcium, OD280/OD315 of Flavanoids, Total Phenols, Phosphate, Chloride, Color Intens
ity, Magnesium, Sugar-free Extract, Flavanoids
[1] "The best AIC result is achieved with  10  clusters."
[1] "The best BIC result is achieved with  7  clusters."

Selected features:  Magnesium, pH, OD280/OD315 of Flavanoids, Non-flavanoid Phenols, 2-3-Butanediol, OD280/OD315 o
f Diluted Wines, Fixed Acidity, Proanthocyanins, Total Nitrogen, Glycerol
[1] "The best AIC result is achieved with  8  clusters."
[1] "The best BIC result is achieved with  10  clusters."

Selected features:  Alcalinity of Ash, Total Nitrogen, Calcium, Proline, Flavanoids, pH, Color Intensity, Malic Ac
id, Sugar-free Extract, 2-3-Butanediol
[1] "The best AIC result is achieved with  10  clusters."
[1] "The best BIC result is achieved with  5  clusters."

Selected features:  Methanol, pH, Uronic Acids, Flavanoids, Glycerol, Color Intensity, OD280/OD315 of Flavanoids,
Ash, Tartaric Acid, 2-3-Butanediol
[1] "The best AIC result is achieved with  8  clusters."
[1] "The best BIC result is achieved with  6  clusters."
```

Analysis

As one could have expected, we note that both criteria fail on the high dimensional, 10-features, case as they favor very high number of clusters instead of 3 clusters. We notice however that the BIC performs better than the AIC as it tends to yield lower number of clusters (over multiple runs).

Select model on 5-features models

In [ ]:
```
for (perm in 1:nrow(five_perms)) {
  cat("\nSelected features: ", paste(five_perms[perm,], collapse=", "), "\n")
  compute_aic(as.matrix(wine_features[five_perms[perm,]]), print_steps=FALSE)
  compute_bic(as.matrix(wine_features[five_perms[perm,]]), print_steps=FALSE)
}
```

```
Selected features:  Proline, Potassium, Fixed Acidity, Alcohol, Total Phenols
[1] "The best AIC result is achieved with  10  clusters."
[1] "The best BIC result is achieved with  9  clusters."

Selected features:  Phosphate, Proanthocyanins, Fixed Acidity, Total Nitrogen, Calcium
[1] "The best AIC result is achieved with  6  clusters."
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Potassium, Tartaric Acid, Ash, Methanol, 2-3-Butanediol
[1] "The best AIC result is achieved with  10  clusters."
[1] "The best BIC result is achieved with  10  clusters."

Selected features:  Chloride, Ash, Fixed Acidity, OD280/OD315 of Flavanoids, pH
[1] "The best AIC result is achieved with  6  clusters."
[1] "The best BIC result is achieved with  9  clusters."

Selected features:  Sugar-free Extract, Proline, Hue, OD280/OD315 of Flavanoids, Proanthocyanins
[1] "The best AIC result is achieved with  9  clusters."
[1] "The best BIC result is achieved with  3  clusters."
```

Analysis

We see that is the case of 5 features, the number of clusters lowers a bit for the BIC, while it remains high for the AIC (over multiple runs). This hints that the BIC performs better in this case.

Select model on 4-features models

As we have seen that BIC consistently performs better than AIC on average, we choose to drop AIC. This also comes with a significant increase in runtime, which is appreciated because running EM's on multiple number of clusters multiples out quickly and through combinatorics makes the runtime undoable. Removing AIC (almost) divides this time by 2.

In [ ]:
```
for (perm in sample(1:nrow(four_perms), 20)) {
  cat("\nSelected features: ", paste(four_perms[perm,], collapse=", "), "\n")
  # compute_aic(as.matrix(wine_features[four_perms[perm,]]), print_steps=FALSE)
  compute_bic(as.matrix(wine_features[four_perms[perm,]]), print_steps=FALSE)
}
```

```
Selected features:  Fixed Acidity, OD280/OD315 of Flavanoids, pH, Chloride
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Potassium, Ash, Tartaric Acid, 2-3-Butanediol
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Sugar-free Extract, OD280/OD315 of Flavanoids, Proline, Hue
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Phosphate, Total Nitrogen, Fixed Acidity, Calcium
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Tartaric Acid, Ash, 2-3-Butanediol, Methanol
[1] "The best BIC result is achieved with  9  clusters."

Selected features:  Proline, Total Phenols, Alcohol, Fixed Acidity
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Fixed Acidity, OD280/OD315 of Flavanoids, Ash, pH
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Ash, Methanol, Tartaric Acid, Potassium
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Sugar-free Extract, Hue, OD280/OD315 of Flavanoids, Proline
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Proline, Proanthocyanins, Sugar-free Extract, Hue
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  pH, Fixed Acidity, Chloride, OD280/OD315 of Flavanoids
[1] "The best BIC result is achieved with  7  clusters."

Selected features:  pH, Ash, Chloride, OD280/OD315 of Flavanoids
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  OD280/OD315 of Flavanoids, Proanthocyanins, Sugar-free Extract, Hue
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  OD280/OD315 of Flavanoids, Ash, Chloride, Fixed Acidity
[1] "The best BIC result is achieved with  9  clusters."

Selected features:  Methanol, Potassium, Ash, Tartaric Acid
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Phosphate, Total Nitrogen, Calcium, Proanthocyanins
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Tartaric Acid, Methanol, 2-3-Butanediol, Potassium
[1] "The best BIC result is achieved with  8  clusters."

Selected features:  Tartaric Acid, Methanol, Potassium, 2-3-Butanediol
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  2-3-Butanediol, Tartaric Acid, Methanol, Potassium
[1] "The best BIC result is achieved with  10  clusters."

Selected features:  pH, Fixed Acidity, Ash, OD280/OD315 of Flavanoids
[1] "The best BIC result is achieved with  3  clusters."
```

Analysis

We notice that as we lower the dimension, a greater proportion of the cases run suggest that 3 clusters seems optimal. This validates our hypothesis that EM struggles with high-dimensional, low-quantity data.

Select model on 3-features models

In [ ]:
```
for (perm in sample(1:nrow(three_perms), 20)) {
  cat("\nSelected features: ", paste(three_perms[perm,], collapse=", "), "\n")
  # compute_aic(as.matrix(wine_features[three_perms[perm,]]), print_steps=FALSE)
  compute_bic(as.matrix(wine_features[three_perms[perm,]]), print_steps=FALSE)
}
```

```
Selected features:  Potassium, Alcohol, Proline
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Calcium, Phosphate, Total Nitrogen
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Potassium, Proline, Total Phenols
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Proanthocyanins, Proline, Sugar-free Extract
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Proline, Hue, Sugar-free Extract
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Tartaric Acid, Ash, Potassium
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Potassium, Tartaric Acid, Methanol
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Alcohol, Proline, Total Phenols
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Proline, Total Phenols, Alcohol
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Fixed Acidity, Alcohol, Total Phenols
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  OD280/OD315 of Flavanoids, Sugar-free Extract, Proanthocyanins
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Hue, Sugar-free Extract, Proanthocyanins
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Sugar-free Extract, Hue, OD280/OD315 of Flavanoids
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Methanol, Ash, Potassium
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Fixed Acidity, Total Nitrogen, Phosphate
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Ash, Chloride, OD280/OD315 of Flavanoids
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Fixed Acidity, Ash, pH
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Fixed Acidity, Potassium, Alcohol
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  OD280/OD315 of Flavanoids, Chloride, pH
[1] "The best BIC result is achieved with  3  clusters."

Selected features:  Proanthocyanins, OD280/OD315 of Flavanoids, Proline
[1] "The best BIC result is achieved with  3  clusters."
```

Analysis

Even more than in the previous case, the algorithm suggests 3 clusters as the optimal set up in almost all cases. This reassures us even further and concludes the analysis.

Conclusion

We saw that over multiple cell runs, the performance of EM seems to improve as we remove features from the high dimensional set up. This is true in terms of BIC, but also somewhat in terms of AIC. We saw that in the high dimensional set up, the EM algorithm will favor more clusters and will be unable to make sense of such little information. Given the size of the data at hand, we saw that 2 or 3 features seem to get the closest to the right number of clusters when using the BIC criterion.

As a data scientist in the wild, I would therefore tend to limit my number of features to only the most (very) primordial ones. Depending on the size of the dataset, this may be more than 2 or 3 as it was in this example, but most certainly something like the lower the better.