Education is the most powerful weapon which you can use to change the world. – Nelson Mandela

Clustering

(SEGMENTATION)

Clustering

- Unsupervised: no target variable for training
- Partition the data into groups (clusters) so that:
  - Observations within a cluster are similar in some sense
  - Observations in different clusters are different in some sense
- There is no one correct answer, though there are good and bad cluster solutions
- No method works best all the time

Examples of Clustering (segmentation)

- Customer segmentation: groups of customers with similar shopping or buying patterns
- Dimension reduction:
  - Cluster individuals together and use cluster variable as proxy for demographic or behavioral variables
- Gather stores with similar characteristics for sales forecasting
- Find topics (clusters of words) in text data
- Find communities in social networks

Hard versus Fuzzy

Hard: objects can belong to only one cluster

- k-means
- DBSCAN
- Hierarchical

Fuzzy: objects can belong to more than one cluster (usually with some probability)

- Fuzzy C-means (FCM)
- Gaussian Mixture Models / Expectation-Maximization (EM)

Hierarchical versus Flat

Hierarchical: clusters form a tree so you can visually see which clusters are most similar to each other.

- *Agglomerative*: points start out as individual clusters, and they are combined until everything is in one cluster. (ex: Linkages - coming next class)
- *Divisive*: All points start in same cluster and at each step a cluster is divided into two clusters. (ex: DIANA)

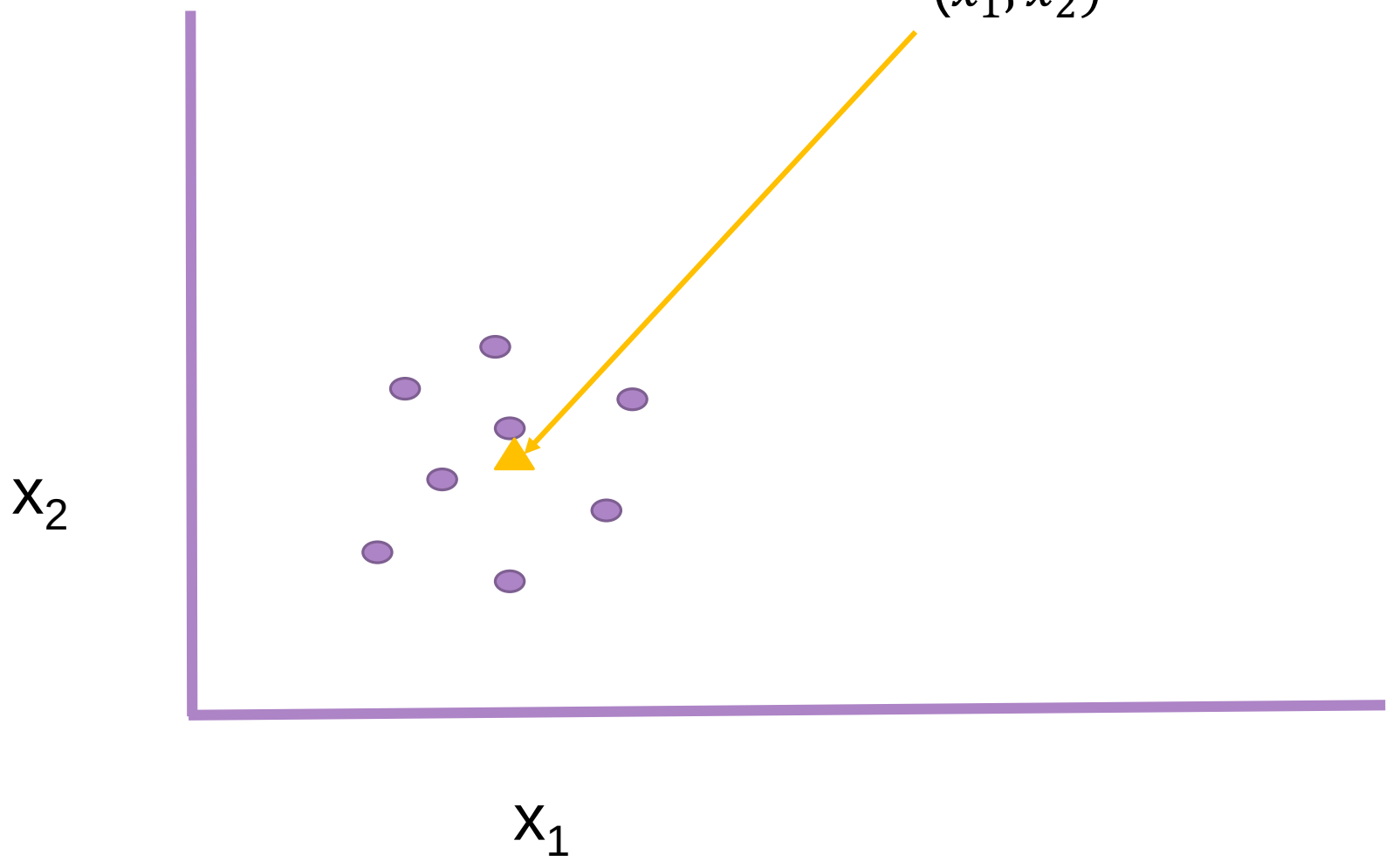
Flat: Clusters are created according to some other process, usually iteratively updating cluster assignments (usually specify the number of clusters apriori)

K-Means

MOST POPULAR CLUSTERING METHOD

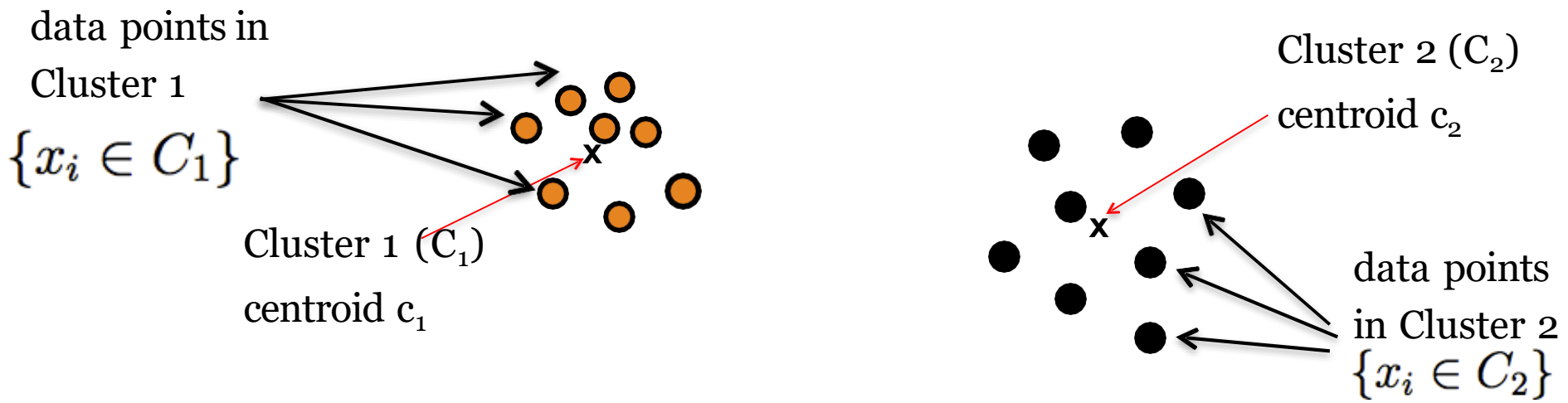
Centroid-Mean of a group of observations

$(\bar{x}_1, \bar{x}_2)$



k-Means Clustering

- The most popular clustering algorithm



- Tries to minimize the sum of squared distances from each point to its cluster centroid. (Global objective function)

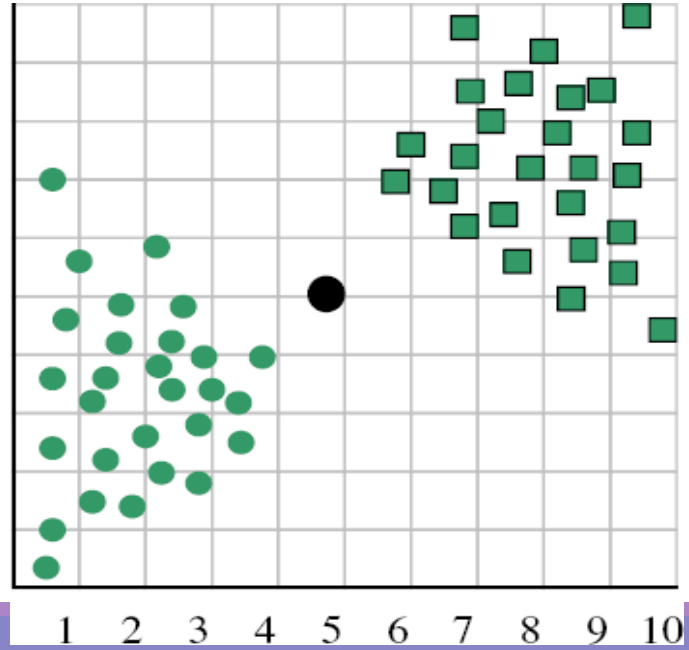
$$\sum_{C_k} \sum_{x_i \in C_k} \|x_i - c_k\|^2$$

K-means algorithm

- Start with k “seed points”
  - Randomly initialized (most software)
- Assign each data point to the closest seed point.
- The seed point then represents a cluster of data
- Reset seed points to be the centroids of the cluster
- Repeat steps 2-4 updating the cluster centroids until they do not change.

Determining Number of Clusters (SSE)

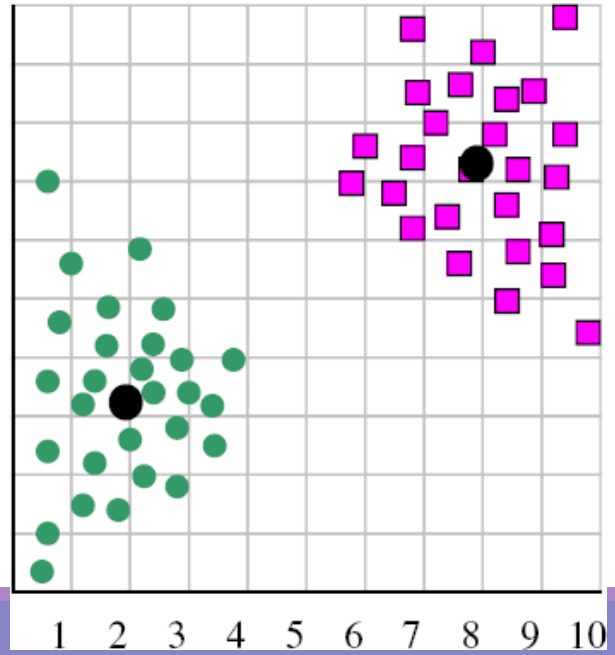
- Try the algorithm with k=1,2,3,…
- Examine the objective function values
- Look for a place where the marginal benefit to objective function for adding a cluster becomes small



k=1 objective function (SSE) is 902

Determining Number of Clusters (SSE)

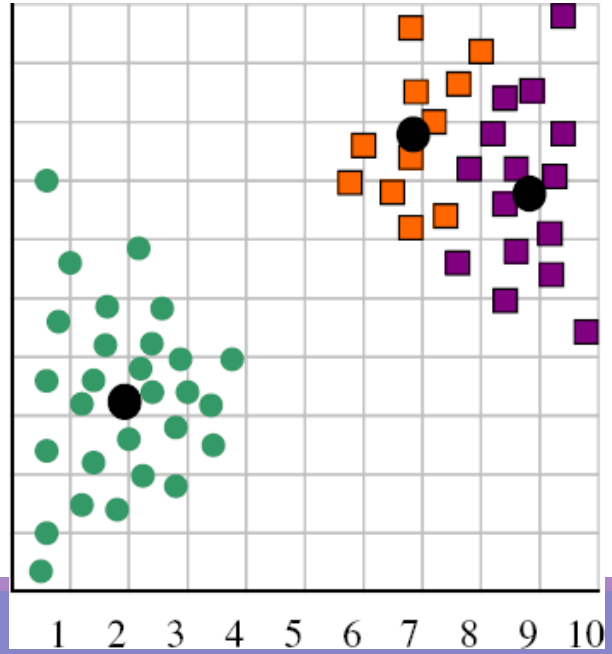
- Try the algorithm with k=1,2,3,…
- Examine the objective function values
- Look for a place where the marginal benefit to objective function for adding a cluster becomes small



k=2 objective function (SSE) is 213

Determining Number of Clusters (SSE)

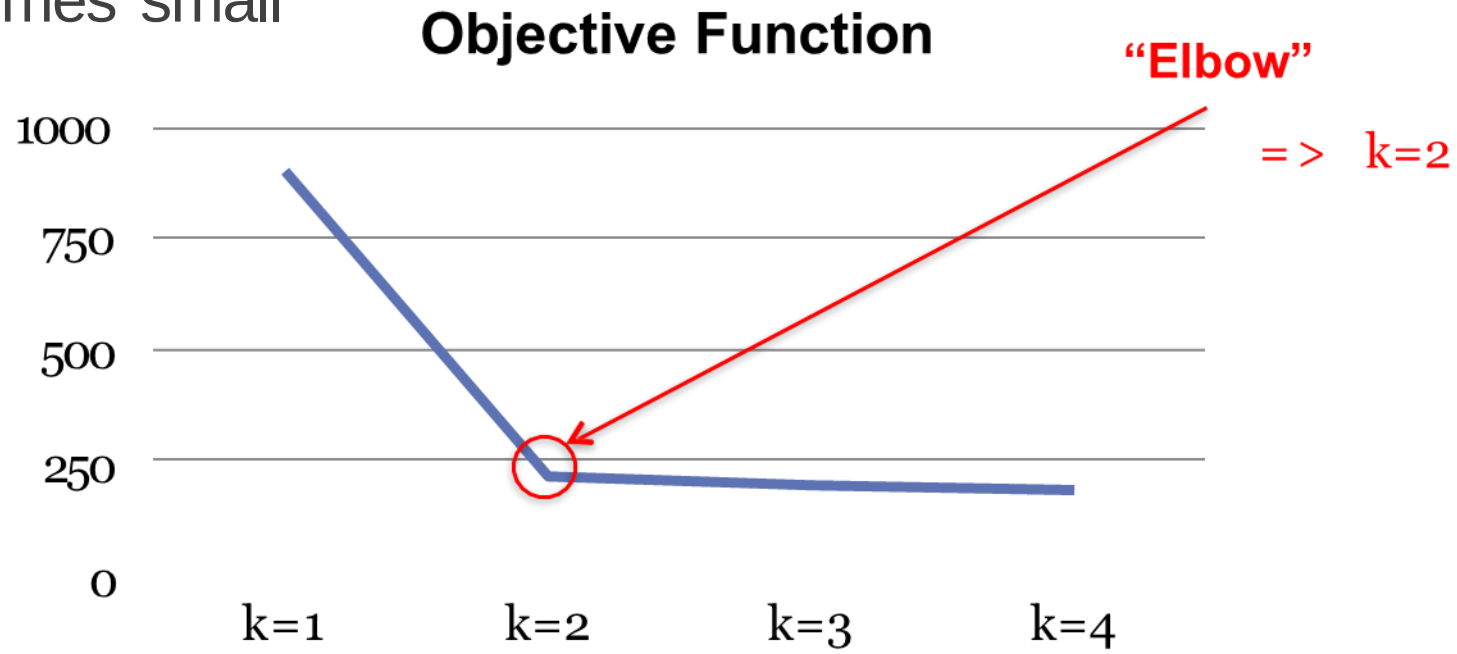
- Try the algorithm with k=1,2,3,…
- Examine the objective function values
- Look for a place where the marginal benefit to objective function for adding a cluster becomes small



k=3 objective function (SSE) is 193

Determining Number of Clusters (SSE)

- Try the algorithm with k=1,2,3,…
- Examine the objective function values
- Look for a place where the marginal benefit to objective function for adding a cluster becomes small



K-means summary

Disadvantages

- Dependent on initialization (initial seeds)
- Can be sensitive to outliers
  - If problem, should consider k-medoids
- Have to input the number of clusters
- Difficulty detecting non-spheroidal (globular) clusters

Advantages

- Modest time/storage requirements.
- Shown you can terminate method after small number of iterations with good results.
- Good for wide variety of data types

Example

ARREST DATA

USArrests data set

Data set is already in R

Has 50 observations (one observation per state)

Provides information on arrests per 100,000 in each state in assault, murder and rape

Also contains information on percent of state's population living in an urban area

Data is from 1973

Preprocessing

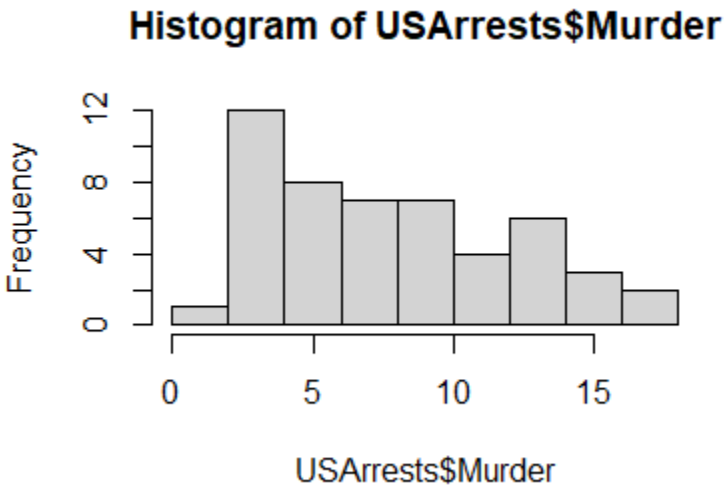
You will need to do some data exploration BEFORE trying to cluster the data

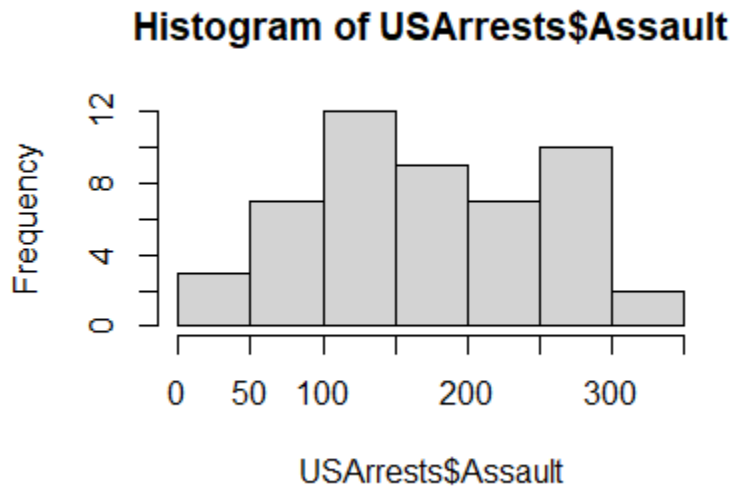
- **Missing values**
  - you will either need to impute missing values or remove that variable or observation
- **Categorical variables**
  - Do you need to bin categorical variables?
  - Need to create dummy variables for ALL categorical variables
- **Continuous variables**
  - If outliers or heavy skewness, potentially consider transformation
  - At a minimum, center the continuous variables (better to standardized, for example z-scores…this would happen AFTER any transformations are made)

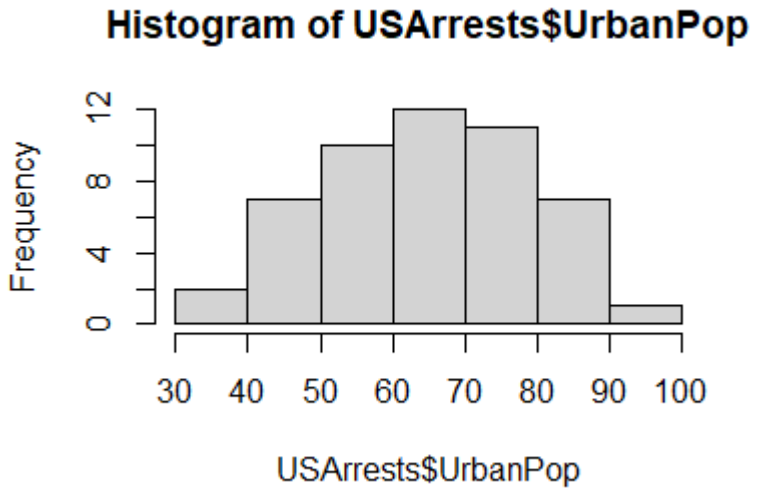
- You can try clustering on original data (after scaled and dummy coded, etc) or you can try it on PCA of the variables (especially useful if data is BIG)

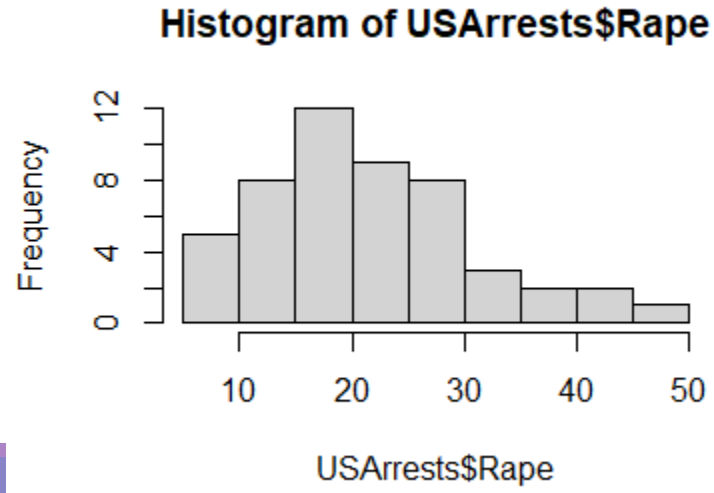
```
summary(USArrests)
hist(USArrests$Murder)
hist(USArrests$Assault)
hist(USArrests$Rape)
hist(USArrests$UrbanPop)
arrest.scal=scale(USArrests)
```

No missing values in data set!!









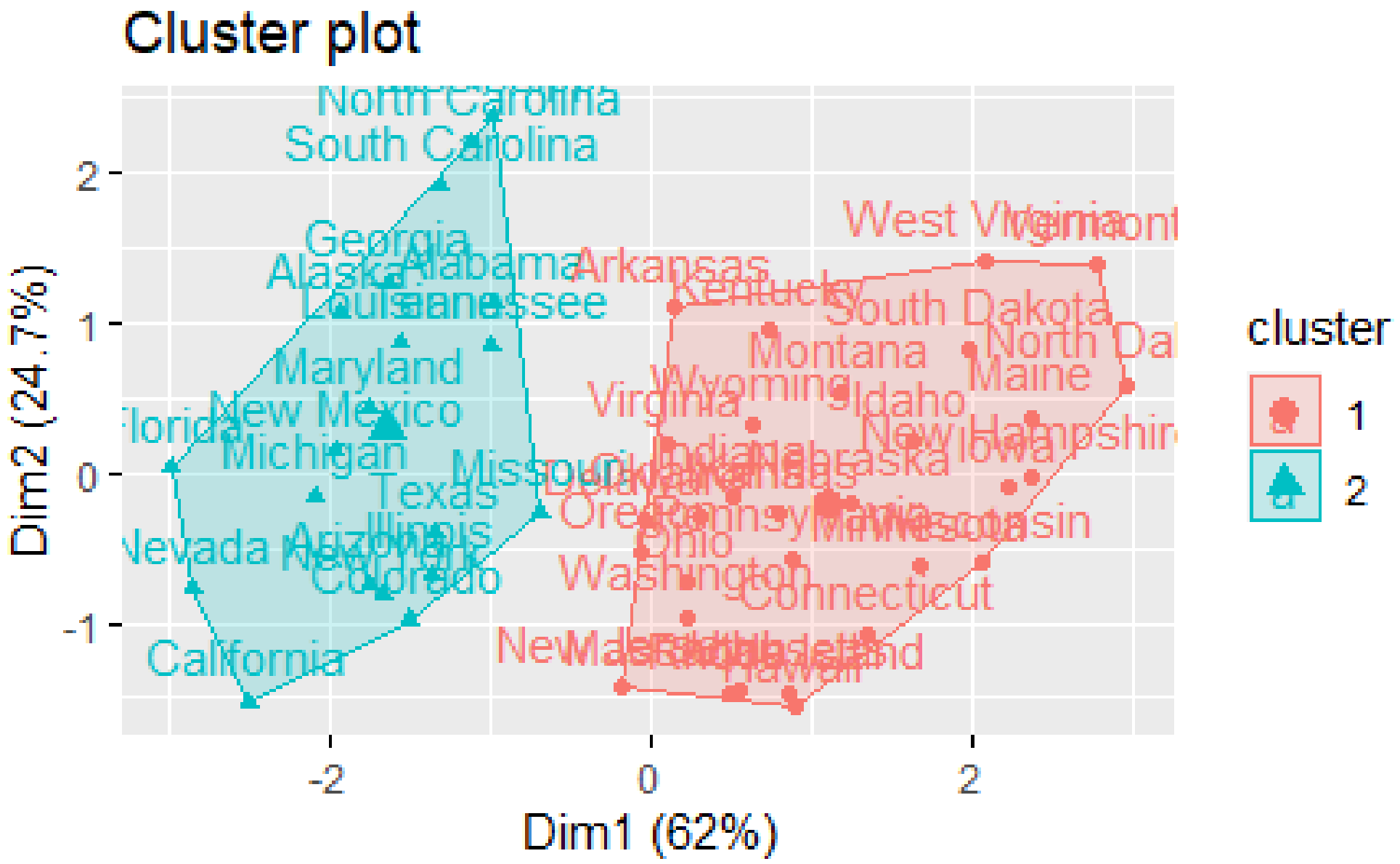
```
clus2=kmeans(arrest.scal,centers=2,nstart = 25)
clus2
```

```
K-means clustering with 2 clusters of sizes 30, 20

Cluster means:
     Murder    Assault   UrbanPop       Rape
1 -0.669956 -0.6758849 -0.1317235 -0.5646433
2  1.004934  1.0138274  0.1975853  0.8469650

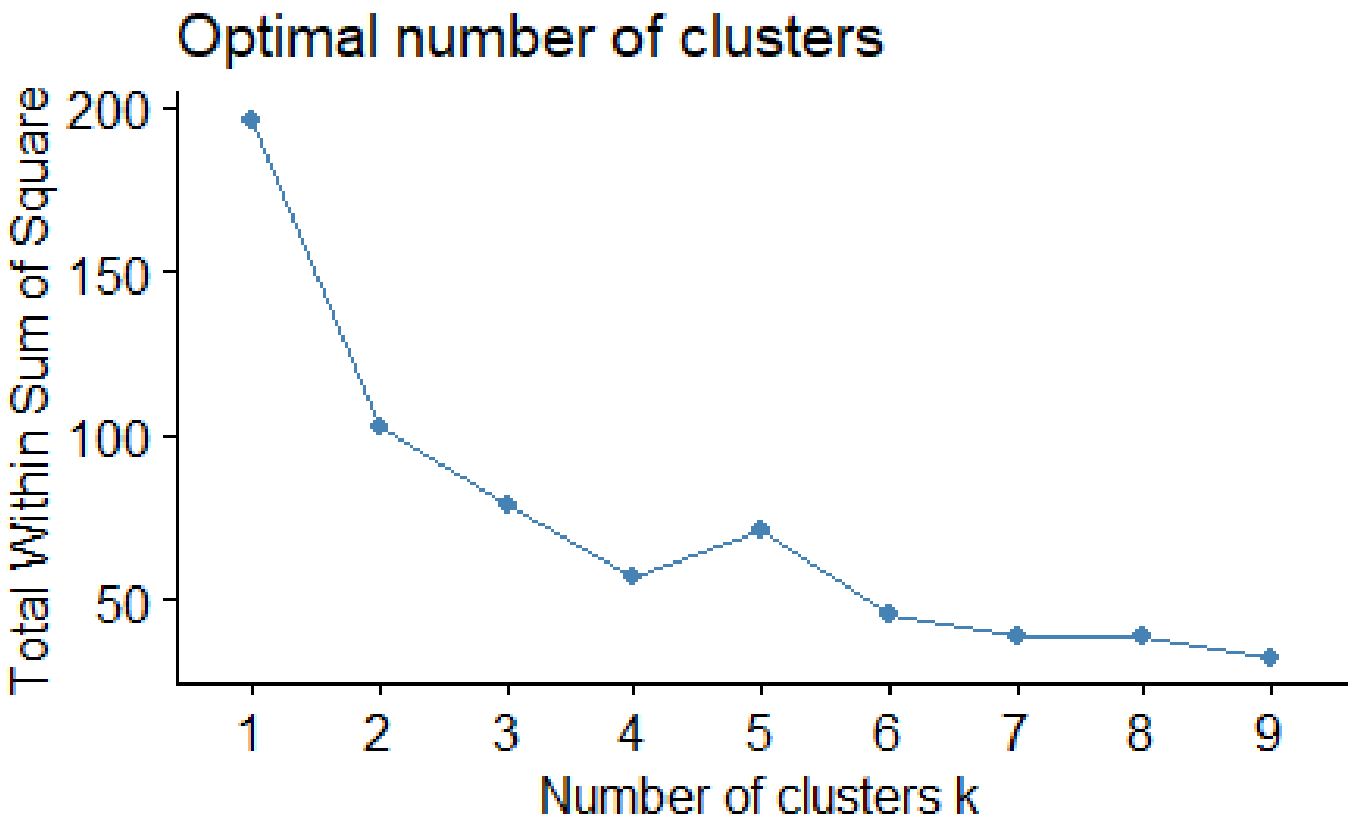
Clustering vector:
    Alabama      Alaska     Arizona    Arkansas
          2           2           2           1
 California    Colorado Connecticut    Delaware
          2           2           1           1
    Florida     Georgia      Hawaii       Idaho
          2           2           1           1
```

fviz_cluster(clus2, data = arrest.scal)



```
set.seed(12964)

fviz_nbclust(arrest.scal, kmeans, method = "wss",k.max = 9,)
```



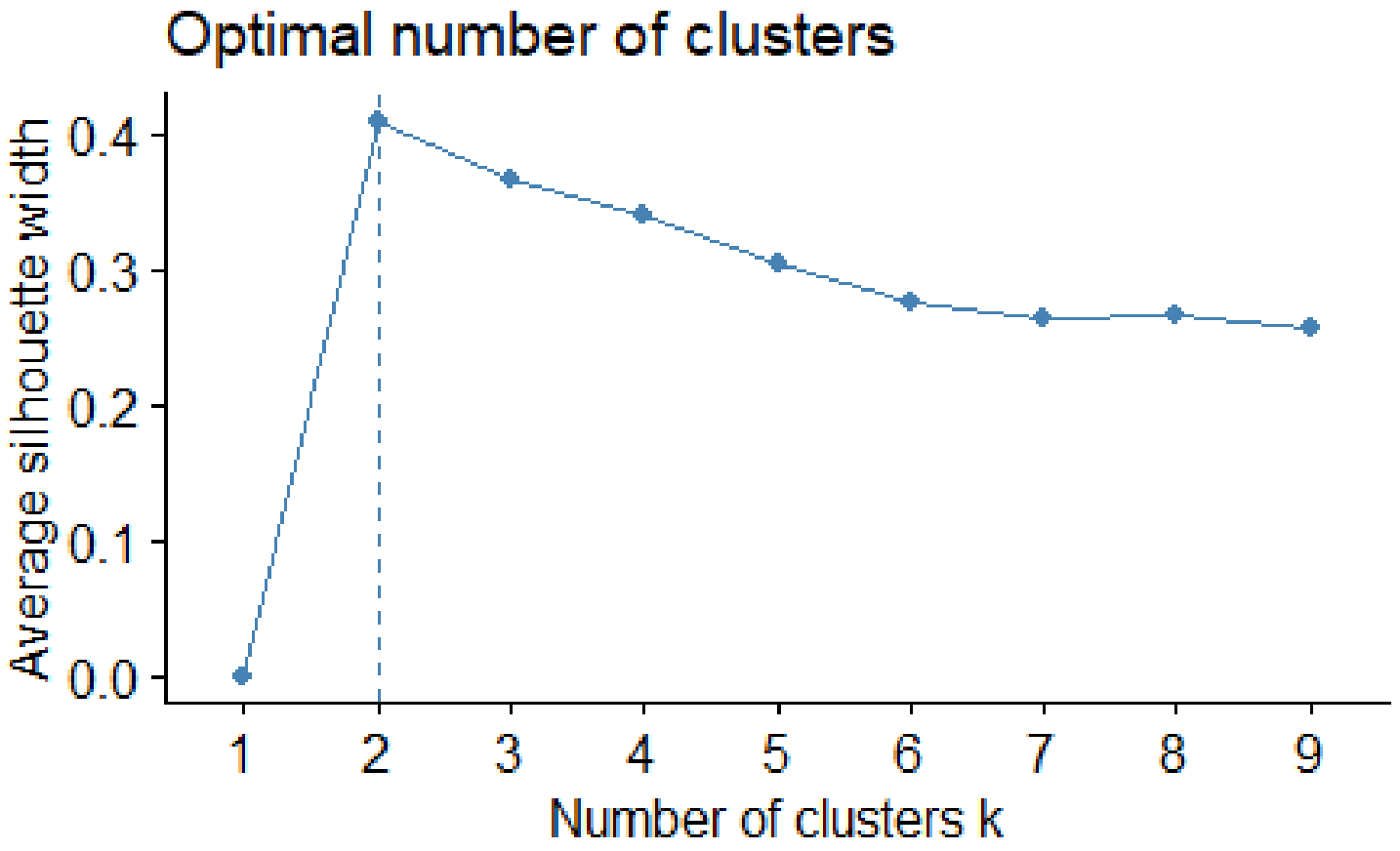
Silhouette method

Another method that can be used to define the number of clusters is the Silhouette method.

This method estimates how well each observation falls within its cluster (looks at the distance the point is to all other points in that cluster and compare it to the distance from that point to points in other clusters).

Want to find the number of clusters that maximize this ratio (get close to 1)

```
fviz_nbclust(arrest.scal, kmeans, method = "silhouette",k.max = 9)
```



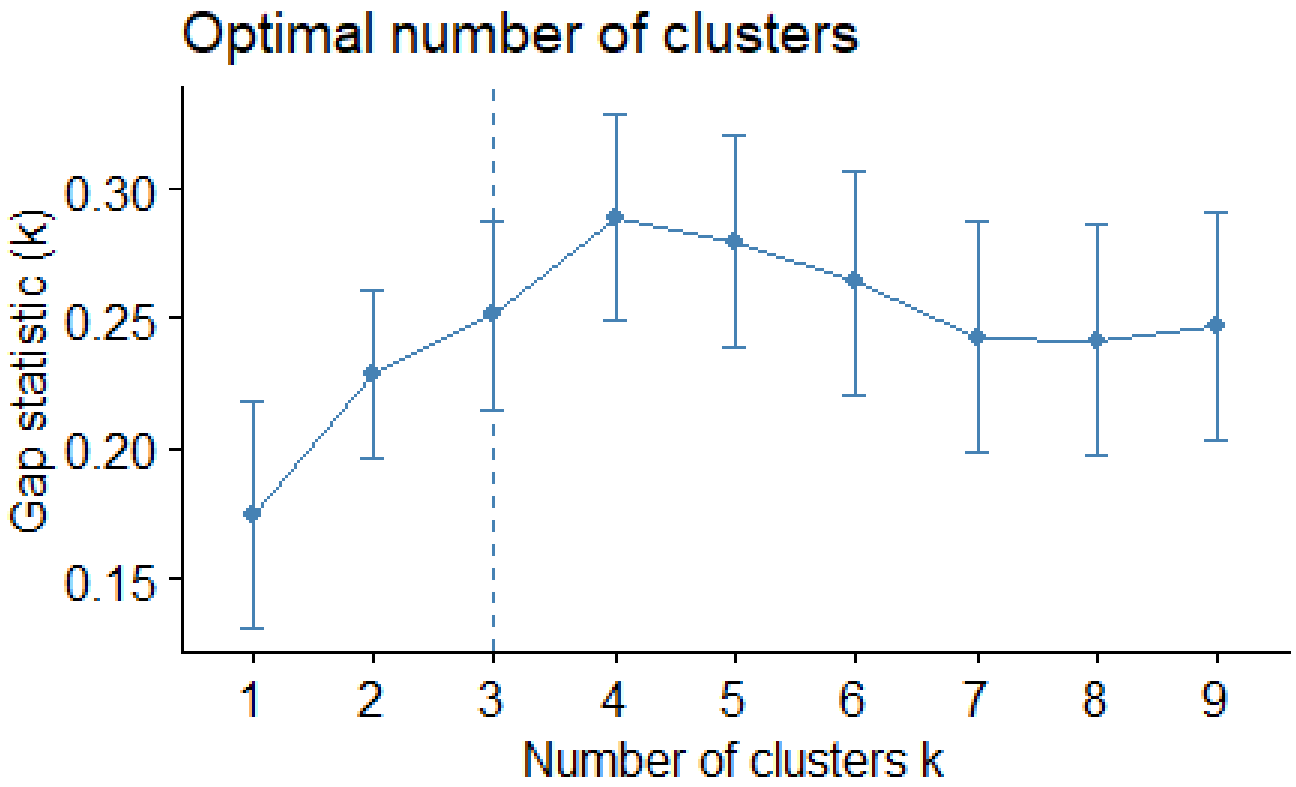
Gap statistic

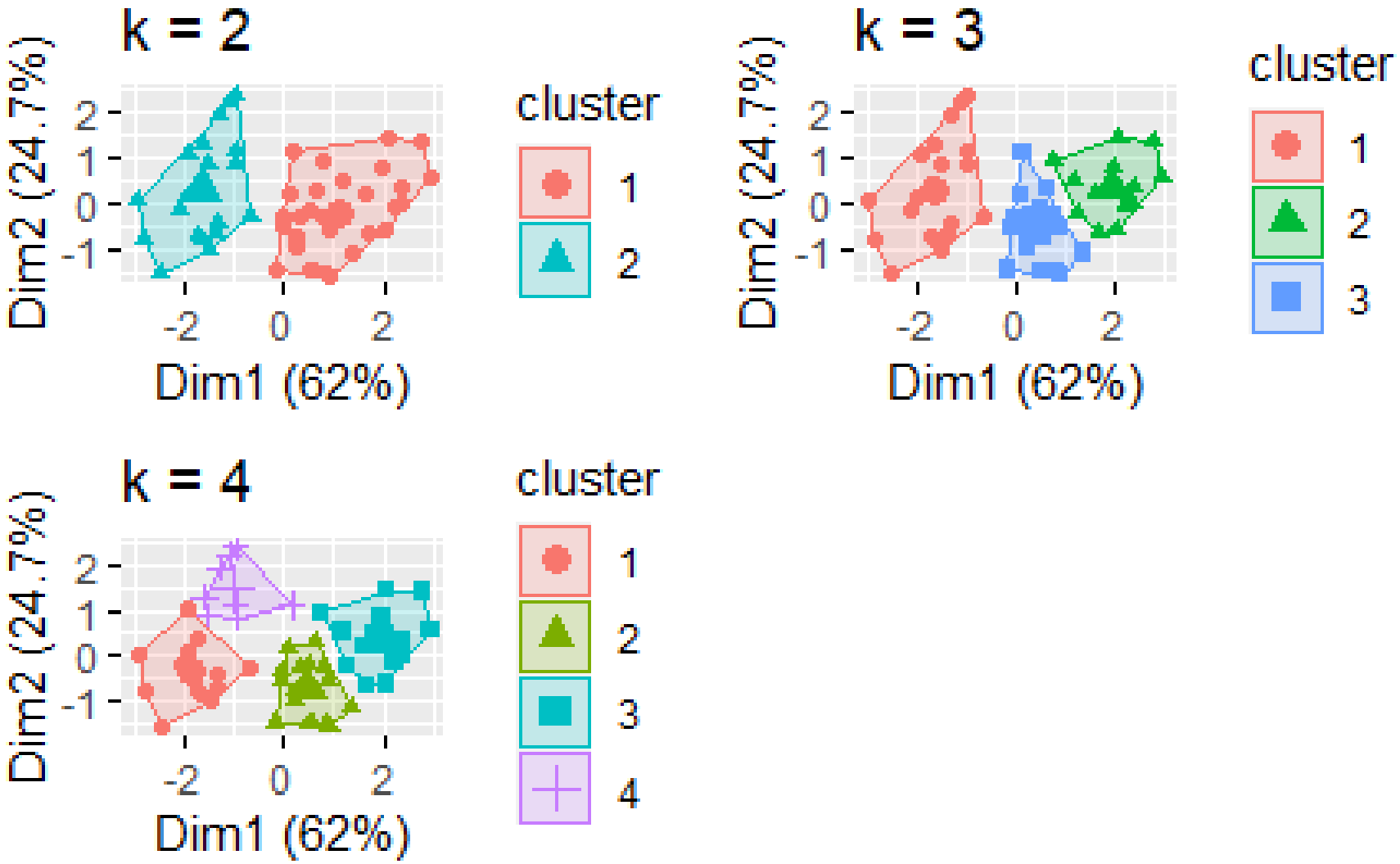
The gap statistic compares the total intracluster variation for different values of *k* with their expected values under null reference distribution of the data (i.e. a distribution with no obvious clustering).

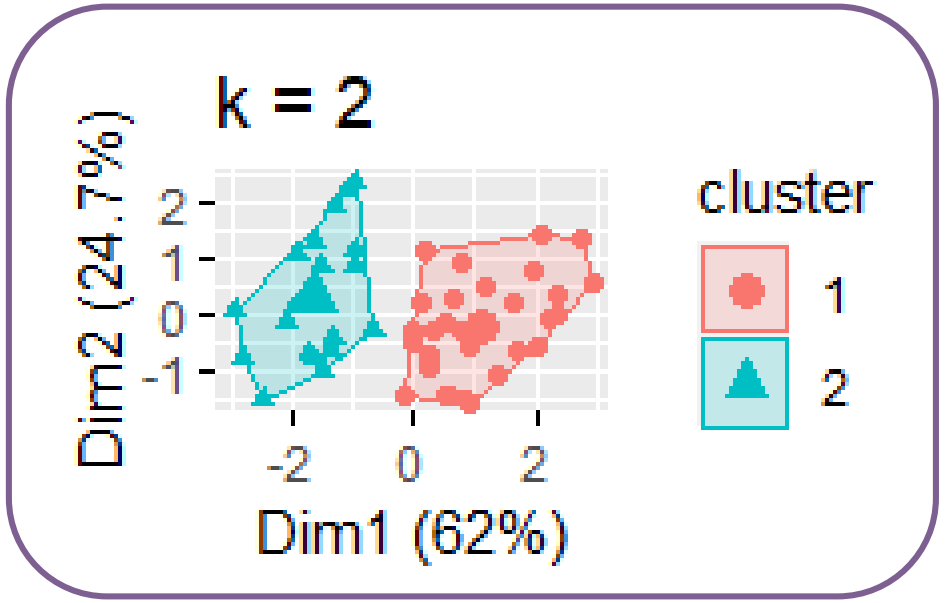
The reference data set is generated by sampling points uniformly from the minimum to the maximum value for each variable. We then choose B bootstrap samples from this reference distribution to compare to the data (compare using intracluster variation).

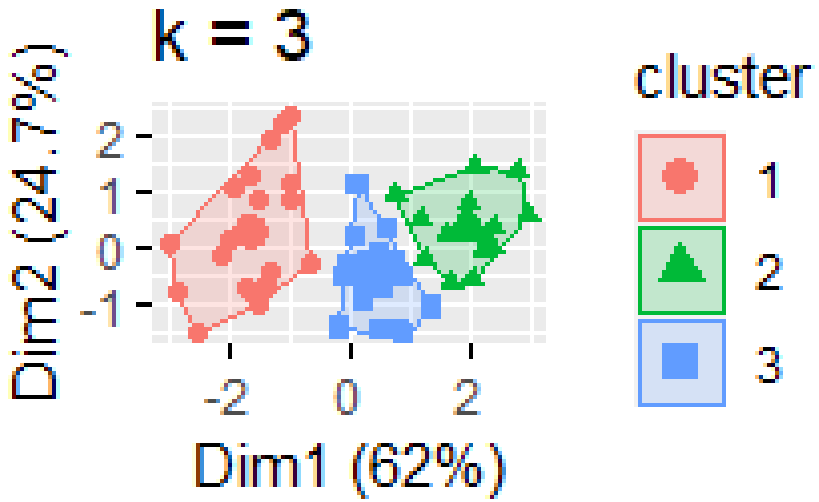
The “best” number of clusters is the value for k in which the gap statistics first exceeds a set critical level.

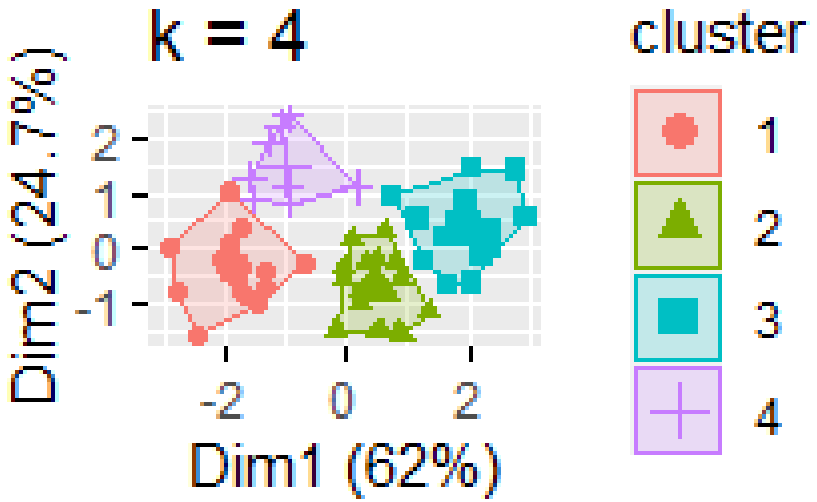
```
set.seed(123)
gap_stat = clusGap(arrest.scal, FUN = kmeans, nstart = 25, K.max = 9, B = 50)
fviz_gap_stat(gap_stat)
```




k = 2
Dim2 (24.7%)
Dim1 (62%)
cluster
1
2
k = 3
Dim2 (24.7%)
Dim1 (62%)
cluster
1
2
3
k = 4
Dim2 (24.7%)
Dim1 (62%)
cluster
1
2
3
4


k = 2
Dim2 (24.7%)
2
1
0
-1
-2
0
2
Dim1 (62%)
cluster
1
2


k = 3
Dim2 (24.7%)
2
1
0
-1
-2
0
2
Dim1 (62%)
cluster
1
2
3


k = 4
Dim2 (24.7%)
2
1
0
-1
-2
0
2
Dim1 (62%)
cluster
1
2
3
4

```
profile.kmeans=cbind(USArrests,k2$cluster)

all.k=profile.kmeans %>% group_by(k2$cluster) %>%

summarise(mean.assault=mean(Assault),mean.murder=m
ean(Murder),mean.rape=mean(Rape),mean.pop=mean(U
rbanPop))
```

NOW, go back to original data to summarize the clusters!!

cluster`	assault	murder	rape	pop
1	114.	4.87	15.9	63.6
2	255.	12.2	29.2	68.4

SAFE HAVENS

```
profile.kmeans=cbind(USArrests,k2$cluster)

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```

NOW, go back to original data to summarize the clusters!!

cluster`	assault	murder	rape	pop
1	114.	4.87	15.9	63.6
2	255.	12.2	29.2	68.4

RISKY BUSINESS

INTERESTING LIBRARY…outputs 24 measures for clustering

NbClust(arrest.scal,method="kmeans",min.nc=2,max.nc = 4)

```
*******************************************************************
*
* Among all indices:
* 13 proposed 2 as the best number of clusters
* 9 proposed 3 as the best number of clusters
* 2 proposed 4 as the best number of clusters

                   ***** Conclusion *****

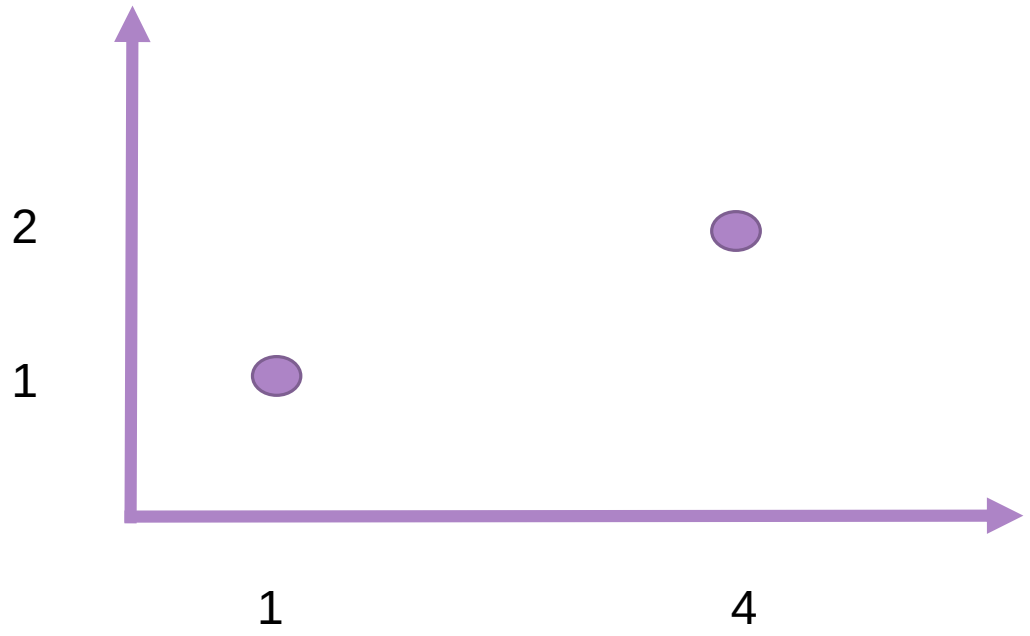
* According to the majority rule, the best number of
clusters is  2
```

http://www.jstatsoft.org/v61/i06/

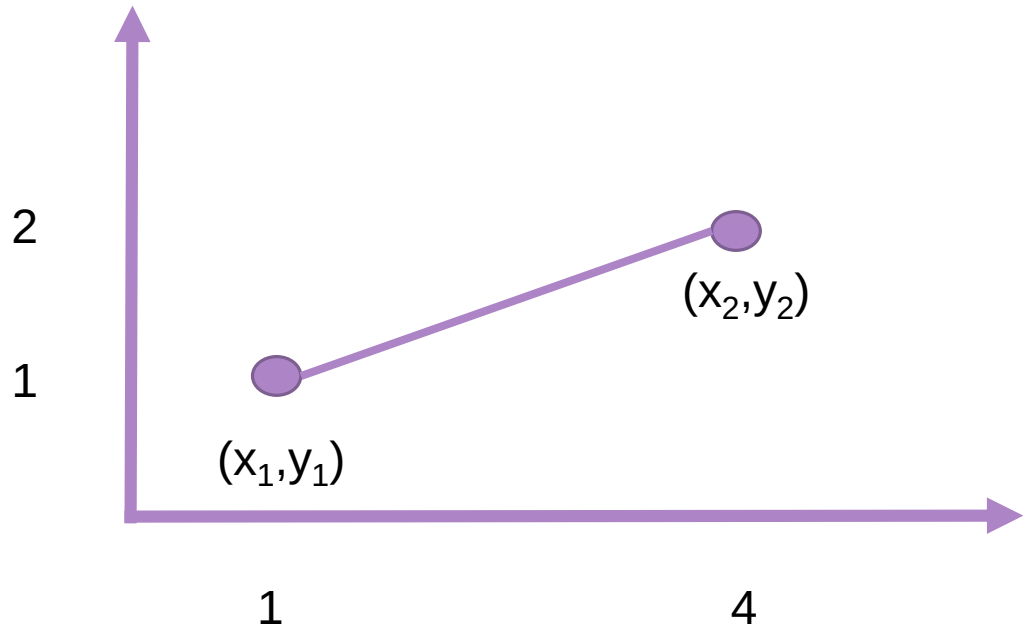
Hierarchical Clustering

AGGLOMERATIVE

Distance measures



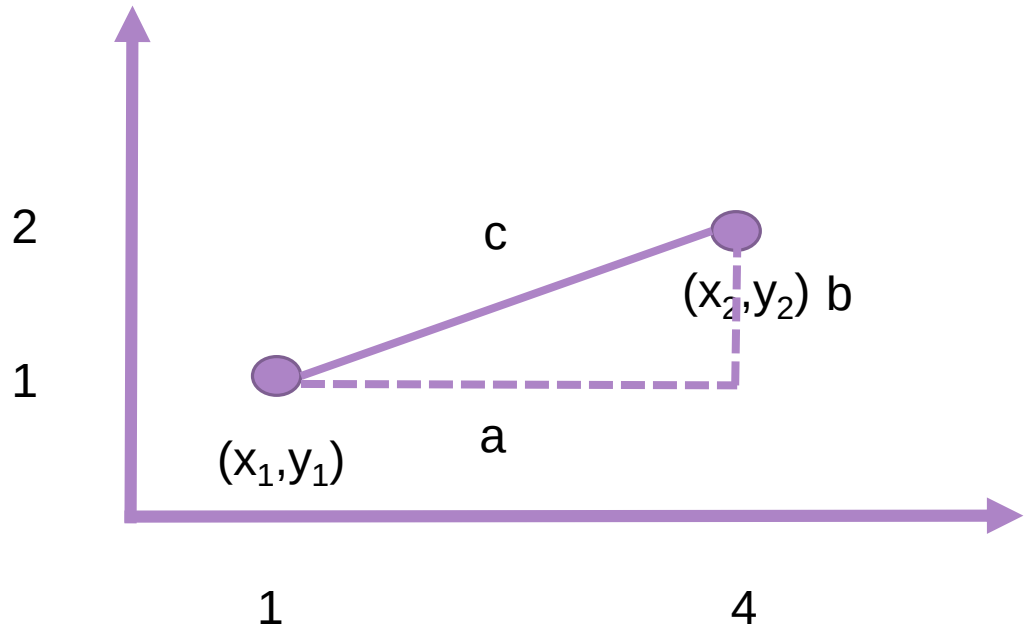
Distance measures



Euclidean distance between two points is:

$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Distance measures

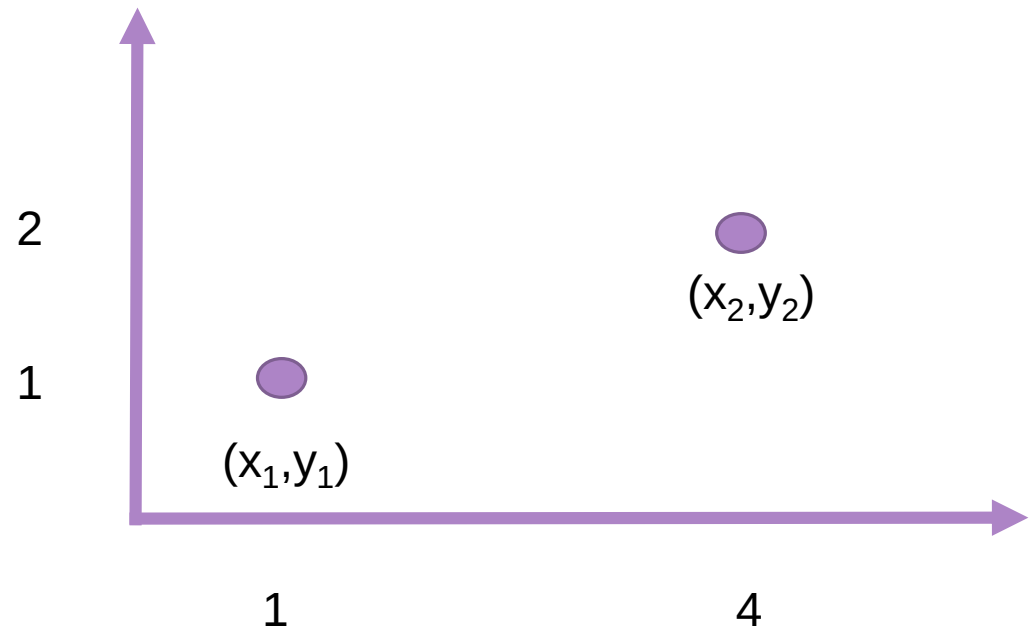


Euclidean distance between two points is:

$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Pythagorean theorem: c = $\sqrt{a^2 + b^2}$

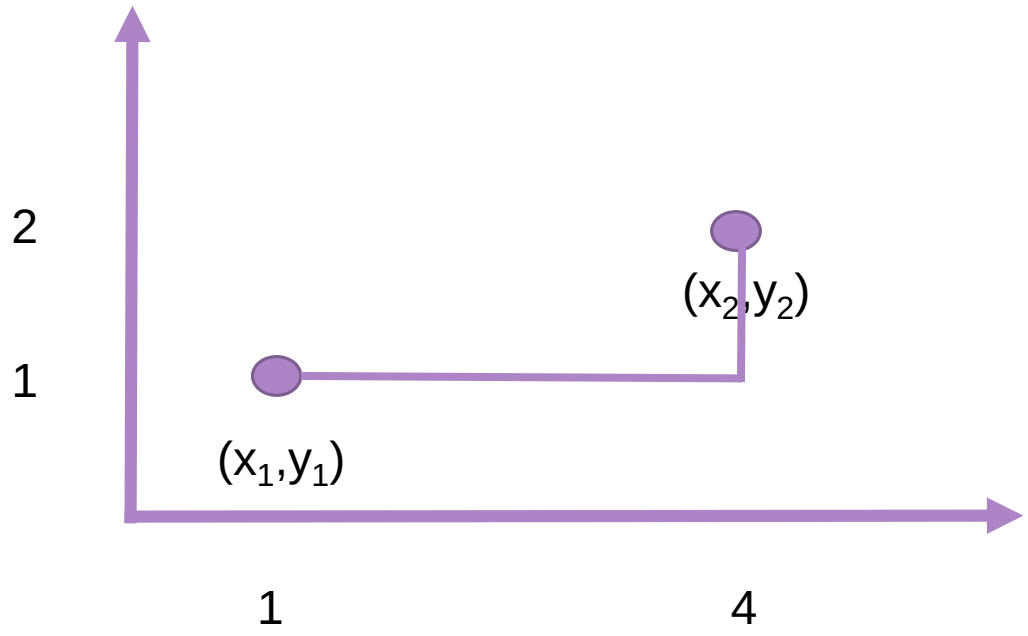
Distance measures



Manhattan distance between two points is:

$$|x_1 - x_2| + |y_1 - y_2|$$

Distance measures



Manhattan distance between two points is:

$$|x_1 - x_2| + |y_1 - y_2|$$

Agglomerative Hierarchical Algorithm

Each point starts as its own cluster (start with n clusters)

1. Calculate the distance between each point (using the specified distance measure)

2. Choose the two points that are the closest and form a cluster (now there are n-1 clusters)

3. Calculate distance between all single points and all clustered points

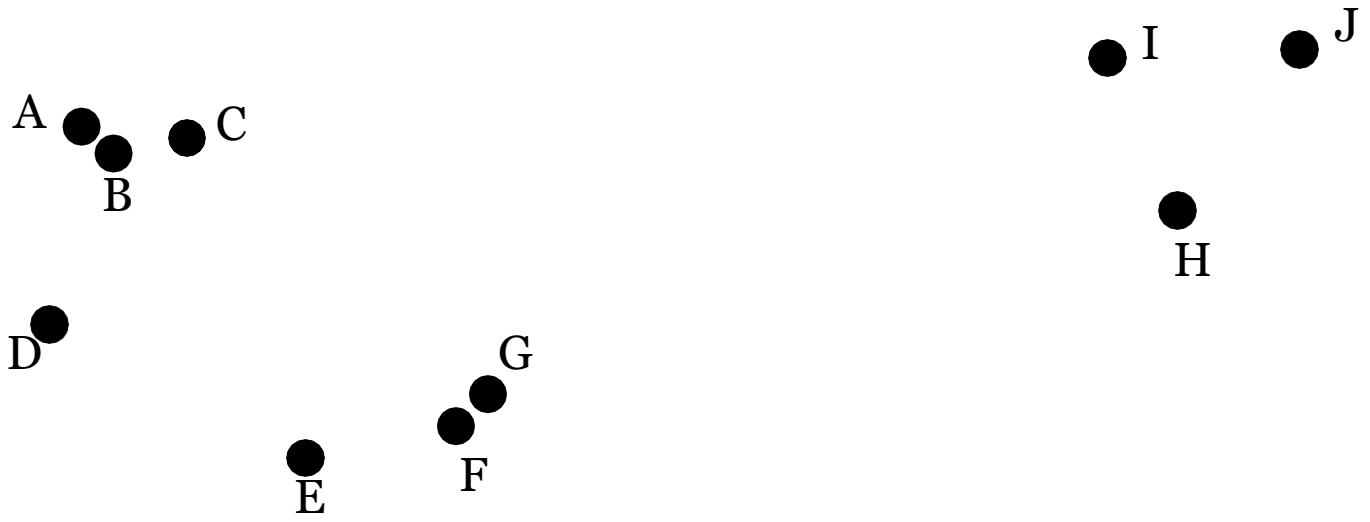
4. Find smallest distance and combine to form a cluster

Repeat steps 3 and 4 until all observations are in one cluster

Hierarchical Clustering

(Agglomerative)

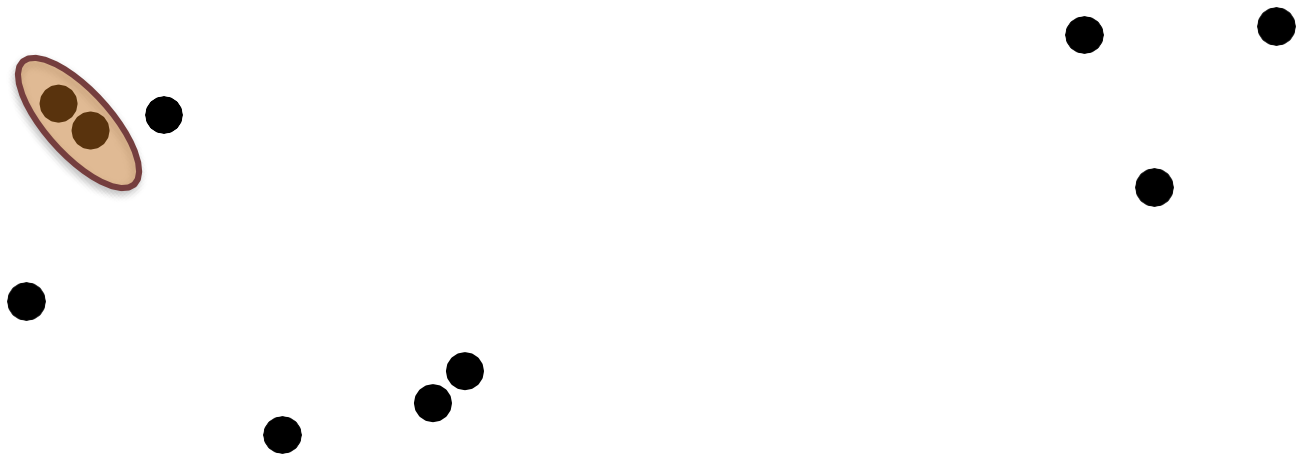
Some Data



Hierarchical Clustering

(Agglomerative)

First Step



Hierarchical Clustering

(Agglomerative)

Second Step

Hierarchical Clustering

(Agglomerative)

Third Step

Hierarchical Clustering

(Agglomerative)

Fourth Step

Hierarchical Clustering

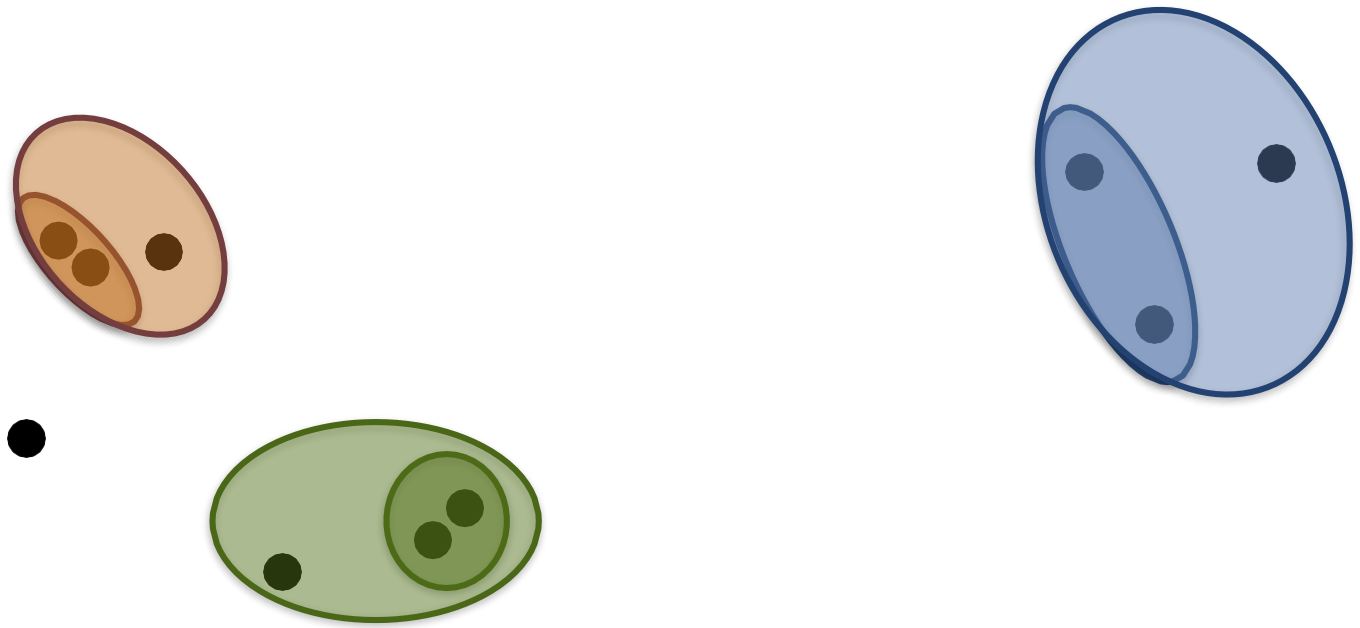
(Agglomerative)

Fifth Step

Hierarchical Clustering

(Agglomerative)

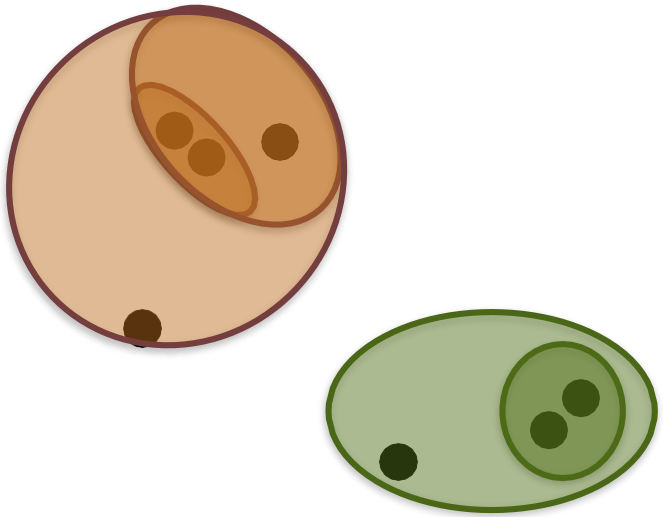
Sixth Step

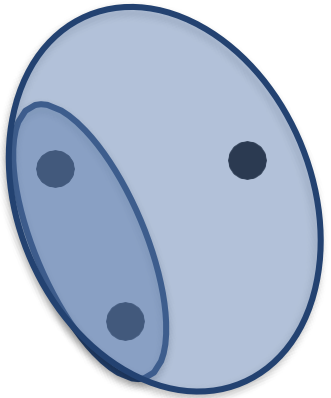


Hierarchical Clustering

(Agglomerative)

Seventh Step



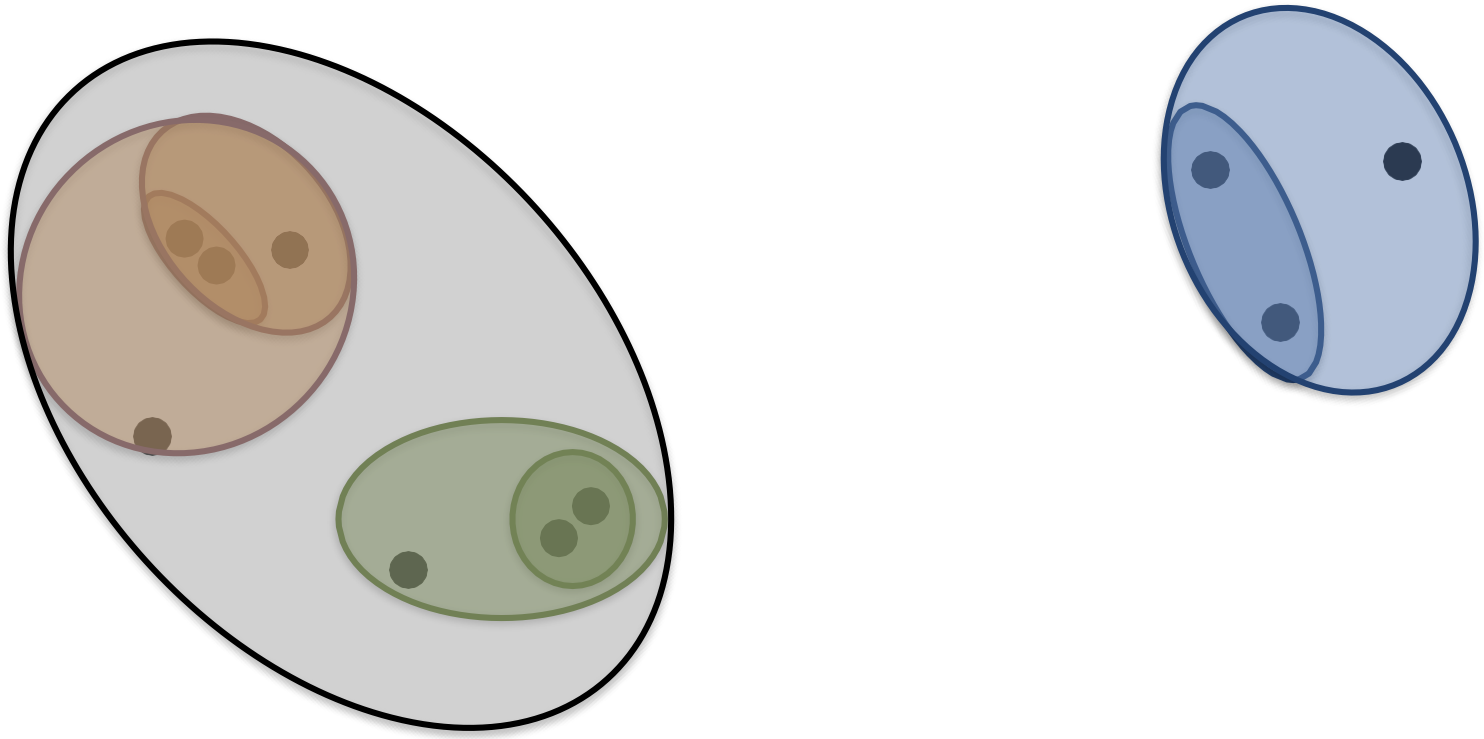


We might have known that we only wanted 3 clusters, in which case we'd stop once we had 3.

Hierarchical Clustering

(Agglomerative)

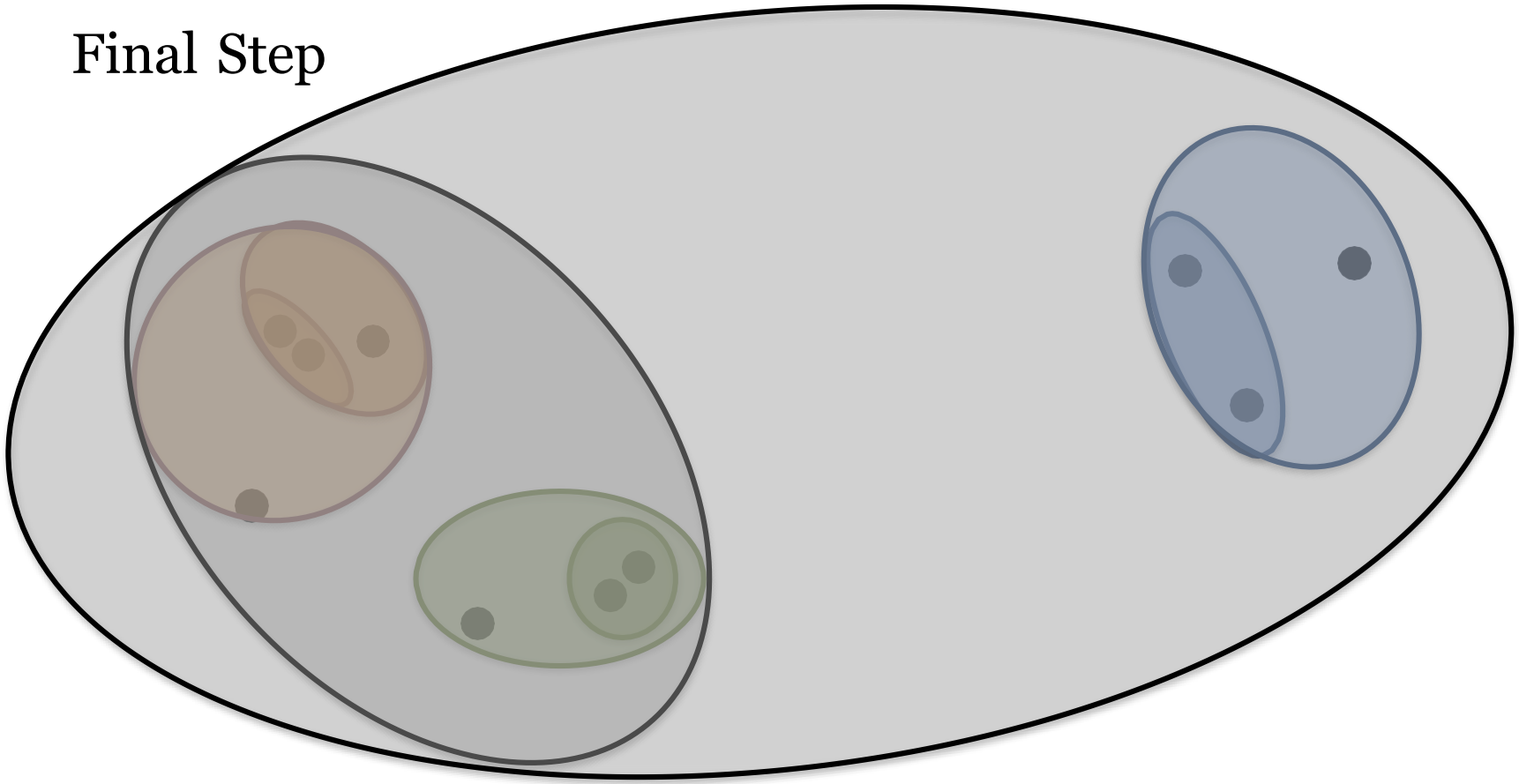
Eighth Step



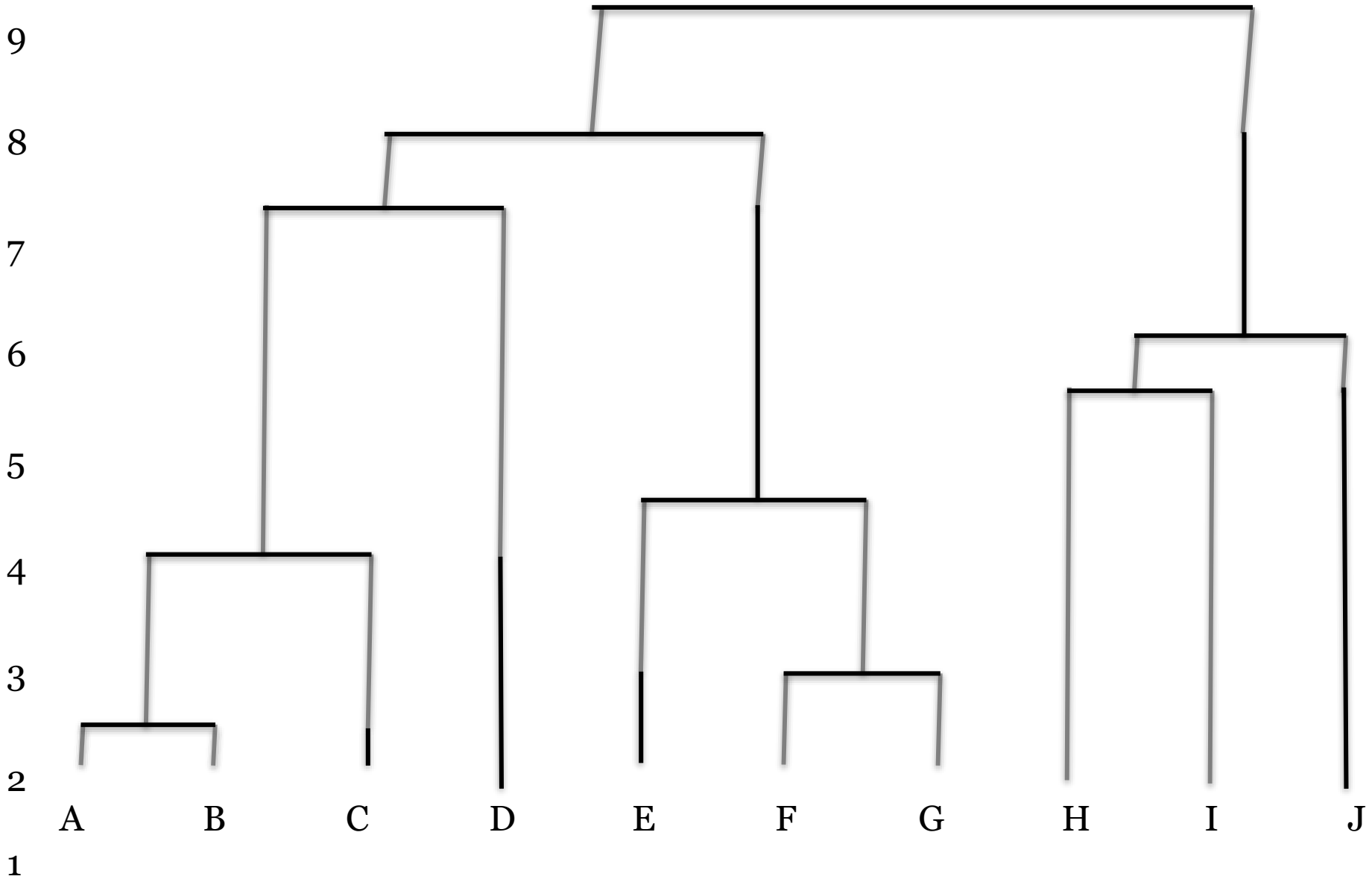
Hierarchical Clustering

(Agglomerative)

Final Step



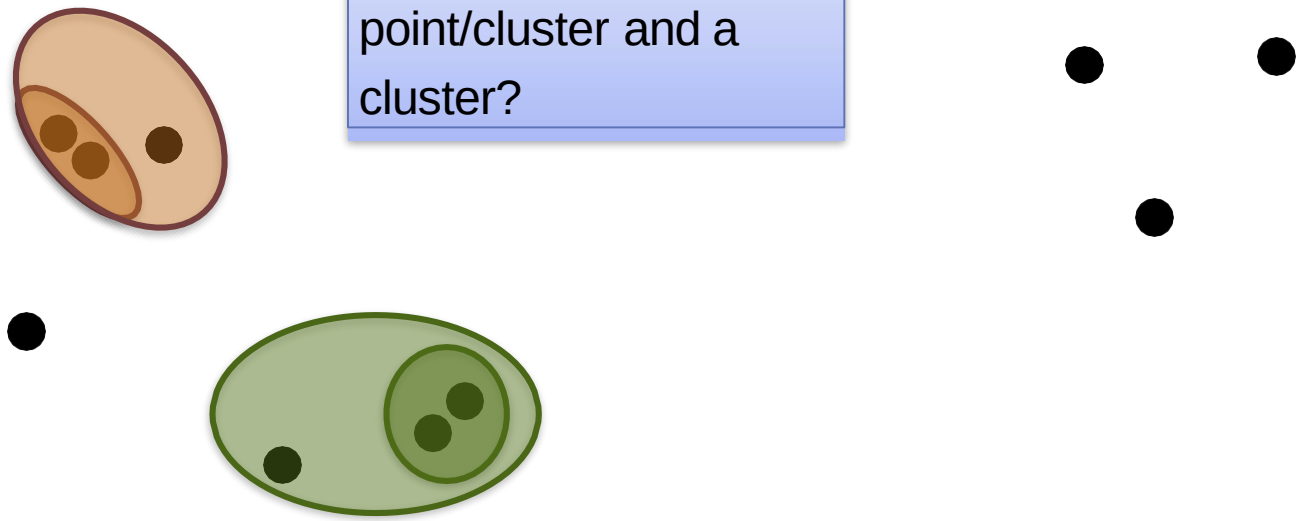
Resulting Dendrogram (not to scale)



Linkages

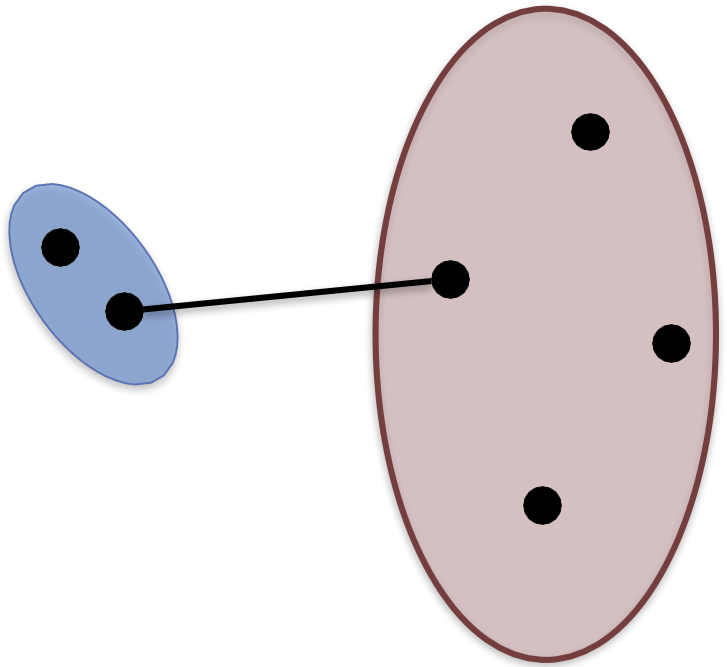
Which clusters/points are closest to each other?

How do I measure the distance between a point/cluster and a cluster?



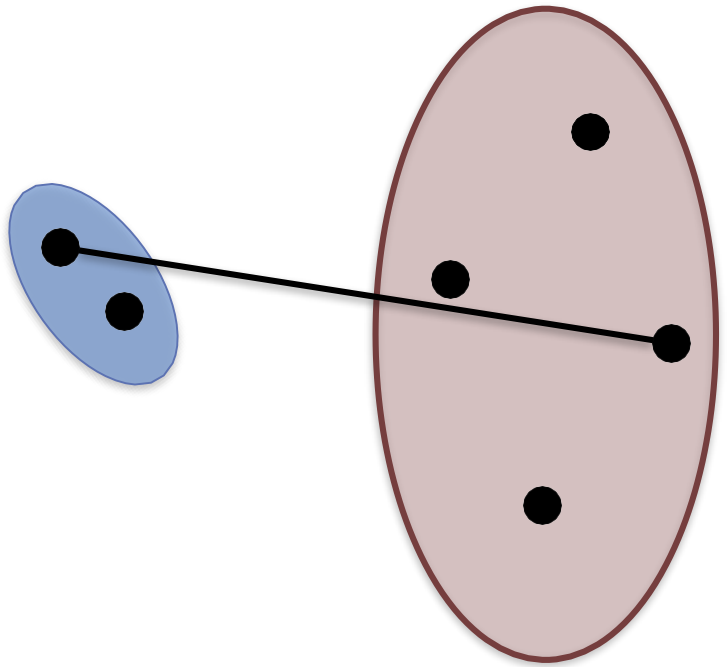
Linkages

Single Linkage: Distance between the closest points in the clusters.



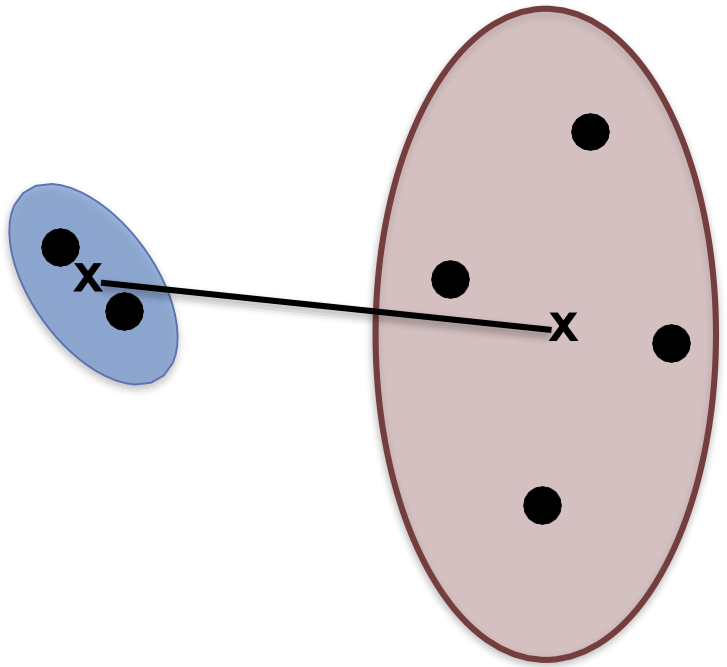
Linkages

Complete Linkage: Distance between the farthest points in the clusters.



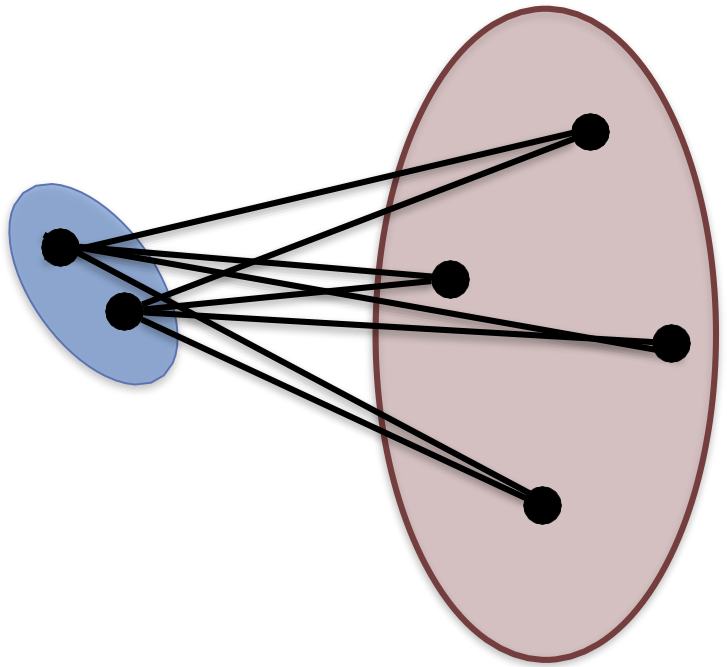
Linkages

Centroid Linkage: Distance between the centroids (means) of each cluster.



Linkages

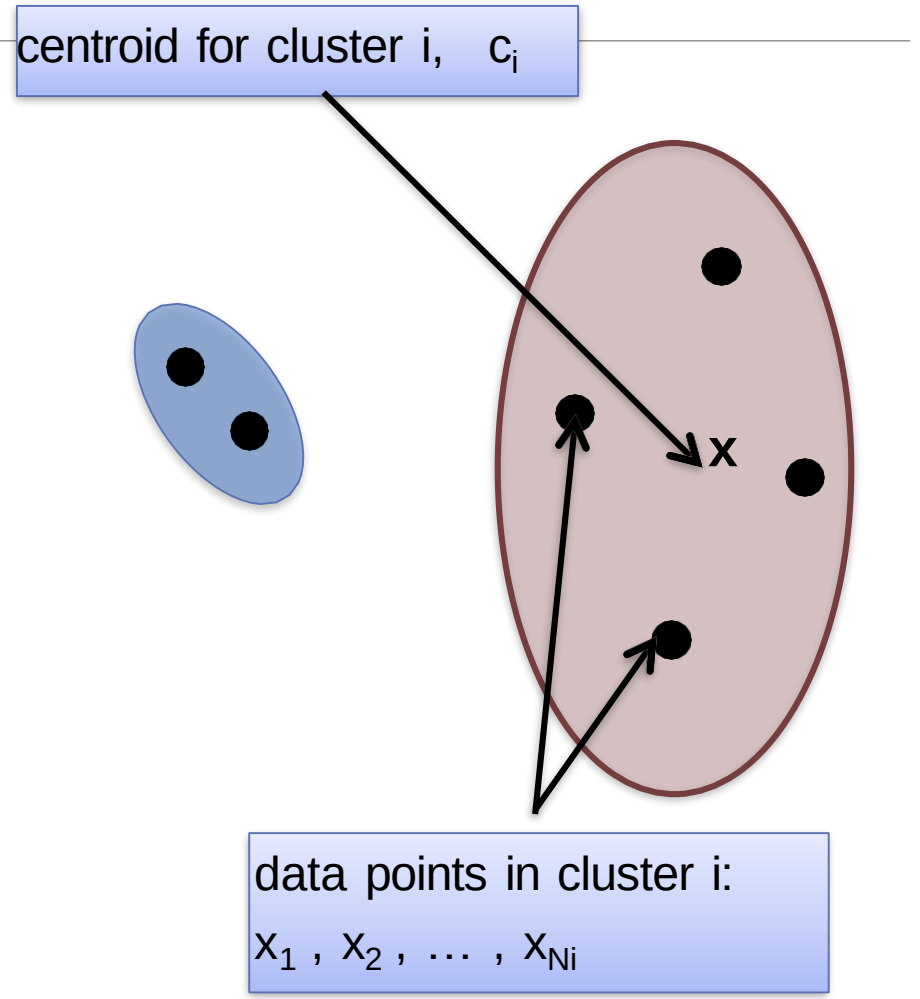
Average Linkage: Average distance between all points in the clusters.



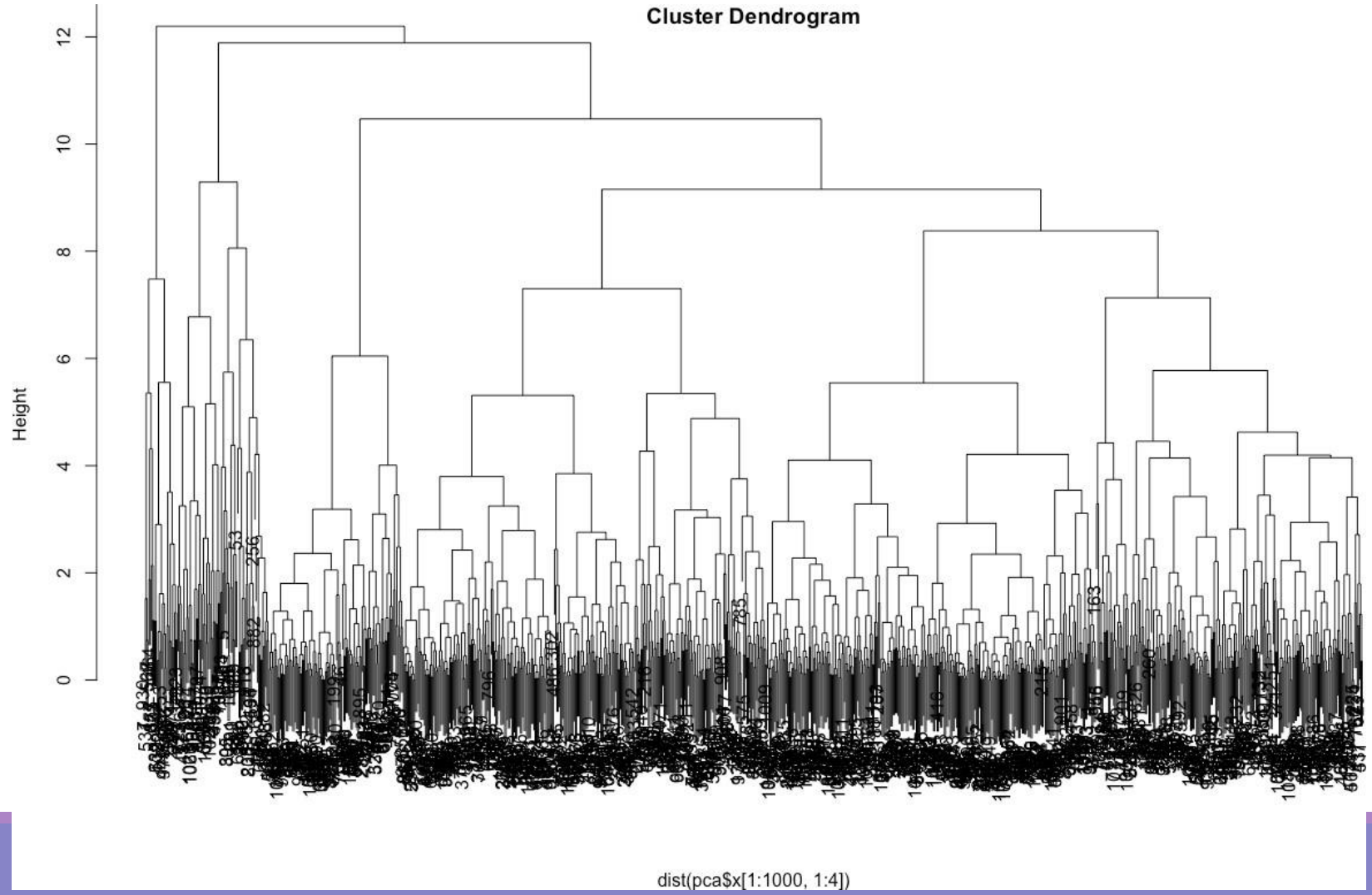
Linkages

Ward's Method: Minimize SSE.

$$\sum_{j=1}^{N_i} \|\mathbf{x}_j - \mathbf{c}_i\|_2$$



Hierarchical Clustering Summary



Hierarchical Clustering Summary

Disadvantages

- Computationally intensive, large storage requirements, **not good for large datasets**
- **Lacks global objective** function: only makes decision based on local criteria.
- **Merging decisions are final**. Once a point is assigned to a cluster, it stays there.
- **Poor performance on noisy** or high-dimensional **data** like text.

Advantages

- **Creates hierarchy (dendrogram)** that can help choose the number of clusters and examine how those clusters relate to each other.
- **Do NOT need to know number of clusters apriori**

US Arrest data

Number of different hierarchical packages in R

We will focus on the cluster package (start with agnes…Agglomerative “Nesting” Hierarchical Clustering) and the Nbclust package

In the cluster package, recommend calculating distances outside of package (more options!!). In this case, you will pass the clustering algorithm the DISTANCE matrix!

Options

DISTANCE (IN DIST)

Euclidean

Manhattan

Maximum

Canberra

Binary

Minkowski

LINKAGE (IN CLUSTER ALGORITHM)

Average

Single

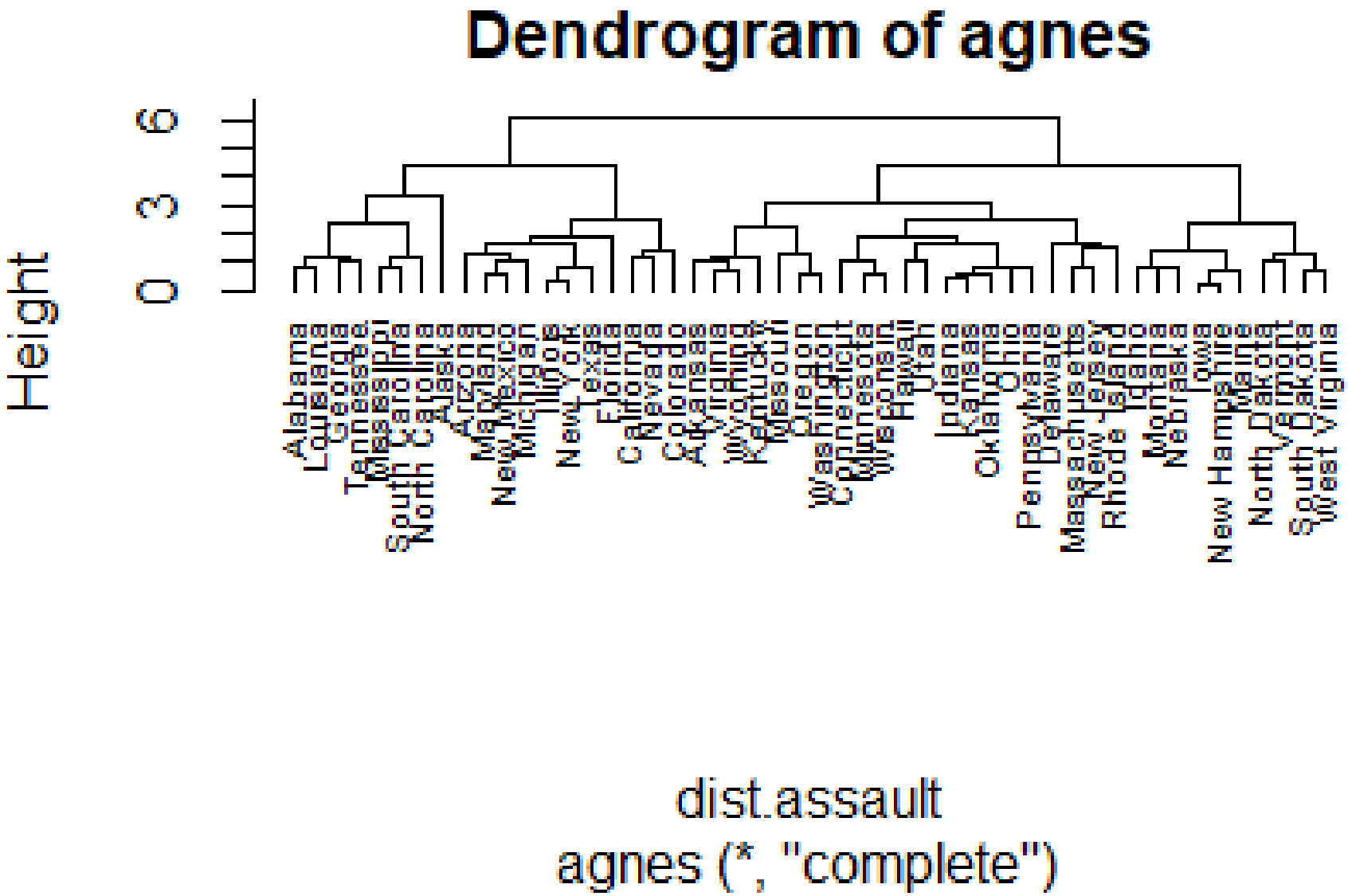
Complete

Ward

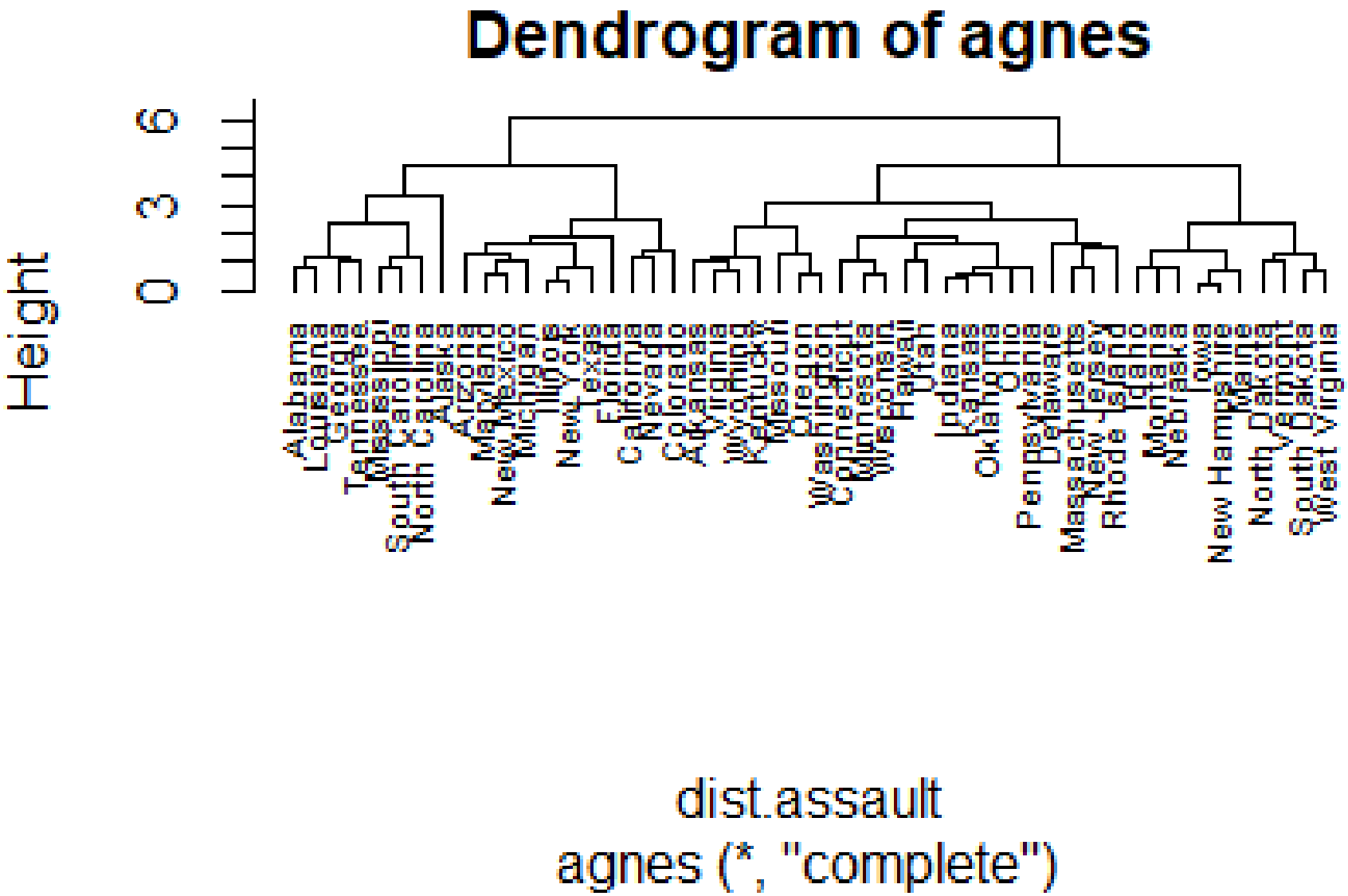
Weighted

Some more advanced options…

```
dist.assault=dist(arrest.scal,method = "euclidean")
h1.comp.eucl=agnes(dist.assault,method="complete")
pltree(h1.comp.eucl, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
```



```
dist.assault=dist(arrest.scal,method = "euclidean")
h1.comp.eucl=agnes(dist.assault,method="complete")
pltree(h1.comp.eucl, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
```



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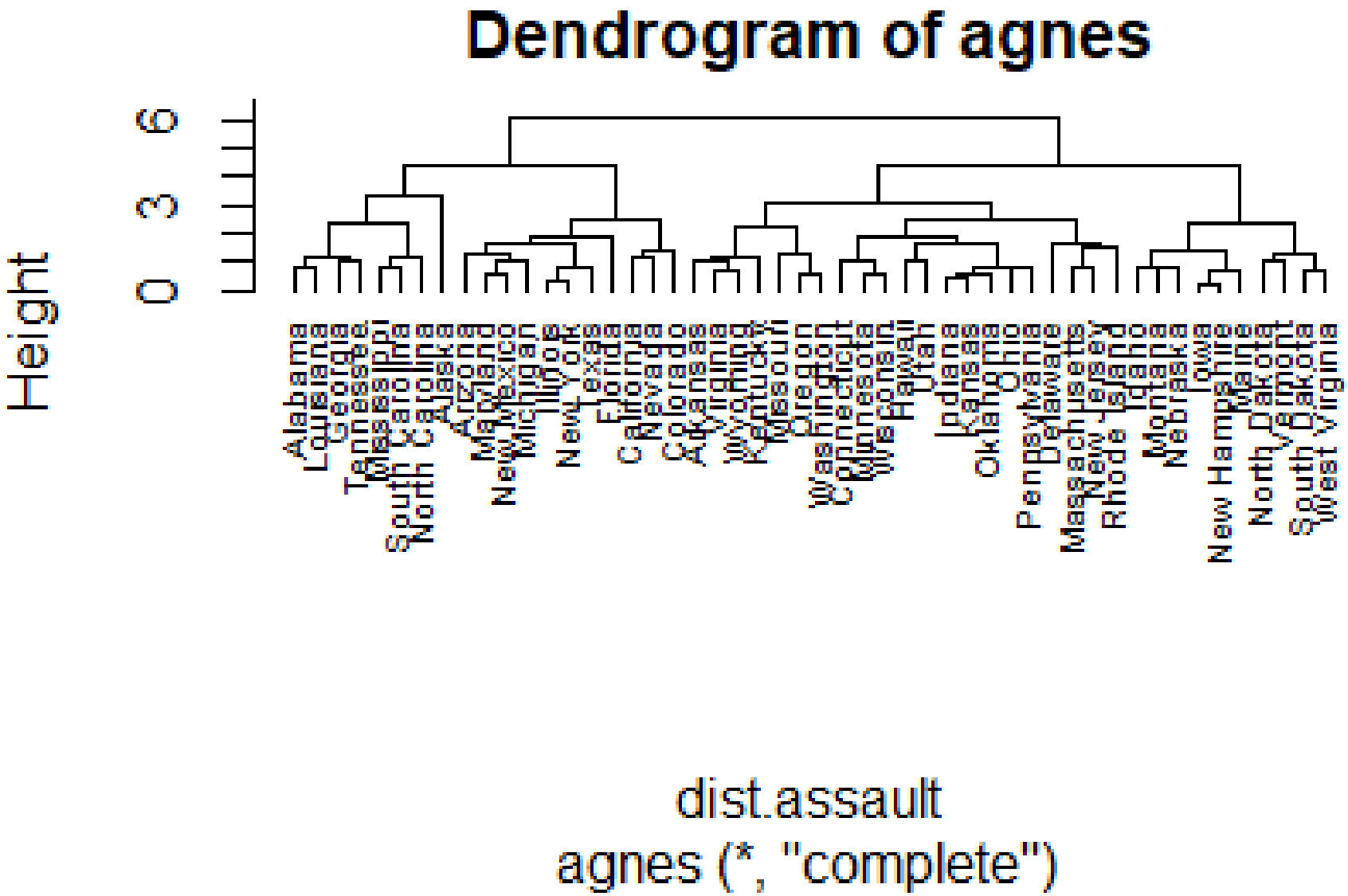

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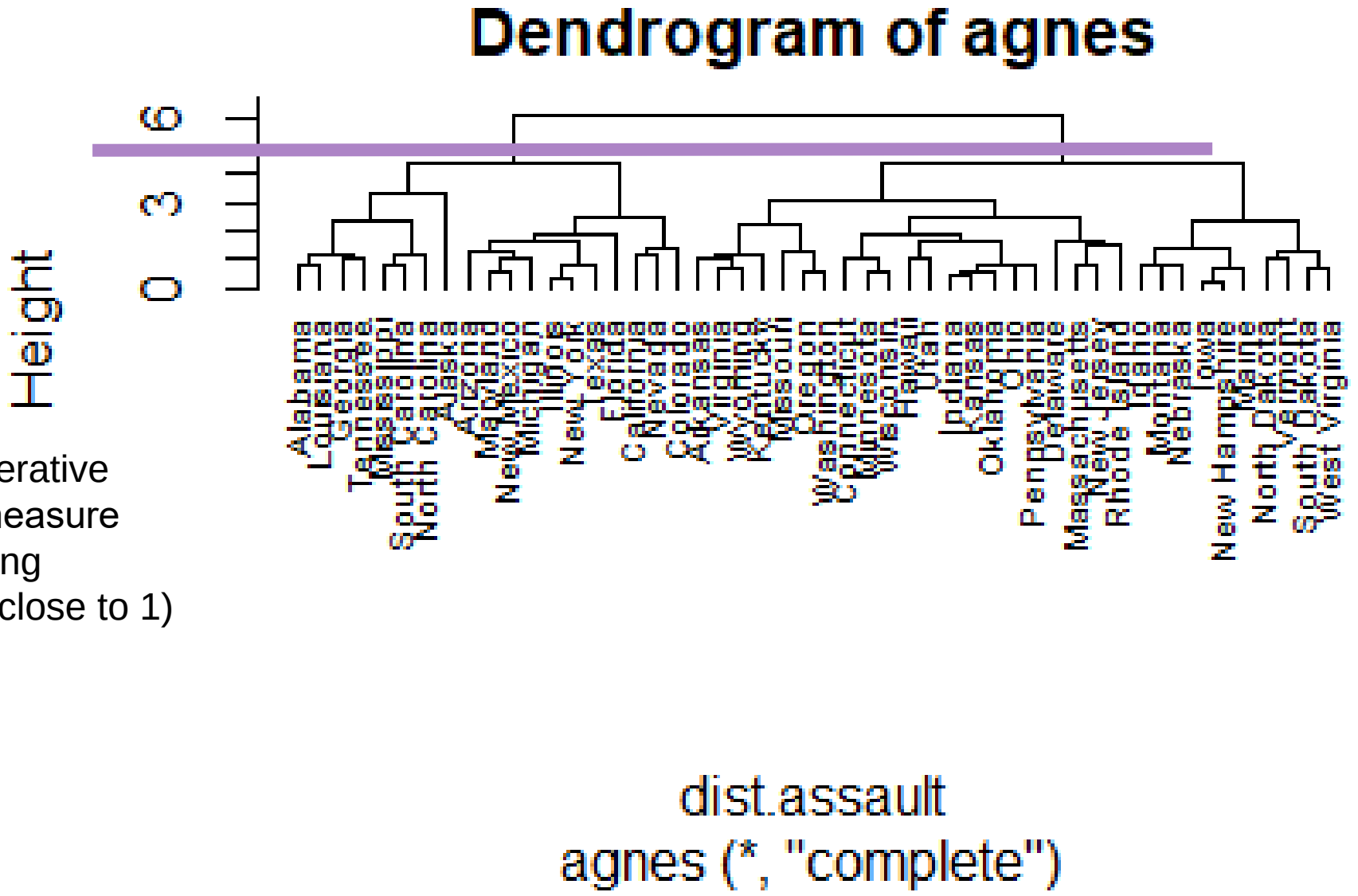
h1.comp.eucl=agnes(dist.assault,method="complete")
pltree(h1.comp.eucl, cex = 0.6, hang = -1, main = "Dendrogram of agnes")
```



h1.comp.eucl$ac
[1] 0.8531583

This is called the agglomerative coefficient…provides a measure of how strong the clustering structure is (want values close to 1)

Results from hierarchical clustering

You will most likely get different results when

1. You use different distance metrics
2. You use different linkage methods
3. Use scaled data versus PCA versus different types of standardization

Create algorithm to run through possibilities:

```
m <- c( "average", "single", "complete", "ward")
names(m) <- c( "average", "single", "complete", "ward")

# function to compute coefficient
ac <- function(x) {
  agnes(dist.assault, method = x)$ac
}

map_dbl(m, ac)
```

```
  average    single  complete      ward 
0.7379371 0.6276128 0.8531583 0.9346210 
```

CAUTION

Want best algorithm for business sense (creates the most sensible clusters). This might not be the best mathematical cluster!! You will need to explore profiles to see which makes the most sense!!

Create clusters in hierarchical

```
h2=agnes(dist.assault,method="ward")
h2_clus <- cutree(h2, k = 2)
H2_clus
```

```
[1] 1 1 1 2 1 1 2 2 1 1 2 2 1 2 2 2 2 1 2 1 2 1 2 1 2 2 2 1 2
[30] 2 1 1 1 2 2 2 2 2 2 1 2 1 1 2 2 2 2 2 2 2
```

Other options in cluster package

Diana – divisive hierarchical clustering

Pam – Partitioning around Medoids

Clara - Clustering Large applications

Mona - Monothetic Analysis Clustering of Binary Variables

NbClust with hierarchical clustering

NbClust(arrest.scal,distance="euclidean",method="complete",min.nc=2,max.nc = 4)

```
*******************************************************************
*
* Among all indices:
* 9 proposed 2 as the best number of clusters
* 9 proposed 3 as the best number of clusters
* 5 proposed 4 as the best number of clusters

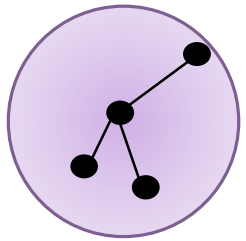
                   ***** Conclusion *****

* According to the majority rule, the best number of
clusters is  2
```

DBSCAN

Density-based spatial clustering of applications with noise

Groups together points that are close to each other based on a distance measure, a minimum number of points (“neighbors”) and a “neighborhood about each point”



Points not “near” other points will be deemed an “outlier”
A “cluster” of points must have a minimum number of points around it to be considered a cluster

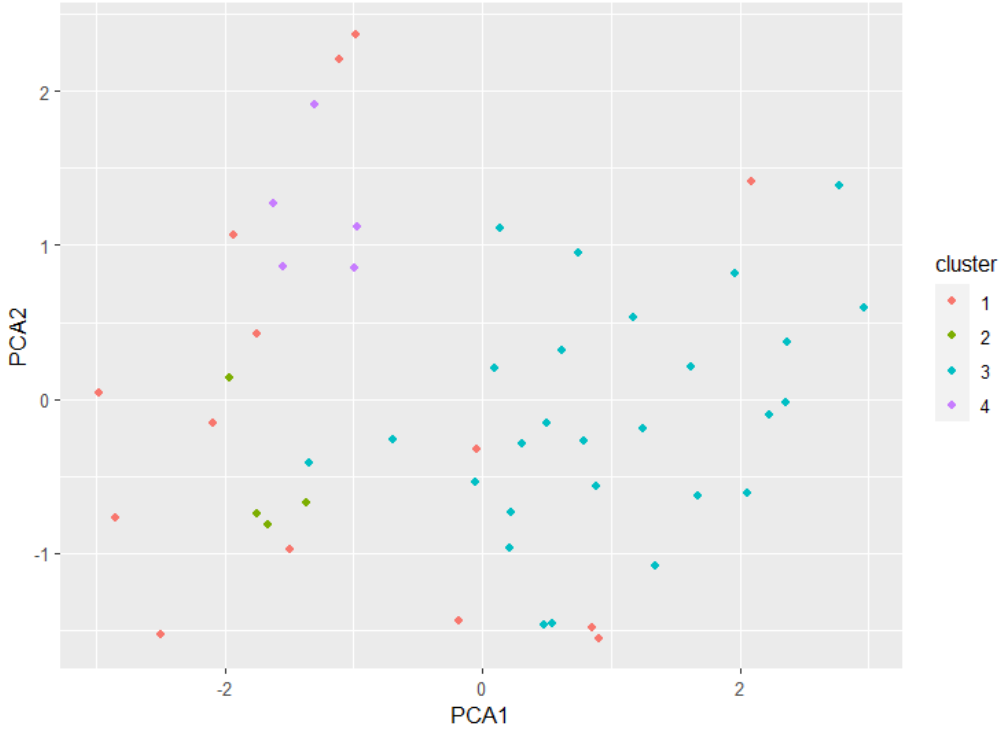
Example how it works….

https://www.kdnuggets.com/2020/04/dbscan-clustering-algorithm-machine-learning.html

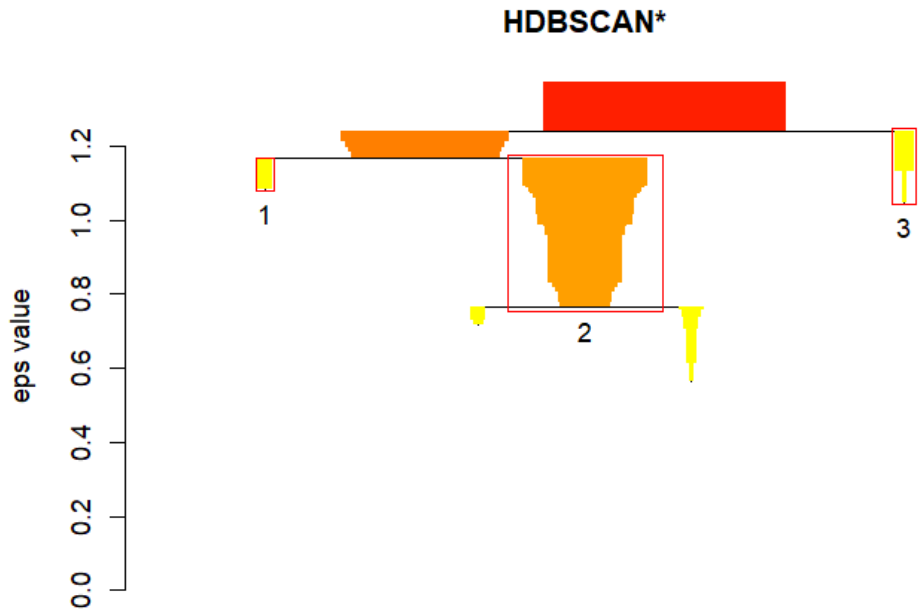
HDBSCAN (hierarchical)

minPts – usually try d +1 (d=number of dimensions…here d=4….d=4 works better than d=5)

```
scan1<-hdbscan(arrest.scal,minPts=4)
pca_ex=prcomp(arrest.scal,scale=F)
scan1data=cbind.data.frame(pca_ex$x[,1],pca_ex$x[
,2],as.factor(scan1$cluster+1))
colnames(scan1data)=c("PCA1","PCA2","cluster")
ggplot(scan1data,aes(x=PCA1,y=PCA2,color=cluster
))+geom_point()+ scale_fill_brewer(palette =
"Dark2")
```



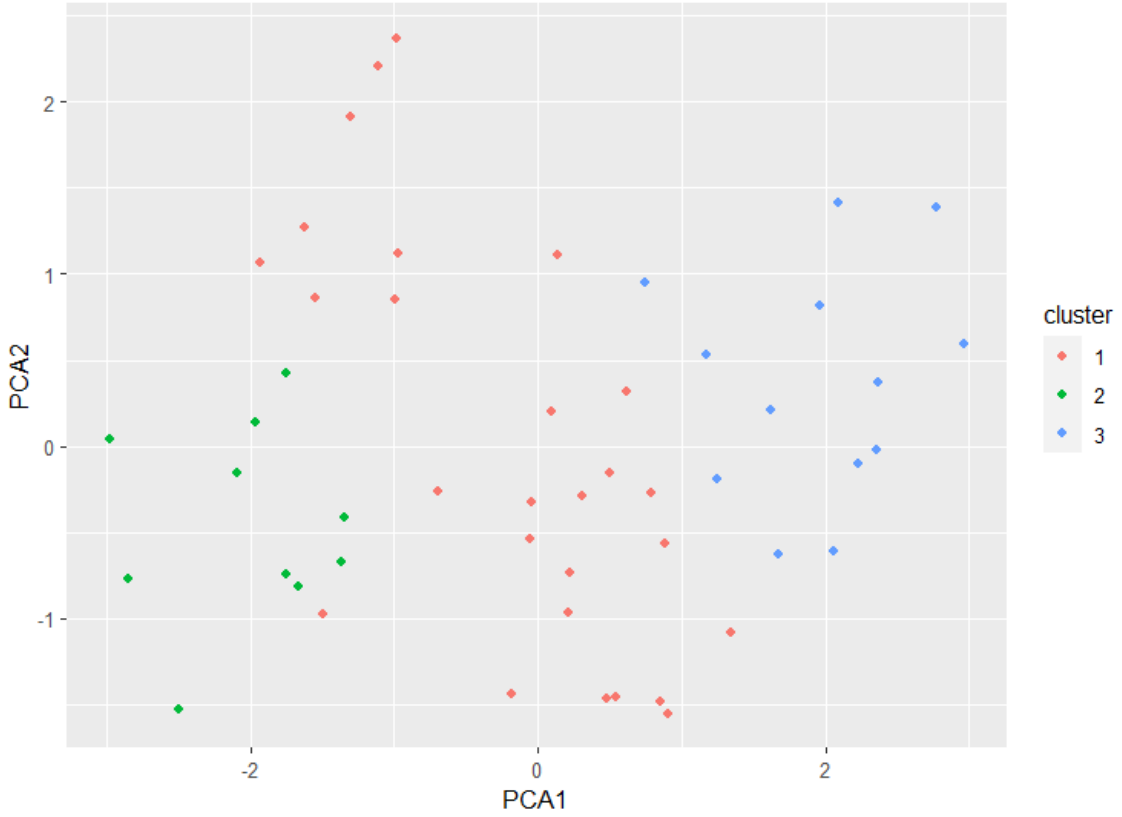
plot(scan1,show_flat=T)



https://hdbscan.readthedocs.io/en/latest/how_hdbscan_works.html

```
d=dist(arrest.scal,method = "canberra")
res.dbscan=dbscan(d,eps=1.2,minPts=4)
res.dbscan

scan1data=cbind.data.frame(pca_ex$x[,1],pca_ex$x[,2],a
s.factor(res.dbscan$cluster+1))
colnames(scan1data)=c("PCA1","PCA2","cluster")
ggplot(scan1data,aes(x=PCA1,y=PCA2,color=cluster))+g
eom_point()+ scale_fill_brewer(palette = "Dark2")
```



Variable Clustering

Variable Clustering in R

Goal: We would like to cluster variables that are related (reduce reduncies/multicollinearity)

This is a form of dimension reduction (can aid in analysis)

In R, the package is ClustOfVar…you can do hierarchical clustering (agglomerative in R….SAS and Python do divisive) or kmeans

Uses eigenvalues to identify similar variables and to assess the goodness of the partition

Can handle quantitative and qualitative variables (you need to split these into two data matrices first)

Example

TELCO CHURN DATA

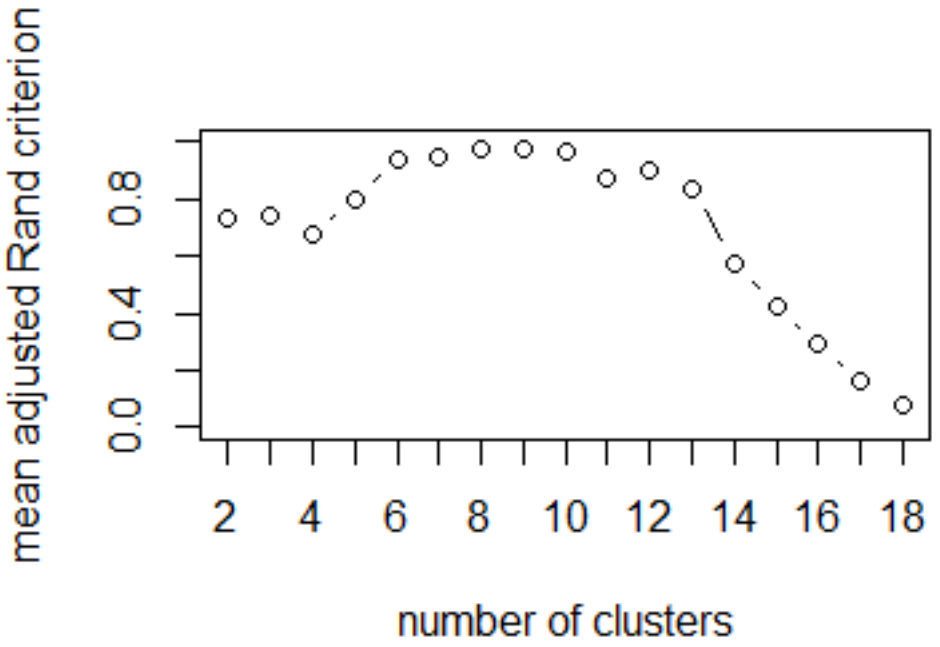
Preprossing

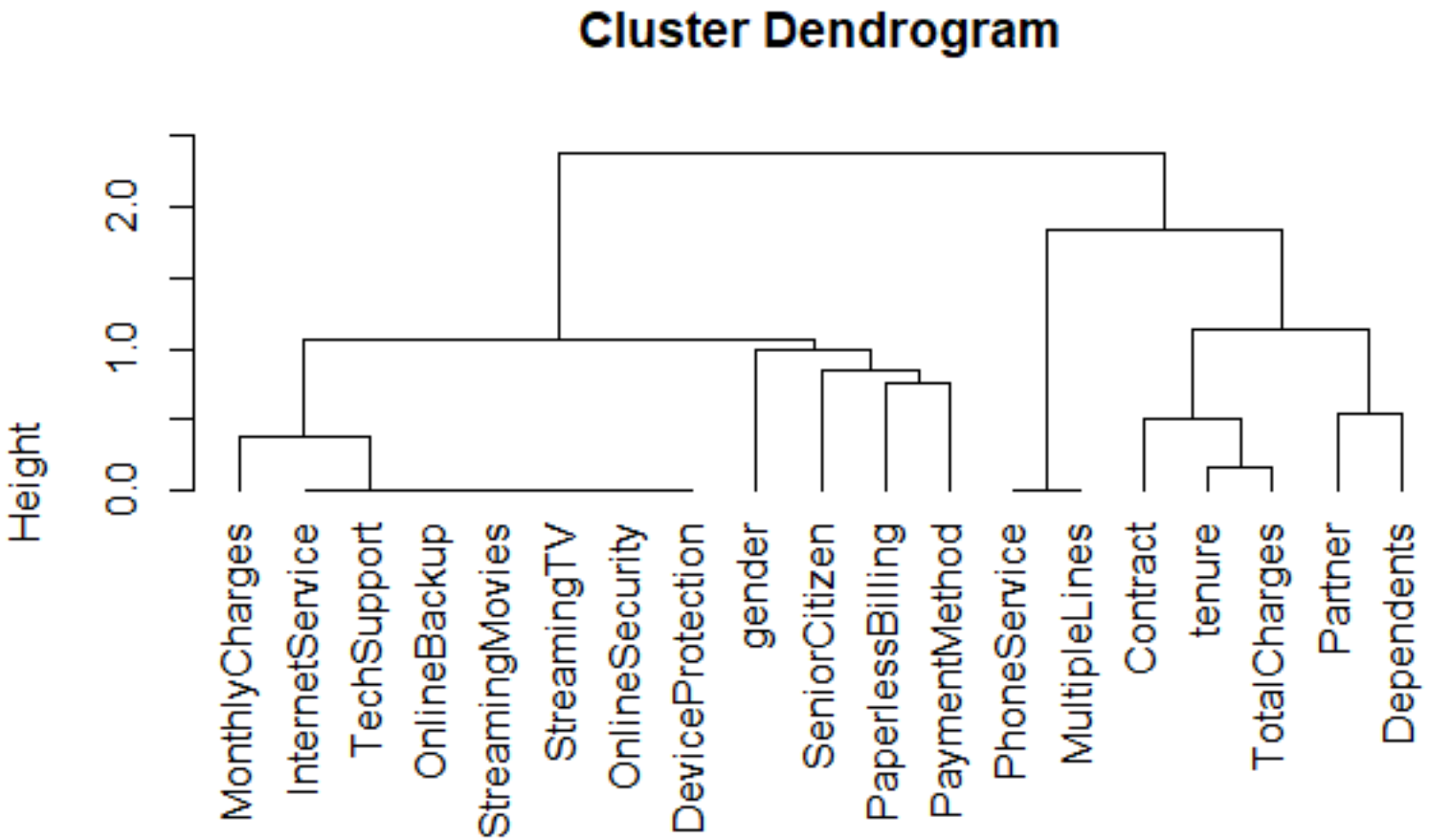
Split into quantitative and qualitative variables (no need to dummy code…all is done within algorithm)

Impute missing values (in this case, makes sense to replace missing values in total charges with 0)

```
telco[is.na(telco)] = 0
quant.var=telco[,c(3,6,19,20)]
qual.var=telco[,c(2,4,5,7:18)]

var.clust.h=hclustvar(quant.var, qual.var)
stab=stability(var.clust.h,B=50)
plot(stab)
```




Cluster Dendrogram
Height
0.0
1.0
2.0
MonthlyCharges
InternetService
TechSupport
OnlineBackup
StreamingMovies
StreamingTV
OnlineSecurity
DeviceProtection
gender
SeniorCitizen
PaperlessBilling
PaymentMethod
PhoneService
MultipleLines
Contract
tenure
TotalCharges
Partner
Dependents

h6=cutreevar(var.clust.h, 6)

h6$cluster

SeniorCitizen	tenure	MonthlyCharges
1	2	3
TotalCharges	**gender**	**Partner**
2	4	5
Dependents	PhoneService	MultipleLines
5	6	6
InternetService	OnlineSecurity	OnlineBackup
3	3	3
DeviceProtection	TechSupport	StreamingTV
3	3	3
StreamingMovies	Contract	PaperlessBilling
3	2	1
PaymentMethod		
1		

Questions?