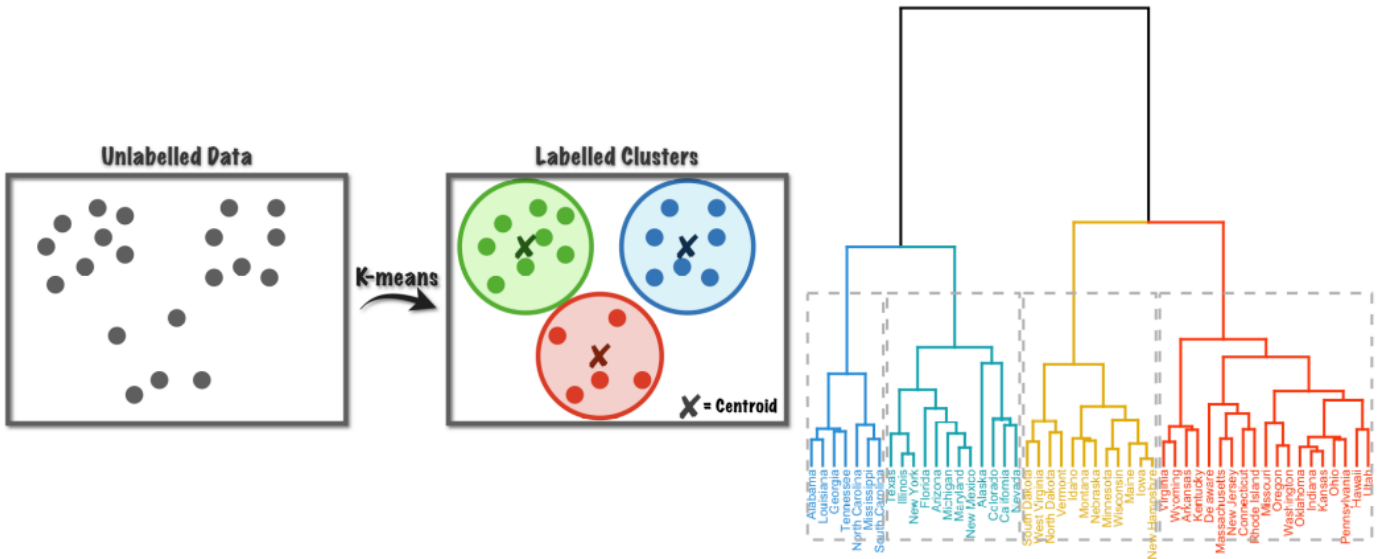
Clustering

PSY-GS 8875 Behavioral Data Science



Overview

Overview: Week 7

Readings

- ESL Chapters: 14.3
- HML Chapters: 20 and 21

Optional

- Steinley - 2006
- Forbes et al. - 2023

- Distances
- k-Means/Mediods Clustering
- Cluster Selection
- Cluster Comparison
- Hierarchical Clustering
- Activity: Schools that pay

Motivating Data

Motivating Data

Wall Street Journal in 2008 put out data on median salary for different universities across the United States

Across 320 universities sampled, we want to know:

- Do universities tend to organize by region?
- Does Vanderbilt cluster with universities it likes to compare itself to (e.g., Harvard, Yale)?

Set up data

```
# Load packages
library(ggplot2); library(factoextra); library(cluster)
library(NbClust); library(igraph); library(EGAnet)

# Set seed
set.seed(42)

# Load data
salary <- read.csv("../../data/university_salary/schools_that_pay.csv")

# Select complete data (no missing values)
salary_voi <- salary[,-c(5, 8)]

# Regions
unique(salary_voi$region)
```

```
[1] "California"    "Western"       "Midwestern"    "Southern"      "Northeastern"
```

Set up data

```
# Extract numeric values
salary_numeric <- salary_voi[,-c(1:2)]

# Scale numeric values
salary_numeric <- scale(salary_numeric)
# Not necessary with Gower's Distance *BUT*
# necessary for many distances used in clustering
```

Clustering

Clustering

clustering: identifying sets of observations or variables that are "like" each other based on their variables or observations

- *Most often*, clustering refers to identifying sets of observations that are similar in their values across one or more variables
- *Sometimes*, clustering refers to identifying sets of variables that are similar in their values across many observations
- *Always*, clustering refers to identifying sets of data that are alike

Clustering

Purpose

- For our purposes, we will refer **clustering** as the identification of sets of observations that are similar in their values across one or more variables

- Goal: find sub-groups of observations that have *meaningful* differences

Distances

- Most clustering algorithms work on some kind of "distance" between observations

- Distances can be computed in many different ways including...
  - Actual distance measures: Euclidean, Manhattan, etc.
  - Correlations
  - Information theory: entropy, divergences (e.g., Kullback-Leibler)

- Distances are how *dissimilar* two observations are (across variables)

- 1 minus a distance is how *similar* two observations are (across variables)

Euclidean Distance

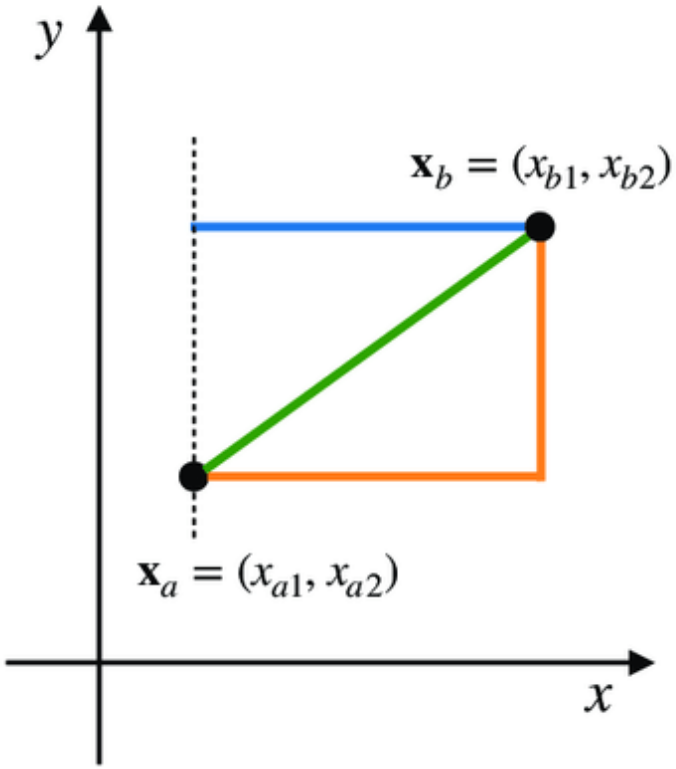
$$d(i,j) = \sqrt{\sum_{k=1}^{n}(x_{i,k} - x_{j,k})^2},$$

Euclidean Distance

$$d(i,j) = \sqrt{\sum_{k=1}^{n}(x_{i,k} - x_{j,k})^2},$$

Does this equation look familiar at all?

Common Distances (2-dimensions or variables)



$p = 2$ Euclidean distance

$$\|\mathbf{x}_a - \mathbf{x}_b\|_2 = (|x_{a1} - x_{b1}|^2 + |x_{a2} - x_{b2}|^2)^{\frac{1}{2}}$$

$p = 1$ Manhattan distance

$$\|\mathbf{x}_a - \mathbf{x}_b\|_M = |x_{a1} - x_{b1}| + |x_{a2} - x_{b2}|$$

$p = \infty$ Chebyshev distance

$$\|\mathbf{x}_a - \mathbf{x}_b\|_\infty = \max\{|x_{a1} - x_{b1}|, |x_{a2} - x_{b2}|\}$$

Euclidean distance is, by far, the most commonly used

One problem though... Euclidean distance is intended for continuous variables

- Continuous data aren't common in the social sciences
- It's not uncommon to have mixed data types (continuous, ordinal, and binary)

Gower's Distance (Gower, 1971)

$$d(i,j) = 1 - \left(\frac{\sum_{k=1}^{n} w_k \cdot s_k(i,j)}{\sum_{k=1}^{n} w_k} \right),$$

where

- $s_k(i,j)$ = similarity scores between i and j for variable k
- w_k = weight assigned to k (usually equal to 1)

General form for the average of partial similarities

Continuous Variables

$$s_k(i,j) = 1 - \frac{|x_{i,k} - x_{j,k}|}{R_k},$$

where

- R_k = range of variable k across all values (normalizing term)

Ordinal Variables

$$s_k(i,j) = 1 - \frac{r_{ik} - r_{jk}}{n_k - 1},$$

where

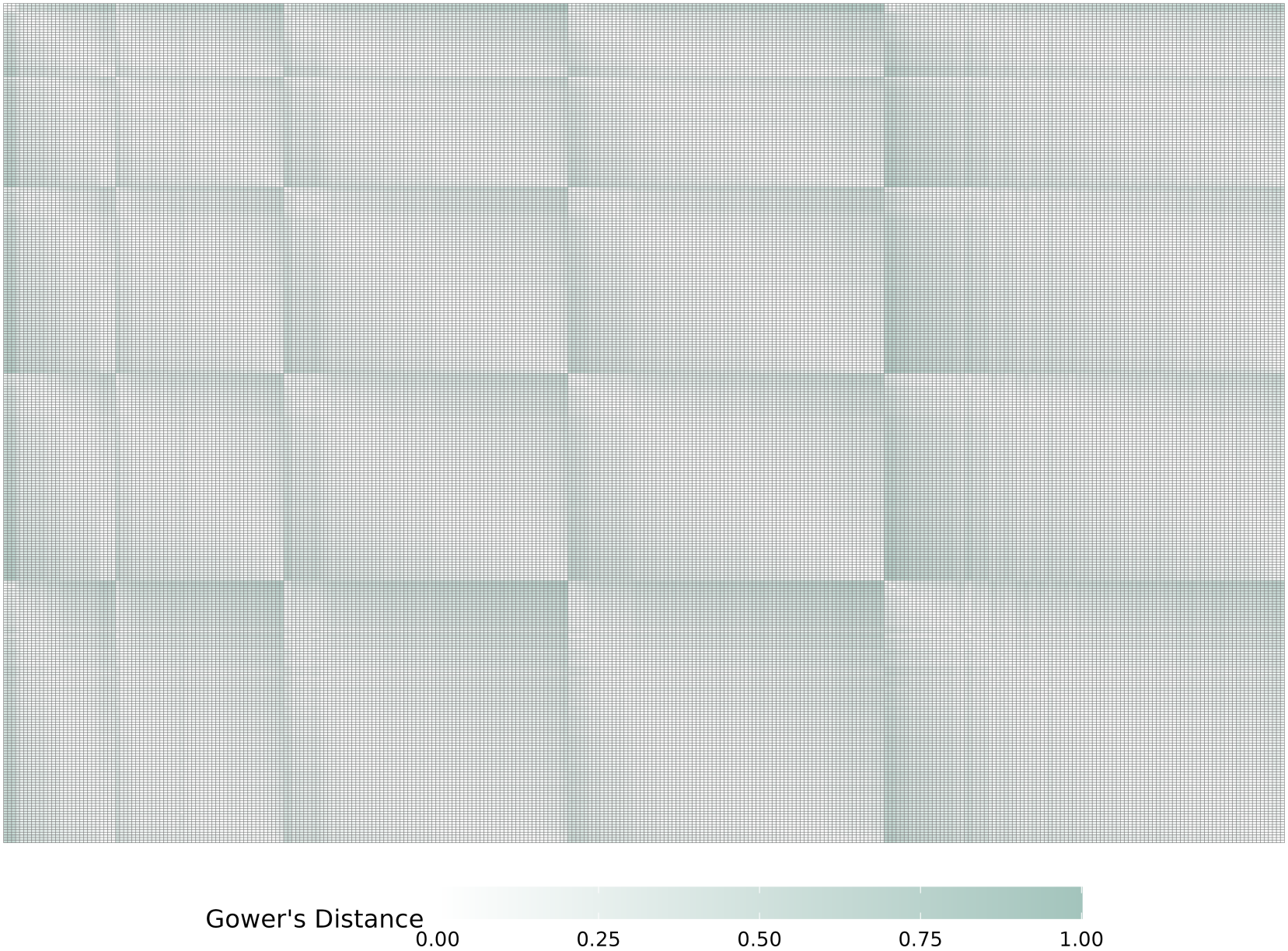
- r = ranks of variable k for observations
- n_k = number of distinct ranks of variable k

Gower's Distance

- Useful, general-purpose distance for mixed data types
- Roughly consistent with other distance measures with continuous data:
  - Manhattan: equivalent when performing $(1 - s_k) \times R_k$
  - Euclidean: scales similarly (though no direct translation in math)
- Can be made to **metric** by taking the square root
  - non-negativity: always positive values
  - symmetric: $d(i, j) = d(j, i)$
  - triangle inequality: $d(i, j) \leq d(i, k) + d(k, j)$
  - zero when values are identical

Compute Gower's Distance

```
# Convert to distance (from {cluster} package)
salary_distance <- daisy(salary_numeric, metric = "gower")

# Visualize
EGAnet:::ggsymmetric(salary_distance) +
  scale_fill_gradient2(
    name = "Gower's Distance",  limits = c(0, 1),
    low = "lightgrey", high = "#A3C4BC"
  ) + theme(
    axis.text = element_blank(), axis.title = element_blank(),
    axis.ticks = element_blank(), legend.position = "bottom",
    legend.key.width = unit(2, "cm"),
    legend.key.height = unit(0.5, "cm")
  )
```


Gower's Distance
0.00
0.25
0.50
0.75
1.00

k-means/k-mediods

Goal: minimize the *mean*/*median* distance between observations using k clusters

- k-means/k-mediods minimizes this objective in an *unsupervised* manner

- **unsupervised learning**: using statistical patterns, without known labels, to learn the data-driven labels

- We'll focus on k-means but we can swap out "median" with "mean" at any point for k-mediods
    - Often, k-mediods is preferred because the median tends to be more robust to outliers

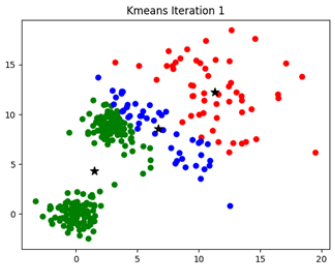
How does k-means "learn" the labels or sub-groups of the data?

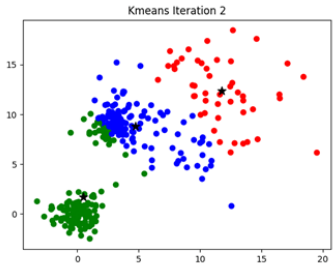
Algorithm

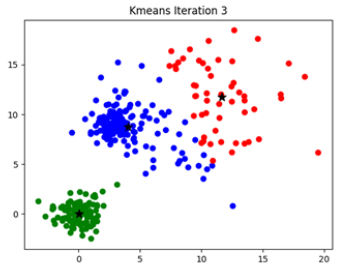
- Step 1: Decide on the number of clusters (k)
- Step 2: Initialize centroids (for k-means) or medoids (for k-medoids) such as selecting random observations as the k centroids
- Step 3: Compute a "centroid" for each cluster representing p variable means (k-means) and the medoid for each cluster (k-mediods)

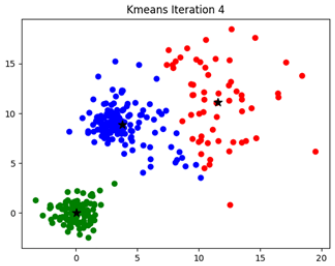
  Step 4: Assign each observation to the cluster whose centroid (or medoid) is closest in terms of Euclidean distance.

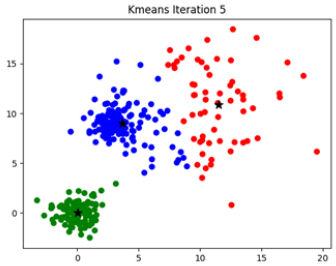
  Step 5: Repeat Steps 3 and 4 until there are no changes in centroid positions or cluster assignments.

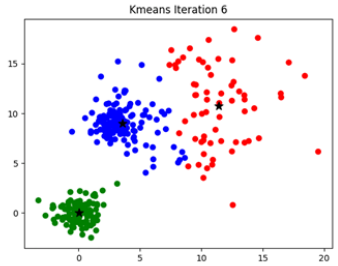

Kmeans Iteration 1

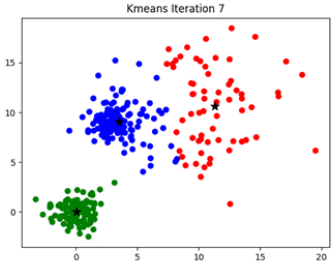

Kmeans Iteration 2

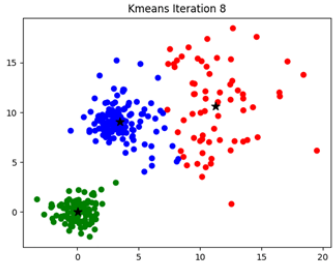

Kmeans Iteration 3

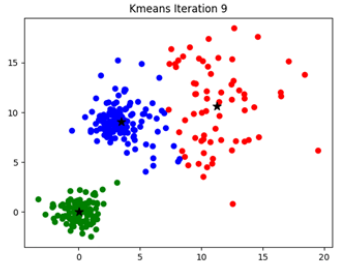

Kmeans Iteration 4

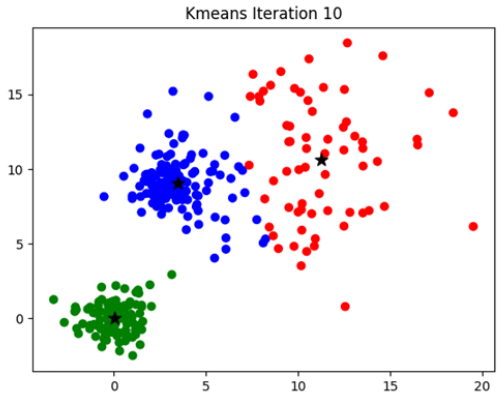

Kmeans Iteration 5


Kmeans Iteration 6


Kmeans Iteration 7


Kmeans Iteration 8


Kmeans Iteration 9


Kmeans Iteration 10

Step 1: Decide on number of clusters (k)

- Are there any expected sub-groups in the data?
  - Pre-defined categories: regions of the country
  - High/low: personality trait profiles
  - Different samples: control/experimental
- If no expectation, then the groups can be "learned" from the data by some objective function (e.g., mean square error)

Step 2: Randomly assign 1-k values to observations

- This step is done within the algorithm
- If there is some theory, then starting values can be provided
- Otherwise, one or more sets of random values will be used and return the clusters that best minimize the objective function

Step 3: Compute a "centroid" for each cluster representing p variable means

- The initial centroids are the (random) starting values
- With initial centroids placed, the goal is to minimize the within-cluster sum of squared distances

$$\arg \min_{W(C_k)} \sum_{k=1}^{K} W(C_k) = \sum_{i \in C_k} d(x_i, \mu_k)^2$$

- C_k = set of all observations in the k^{th} cluster
- $d(x_i, \mu_k)$ = distance between observation i and the centroid μ_k of cluster C_k

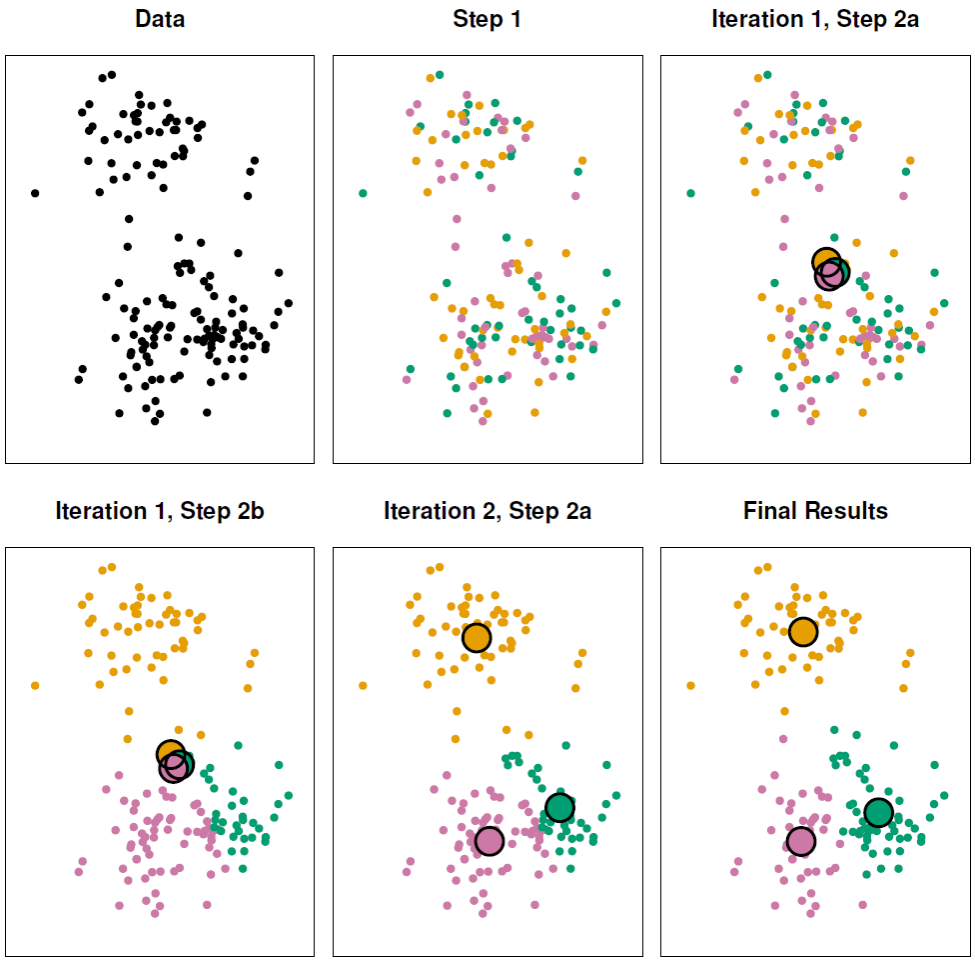
This equation represents the total within-cluster sum of squared distances

Step 4: Assign each observation to the cluster whose centroid is closest

- The centroid will move after Step 3 based on how best the total within-cluster sum of squared distances can be minimized

Step 5: Repeat Step 3 (computing distances) and Step 4 (moving centroids) until there are no changes

Simple Steps

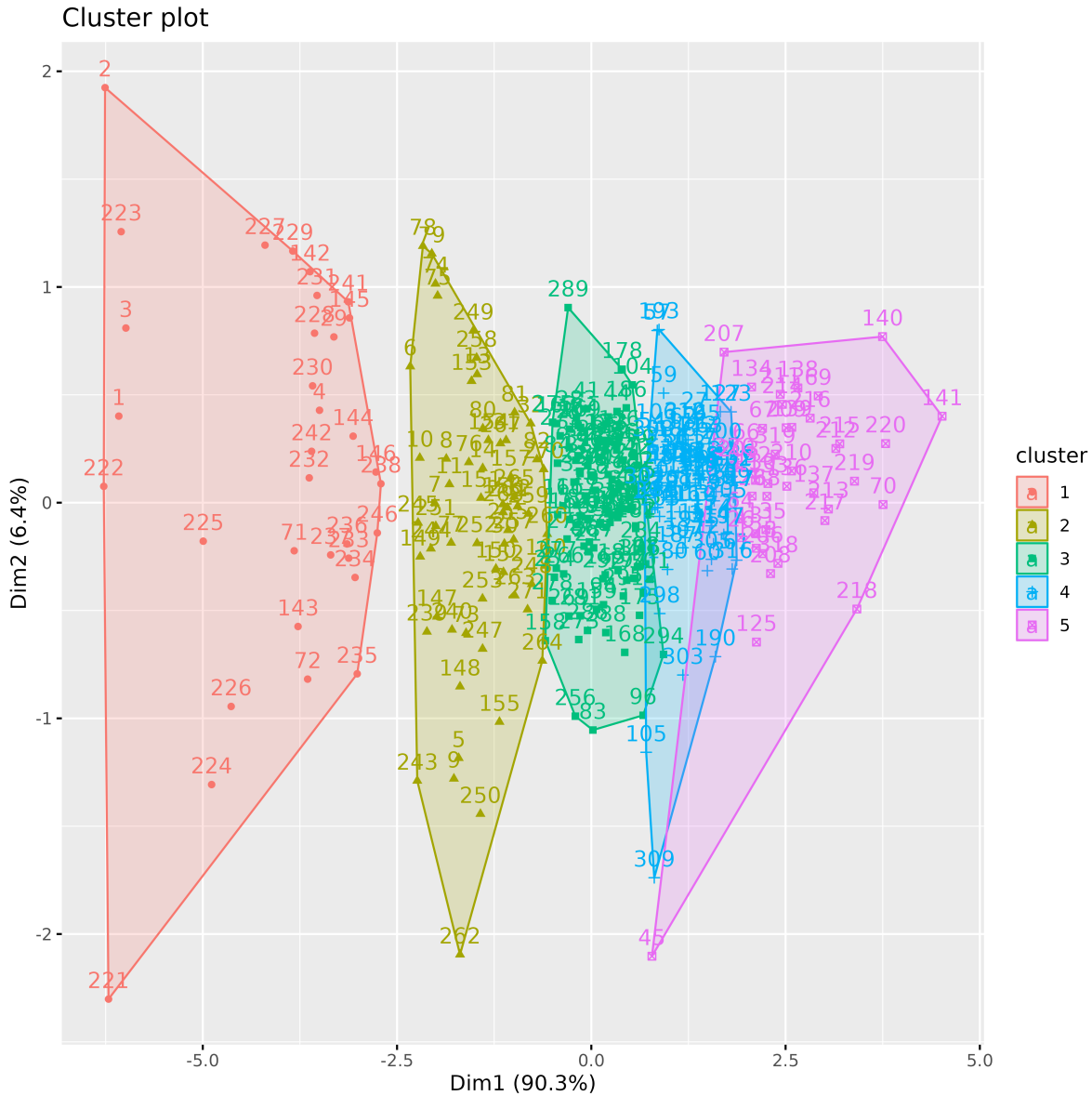


Different Starting Values

Applying k-mediods

```
# Perform k-mediods based on number regions
theoretical_run <- pam(
  x = salary_distance, # supply distance
  k = 5, # number of clusters
  nstart = 25 # number of random starting values
)

# Median observations
salary_voi[theoretical_run$medoids,]

# Need to supply data back to object
theoretical_run$data <- salary_numeric

# Let's visualize
fviz_cluster(theoretical_run)
```

```
                                        school_name       region
232                             Cornell University Northeastern
156                University of Texas (UT) - Austin     Southern
93                       Ohio State University (OSU)   Midwestern
191 University of North Carolina at Charlotte (UNCC)     Southern
136                             Kent State University   Midwestern
    starting_median mid_career_median mid_career_25 mid_career_75
232           60300             110000         79800        160000
156           49700              93900         67400        129000
93            44900              83700         60700        116000
191           43100              74000         53200         99500
136           38700              62600         45800         87000
```

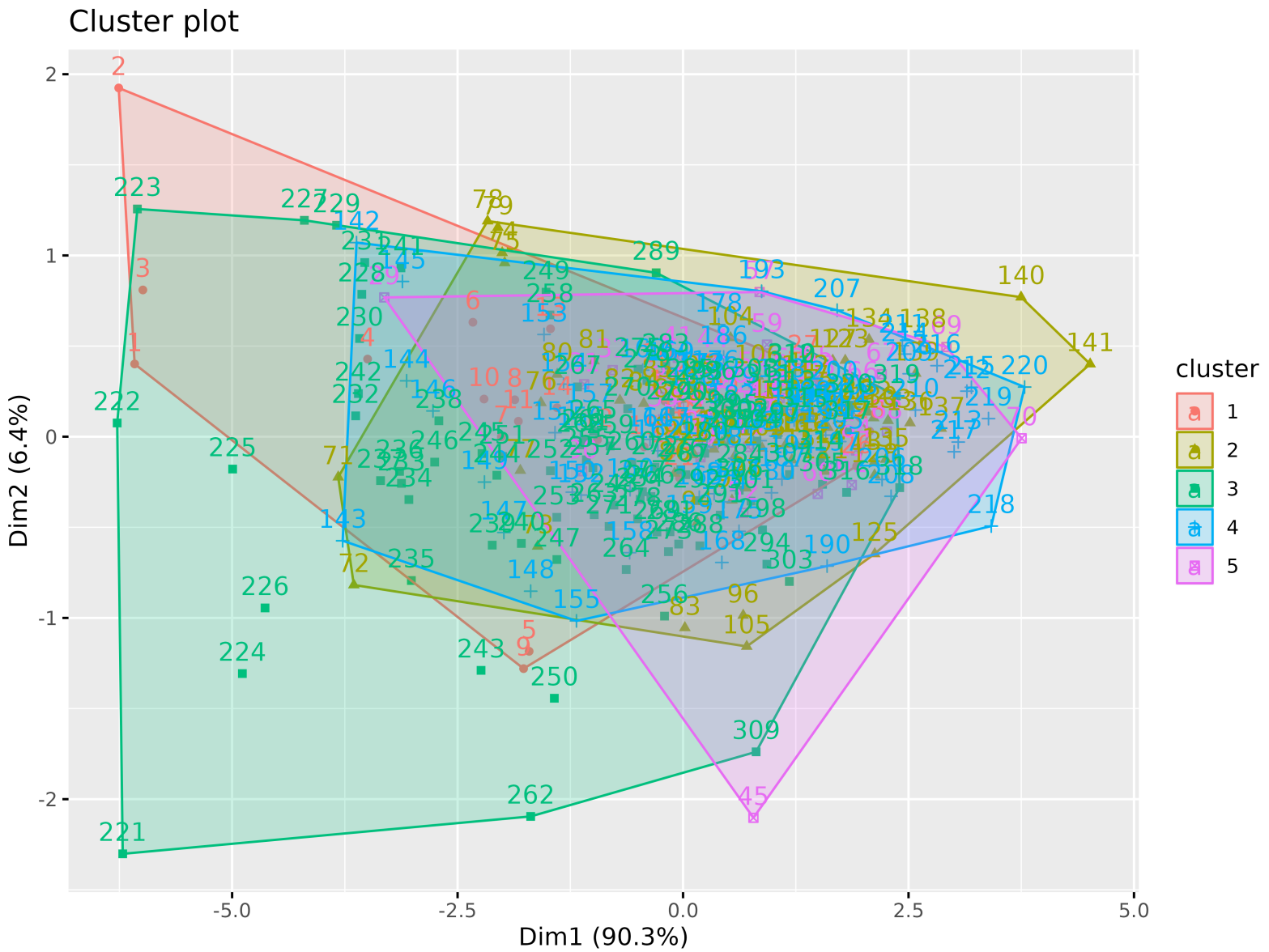

Cluster plot
Dim2 (6.4%)
Dim1 (90.3%)
2
1
0
-1
-2
-5.0
-2.5
0.0
2.5
5.0
cluster
1
2
3
4
5

Cluster Comparison

How do these clusters compare with the five regions these universities were drawn from?

Visualize using "theoretical" clusters

```
# Make copy of theoretical
actual <- theoretical_run

# Replace clusters
actual$clustering <- as.numeric(factor(salary_voi$region))

# What does the region clusters look like?
fviz_cluster(object = actual, data = salary_numeric)
```


Cluster plot
Dim2 (6.4%)
Dim1 (90.3%)
2
1
0
-1
-2
-5.0
-2.5
0.0
2.5
5.0
cluster
1
2
3
4
5

How do these clusters compare with the five regions these universities were drawn from?

- Adjusted Rand Index (ARI): best for larger and balanced clusters
  - -1 $<$ ARI $<$ 0: negative relationship between clustering
  - ARI $=$ 0: clustering is no different than random
  - 0 $<$ ARI $<$ 1: positive similarity between clustering

$$ARI = \frac{\sum_{ij}\binom{n_{ij}}{2} - \left[\sum_i \binom{a_i}{2}\sum_j \binom{b_j}{2}\right]/\binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}\right] - \left[\sum_i \binom{a_i}{2}\sum_j \binom{b_j}{2}\right]/\binom{n}{2}}$$

where

- n_{ij} = elements in both cluster i and cluster j
- a_i = elements in cluster i
- b_j = elements in cluster j
- n = total elements
- $\binom{n}{2} = \frac{n(n-1)}{2}$

How do these clusters compare with the five regions these universities were drawn from?

- Normalized Mutual Information (NMI): best for smaller and unbalanced clusters
  - NMI $= 0$: no relationship between clusters
  - $0 <$ NMI < 1: positive similarity between clusters
  - NMI $= 1$: identical clusters

$$NMI(U, V) = \frac{2 \cdot I(U;V)}{H(U)+H(V)}$$

where

- H = entropy

$$\sum_{i=1}^{K} p_k \log(p_k)$$

- $I(U; V)$ = mutual information

$$\sum_{i=1}^{K_U} \sum_{j=1}^{K_V} p(i,j) \log \left(\frac{p(i,j)}{p(i)p(j)} \right)$$

Compare Empirical with Regions

```
## Adjusted Rand Index
compare(
  actual$clustering, theoretical_run$clustering,
  method = "adjusted.rand"
)
```

```
[1] 0.01825695
```

```
## Normalized Mutual Information
compare(
  actual$clustering, theoretical_run$clustering,
  method = "nmi"
)
```

```
[1] 0.06156435
```

Selecting Clusters

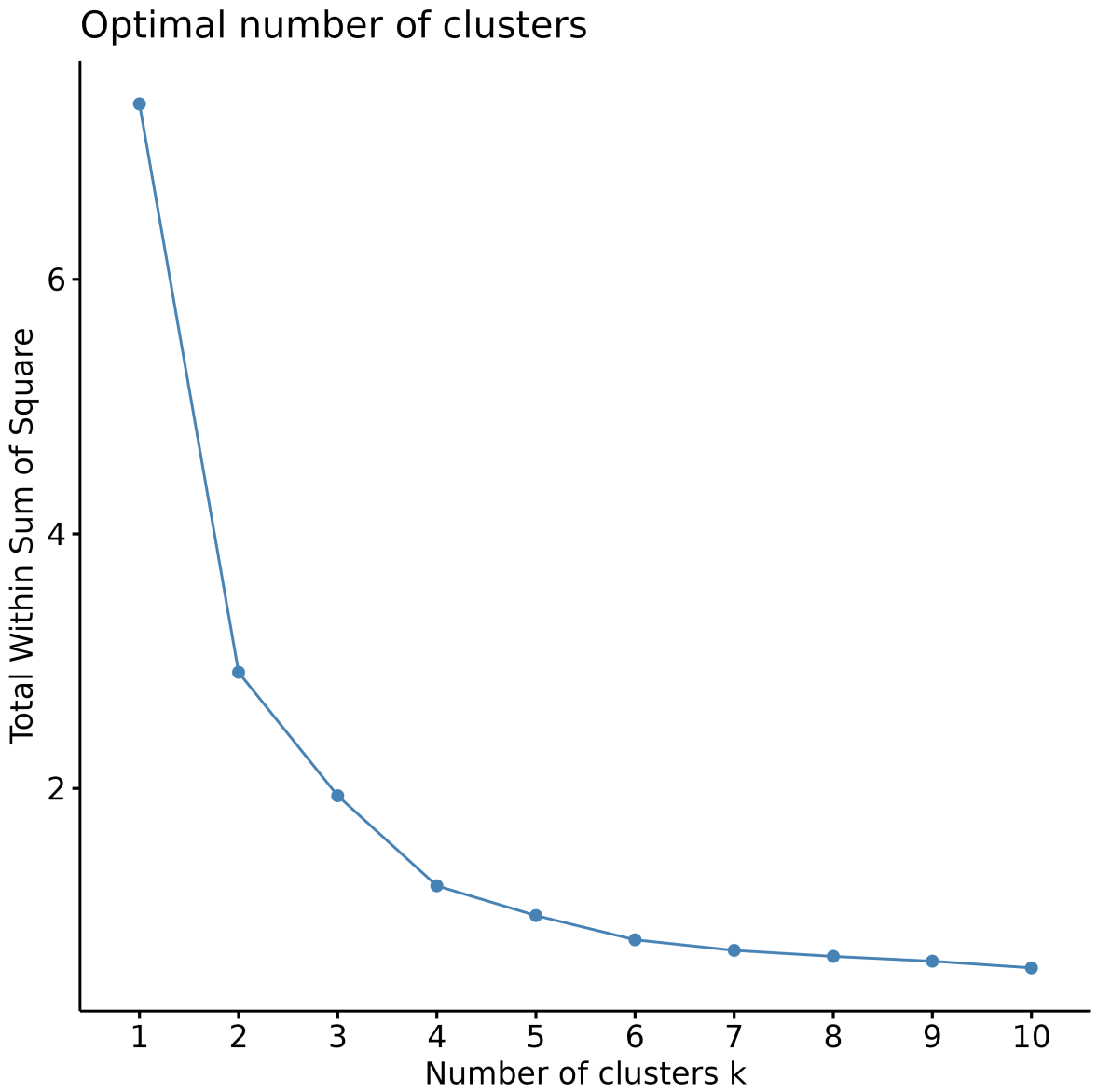
- Selecting the number of clusters is a key part of clustering methods
- Although we can set the number of clusters ourselves, there are methods that can help us select the number
- **Grid search** or fitting over a range of possible cluster values (e.g., 2-8 clusters) is usually employed

What do you expect to happen to the within-cluster variance (distance) as the number of clusters increases?

"Elbow" Approach

- Goal: identify a "drop off" and "leveling out" of within-cluster variance across the range of clusters

```
# Plot "elbow" method
fviz_nbclust(
  x = salary_numeric, # supply data
  FUNcluster = pam, # cluster function
  diss = salary_distance, # supply distance
  method = "wss", # within-cluster sum of squares
  k = 10,  # maximum number of clusters
  nstart = 25 # same as our k-mediods setup
)
```


Optimal number of clusters
Total Within Sum of Square
2
4
6
1
2
3
4
5
6
7
8
9
10
Number of clusters k

Statistical Approaches

- There is a vast number of statistical approaches
- {NbClust} package boasts 30 different methods
- Common methods include:
  - Silhoutte method
  - Gap statistic

Silhoutte Method

$$a(i) = \frac{1}{|C_I| - 1} \sum_{j \in C_I, i \neq j} d(i, j)$$

- C_I = number of points in cluster i
- $d(i, j)$ = distance (e.g., Euclidean) between points i and i

Silhoutte Method

$$b(i) = min_{J \neq I} \frac{1}{|C_J|} \sum_{j \in C_J} d(i,j)$$

- C_J = number of points in cluster j
- $d(i,j)$ = distance (e.g., Euclidean) between points i and i

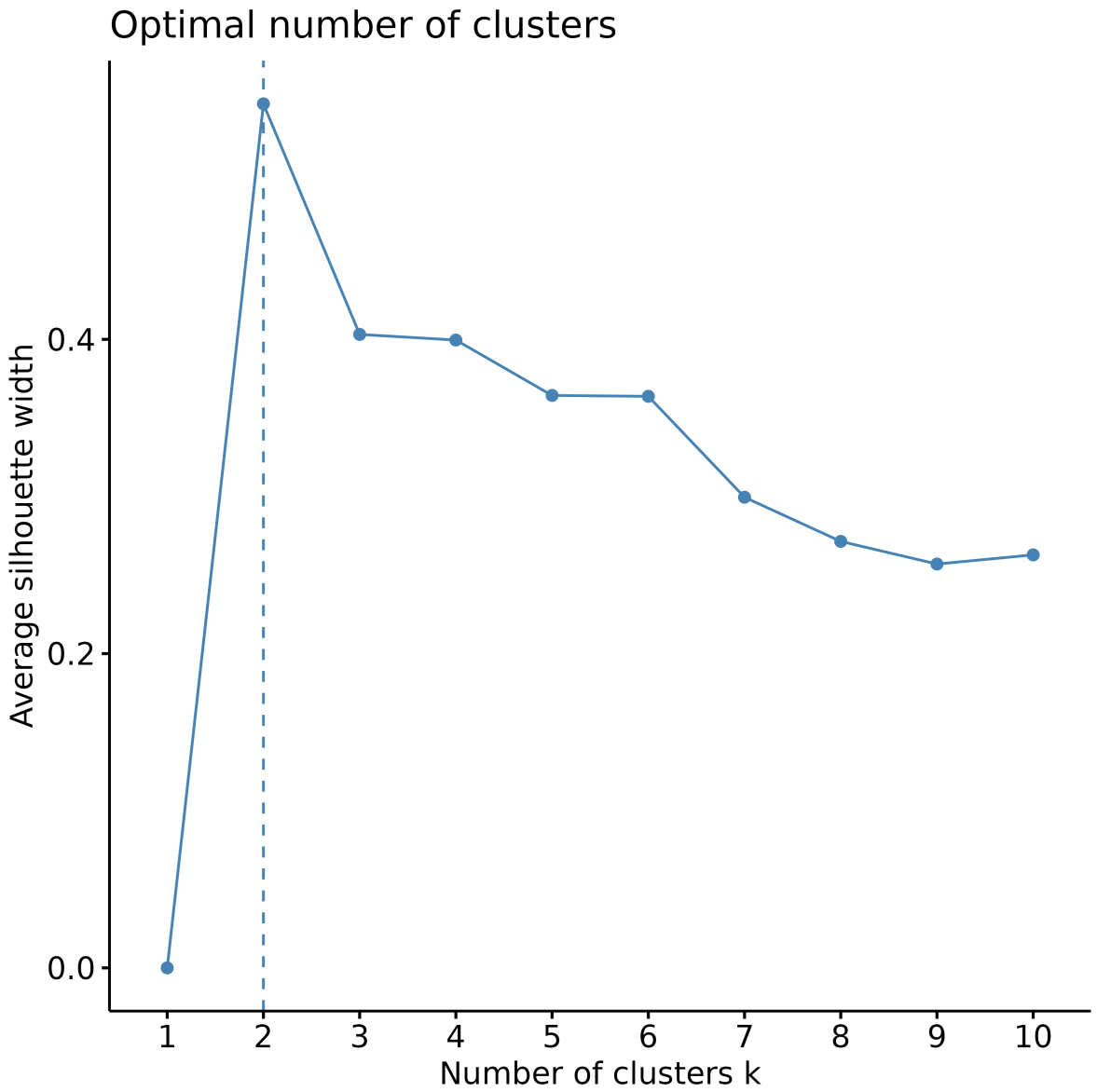
Silhoutte Method

$$s(i) = \frac{b(i) - a(i)}{max\{a(i), b(i)\}}$$

- Average silhouette is used for each number of clusters
- Select clusters that **maximize** average silhouette

Silhouette Method

```
# Plot "elbow" method
fviz_nbclust(
  x = salary_numeric, # supply data
  FUNcluster = pam, # cluster function
  diss = salary_distance, # supply distance
  method = "wss", # within-cluster sum of squares
  k = 10,  # maximum number of clusters
  nstart = 25 # same as our k-mediods setup
)
```


Optimal number of clusters
Average silhouette width
0.0
0.2
0.4
1
2
3
4
5
6
7
8
9
10
Number of clusters k

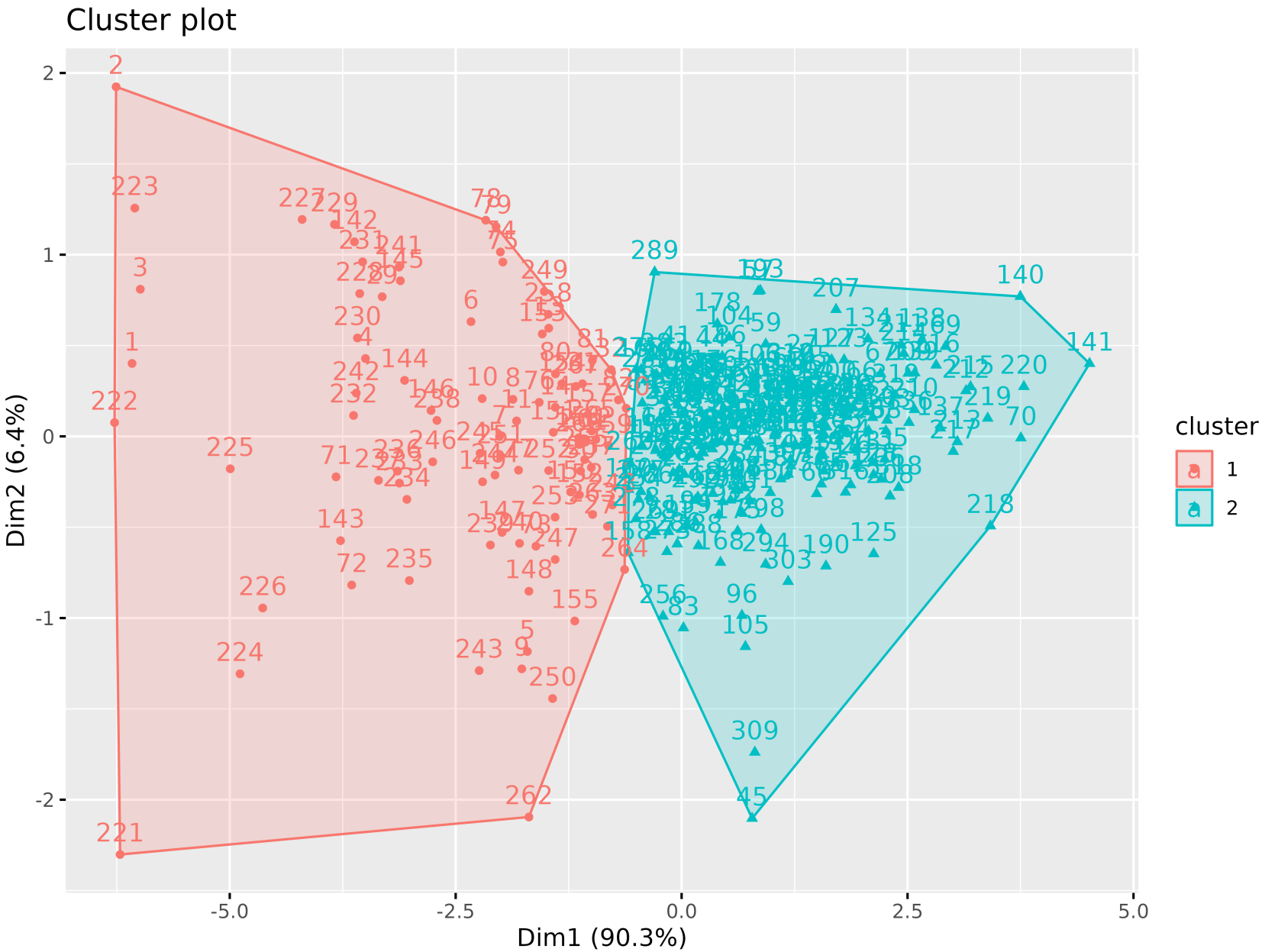
Majority Method

```
# {NbClust} has over 30 different metrics to evaluate
# the number of clusters -- majority approach:
majority <- NbClust(
  data = salary_numeric, # supply data
  diss = salary_distance, # supply distance
  distance = NULL, # using our own distance
  max.nc = 10, # maximum number of clusters
  method = "median", # perhaps more consistent with mediods
  index = "all" # all metrics
)
```

```
* Among all indices:
 * 9 proposed 2 as the best number of clusters
 * 3 proposed 3 as the best number of clusters
 * 1 proposed 4 as the best number of clusters
 * 2 proposed 5 as the best number of clusters
 * 4 proposed 6 as the best number of clusters
 * 3 proposed 8 as the best number of clusters
 * 2 proposed 10 as the best number of clusters

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

Final Solution

```r
# Perform k-mediods with silhouette
silhouette_run <- pam(
  x = salary_distance, # supply distance
  k = 2, # number of clusters
  nstart = 25 # number of random starting values
)

# Need to supply data back to object
silhouette_run$data <- salary_numeric

# Plot
fviz_cluster(silhouette_run, salary_numeric)
```


Cluster plot
Dim2 (6.4%)
Dim1 (90.3%)
2
1
0
-1
-2
-5.0
-2.5
0.0
2.5
5.0
cluster
1
2

Mediods

```
# Median observations
salary_voi[silhouette_run$medoids,]
```

```
                                        school_name     region starting_median
7   University of California at Los Angeles (UCLA) California           52600
185                 West Virginia University (WVU)   Southern           43100
    mid_career_median mid_career_25 mid_career_75
7              101000         72500        139000
185             78100         55700        106000
```

```
# Higher versus lower outcome in terms of median salary
```

Where did Vanderbilt fall?

```
# Where does Vanderbilt come out?
silhouette_run$cluster[grepl("Vanderbilt", salary$school_name)]
```

```
[1] 1
```

In-class Activity

1. Perform hierarchical clustering on the `salary_data` using `salary_distance` (Gower's distance)
2. Apply the Silhouette Method to determine the number of clusters
3. Extract clusters using `cutree`
4. Visualize clusters

Hierarchical

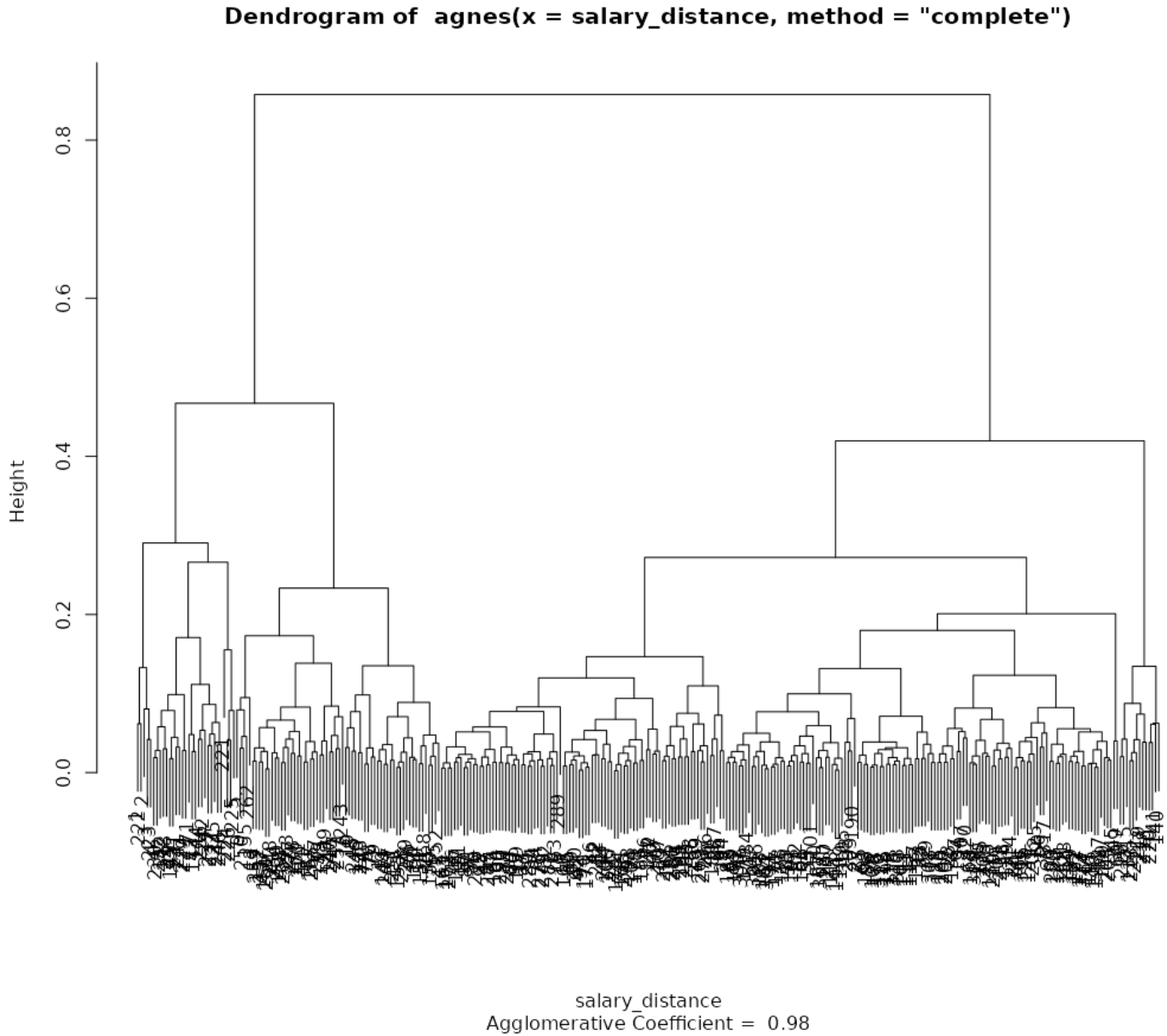
Goal: bring together/split "like" observations based on distance, one observation/cluster at a time

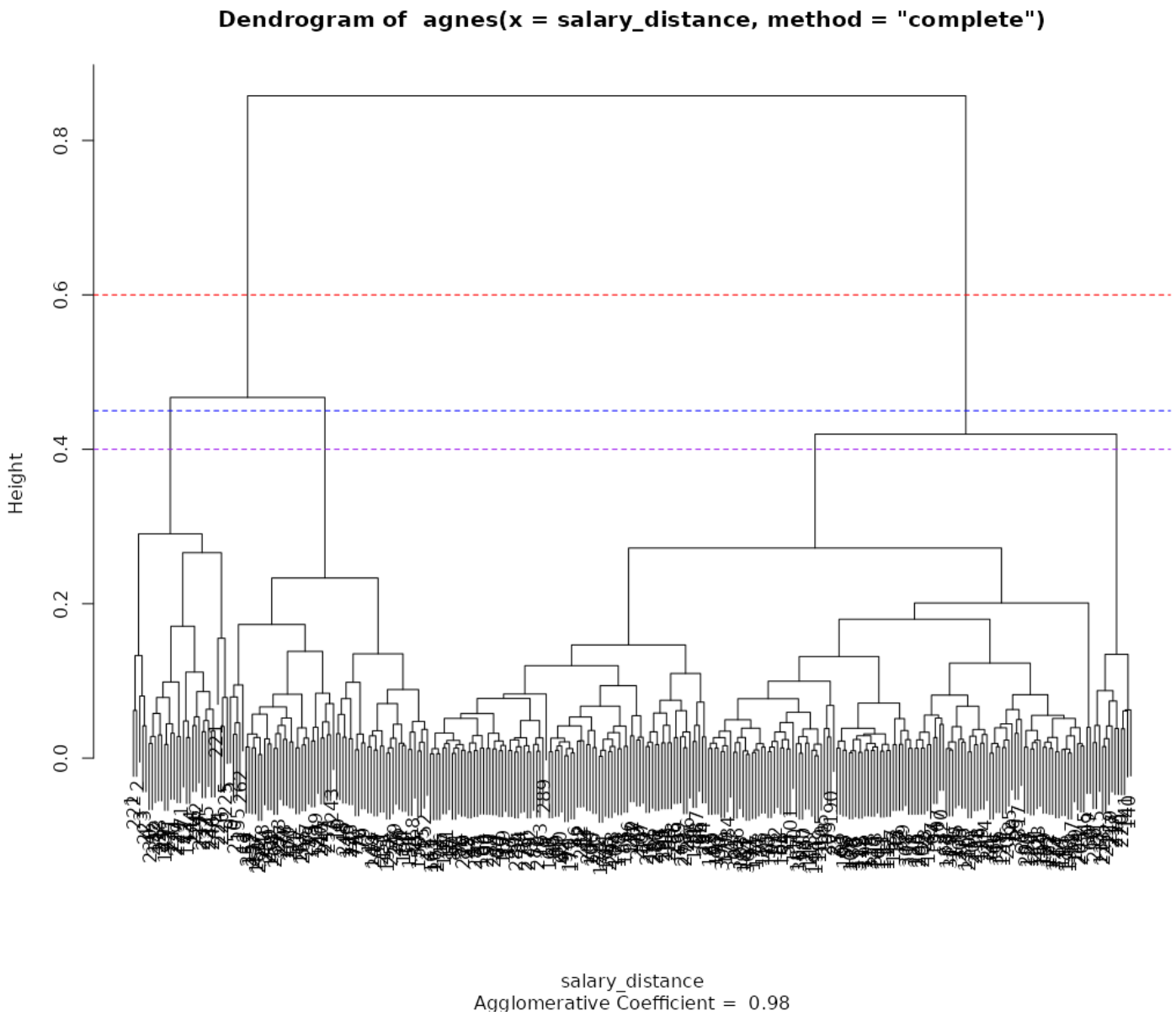
Like *k*-means/mediods, hierarchical "learns" in an *unsupervised* manner

How does hierarchical clustering "learn" the labels or sub-groups of the data?

Algorithm

- Step 1: Decide on either agglomerative ("bottom-up") or divisive ("top-down") method
- Step 2: Compute (dis)similarity or *distance* measure between observations
- Step 3: Use a *linkage* function to join/split observations
- Step 4: Join/split observations/clusters that are most (dis)similar of all possible distance values
- Step 5: Repeat Steps 4 until there is one cluster or individual observations


Dendrogram of agnes(x = salary_distance, method = "complete")
Height
0.0
0.2
0.4
0.6
0.8
salary_distance
Agglomerative Coefficient = 0.98


Dendrogram of agnes(x = salary_distance, method = "complete")
Height
0.0
0.2
0.4
0.6
0.8
salary_distance
Agglomerative Coefficient = 0.98

Step 1: Decide on agglomerative or divisive method

- agglomerative: starts with individual observations and joins them, one-by-one, until all observations form a single cluster ("bottom-up")

- divisive: starts with all observations in a single cluster and splits them, one-by-one, until all observations are individual observations ("top-down")

Step 2: Compute (dis)similarity or *distance* measure between observations

Step 3: Use a *linkage* function

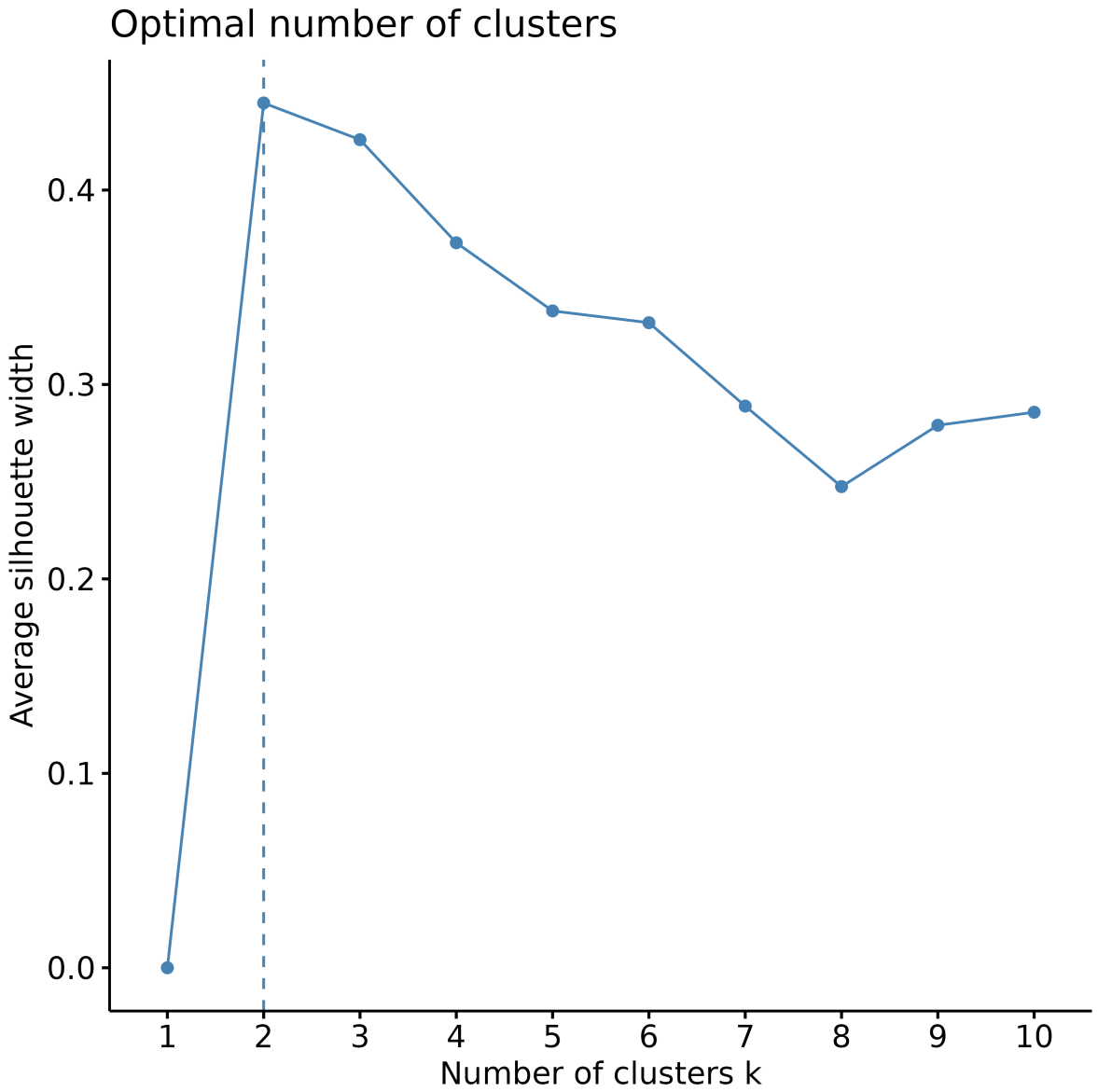
Method	Equation	Description
Single	$min_{i,j} d(\mathbf{X_i}, \mathbf{Y_j})$	minimize distance between clusters
Complete	$max_{i,j} d(\mathbf{X_i}, \mathbf{Y_j})$	maximize distance between clusters
Average	$\frac{\sum_{i=1}^{k} \sum j = 1^{l} d(\mathbf{X_i}, \mathbf{Y_j})}{kl}$	average distance between clusters
Centroid	$d(\bar{x}, \bar{y})$	distance between average location of cluster points
Ward's D	too complex for this table	minimizes sum of squares (like K-means)

Step 4: Join/split observations/clusters that are most (dis)similar of all possible distance values

Step 5: Repeat Steps 4 until there is one cluster or individual observations

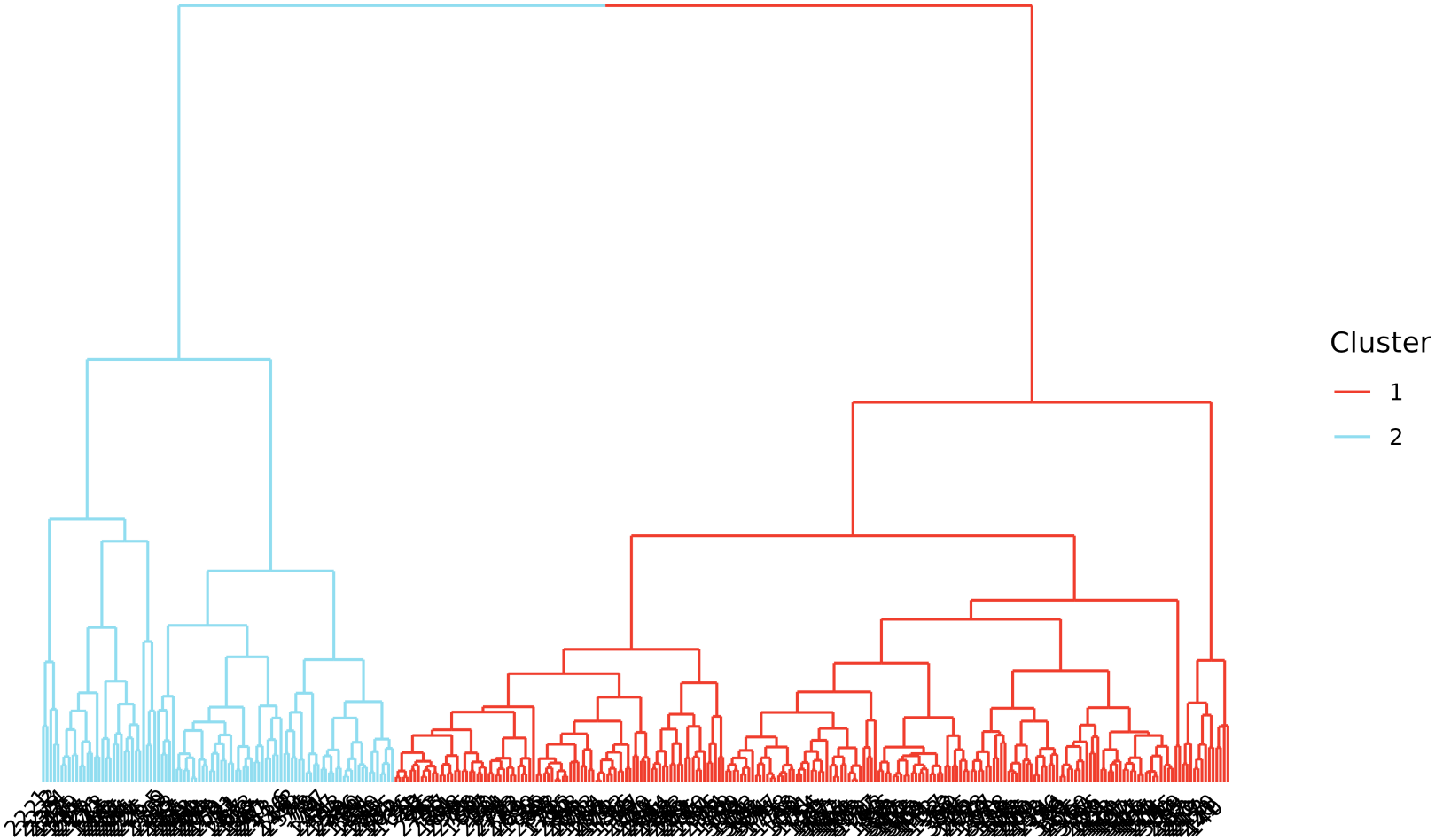
Selecting Clusters: same as *k*-means/mediods

```
# Plot silhouette method
fviz_nbclust(
  x = salary_numeric, # supply data
  FUNcluster = hcut, # cluster function
  hc_func = "agnes", # ensures same approach
  hc_method = "complete", # ensures same approach
  diss = salary_distance, # supply distance
  method = "silhouette" # within-cluster sum of squares
)
```


Optimal number of clusters
Average silhouette width
0.0
0.1
0.2
0.3
0.4
1
2
3
4
5
6
7
8
9
10
Number of clusters k

Selecting Clusters: make the "cut"

```
# Get agglomerative clusters based on silhouette
silhouette_clusters <- cutree(hierarchical, k = 2)

# Plot with clusters
pseudo_info <- list(
  clusters = silhouette_clusters,
  clusterTree = hierarchical,
  JSD = as.matrix(salary_distance)
)

# Set class
class(pseudo_info) <- "infoCluster"

# Plot
plot(pseudo_info)
```


Cluster
1
2

At Home Activity

Bipolar/Depression Dataset [source]

- Actual outcome: `Expert.Diagnose` (`"Normal"`, `"Depression"`, `"Bipolar Type-1"`, `"Bipolar Type-2"`)
- Variables of interest:
  - binary (yes/no): `Mood.Swing`, `Suicidal.thoughts`, `Anorxia`, `Authority.Respect`, `Try.Explanation`, `Aggressive.Response`, `Ignore...Move.On`, `Nervous.Break.down`, `Admit.Mistakes`, `Overthinking`
  - ordinal (1-4): `Sadness`, `Euphoric`, `Exhausted`, `Sleep.dissorder`
  - continuous (1-10): `Sexual.Activity`, `Concentration`, `Optimisim`

Goal: use the variables of interest to derive clusters and compare them to the `Expert.Diagnose`

At Home Activity

- Using the `bipolar_depression_clean.csv`,
  - Use columns 2-18 as your features (see previous slide)
- Apply *either* k-mediods or hierarchical clustering
  - Compute Gower's distance
  - Perform silhouette or majority (use `"median"`) method
  - Visualize
- Compare clusters derived from your analysis with `Expert.Diagnose`
  - Compute Adjusted Rand Index
  - Compute Normalized Mutual Information

Readings for Next Week

Readings

- ESL Chapters: 17.1-17.3
- Epskamp and Fried - 2018
- Golino and Epskamp - 2017

Optional

- Pons and Latapy -2006
- Christensen - 2024
- Schmittmann et al. - 2013
- Blondel et al. - 2008
- Christensen et al. - 2023 - community
- Golino et al. - 2020