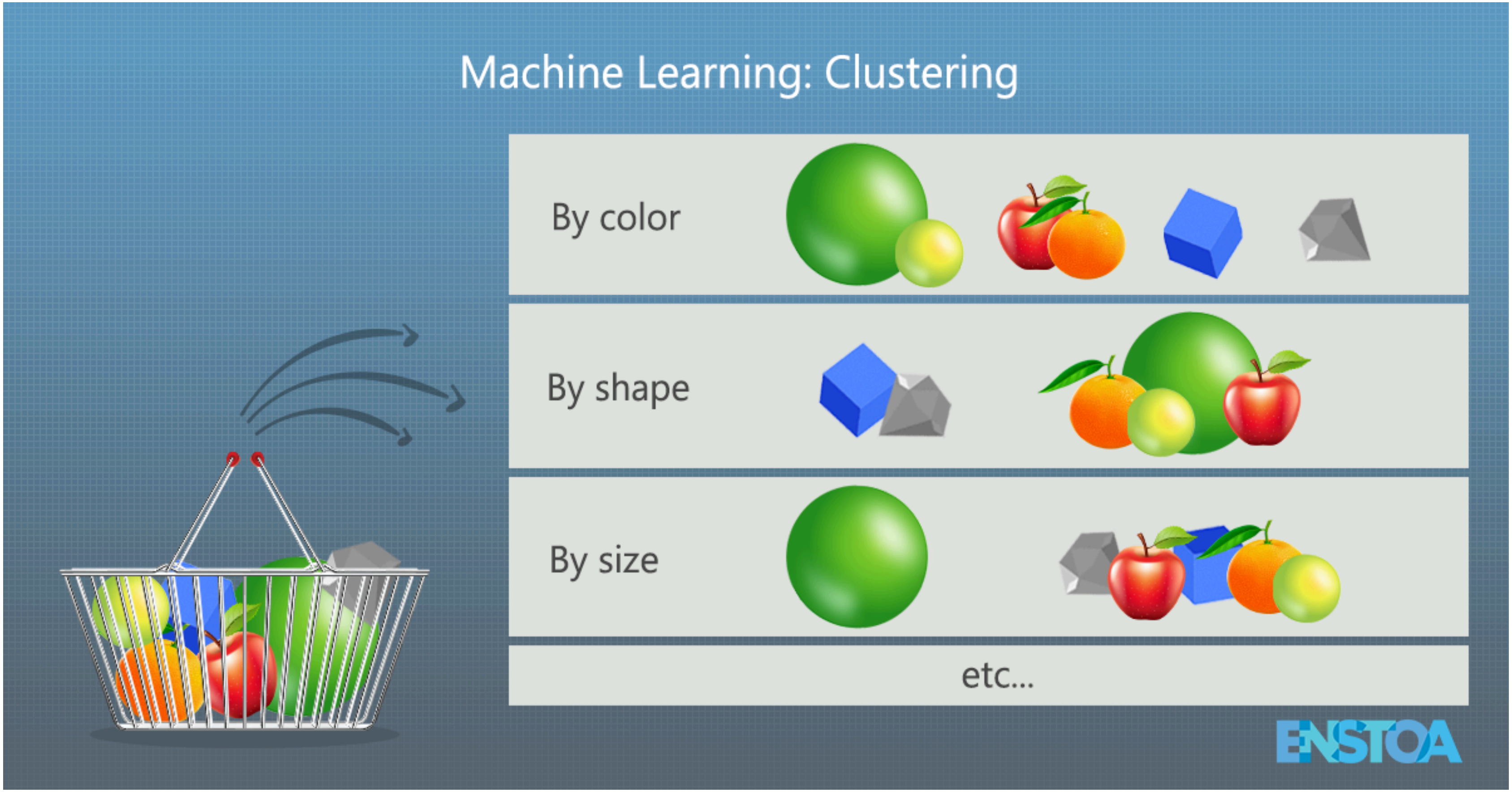
# K-means Clustering

Son Nguyen

# What is clustering?

Clustering is grouping data points into groups where data points in one group are `similar` to each other.

# What is clustering?



# Methods of Clustering

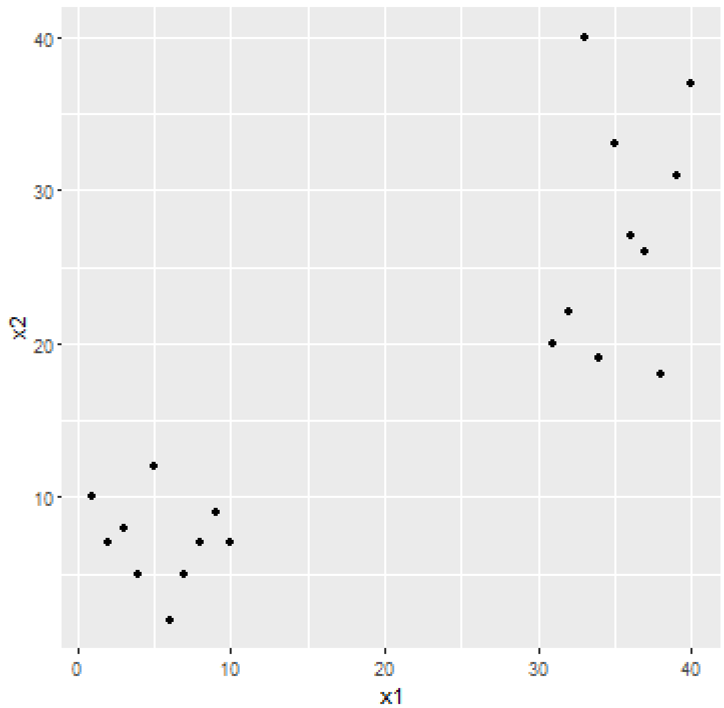
We will cover two clustering methods:

- K-means clustering and
- Hierarchical clustering

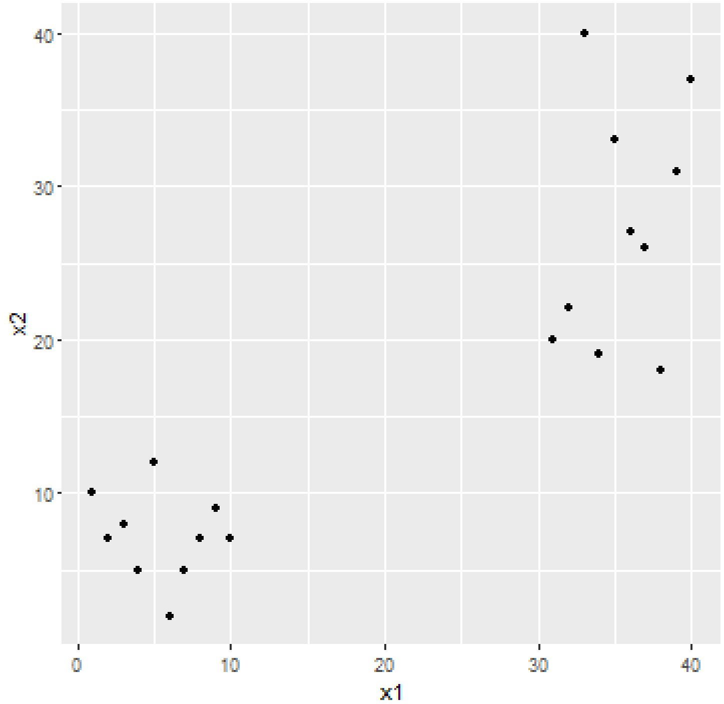
# K-means Clustering

- Data
- Visualize Data
- Result of K-means clustering

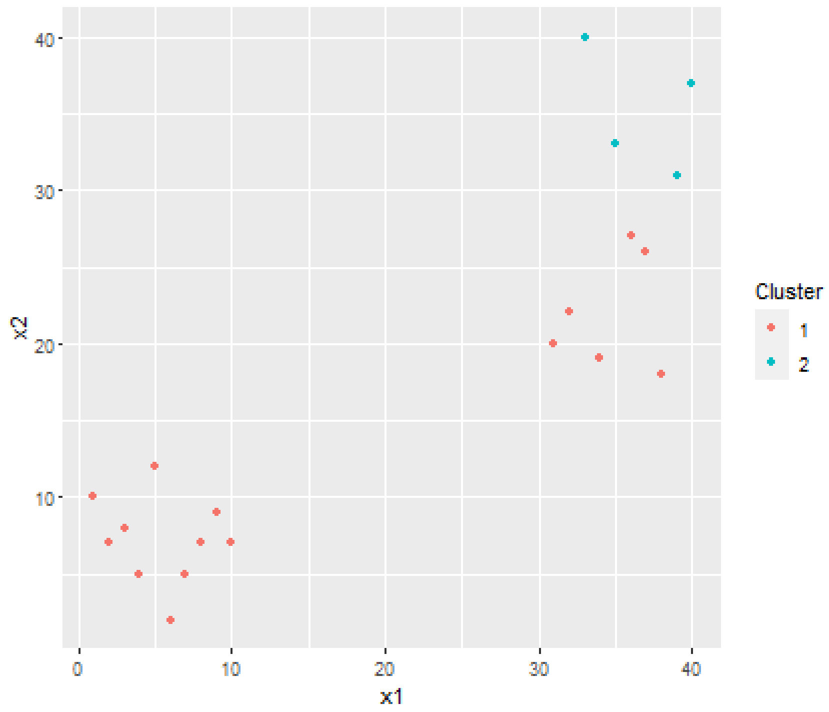
# Step 1



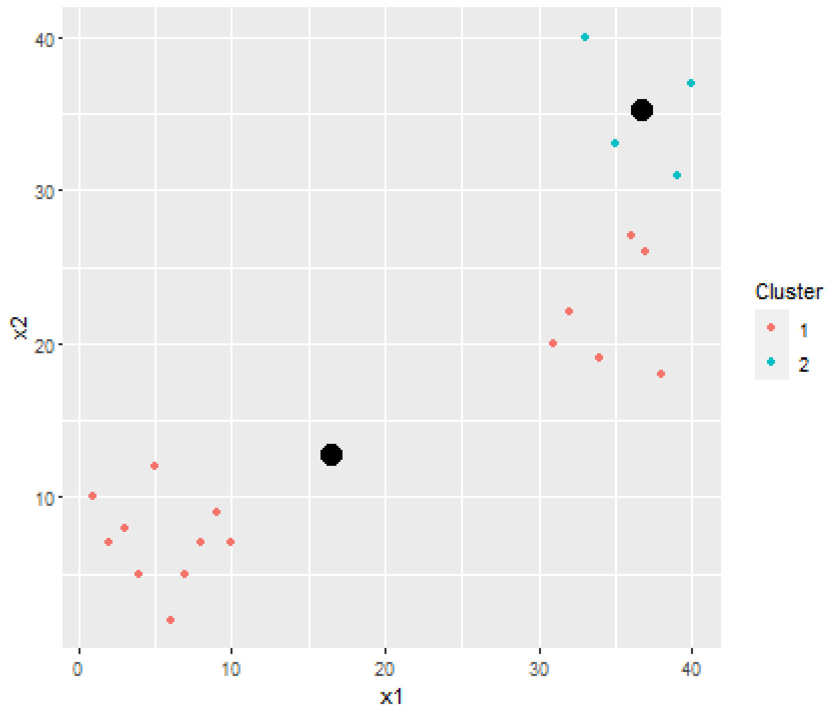
# Step 1: Randomly select centroids



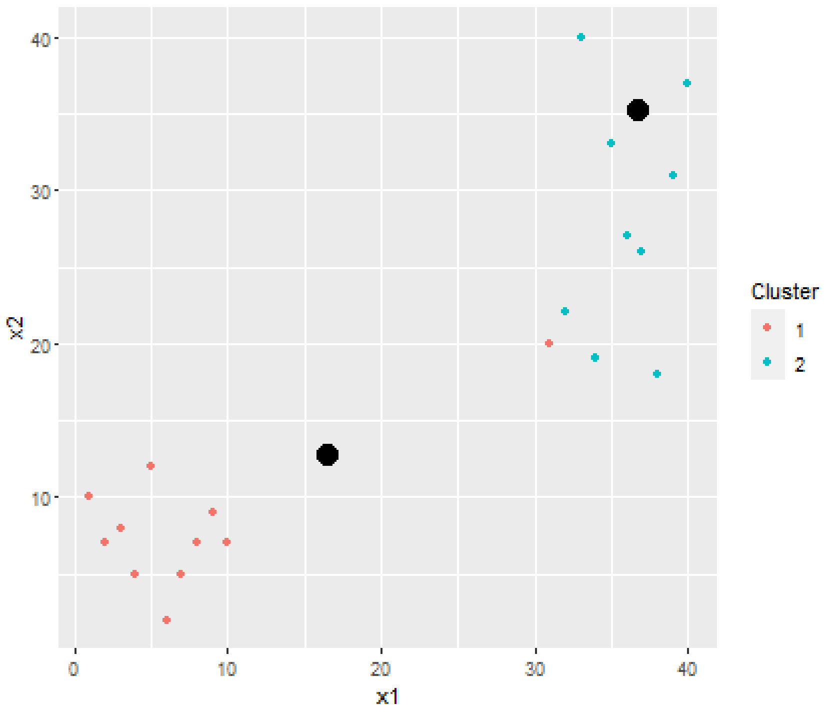
# Step 1: Collect points for each clusters



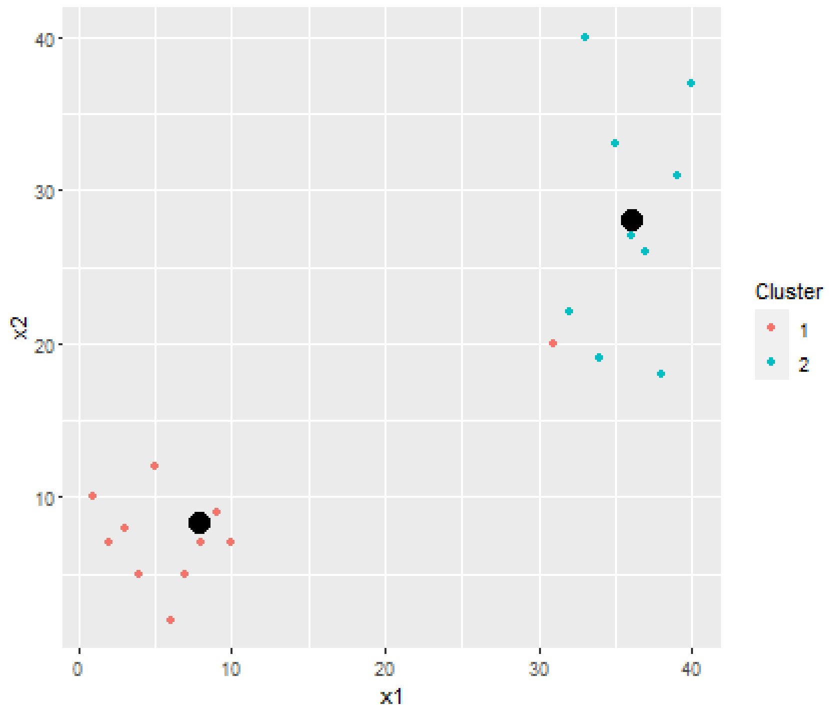
# Locate centroids



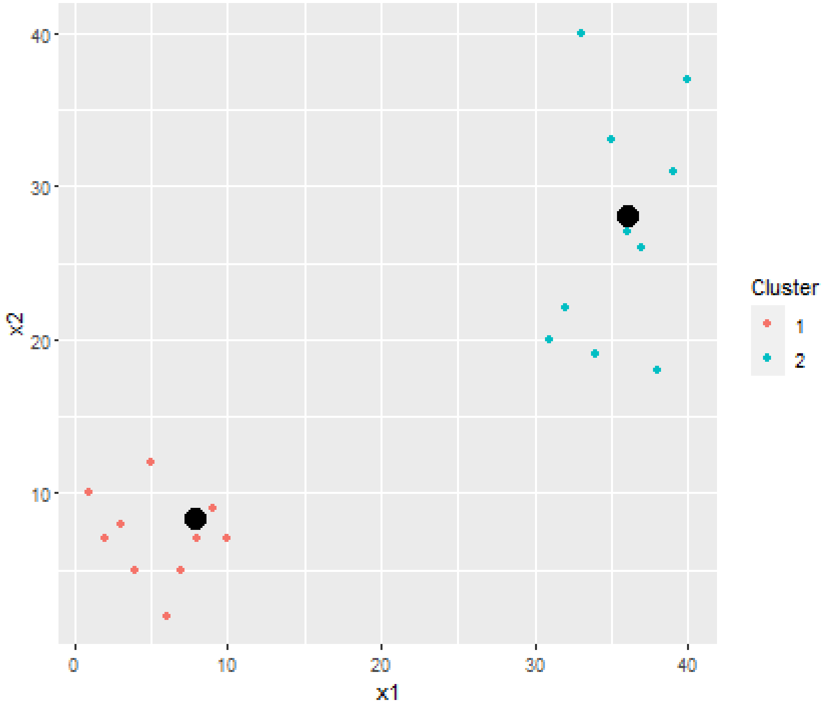
# Collect points for each clusters



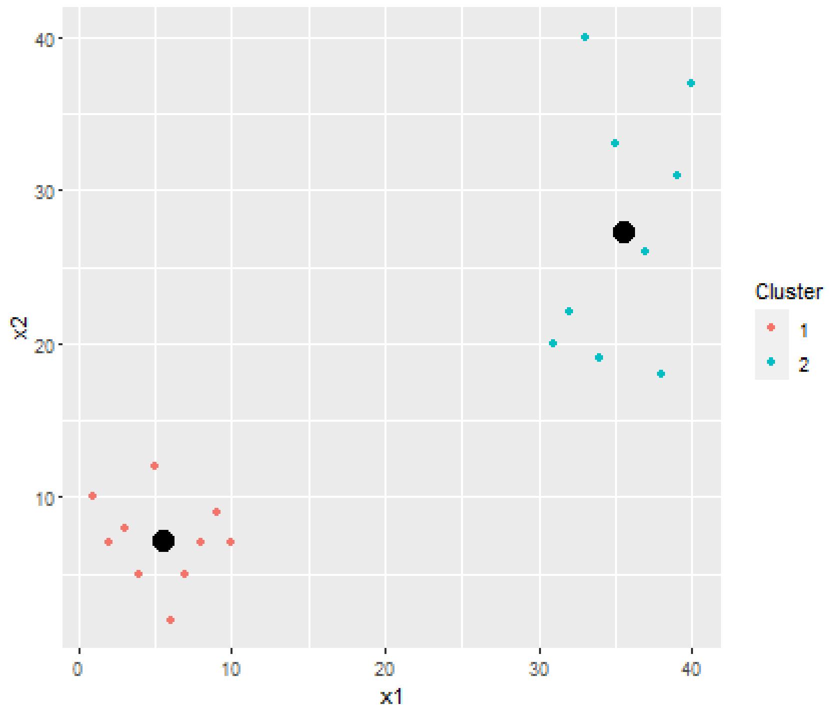
# Relocate centroids



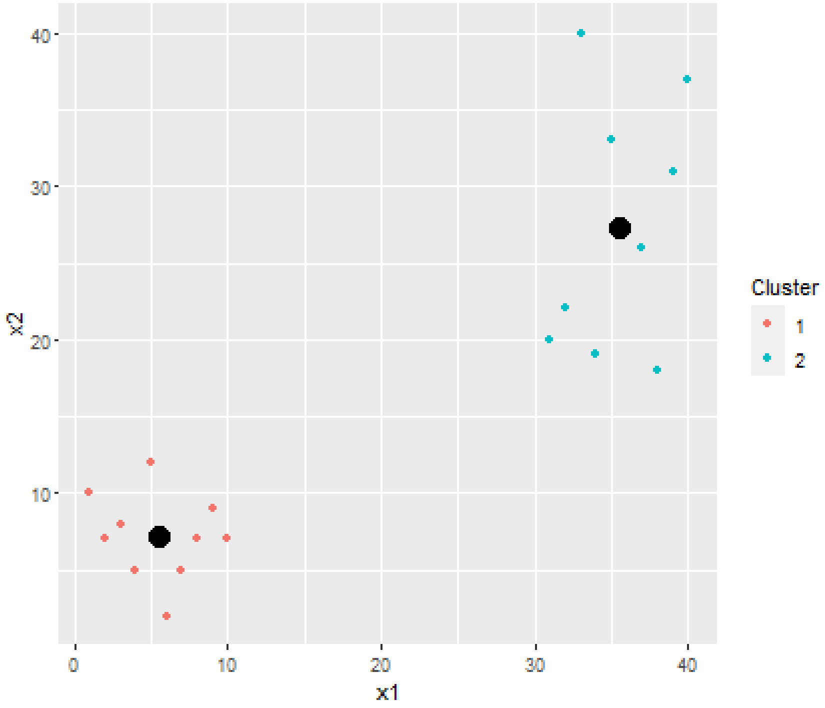
# Collect points for each clusters



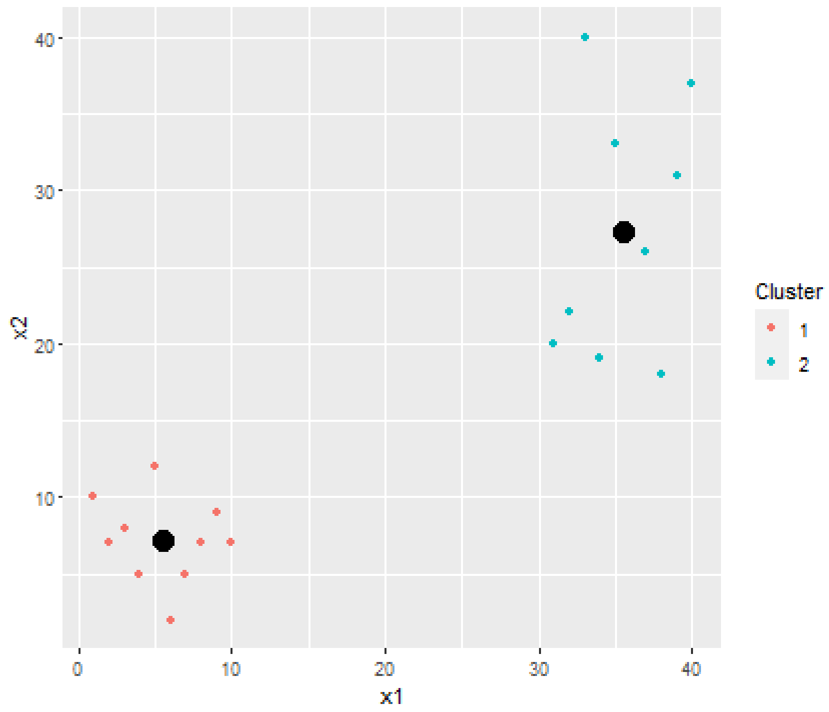
# Relocate centroids



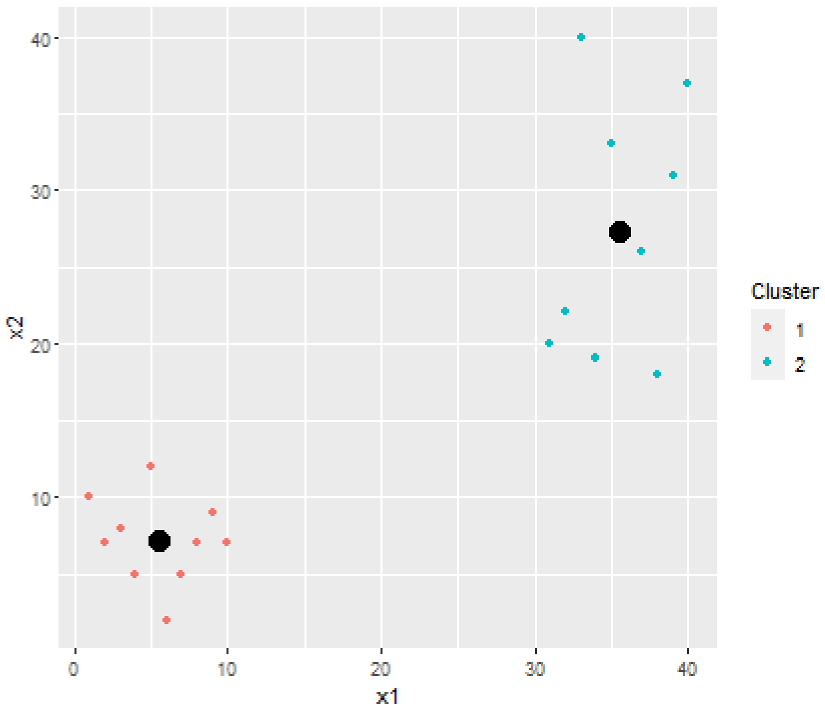
# Collect points for each clusters



# Relocate centroids

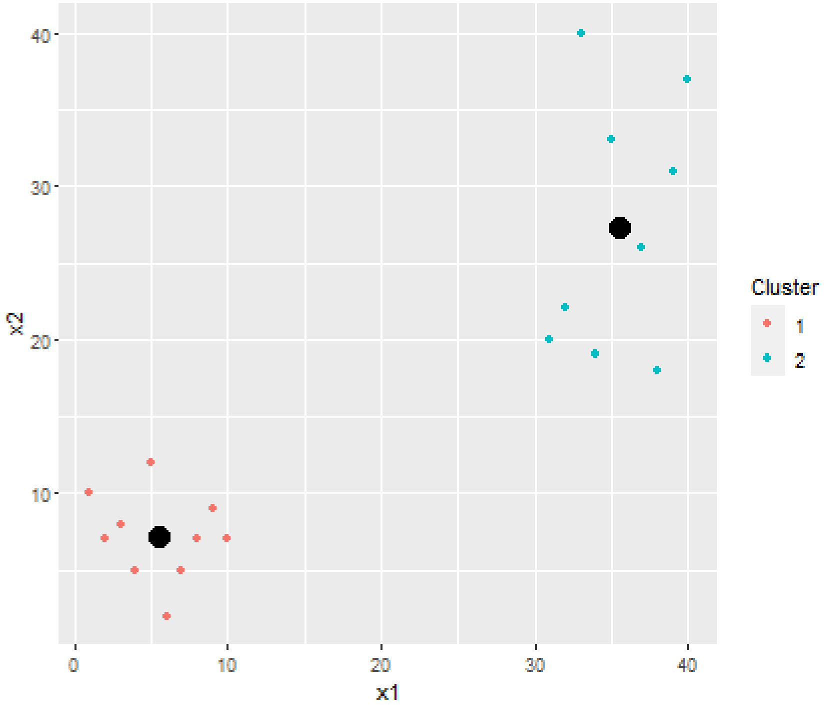


# Step 2: Collect points for each clusters

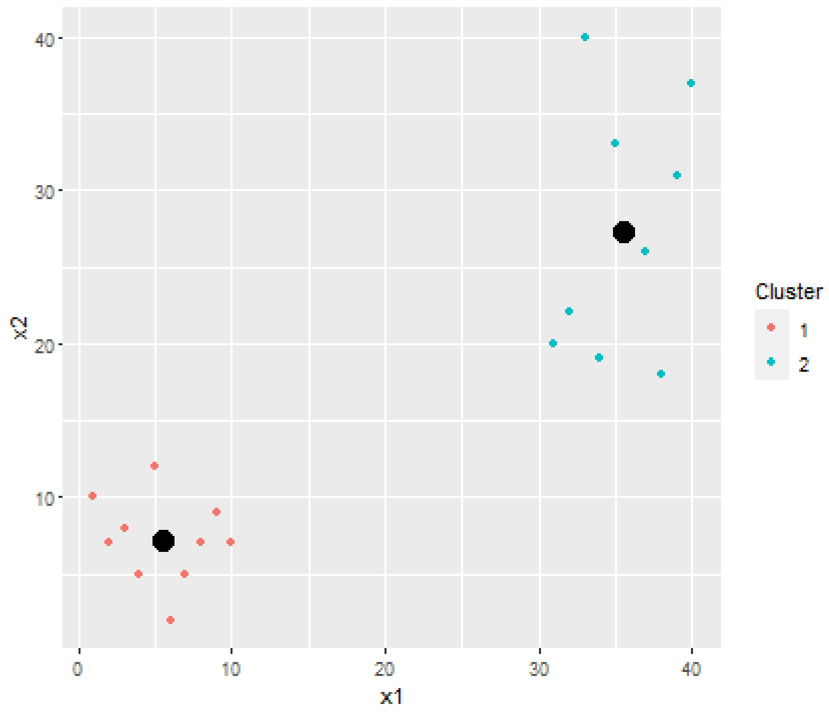


| GPA | Screen Time |
|---|---|
| 3.9 | 90 |
| 4.0 | 150 |
| 3.0 | 140 |
| 2.0 | 139 |

# Step 2: Relocate centroids



# Step 2: Collect points for each clusters



# Centroids

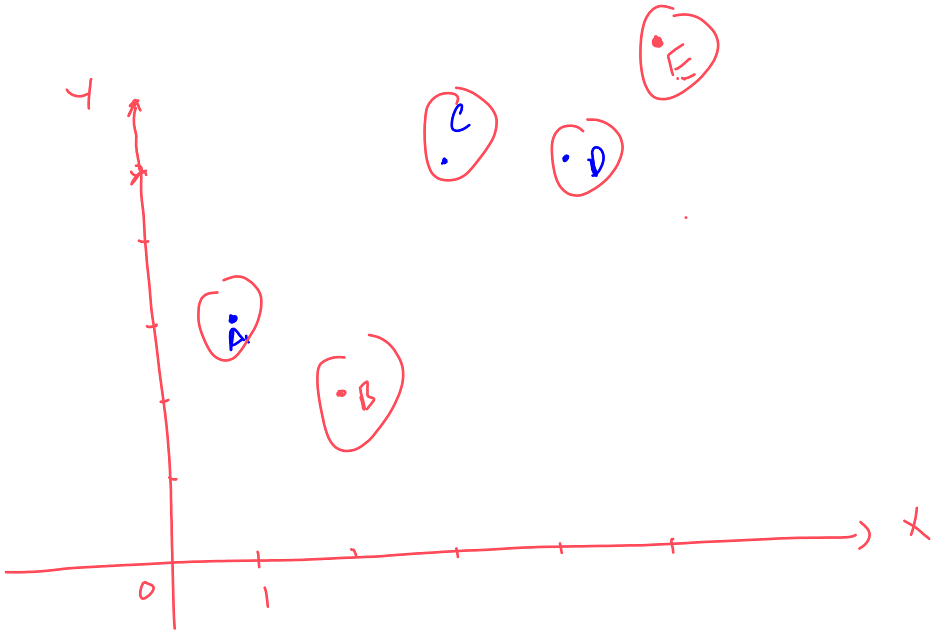
| Cluster | x1 | x2 |
|---|---|---|
| 1 | 5.5 | 7.2 |
| 2 | 35.5 | 27.3 |

# K-means Algorithm

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

# Dataset

| Point | x | y |
|---|---|---|
| A | 1 | 3 |
| B | 2 | 2 |
| C | 3 | 5 |
| D | 4 | 5 |
| E | 5 | 6 |



# Randomly Assign Cluster to Points

| Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 2 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 1 | D | 4 | 5 |
| 2 | E | 5 | 6 |

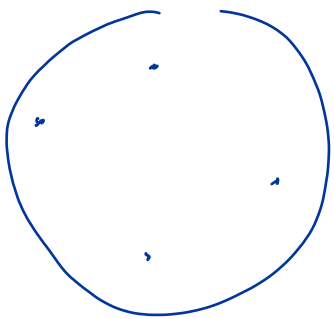
# Determine Centroids

| Cluster | Point | x | y | M_1x | M_1y | M_2x | M_2y |
|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.67 | 4.33 | 3.5 | 4 |
| 2 | B | 2 | 2 | 2.67 | 4.33 | 3.5 | 4 |
| 1 | C | 3 | 5 | 2.67 | 4.33 | 3.5 | 4 |
| 1 | D | 4 | 5 | 2.67 | 4.33 | 3.5 | 4 |
| 2 | E | 5 | 6 | 2.67 | 4.33 | 3.5 | 4 |

- Centroid 1: $M_1 = \frac{A+C+D}{3} = \frac{(1,3)+(3,5)+(4,5)}{3} = \frac{(8,13)}{3} = (2.67, 4.33)$
- Centroid 2: $M_2 = \frac{B+E}{\underset{2}{\cancel{3}}} = \frac{(2,2)+(5,6)}{2} = \frac{(7,8)}{2} = (3.5, 4)$

# Distance to Centroids

| Cluster | Point | x | y | M_1x | M_1y | M_2x | M_2y | dc1 | dc2 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.67 | 4.33 | 3.5 | 4 | 2.13 | 2.69 |
| 2 | B | 2 | 2 | 2.67 | 4.33 | 3.5 | 4 | 2.42 | 2.50 |
| 1 | C | 3 | 5 | 2.67 | 4.33 | 3.5 | 4 | 0.75 | 1.12 |
| 1 | D | 4 | 5 | 2.67 | 4.33 | 3.5 | 4 | 1.49 | 1.12 |
| 2 | E | 5 | 6 | 2.67 | 4.33 | 3.5 | 4 | 2.87 | 2.50 |



- $AM_1 = \sqrt{(1-2.67)^2 + (3-4.33)^2} = 2.13$ and so on
- Variance within Cluster 1 = $V_1 = AM_1^2 + CM_1^2 + DM_1^2 = 7.3195$
- Variance within Cluster 2 = $V_2 = BM_2^2 + DM_2^2 = 12.5$

- Total Variance = $V_1 + V_2 = 19.83$

# Compare Distances to Centroids

| Cluster | Point | x | y | dc1 | dc2 | min_distance |
|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.13 | 2.69 | 2.13 |
| 2 | B | 2 | 2 | 2.42 | 2.50 | 2.42 |
| 1 | C | 3 | 5 | 0.75 | 1.12 | 0.75 |
| 1 | D | 4 | 5 | 1.49 | 1.12 | 1.12 |
| 2 | E | 5 | 6 | 2.87 | 2.50 | 2.50 |

# Reassign Clusters

| Cluster | Point | x | y | dc1 | dc2 | min_distance | New_Cluster |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | A | 1 | 3 | 2.13 | 2.69 | 2.13 | 1 |
| 2 | B | 2 | 2 | 2.42 | 2.50 | 2.42 | 1 |
| 1 | C | 3 | 5 | 0.75 | 1.12 | 0.75 | 1 |
| 1 | D | 4 | 5 | 1.49 | 1.12 | 1.12 | 2 |
| 2 | E | 5 | 6 | 2.87 | 2.50 | 2.50 | 2 |

- New cluster 1 = {A, B, C}
- New cluster 2 = {D, E}
- Total Variance = $AN_1^2 + BN_1^2 + CN_1^2 + DN_2^2 + EN_2^2 = 7.67$

# Reassign Clusters

| Cluster | Point | x | y | dc1 | dc2 | min_distance | New_Cluster |
|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.13 | 2.69 | 2.13 | 1 |
| 2 | B | 2 | 2 | 2.42 | 2.50 | 2.42 | 1 |
| 1 | C | 3 | 5 | 0.75 | 1.12 | 0.75 | 1 |
| 1 | D | 4 | 5 | 1.49 | 1.12 | 1.12 | 2 |
| 2 | E | 5 | 6 | 2.87 | 2.50 | 2.50 | 2 |

- New cluster 1 = {A, B, C}
- New cluster 2 = {D, E}
- Total Variance = $AN_1^2 + BN_1^2 + CN_1^2 + DN_2^2 + EN_2^2 = 7.67$
- The process continues until there is no change in the total variance
- The total variance will be reduced to its minimum.

# Step 1: Total Variance within

| Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 2 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 1 | D | 4 | 5 |
| 2 | E | 5 | 6 |

- Total Variance within 19.83

# Step 2: Total Variance within

| New_Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 1 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 2 | D | 4 | 5 |
| 2 | E | 5 | 6 |

- Total Variance within 7.67

# Step 2: Total Variance within

| New_Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 1 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 2 | D | 4 | 5 |
| 2 | E | 5 | 6 |

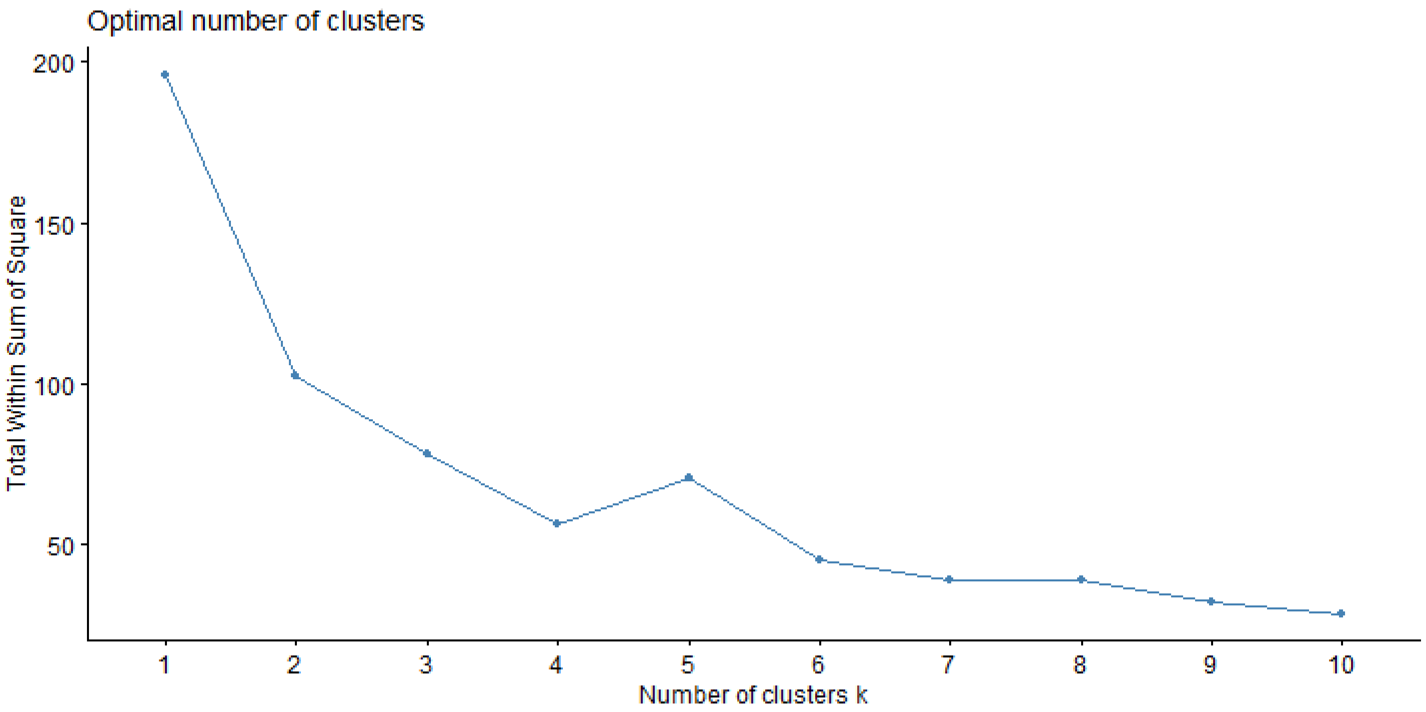
- Total Variance within 7.67
- The process continues until there is no change in the total variance
- The total variance will be reduced to its minimum.

# Terminology

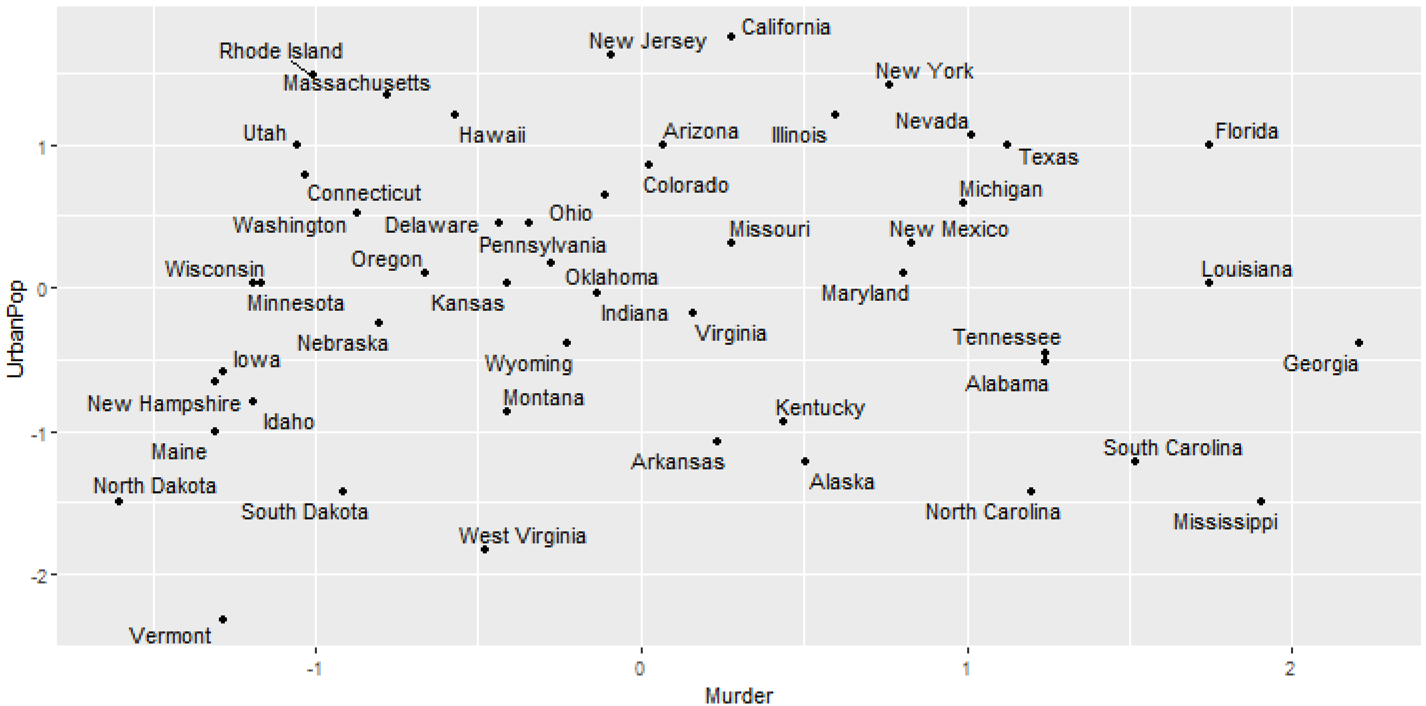
- Total Variance also called the total within sum square or the within-cluster sum of squares (WCSS) or WSS

# Mumber of clusters? Elbow method!

- Plot the WSS
- Decide the `elbow` of the graph



```
##                 Murder   Assault   UrbanPop         Rape cluster
## Alabama    1.24256408 0.7828393 -0.5209066 -0.003416473       4
## Alaska     0.50786248 1.1068225 -1.2117642  2.484202941       4
## Arizona    0.07163341 1.4788032  0.9989801  1.042878388       4
## Arkansas   0.23234938 0.2308680 -1.0735927 -0.184916602       3
## California 0.27826823 1.2628144  1.7589234  2.067820292       4
## Colorado   0.02571456 0.3988593  0.8608085  1.864967207       4
```



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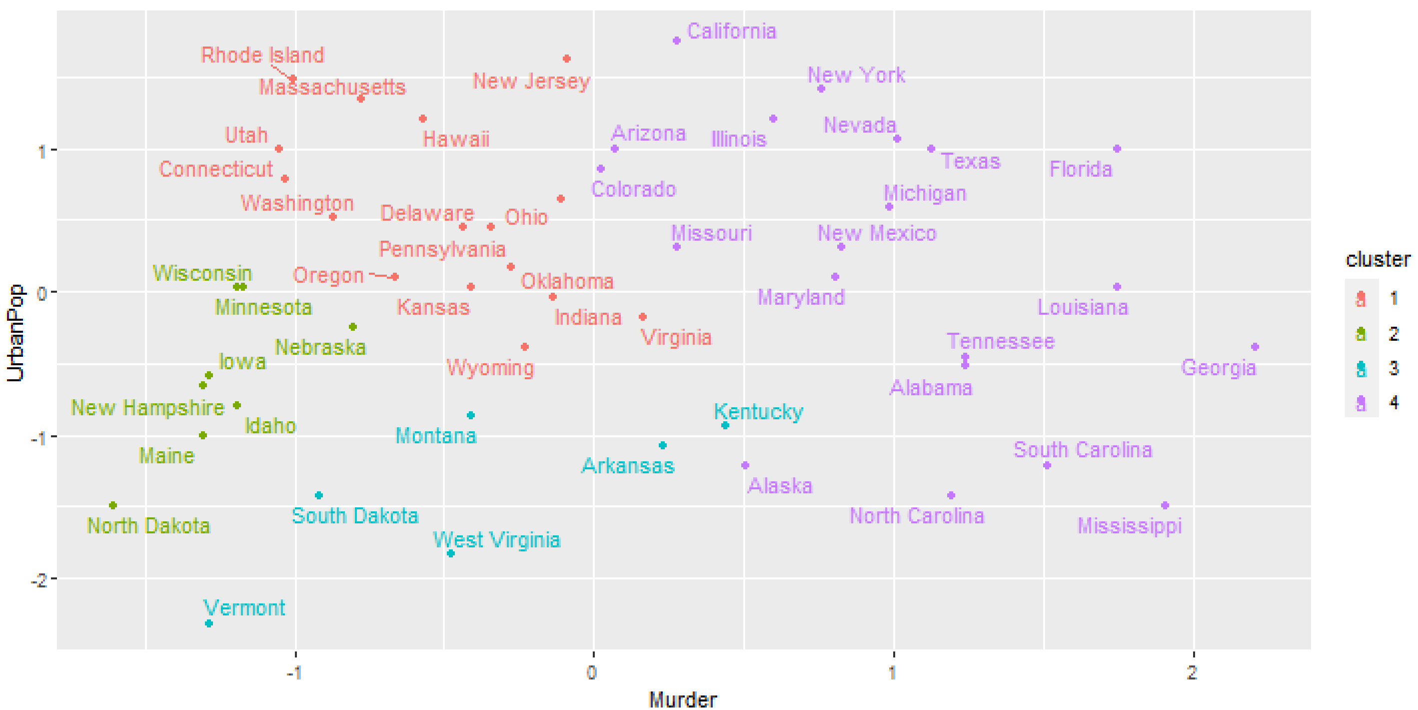

cluster
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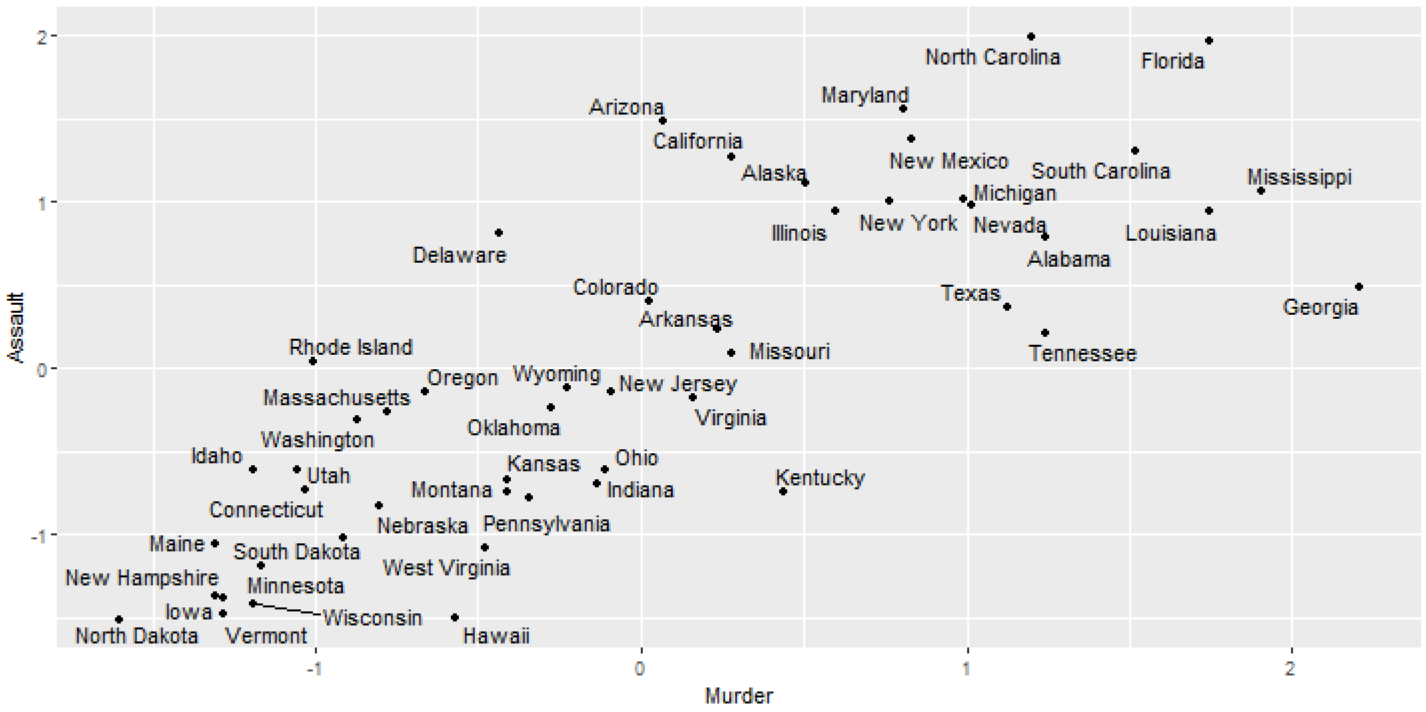
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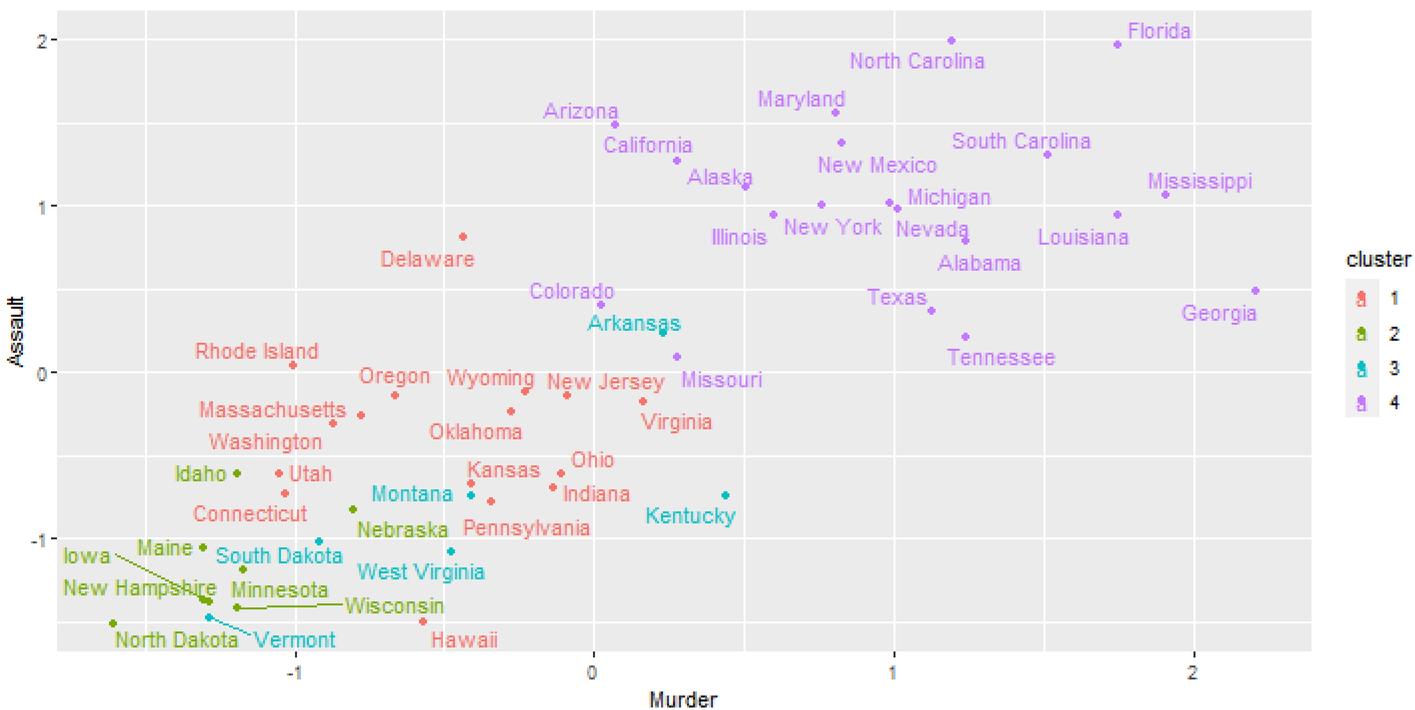

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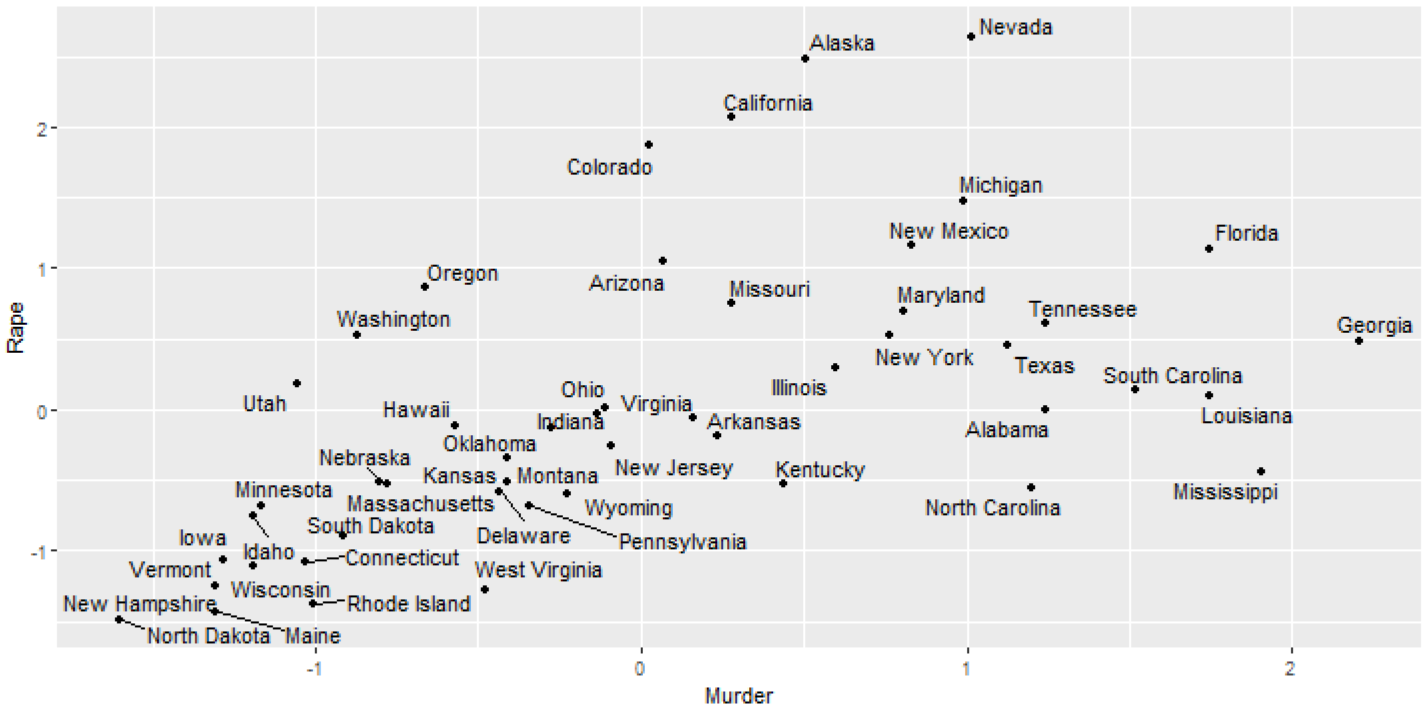
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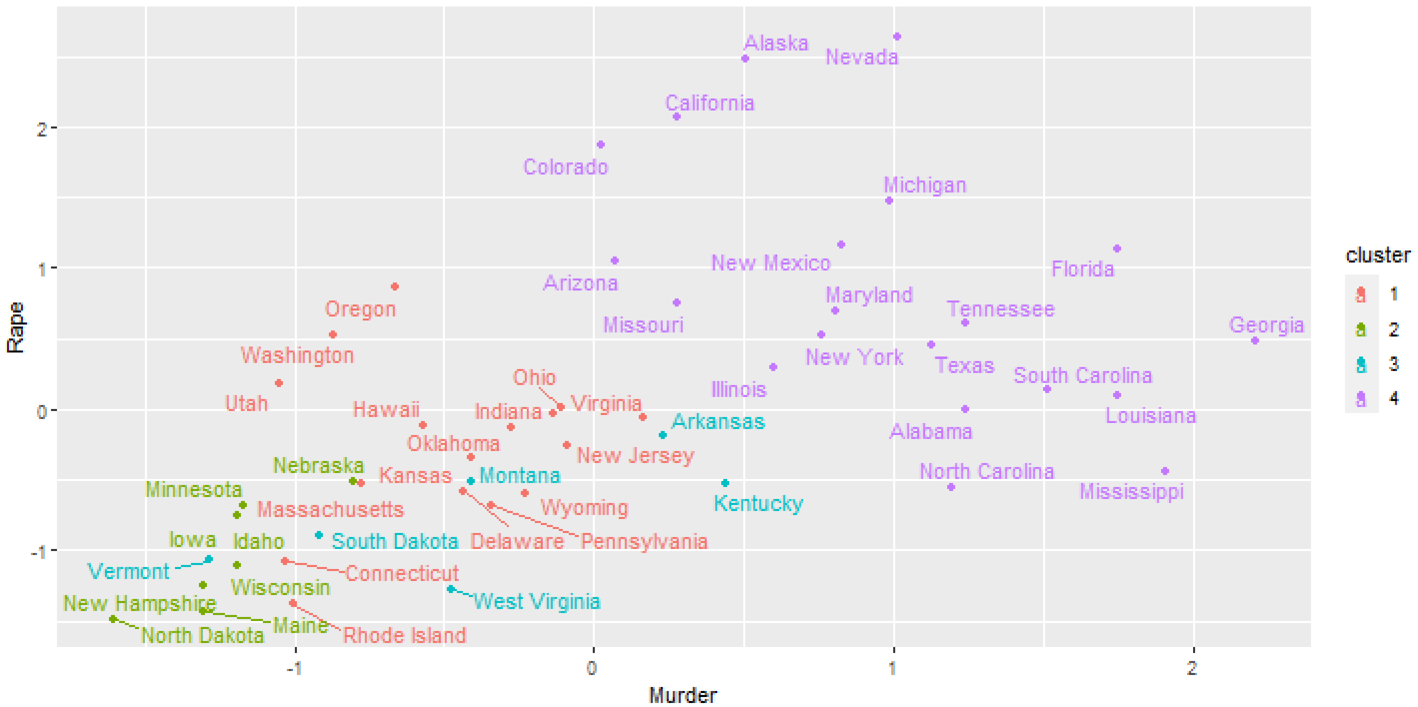
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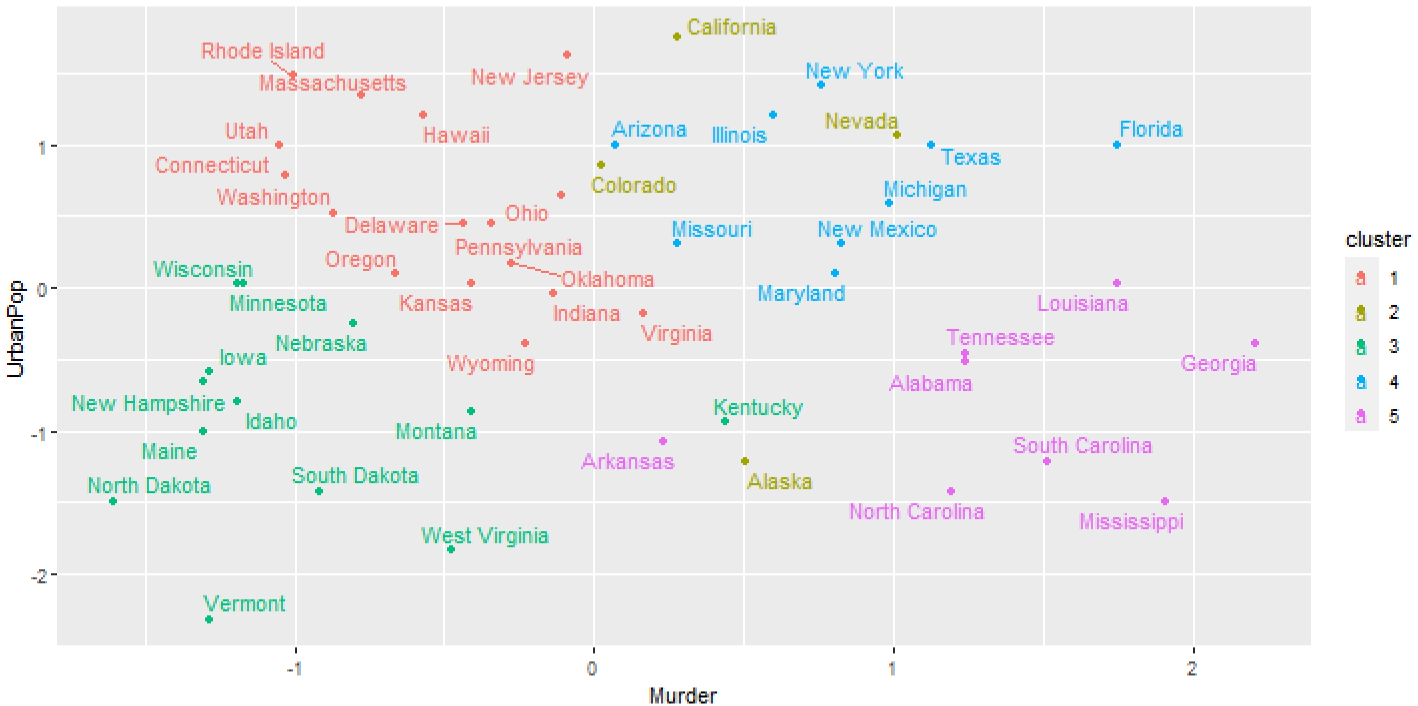
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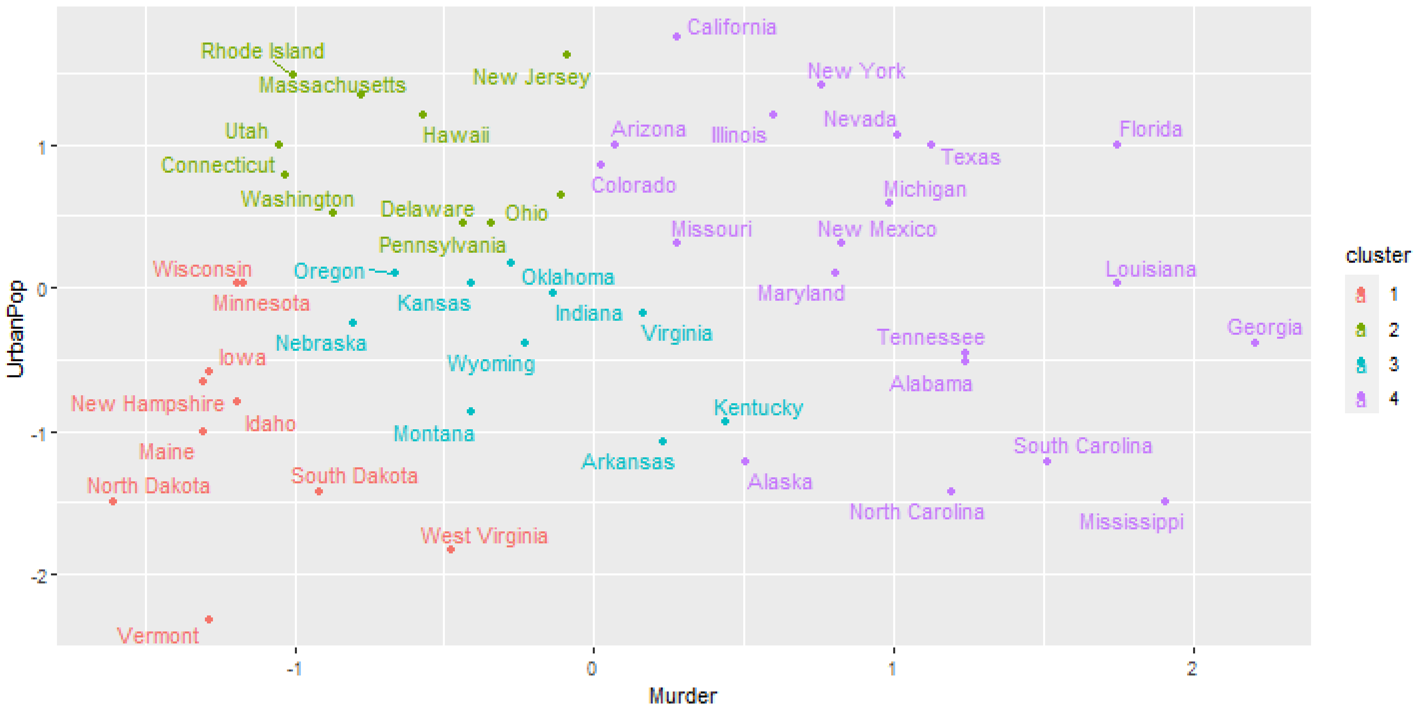

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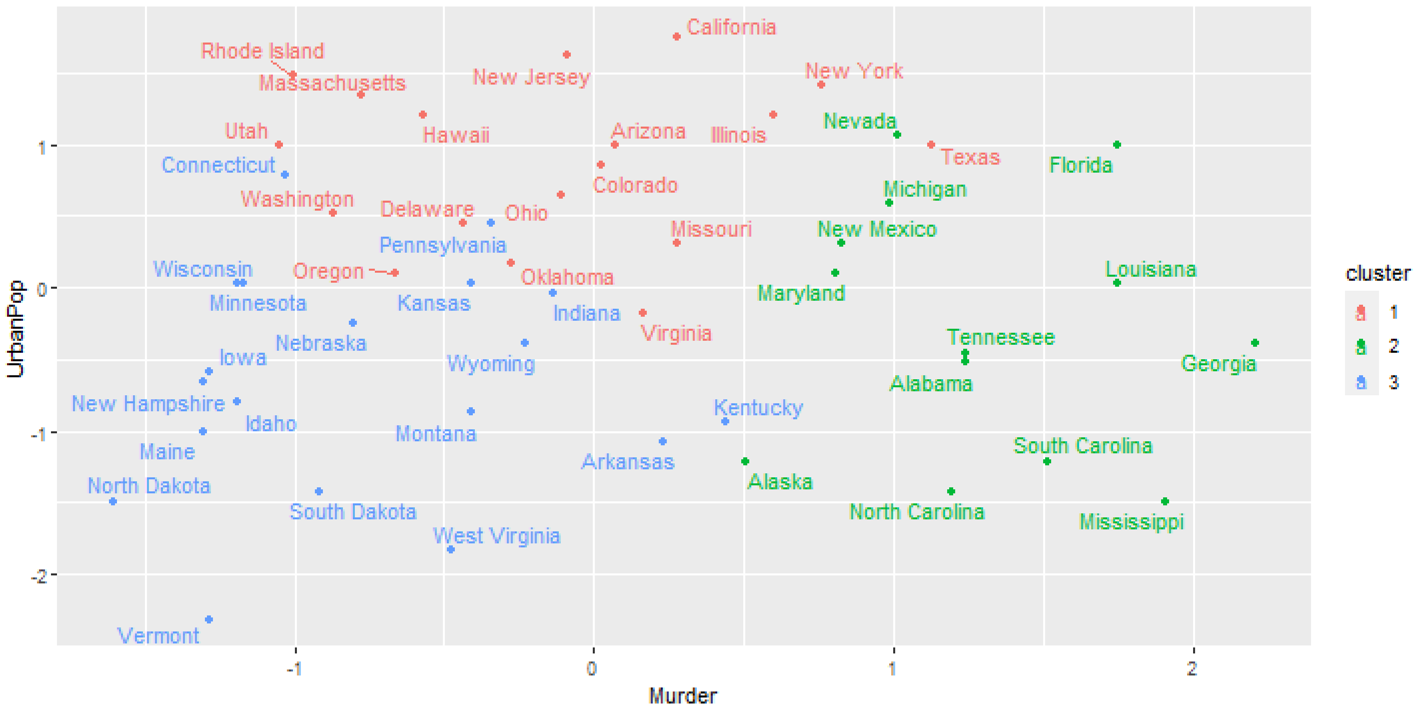

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cluster
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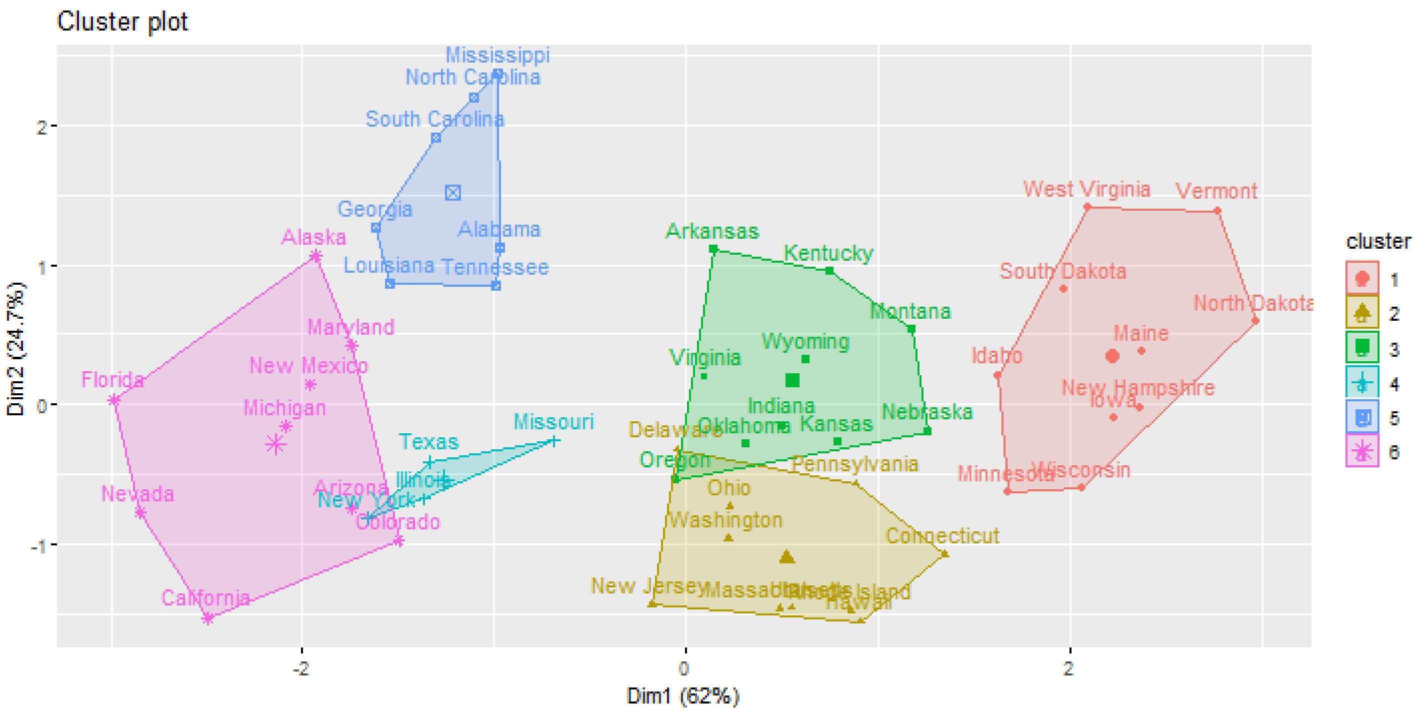
# Principal Components

- Since we have four variables, we could have 6 different plots to visualize the clustring
- The more variables we have, the more plot we can have
- It is easier to contain all the variables in a few variables, then make plots.
- One way to do this is to use principal components analysis. The first two principals may contain most of the information of in the dataset.



Cluster plot
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New Hampshire
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Dim1 (62%)
Dim2 (24.7%)
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-1
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cluster
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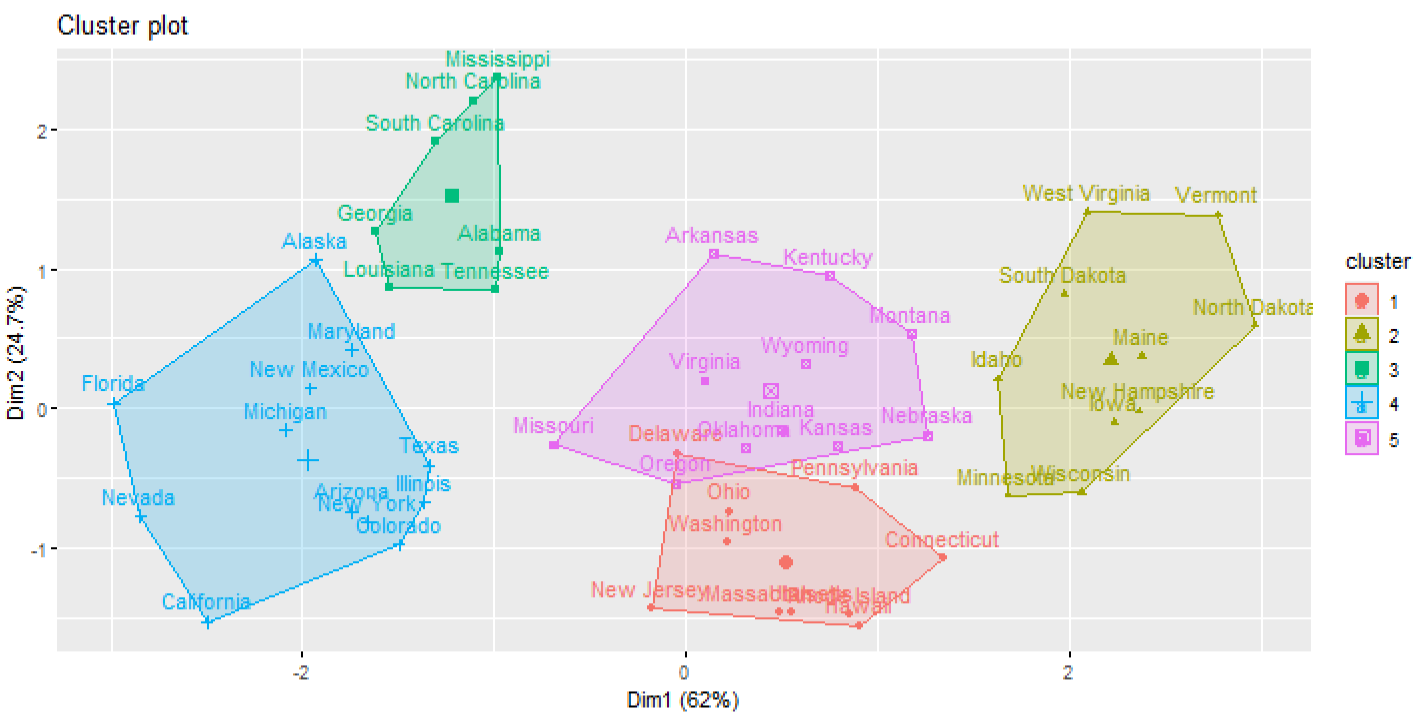

Cluster plot
Dim1 (62%)
Dim2 (24.7%)
cluster
1
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Mississippi
North Carolina
South Carolina
Georgia
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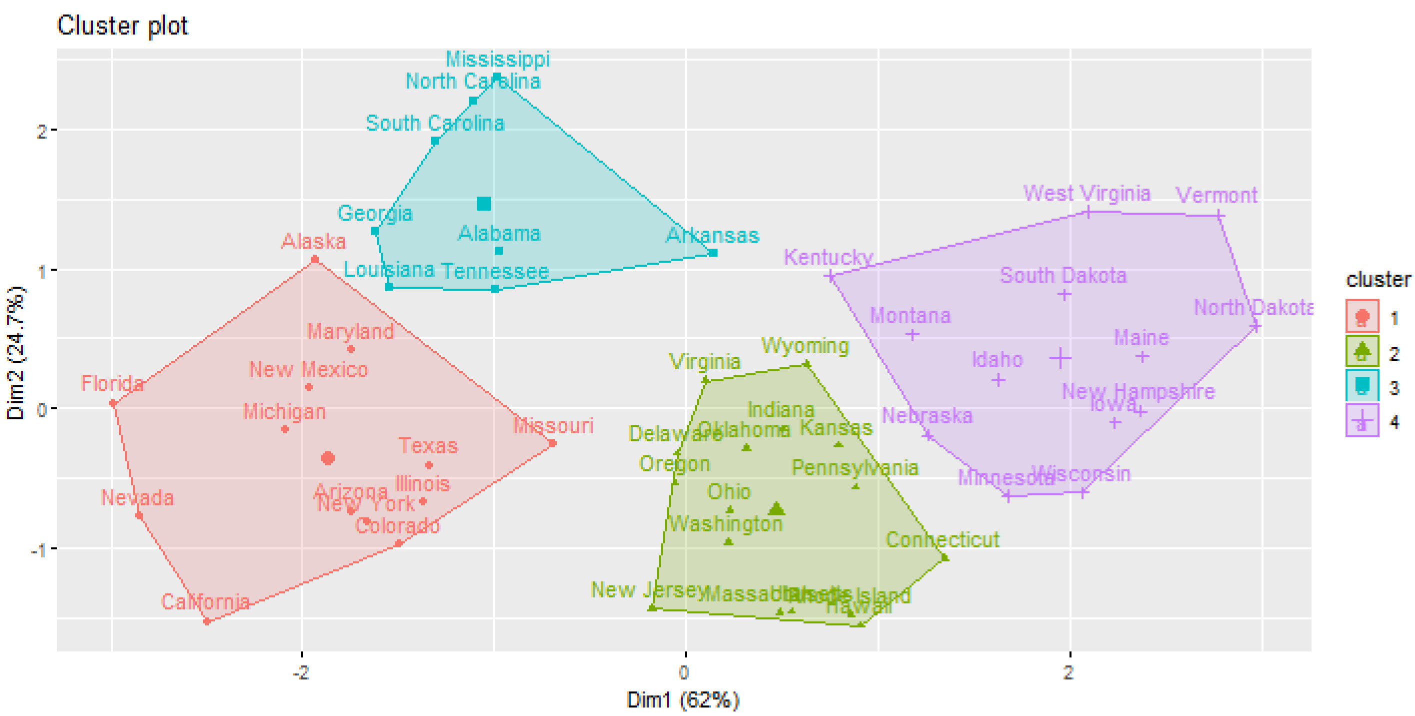
Cluster plot
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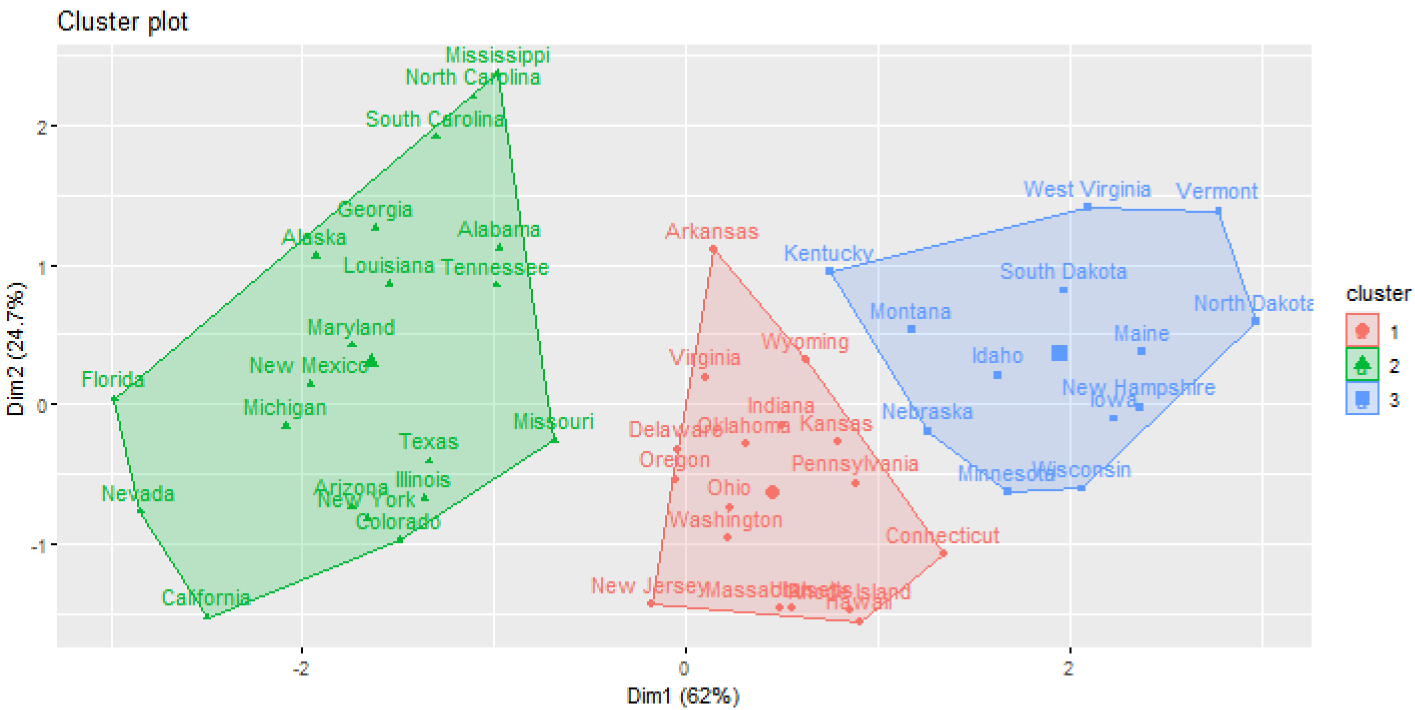
California
West Virginia
Vermont
Kentucky
South Dakota
North Dakota
Montana
Maine
Idaho
New Hampshire
Iowa
Nebraska
Minnesota
Wisconsin
Wyoming
Virginia
Indiana
Delaware
Oklahoma
Kansas
Oregon
Pennsylvania
Ohio
Washington
Connecticut
New Jersey
Hawaii
Dim1 (62%)
Dim2 (24.7%)
cluster
1
2
3
4
-2
0
2
-1
1



Cluster plot
Dim2 (24.7%)
Dim1 (62%)
2
1
0
-1
-2
0
2
Mississippi
North Carolina
South Carolina
Georgia
Alabama
Alaska
Louisiana
Tennessee
Maryland
New Mexico
Florida
Michigan
Texas
Missouri
Illinois
Arizona
New York
Nevada
Colorado
California
Arkansas
Kentucky
West Virginia
Vermont
South Dakota
Montana
North Dakota
Maine
Wyoming
Idaho
Virginia
New Hampshire
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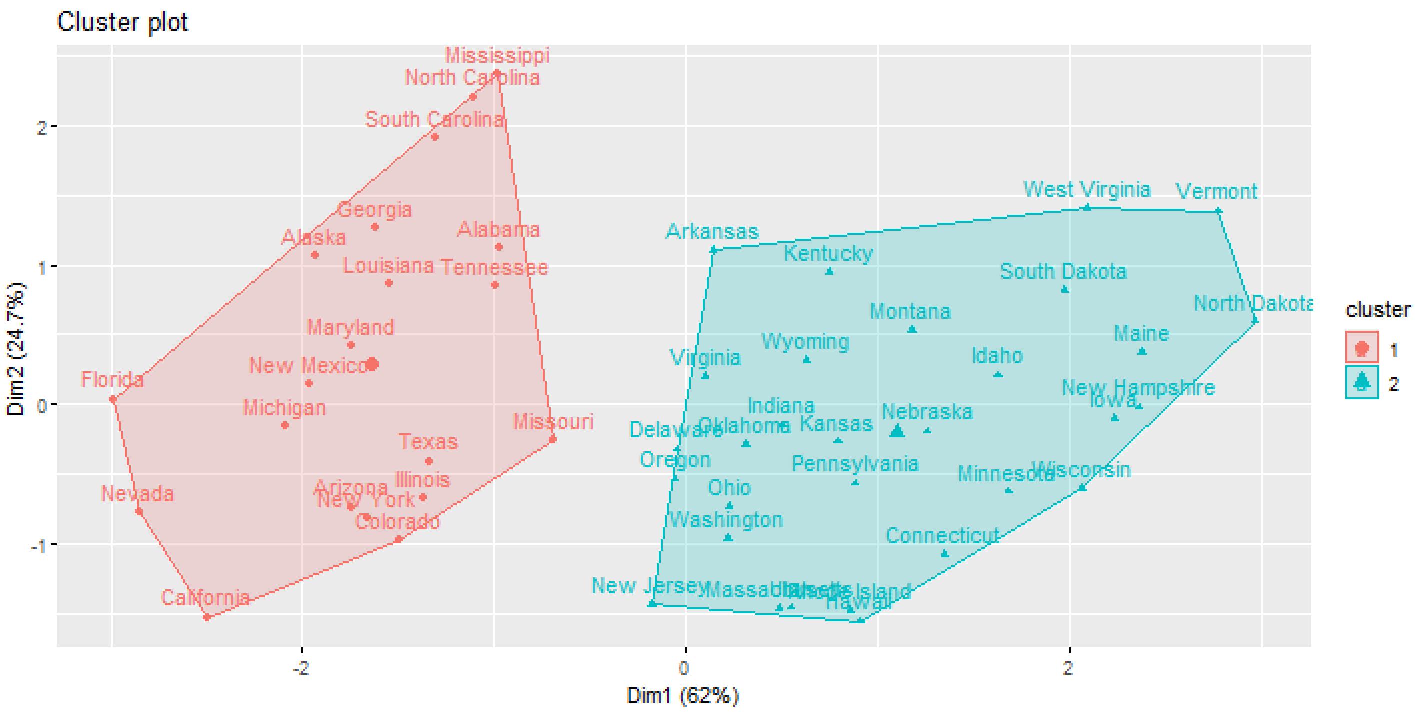
Indiana
Nebraska
Delaware
Oklahoma
Kansas
Oregon
Pennsylvania
Minnesota
Wisconsin
Ohio
Washington
Connecticut
New Jersey
Hawaii
cluster
1
2
3



Cluster plot
Dim1 (62%)
Dim2 (24.7%)
cluster
1
2
-2
0
2
-1
1
Mississippi
North Carolina
South Carolina
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