MA5810: Introduction to Data Mining

Week 4; Collaborate Session 1: Clustering

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Housekeeping

- Collaborate 1 = Tuesday 6.45-8pm (Martha)
- Collaborate 2 = Thursday 6.45-8pm (Martina)

For my Collaborate Sessions, you can get the slides & R code for each week here:

https://github.com/MarthaCooper/MA5810

Subject: MA5810 Intro to Data Mining

MA5810 Learning Outcomes

1. Overview of Data Mining and Examples
2. Unsupervised data mining methods e.g. clustering and outlier detection;
3. Unsupervised and supervised techniques for dimensionality reduction;
4. Supervised data mining methods for pattern classification;
5. Apply these concepts to real data sets using R (Today).

Today's Goals

- Understand how K-means clustering works
- Understand how to obtain the optimal value for K
- Understand the pros and cons of K-means clustering
- Apply K-means clustering on real datasets using R

Unsupervised Learning

A set of statistical tools to understand a set of features, $X_1, \ldots Xp$, without having an associated response variable, Y, to predict.

Data visualization & identification of subgroups

Clustering

A broad class of methods for discovering unknown subgroups (*clusters*) within data

Why Cluster?

- Bioinformatics - identify subtypes of cancer from gene expression data
- Marketing- identify subgroups of shoppers who buy certain products

Cluster Analysis

Clustering looks to find homogeneous subgroups among the observations

Observations should be:

- similar to observations within the same cluster
- different to observations in different cluster

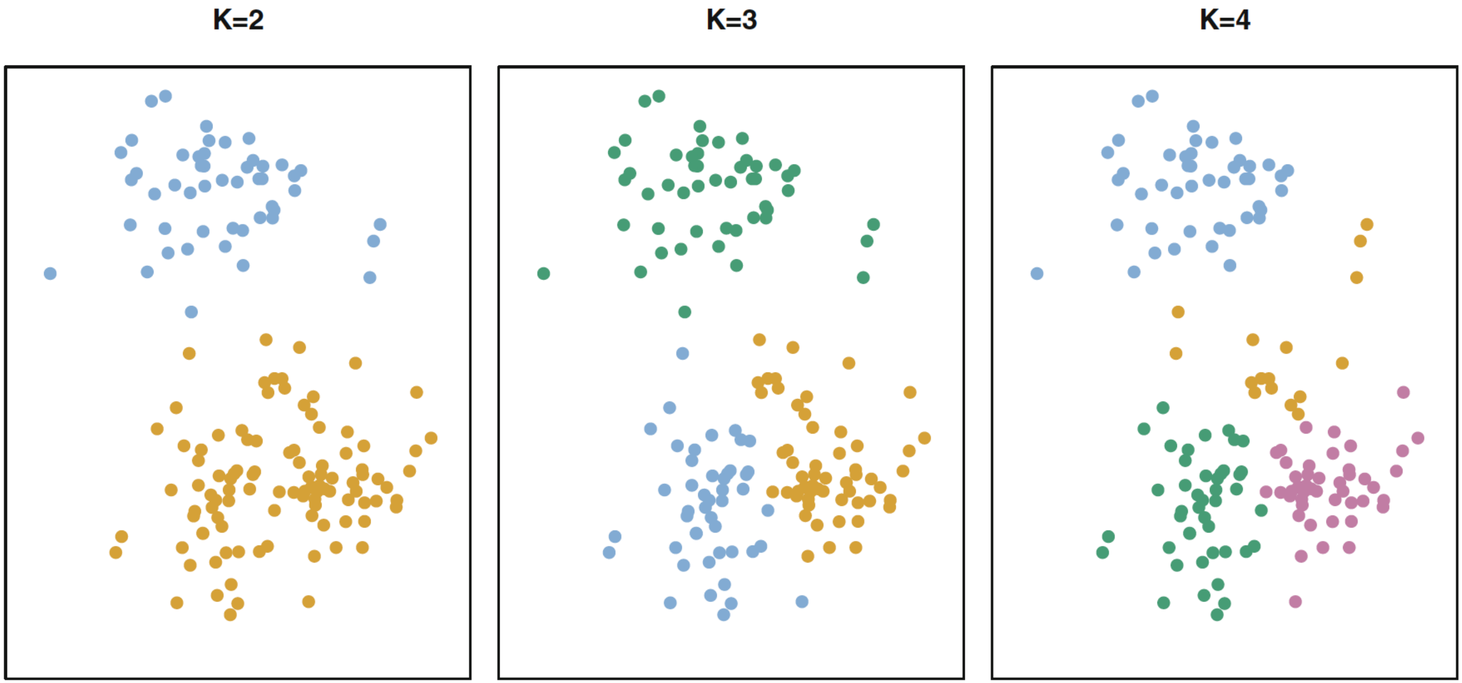
How do we determine these similarities & differences?

Two approaches:

- K-means clustering
- Hierarchical Clustering

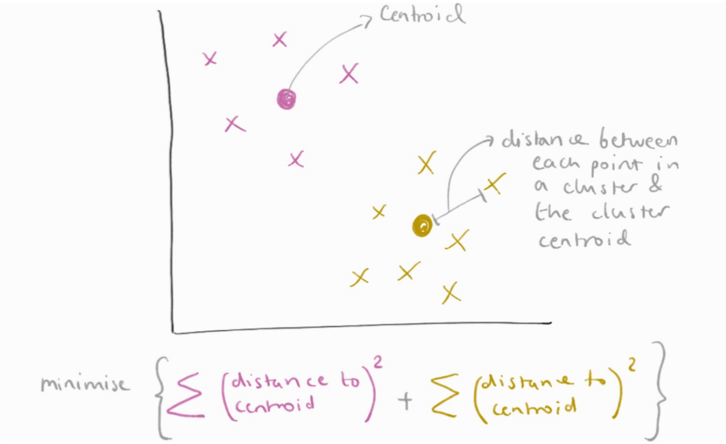
K-Means Clustering

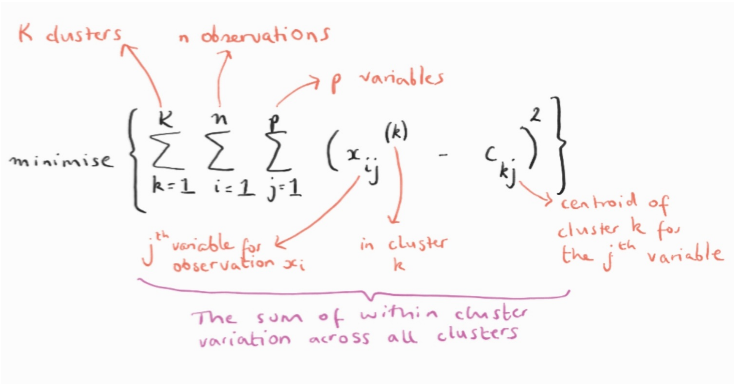
- Partition a dataset into *K* distinct, non-overlapping clusters
- We define the number of clusters, *K*, and the *K*-Means algorithm will assign each observation to *one* of those clusters



How does *K*-means select the best clusters?

- Minimize total within cluster variation





K-means clustering algorithm

Algorithm 10.1 *K-Means Clustering*

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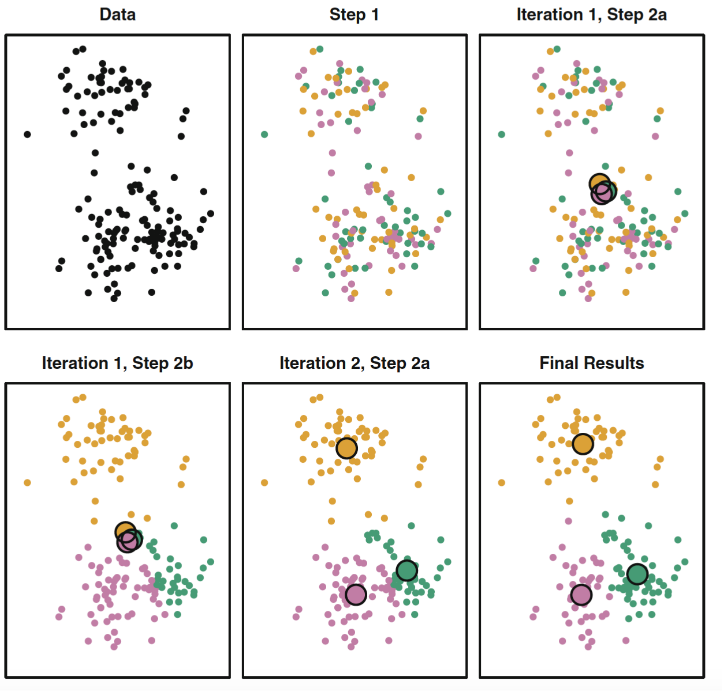
1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
2. Iterate until the cluster assignments stop changing:
   (a) For each of the K clusters, compute the cluster *centroid*. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
   (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).

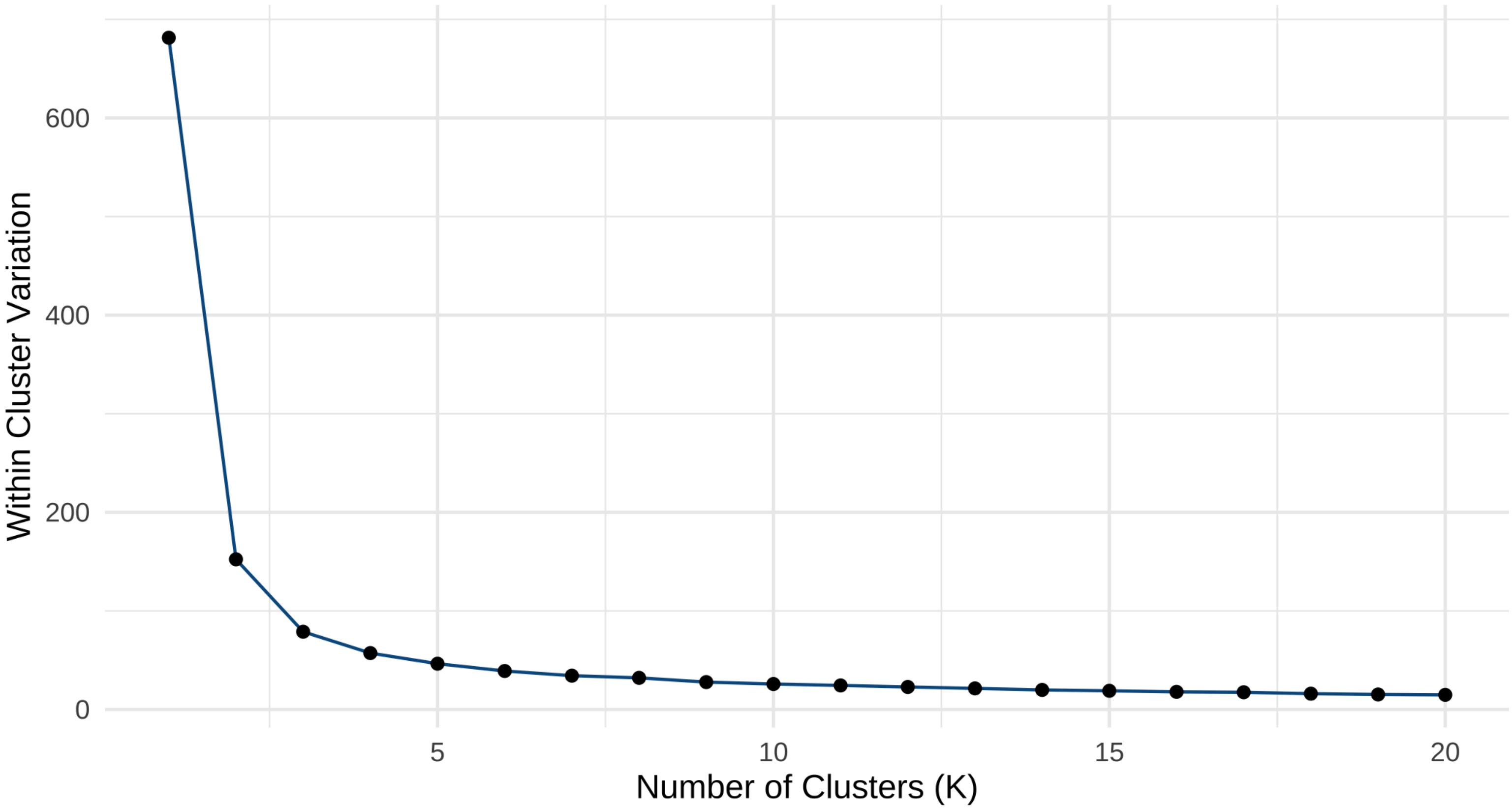


Repeating K-means clustering

- Each solution depends on the *initial, random cluster assignment*
- This is called the local optimum
- Because of this, we should:

    1. Repeat K-means algorithm
    2. Select the iteration that minimizes *within cluster variation*

Choosing *K*



Within Cluster Variation
600
400
200
0
5
10
15
20
Number of Clusters (K)

Pros and Cons

Pros

- Scales to large data sets well
- Doesn't make any assumptions about data distribution
- Generalizes to clusters of different shapes and sizes

Cons

- Subjective
- Interpretation requires domain knowledge
- Exploratory data analysis
- Difficult to assess results

K-means clustering in R

```
library(cluster, warn.conflicts = F, quietly = T) #clustering algorithms
library(factoextra, warn.conflicts = F, quietly = T) #data visualization

head(iris) #data

dat <- iris[,1:4]
dat <- na.omit(dat) #what to do if NA values?
dat_scaled <- scale(dat) #why?

set.seed(6) #why?
kmeans_res <- kmeans(dat_scaled, centers = 3, nstart = 25) #centers? ns
str(kmeans_res)

fviz_cluster(kmeans_res, data = dat_scaled)
```

Interpretation using domain knowledge

- What do the clusters represent?

```
fviz_cluster(kmeans_res, #set up plot
             data = dat_scaled,
             geom = "point", # only shows points and not labels
             shape = 19,# define one shape for all clusters (a circle)
             alpha = 0)+ # make circles see-though
  geom_point(aes(colour = as.factor(kmeans_res$cluster),
                 shape = iris$Species))+ #colour by species
  ggtitle("Comparing Clusters and Iris Species") #add a title
```

- Conclusion?

Choosing K in R

```r
total_sum_squares <- function(k){ #perform kmeans & calculate ss
  kmeans(dat_scaled, centers = k, nstart = 25)$tot.withinss
}

all_ks <- seq(1,20,1) #define a sequence of values for k

choose_k <- sapply(seq_along(all_ks), function(i){ #apply to all values
  total_sum_squares(all_ks[i])
})

choose_k_plot <- data.frame(k = all_ks,  # dataframe for plotting
                            within_cluster_variation = choose_k)
head(choose_k_plot)
ggplot(choose_k_plot, aes(x = k, # plot
                          y = within_cluster_variation))+
  geom_point()+
  geom_line()+
  xlab("Number of Clusters (K)")+
  ylab("Within Cluster Variation")
```

Extra reading

- Chapter 10.3 of James *et al.*, ISLR
- STHDA Factoextra R Package Guide

References

- James *et al.*, ISLR

Slides

- xaringhan, xaringanthemer, remark.js, knitr, R Markdown