STAT 610 project: K-Means Clustering

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December 9 2024

https://github.com/jinglong-w-dotcom/stat610project

##Idea: We have n points (vectors), $x_1, ..., x_n$ in $\mathbb{R}^p$, and divide these points into non-empty K clusters (groups), $C_1, ..., C_K$. Our goal is to minimize the within-cluster variation to make the points within each cluster as close to each other as possible. We defines K-means clustering formula as below:

$$\min_{C_1,...,C_K} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

##Algorithm

Basing on the K-means principle, we design the following 5 functions:

- compute_centers: Calculate cluster centroids. The k-th cluster center $\bar{x}_k$ is the average of all the points in the k-th cluster.

$$\bar{x}_k = \frac{1}{|C_k|} \sum_{i \in C_k} x_i$$

- WCSS: Calculate the wihtin-cluster sum of squares to evaluate clustering compactness (where using Euclidean distance to define the "closest"$\sum_{j=1}^{n}(x_{ij} - x_{i'j})^2$). An iteration reduces out total WCSS, as shown below,

$$\begin{aligned}
\sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 &= \sum_{k=1}^{K} 2 \sum_{i \in C_k} (x_i - \bar{x}_k)^2 \text{ step 2(a)} \\
&= 2 \sum_{i=1}^{n} (x_i - \bar{x}_{k(i)})^2 \text{break the cluster, k(i) means xi is in the k(i)-th cluster} \\
&\geq 2 \sum_{i=1}^{n} (x_i - \bar{x}_{kc(i)})^2 \text{step 2(b), xi assigned to its closest cluster} \\
&= \sum_{k=1}^{K} 2 \sum_{i \in C_k'} (x_i - \bar{x}_k)^2
\end{aligned}$$

- k_means: Perform K-Means Clustering

1.Initialize clusters. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.

2.Iterate until the cluster assignments stop changing:

(a)For each of the K clusters, compute the cluster center, using function compute_centers.

(b)Assign each point to the cluster whose center is closest. We use function WCSS to evaluate the distribution.

- K_means_progresses: Visualize clustering progress
- Kmeans_quality_measure: Compare results for different K value

##compute_centers

Input:

- X is the n x m matrix where each row represents a point.
- *labels* is the n x 1 column vector, representing current cluster assignments for each point.
- K is the number of cluster.

Output:

- *centers* is the k x m matrix of centroids.

```r
# Compute centers for each cluster
compute_centers <- function(X, labels, K) {
  centers <- matrix(NA, nrow = K, ncol = ncol(X))  #initialize a NA mateic
  n <- nrow(X)  # number of data points

  for (k in 1:K) {
    # Get the points in cluster k
    cluster_points <- X[labels == k, , drop = FALSE]
    if (nrow(cluster_points) > 0) {
      # Compute the mean for each feature (column)
      centers[k, ] <- colMeans(cluster_points, na.rm = TRUE)
    }else{
      # Reinitialize center for the empty cluster (randomly choose a point from the sample)
      centers[k, ] <- X[sample(1:n, 1), ]
    }
  }
  return(centers)
}
```

##WCSS(Within-Cluster Sum of Squares)

Input:

- X is the n x m matrix where each row represents a point.
- *labels* is the n x 1 column vector, representing current cluster assignments for each point.
- *centers* is the k x m matrix of centroids.

Output:

- *result* is the value of Within-Cluster Sum of Squares

```
# Function to compute Within-Cluster Sum of Squares,
#i.e. double the sum of squared distances from each point
#to the center of its assigned cluster
WCSS <- function(X, labels, centers) {
  n <- nrow(X)  # number of data points
  squared_dist <- numeric(n)  # to store result

  for (i in 1:n) {
    # Get the index of the assigned cluster for point i
    cluster_index <- labels[i]

    # Get the center of the assigned cluster
    center <- centers[cluster_index, ]

    # Compute the distance from point i to its assigned cluster center
    squared_dist[i] <- sum((X[i, ] - center)^2)
  }

  result <- 2 * sum(squared_dist)

  return(result)
}
```

##k_means

Input:

- X is the n x m matrix where each row represents a point.
- K is the number of cluster.
- *initial_clusters* is the initial cluster assignments.
- *max_iters* is maximum iterations allowed.
- *tol* is convergence tolerance.
- *optimal_simu* is the number of simulation runs to find the best result.

Output:

- *centers* and *clusters*: final cluster assignments.
- *optimal_centers* and$ optimal_clusters$: the final cluster assignments in different simulations.
- *list_cluster* and *list_centers*: the each cluster assignments of k-means process.
- $Within - Cluster\_Sum\_of Squares$: the WCSS of each cluster assignments in k-means process.

```
library(animation)
```

```
## Warning: package 'animation' was built under R version 4.4.2
```

```r
k_means <- function(X, K, initial_clusters = NULL, max_iters = 100, tol = 1e-6,
                    optimal_simu = 100) {
  # Number of samples
  n <- nrow(X)
  if(n < K){
    stop("The number of cluster centers is greater than the number of data points.")
  }

  if(nrow(X) == 0 || ncol(X) == 0){
    stop("Input dataset is empty.")
  }

  if(any(is.na(X))){
    stop("Input dataset contains missing values.")
  }

  if(!is.numeric(X)){
    stop("Input dataset contains non-numeric values.")
  }

    total_wcss <- rep(NA, optimal_simu)
    total_labels <- list()
    total_centers <- list()

    #The initial cluster can affect the final result. Running the algorithm multiple times
    #from different random initial configurations, we can select the optimal result, but this
    #optimal result does not mean minimal.
    for (simulation in 1:optimal_simu) {
      total_labels[[simulation]] <- list()
      total_centers[[simulation]] <- list()

      # Initialize centers
      if (is.null(initial_clusters)) {
        # Randomly assign a cluster number to each observation
        initial_clusters <- sample(1:K, size = n, replace = TRUE)
        centers <- compute_centers(X, initial_clusters, K)
        } else {
          centers <- compute_centers(X, initial_clusters, K)
          }

      for (i in 1:max_iters) {
        # Compute distances from each point to the center of its cluster
        distances <- as.matrix(dist(rbind(X, centers)))[1:n, (n+1):(n+K), drop = FALSE]

        # Assign each point to the nearest center
        labels <- apply(distances, 1, which.min)

        #store the data of labels and center points
        total_labels[[simulation]][[i]] <- labels
        total_centers[[simulation]][[i]] <- centers

        #Recompute centers
        new_centers <- compute_centers(X, labels, K)
```

```
        # Check for convergence (if centers do not change much)
        if (sum((new_centers - centers)^2) < tol) {
          break
          }

        centers <- new_centers
        #new_wcss <- WCSS(X, labels, centers)
      }

      total_wcss[simulation] <- WCSS(X, labels, centers)

    }
    index <- which.min(total_wcss)

    list_cluster <- total_labels[[index]]
    list_centers <- total_centers[[index]]

    optimal_clusters <- lapply(total_labels, function(sublist) tail(sublist, 1)[[1]])
    optimal_centers <- lapply(total_centers, function(sublist) tail(sublist, 1)[[1]])

    clusters <- tail(total_labels[[index]], 1)[[1]]
    centers <- tail(total_centers[[index]], 1)[[1]]

    return(list(centers = centers, clusters = clusters,
                optimal_centers = optimal_centers, optimal_clusters = optimal_clusters,
                total_wcss = total_wcss,
                list_cluster = list_cluster, list_centers = list_centers,
                "Within-Cluster Sum of Squares" = total_wcss[index]))
}
```

##K_means_progresses

Input:

- *klist* is the clustering progress data from k_means function.
- X is the n x m matrix where each row represents a point.

Output:

- a animated GIF

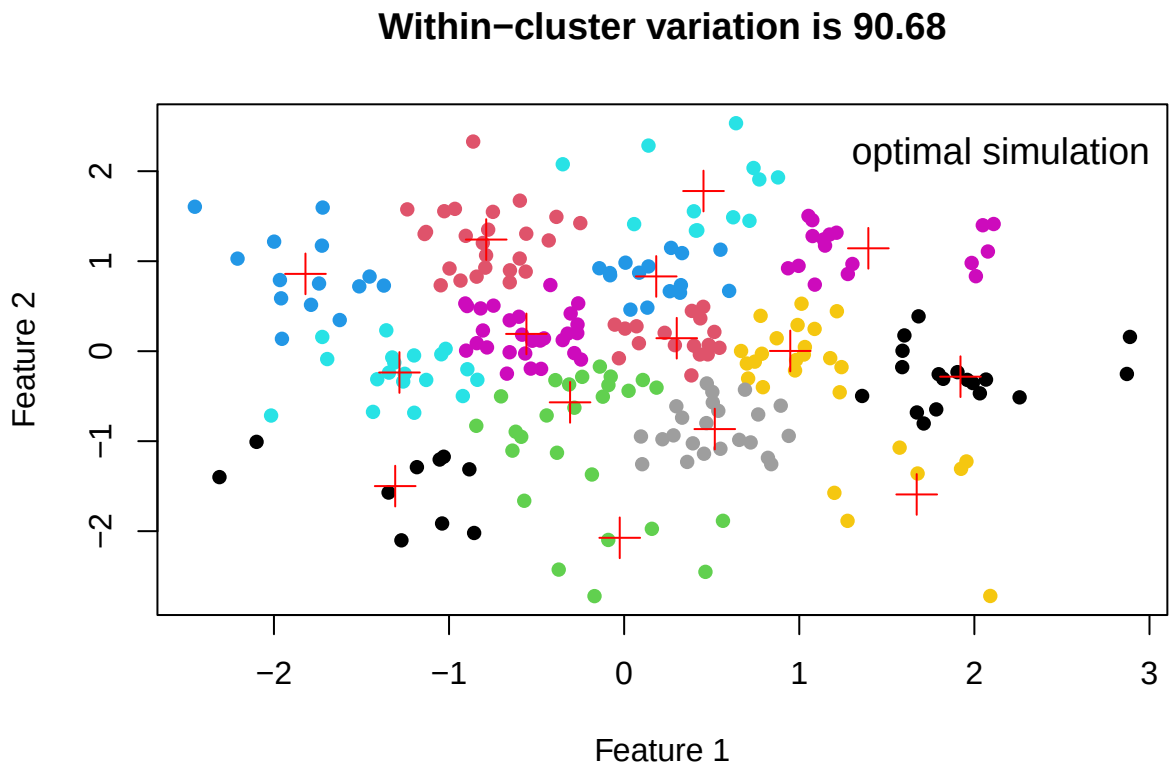
```
K_means_progresses <- function(klist, X){
  total_labels <- klist[["list_cluster"]]
  total_centers <- klist[["list_centers"]]
  library(animation)
  saveGIF({
     # Plot cluster assignments
    for (i in 1:length(total_labels)) {
      current_wcss <- round(WCSS(X, total_labels[[i]], total_centers[[i]]), 2)
      plot(X, col = total_labels[[i]], pch = 16, xlab = 'Feature 1', ylab = 'Feature 2',
           main = paste("Within-cluster variation is", current_wcss))
      legend("topright", legend = paste("Iterations:", i), bty = "n", cex = 1.2, col = "black")
```

```
      points(total_centers[[i]], col = 'red', pch = 3, cex = 2) # Plot centers
      Sys.sleep(0.5) # Pause for visualization
      }
  }, movie.name = "kmeans_progress.gif")
}
```

- From 100 simulations, select the result with the smallest WCSS as the optimal simulation and plot the final results.

```
set.seed(2)
x <- matrix(rnorm(500), ncol = 2)
```

```
km.out <- k_means(X = x, K=15 , max_iters = 1000)
par(mfcol = c(1, 1))
plot(x, col = km.out[["clusters"]], pch = 16, xlab = 'Feature 1', ylab = 'Feature 2',
     main = paste("Within-cluster variation is", round(km.out$`Within-Cluster Sum of Squares`, 2)))
legend("topright", legend = paste("optimal simulation"), bty = "n", cex = 1.2, col = "black")
points(km.out[["centers"]], col = 'red', pch = 3, cex = 2) # Plot centers
```



- Create a animation plots to show the cluster centers and cluster assignment.

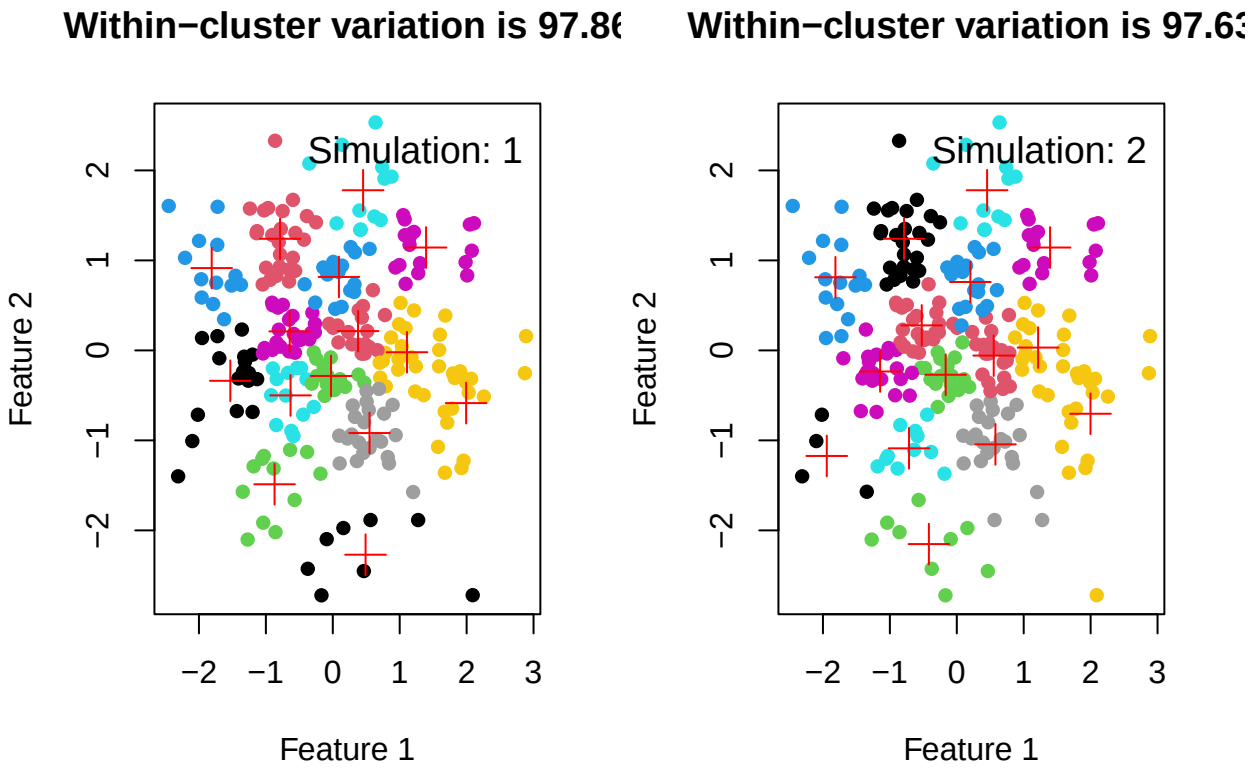
```
K_means_progresses(km.out, x)
```

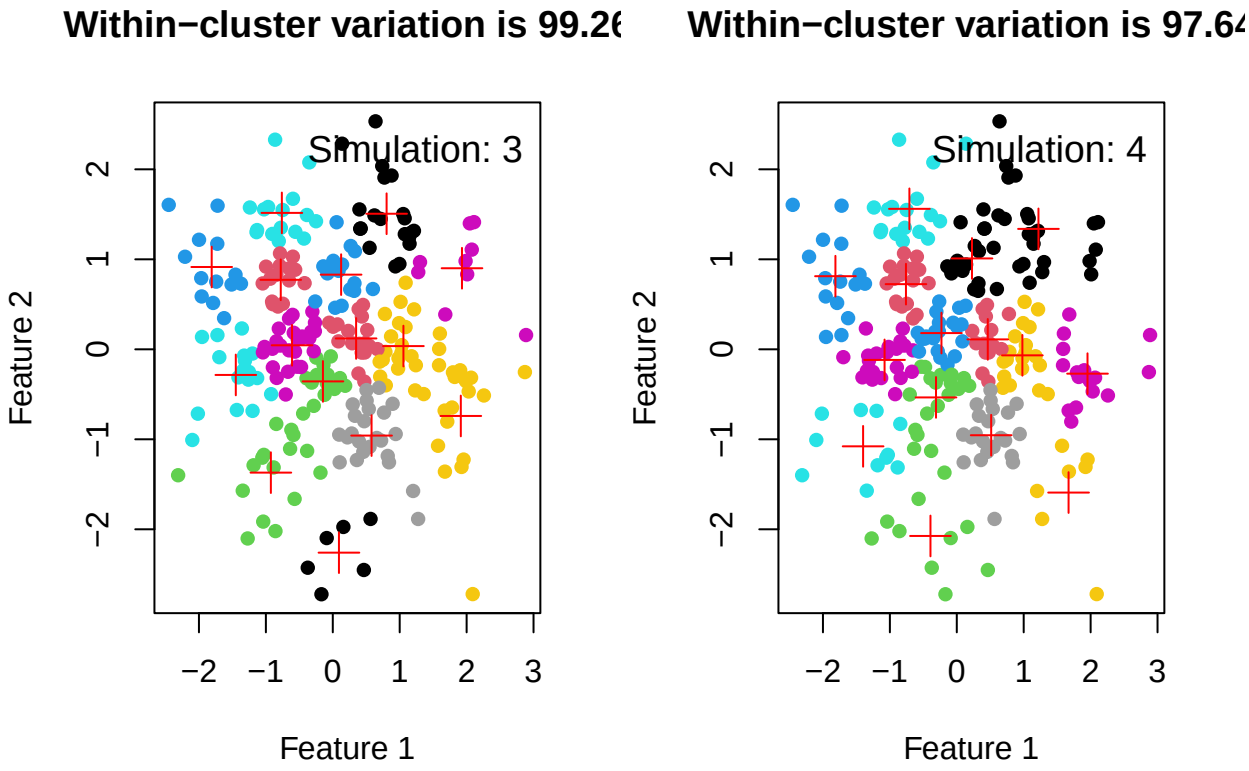
```
## Output at: kmeans_progress.gif
```

```
## [1] TRUE
```

- Show the different results obtained from the 100 times simulation. We can know that each simulation can get different k-means outcome, and its WCSS value is not the same. This is because the initial random assignment points affect the k-means final result.
- Plot the histogram of WCSS value obtained from 100 simulations. The WCSS's distribution is close to normal distribution because of CLT.

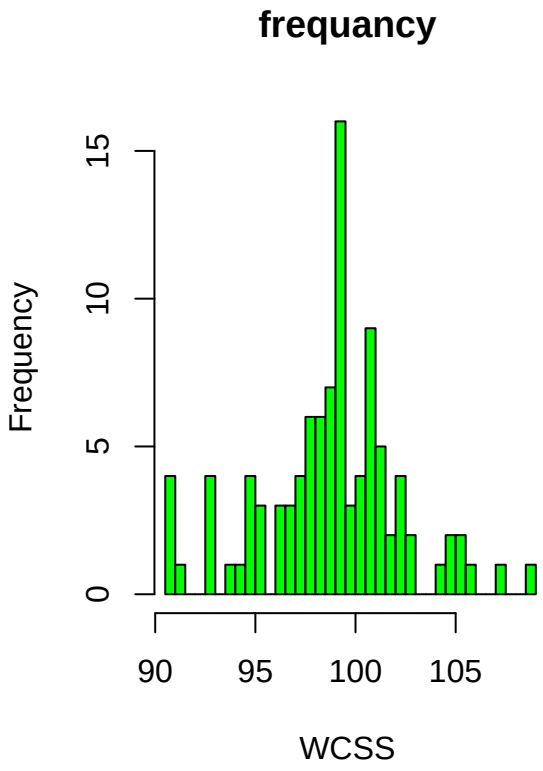
```r
#Since the initial position affects the final result, multiple simulations are performed
#to get the optimal result
par(mfcol = c(1, 2))
for (i in 1:4) {
  current_wcss <- round(km.out[["total_wcss"]][[i]],2)
  plot(x, col = km.out[["optimal_clusters"]][[i]], pch = 16, xlab = 'Feature 1', ylab = 'Feature 2',
       main = paste("Within-cluster variation is", current_wcss))
  legend("topright", legend = paste("Simulation:", i), bty = "n", cex = 1.2, col = "black")
  points(km.out[["optimal_centers"]][[i]], col = 'red', pch = 3, cex = 2) # Plot centers
}
```






```
hist(km.out[["total_wcss"]], breaks = 50, col = "green", xlab = "WCSS",
     xlim = c(min(km.out[["total_wcss"]]), max(km.out[["total_wcss"]])),
     main = "frequancy", freq = TRUE)
summary(km.out[["total_wcss"]])
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##   90.68   97.13   99.15   98.79  100.77  108.51
```



##Kmeans_quality_measure

- Taking a range of values of k and computing WCSS for each k value
- Plot the optimal WCSS results for each value of k
- Plot k value against WCSS

Input:

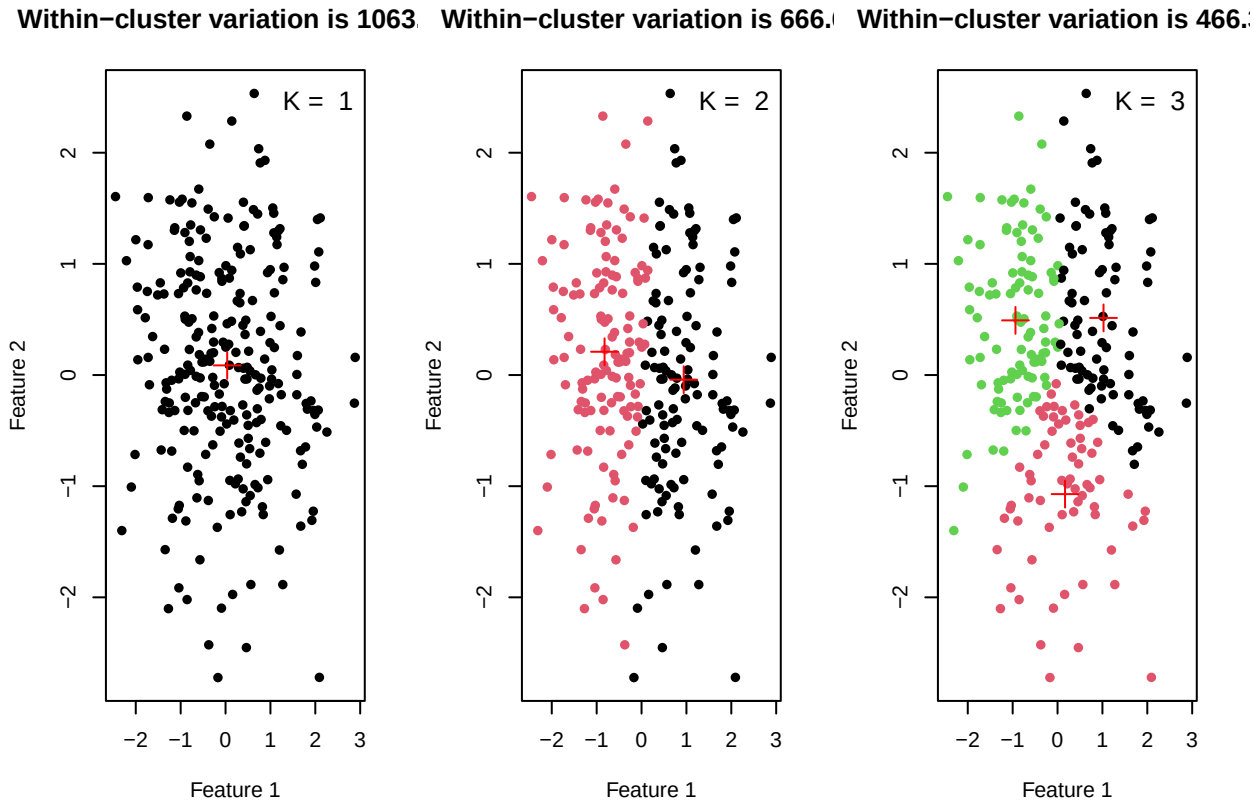
- K_range is the range of values for K to test.
- X is the n x m matrix where each row represents a point.

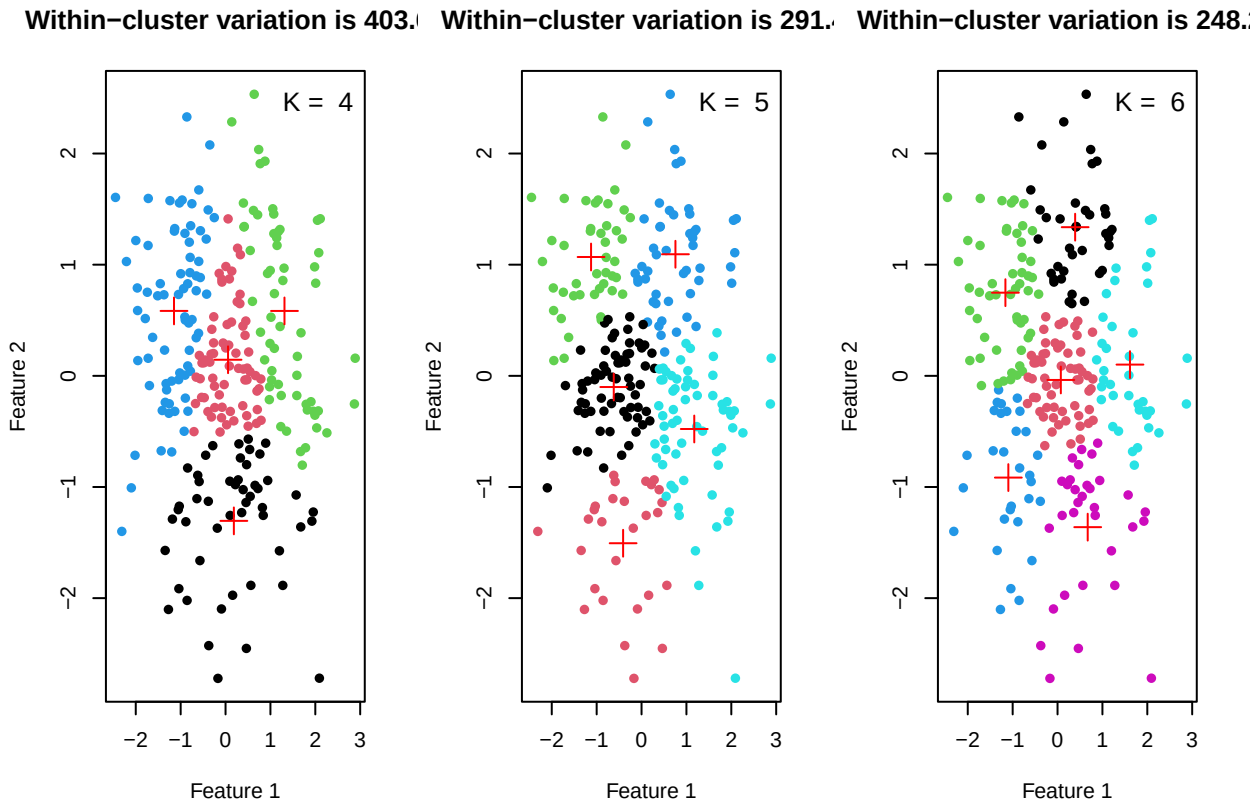
Output:

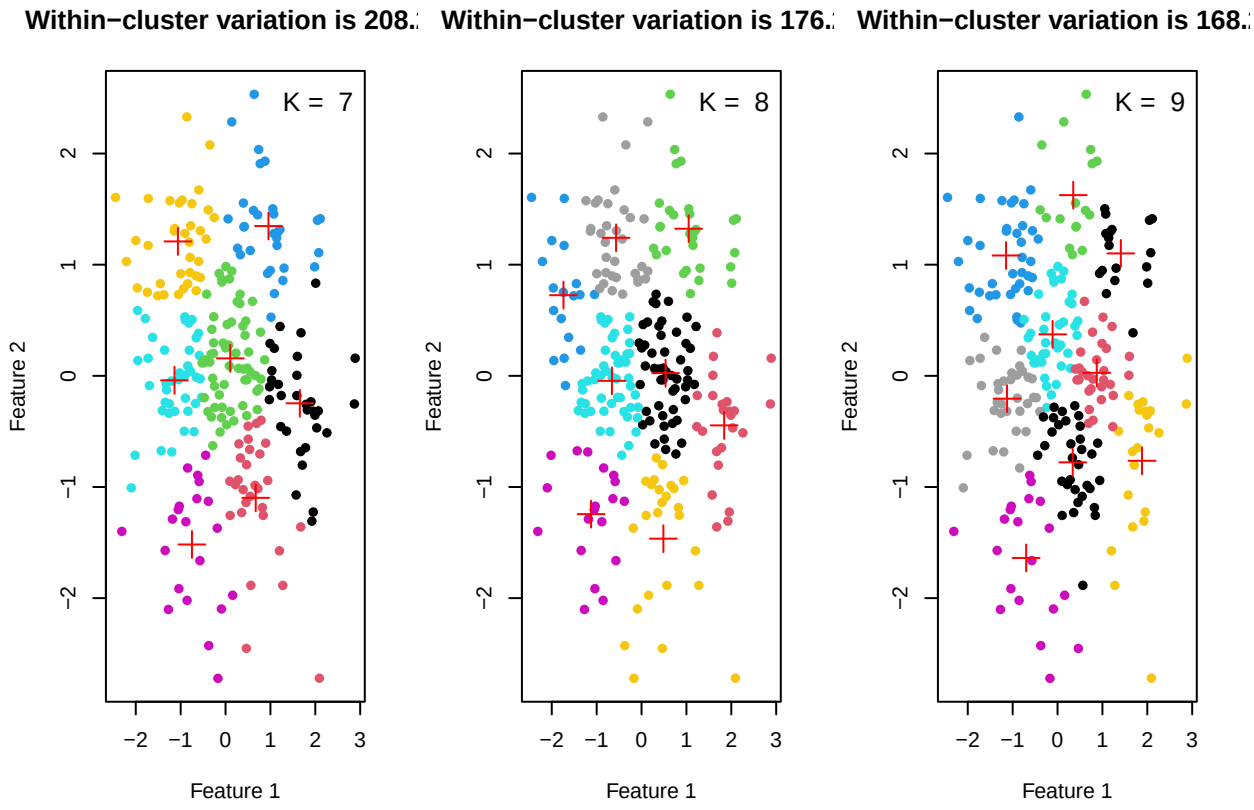
- a plot of k value with WCSS

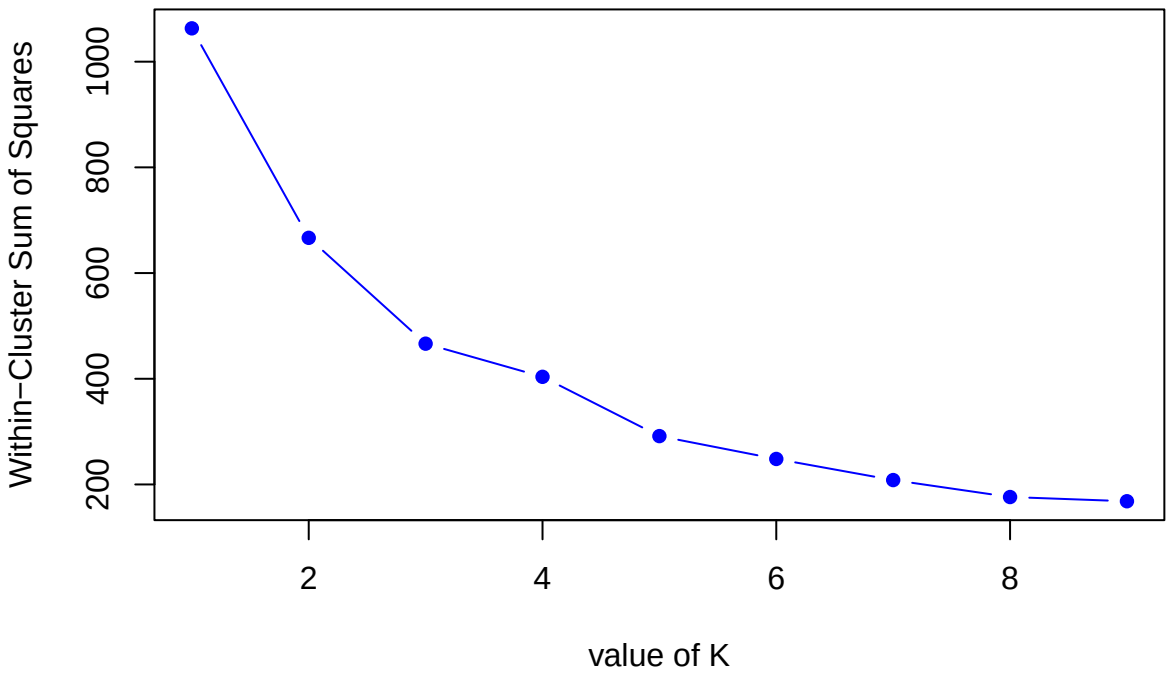
```
Kmeans_quality_measure <- function(K_range, X){
  m <- rep(NA, K_range) #to record the sum of WCk in difference K value
  par(mfcol = c(1, 3))
  for (a in 1:K_range) {
    result <- k_means(X, K = a)
    m[a] <- round(result$`Within-Cluster Sum of Squares`, 2)

    plot(X, col = result[["clusters"]], pch = 16, xlab = 'Feature 1', ylab = 'Feature 2',
```

```r
        main = paste("Within-cluster variation is", round(result$`Within-Cluster Sum of Squares`, 2)))
    legend("topright", legend = paste("K = ", a), bty = "n", cex = 1.2, col = "black")
    points(result[["centers"]], col = 'red', pch = 3, cex = 2) # Plot centers
  }

  k_value <- 1:K_range
  par(mfcol = c(1, 1))
  plot(k_value, m, type = "b", col = "blue", pch = 16, xlab = "value of K",
       ylab = "Within-Cluster Sum of Squares")
  return(m)
}

Kmeans_quality_measure(9, x)
```




Within−cluster variation is 403.
Within−cluster variation is 291.
Within−cluster variation is 248.
K = 4
K = 5
K = 6
Feature 1
Feature 2
−2
−1
0
1
2
3


Within−cluster variation is 208.
Within−cluster variation is 176.
Within−cluster variation is 168.
K = 7
K = 8
K = 9
Feature 1
Feature 2
−2
−1
0
1
2
3




```
## [1] 1063.04  666.64  466.37  403.66  291.49  248.26  208.28  176.22  168.24
```

conclusion: As the k value increases, WCSS value becomes smaller.

##Test

```
#getwd()
library(testthat)
test_dir('.')
```

```
## v | F W  S  OK | Context
## / |          0 | kmeans                                                    \ |          2 | kmea

## \ |         18 | kmeans                                                    [1] "All tests passe
## v |         18 | kmeans [12.4s]
##
## == Results =====================================================================
## Duration: 12.4 s
##
## [ FAIL 0 | WARN 0 | SKIP 0 | PASS 18 ]
```