K-means Clustering

K-means Clustering

- What is clustering?
- Why would we want to cluster?
- How would you determine clusters?
- How can you do this efficiently?

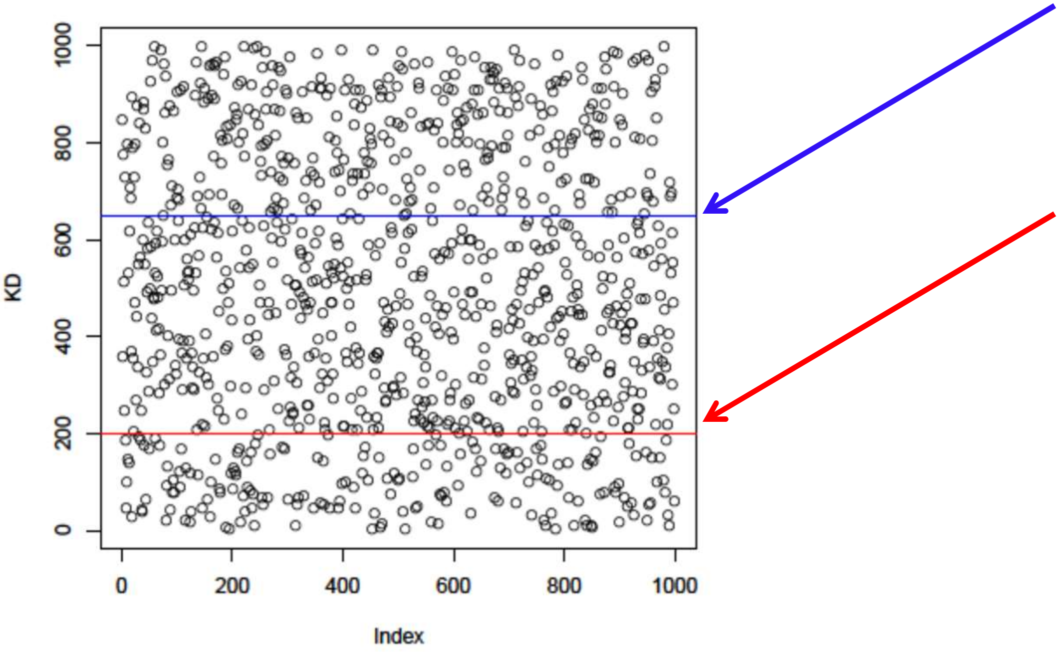
K-means Clustering

- Strengths
  - Simple iterative method
  - User provides “K”
- Weaknesses
  - Often too simple → bad results
  - Difficult to guess the correct “K”

K-means Clustering

Basic Algorithm:

- Step 0: select K
- Step 1: randomly select initial cluster seeds



Seed 1
650

Seed 2
200

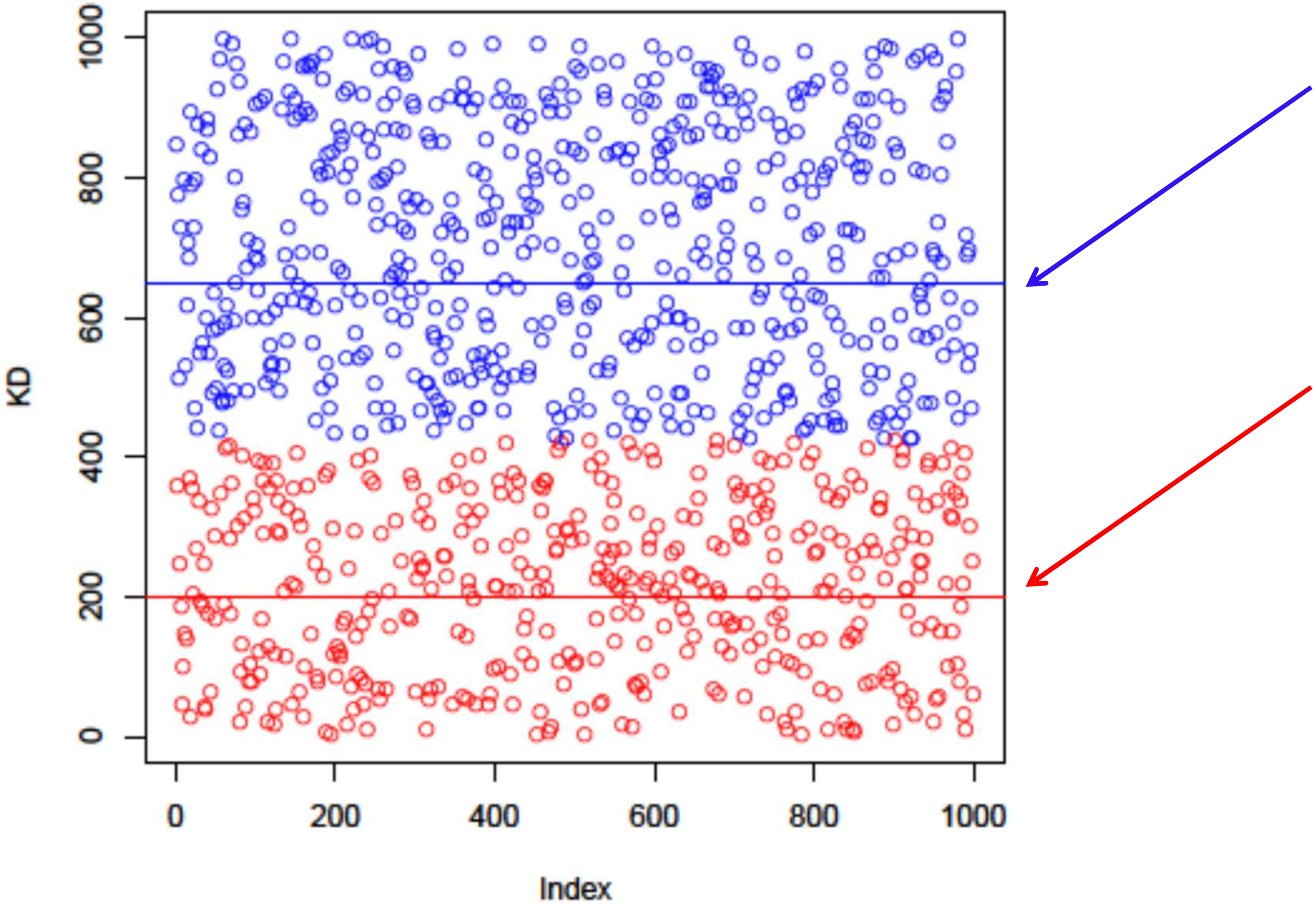
K-means Clustering

- An initial cluster seed represents the “mean value” of its cluster.
- In the preceding figure:
  - Cluster seed 1 = 650
  - Cluster seed 2 = 200

K-means Clustering

- Step 2: calculate distance from each object to each cluster seed.
- What type of distance should we use?
  - Squared Euclidean distance
- Step 3: Assign each object to the closest cluster

K-means Clustering

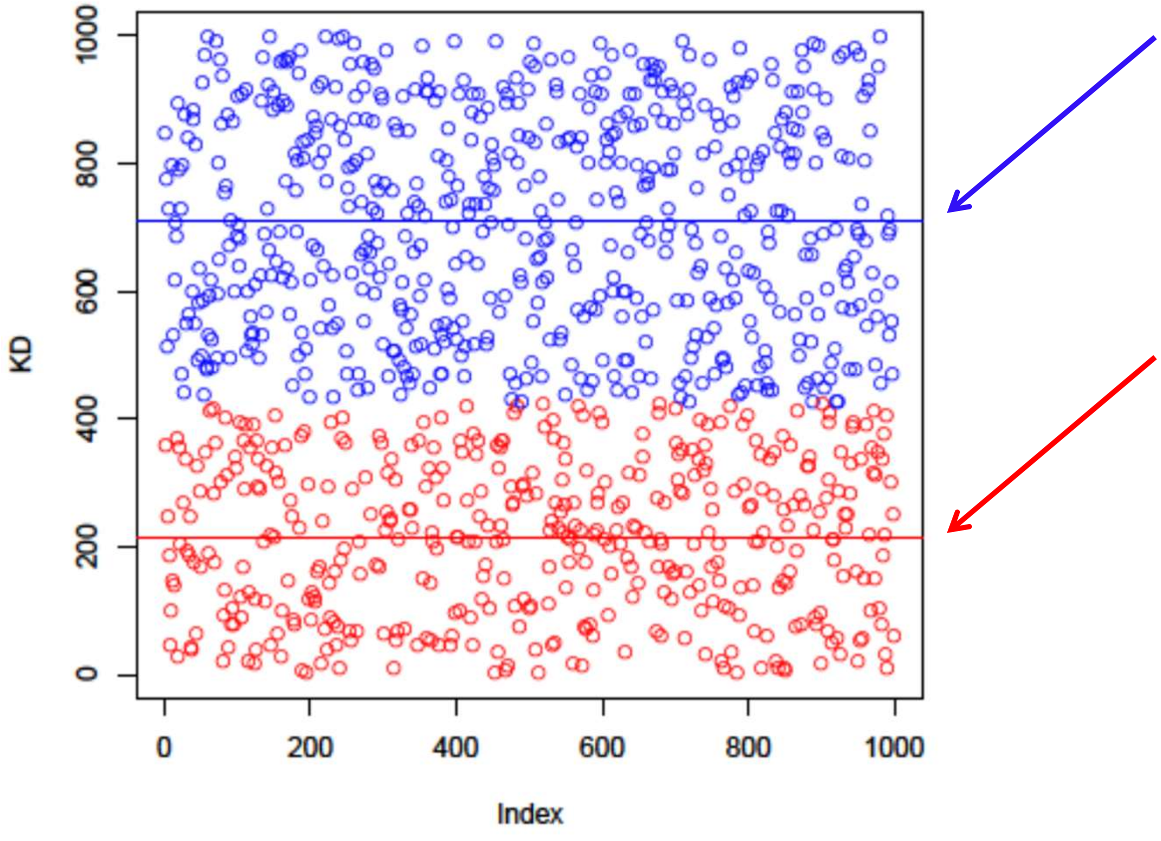


Seed 1

Seed 2

K-means Clustering

- Step 4: Compute the new centroid for each cluster



Cluster Seed 1
708.9

Cluster Seed 2
214.2

K-means Clustering

- Iterate:
  - Calculate distance from objects to cluster centroids.
  - Assign objects to closest cluster
  - Recalculate new centroids
- Stop based on convergence criteria
  - No change in clusters
  - Max iterations

K-means Issues

- Distance measure is squared Euclidean
  - Scale should be similar in all dimensions
    - Rescale data?
  - Not good for nominal data. Why?
- Approach tries to minimize the within-cluster sum of squares error (WCSS)
  - Implicit assumption that SSE is similar for each group

WCSS

- The over all WCSS is given by:

  $$\sum_{i=1}^{k} \sum_{x \in C_i} \|x - \mu_i\|^2$$

- The goal is to find the smallest WCSS
- Does this depend on the initial seed values?
- Possibly.

Bottom Line

- K-means
  - Easy to use
  - Need to know K
  - May need to scale data
  - Good initial method
- Local optima
  - No guarantee of optimal solution
  - Repeat with different starting values

K-Means Lab

Pause this set of slides and switch to lab slides

Other Clustering in R

- Hierarchical Clustering (agglomerative)
  - Create a distance matrix using ‘dist()’
  - Create the hierarchy using ‘hclust()’

- Model Based Clustering
  - Use ‘mclust()’ to create the clusters on the basis of
    - Bayesian Information Criterion (BIC)
    - Parameterized Gaussian mixture models

Hierarchical Clustering

```
# Create the distance matrix
d <- dist(state_income$V2, method = "euclidean")

# Create the hierarchy
fit <- hclust(d, method="ward.D2")

# Plot the histogram
plot(fit)

# cut the tree into 6 clusters
Groups <- cutree(fit, k=6)

# Outline the 6 clusters
rect.hclust(fit, k=6, border="red")
```

Hierarchical Clustering

```
# Other hierarchical methods
sfit <- hclust(d, method="single")
cfit <- hclust(d, method="complete")
afit <- hclust(d, method="average")

# Plot the histogram
op <-  par(mar = c(0, 4, 4, 2), mfrow = c(2, 2))
plot(sfit, labels = FALSE, main = "Single", xlab = "")
plot(cfit, labels = FALSE, main = "Complete", xlab = "")
plot(afit, labels = FALSE, main = "Average", xlab = "")
plot(fit, labels = FALSE, main = "Ward", xlab = "")
```

Model-Based Clusters

This is more complicated that hierarchical or K-means clustering

```
# First load mclust package
#Create the cluster(s)
fit <- Mclust(state_income$V2)

# examine the result(s)
summary(fit)

# plot the result(s)
plot(fit)

#Not very satisfying. Try a different data set
```

Model-Based Clusters

```
# Load in a different data set (iris.data)
#Create the cluster(s)
fit <- Mclust(iris[,-5])

# examine the result
summary(fit)

# plot the result(s)
plot(fit)

# 1: display the model scores vs # clusters
# 2: display the classification based on the best scoring model
# 3: display the uncertainty (based on the best scoring model)
# 4: display the density (based on the best scoring model)
```

(for explanation of mixture models see https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5096736/)