

Cluster Analysis: Discovery

Winter Institute in Data Science

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Matrices and Lists

Supervised and Unsupervised Learning

Hierarchical Clustering

Partitional Clustering

Selecting k

Exercise

Matrices and Lists

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- ▶ `matrix`: rectangular array with a few more restrictions than `data.frame`

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- ▶ `df[, "v1"]`
- ▶ `df[, 6]`
- ▶ `df["v1"]` (keeps col name)

1. Describe list `l1` created below:

```
v1 <- 1:8  
v2 <- letters[1:5]  
m <- matrix(1:9, 3, 3)  
l1 <- list(x = v1, y = v2, z = m)
```

2. What is `l1$y`?
3. What is `l1[[1]]`?
4. What is `l1[[3]][2, 2]`?

Distance Matrix for Clustering

Each cell is a *distance* between unit **row** and unit **column**:

	a	b	c	d
a	0	1	2	3
b	1	0	6	7
c	2	6	0	8
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So, $\|(c, d)\| > \|(a, b)\|$, e.g., $(8 > 1)$

Supervised and Unsupervised Learning

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Supervised: Modeling with **known** outcomes

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Unsupervised: Discovery w/ **unknown** outcomes

Supervised Learning

- ▶ Linear regression (LS)

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(logistic, probit, Poisson, beta)

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- ▶ NLP (predict “bot?” 0/1 from matx of word indicators)

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If you have $y = f(X)$, it's “supervised”.

Unsupervised Learning

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- ▶ Principal components analysis (PCA)
- ▶ (Some neural networks)
- ▶ NLP (derive topics from documents)
- ▶ Clustering algorithms (most)

Clustering is a method of “unsupervised learning” – of trying to derive structure from data when no outcome labels are given.

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 - ▶ (e.g., NE’s *nonpartisan* “Unicameral”)
- ▶ Geographic clustering: daily activities
 - ▶ no “home”/“work”/“leisure” labels

Clustering

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 - ▶ Find best groups at many levels

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Clustering

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 - ▶ Find best groups at many levels
 - ▶ Units in one cluster at each level of hierarchy
- ▶ Partitional clustering
 - ▶ Find splits in full set
 - ▶ Units in only one cluster

Hierarchical Clustering

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Consider a set of units open to cluster discovery,
 $\{a, b, c, d, e\}$

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Divisive clustering

- ▶ Start at $\{a, b, c, d, e\}$

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Divisive clustering

- ▶ Start at $\{a, b, c, d, e\}$
- ▶ Find $\{a, b, d\}$ and $\{c, e\}$

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- ▶ Find $\{a, b, d\}$ and $\{c, e\}$
- ▶ Find $\{a, b\}$, $\{d\}$, and $\{c, e\}$

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- ▶ Find $\{a, b, d\}$ and $\{c, e\}$
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Divisive clustering is “top-down”

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- ▶ Find $\{a, b\}$, $\{c, e\}$, and leave $\{d\}$

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- ▶ ...

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- ▶ Find $\{a, b\}$ and leave $\{c\}, \{d\}, \{e\}$
- ▶ Find $\{a, b\}, \{c, e\}$, and leave $\{d\}$
- ▶ ...
- ▶ End at $\{a, b, c, d, e\}$

Agglomerative clustering is “bottom-up”

Hierarchical Clustering

Each unit is in a clustering at every level.

Agglomerative Hierarchical Clustering

Complete linkage clustering: greedily create clusters

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1. Merge closest pair (into, say, $\{a, b\}$)

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Complete linkage clustering: greedily create clusters

1. Merge closest pair (into, say, $\{a, b\}$)
2. Update **dist**: delete rows/cols for a, b ; add row for $\{a, b\}$
(with max)
3. Merge closest “pair”
4. Update **dist**
5. ...

Agglomerative Hierarchical Complete Linkage Clusters

	a	b	c	d
a	0	1	2	3
b	1	0	6	7
c	2	6	0	8
d	3	7	8	0

Agglomerative Hierarchical Complete Linkage Clusters

	a	b	c	d
a	0	1	2	3
b	1	0	6	7
c	2	6	0	8
d	3	7	8	0

	(a,b)	c	d
(a,b)	0	6	7
c	6	0	8
d	7	8	0

Agglomerative Hierarchical Complete Linkage Clusters

	a	b	c	d
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b	1	0	6	7
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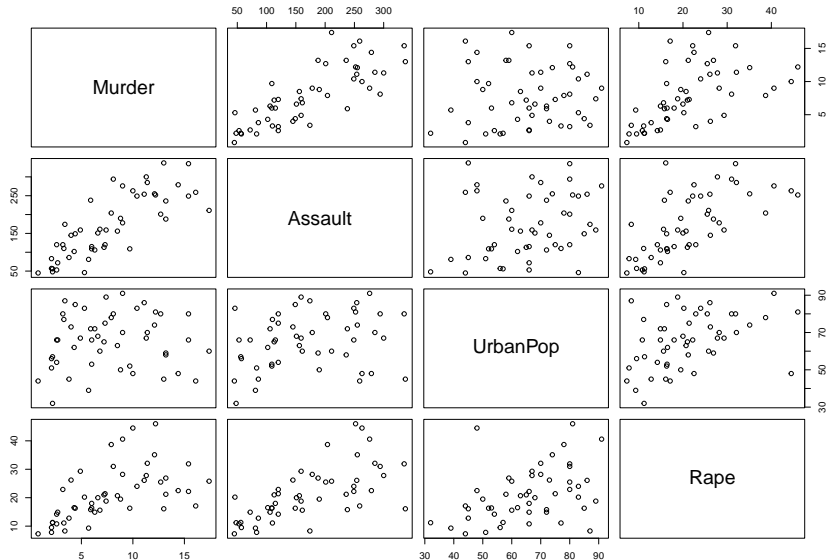
	(a,b)	c	d
(a,b)	0	6	7
c	6	0	8
d	7	8	0

(“friends of friends”)

Agglomerative Hierarchical Clustering

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```
pairs(USArrests)
```



Agglomerative Hierarchical Clustering

```
d <- dist(USArrests, method = "euclidean")  
d |> round(0)
```

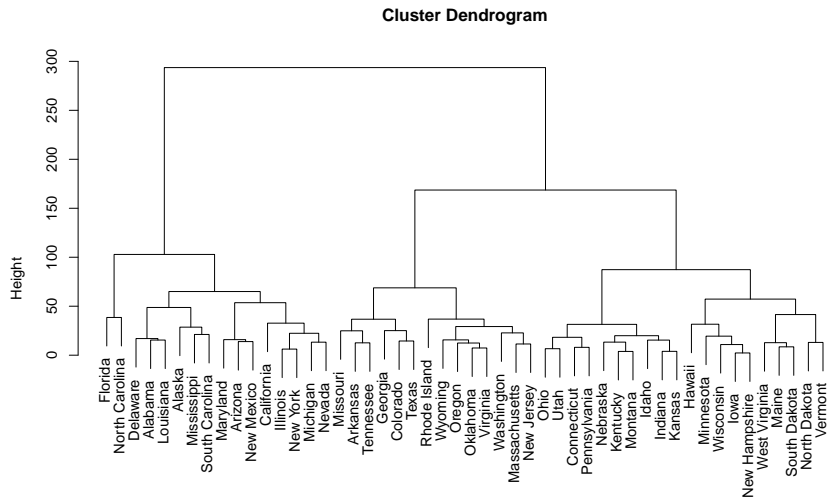
##	Alabama	Alaska	Arizona	Arkansas	California
## Alaska	37				
## Arizona	63	47			
## Arkansas	47	77	109		
## California	56	45	23	98	
## Colorado	42	66	90	37	7
## Connecticut	128	159	185	85	16
## Delaware	17	45	59	53	4
## Florida	102	80	42	149	6
## Georgia	26	57	86	26	7
## Hawaii	192	221	248	148	23
## Idaho	117	146	177	71	16
## Illinois	28	43	46	68	3
## Indiana	123	153	182	78	16
## Iowa	181	210	240	135	22

Agglomerative Hierarchical Clustering

```
hag <- hclust(d, method = "complete")  
plot(hag)
```

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plot(hag)
```



Recluster w/ Alternative Distance Metric: Mahalanobis

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First, define function to make distance matrix:

```
mahal <- function(q, vc){  
  storage <- matrix(NA, nrow(q), nrow(q))  
  q <- as.matrix(q)  
  for(i in 1:nrow(q)){  
    storage[row(q), i] <- mahalanobis(x = q,  
                                       center=q[i, ],  
                                       cov = vc)  
  }  
  return(sqrt(storage))  
}
```

Recluster w/ Alternative Distance Metric: Mahalanobis

```
d_mah <- mahal(USArrests, cov(USArrests))  
row.names(d_mah) <- colnames(d_mah) <- row.names(USArrests)  
d_mah <- as.dist(d_mah)  
d_mah |> round(1)
```

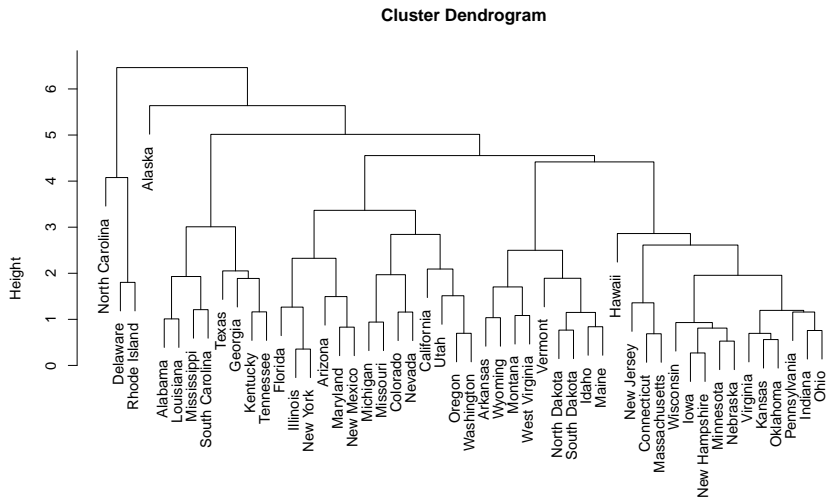
##	Alabama	Alaska	Arizona	Arkansas	California
## Alaska	4.4				
## Arizona	3.2	3.9			
## Arkansas	1.4	3.5	2.7		
## California	3.5	3.6	1.7	3.3	
## Colorado	3.3	2.8	2.6	2.9	1.5
## Connecticut	2.8	5.4	2.9	2.6	3.0
## Delaware	3.0	5.0	1.7	2.6	3.0
## Florida	1.8	4.6	2.3	2.5	2.0
## Georgia	2.2	5.4	5.0	3.3	4.0
## Hawaii	3.5	5.6	4.5	3.8	3.0
## Idaho	2.7	3.8	2.5	1.5	3.0
## Illinois	2.0	4.9	2.1	2.4	2.0

Recluster w/ Alternative Distance Metric: Mahalanobis

```
hag <- hclust(d_mah, method = "complete")  
plot(hag)
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Recluster w/ Alternative Distance Metric: Mahalanobis

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- ▶ (`Assault` has large variance, and cor w/ `UrbanPop`)

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- ▶ Small differences in **Assault** get over-weighted if euclidean dist
- ▶ (**Assault** has large variance, and cor w/ **UrbanPop**)
- ▶ Mahalanobis dist allows vars on different scales to all contribute.

Agglomerative Hierarchical Clustering

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- ▶ (`Assault` has large variance, and cor w/ `UrbanPop`)
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- ▶ E.g., `euclidean` clusters

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- ▶ E.g., euclidean clusters

##		Murder	Assault	UrbanPop	Rape
##	Ohio	7.3	120	75	21.4
##	Utah	3.2	120	80	22.9

Agglomerative Hierarchical Clustering

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- ▶ (**Assault** has large variance, and cor w/ **UrbanPop**)
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##		Murder	Assault	UrbanPop	Rape
##	Ohio	7.3	120	75	21.4
##	Utah	3.2	120	80	22.9

versus

##		Murder	Assault	UrbanPop	Rape
##	Indiana	7.2	113	65	21.0
##	Ohio	7.3	120	75	21.4

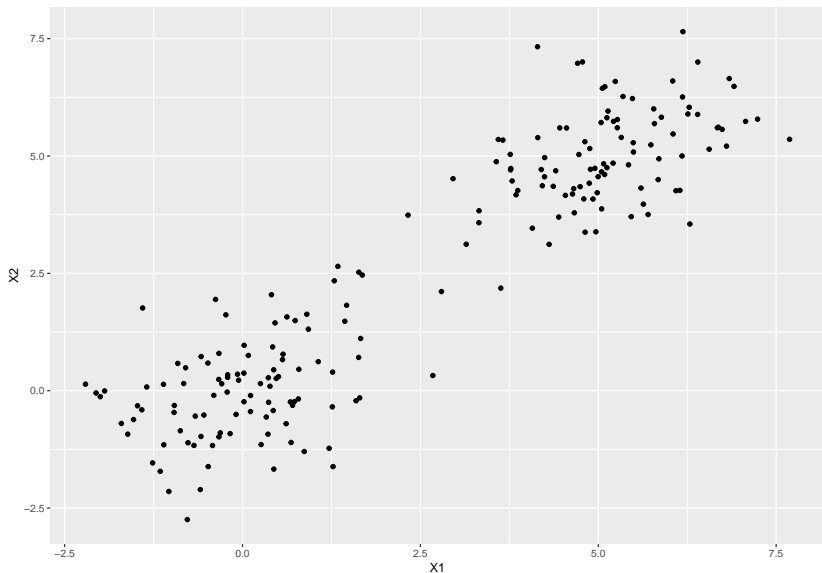
Partitional Clustering

k -means

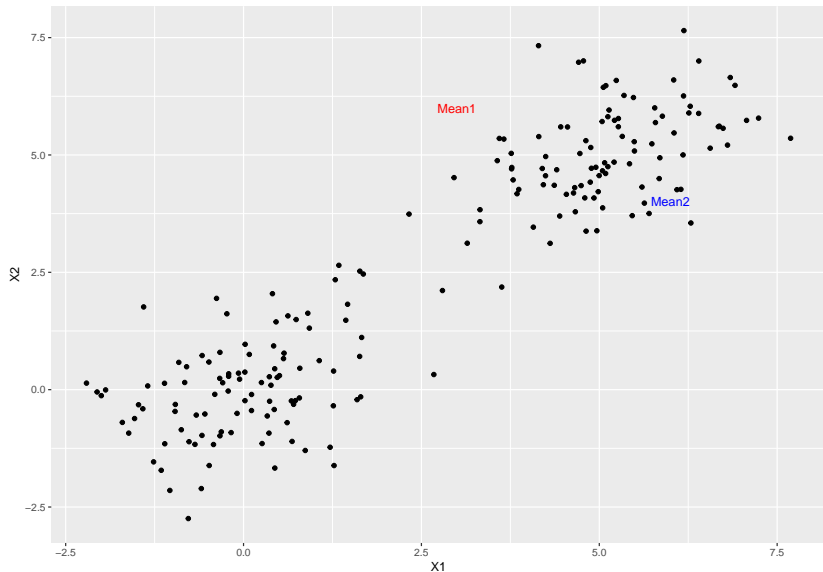
0. Standardize variables, or ensure comparable scales.
(A diff of 1 unit on x_1 should \approx a diff of 1 unit on x_2 .)
1. Choose k , the number of clusters to identify.
2. Select the location of a center for each cluster.
3. Assign each observation to the cluster defined by the center closest to it.
4. Relocate each cluster's center to the mean of the observations currently in that cluster.
5. Repeat 3. and 4. until no observations gets assigned to a new cluster.

Suppose we have a set of points measured in a two-dimensional space, with X_1 and X_2 on comparable scales.

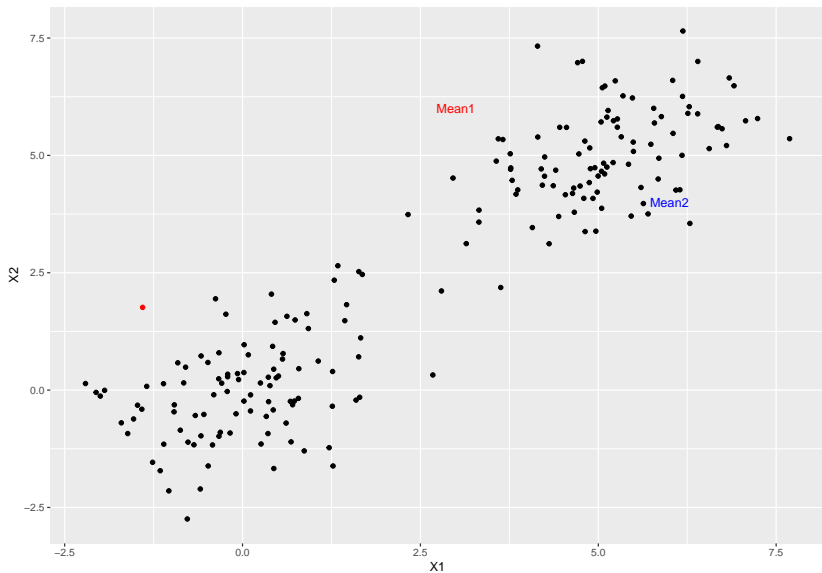
We will find $k = 2$ clusters. Ideas?



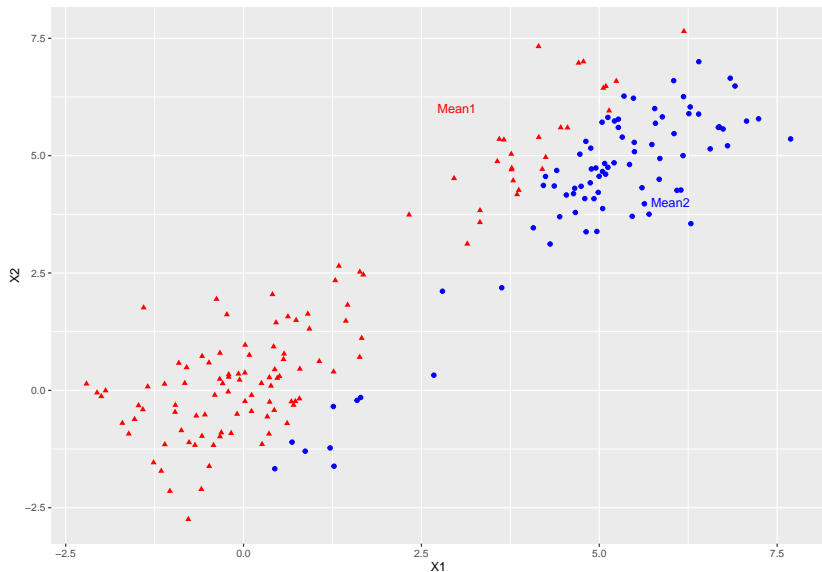
2. Let's randomly select two centroids:



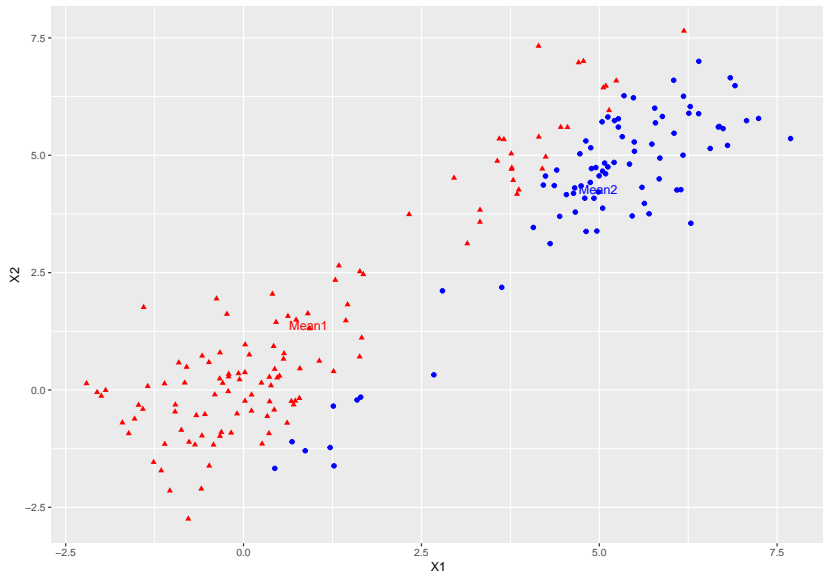
Where “should” this point go?



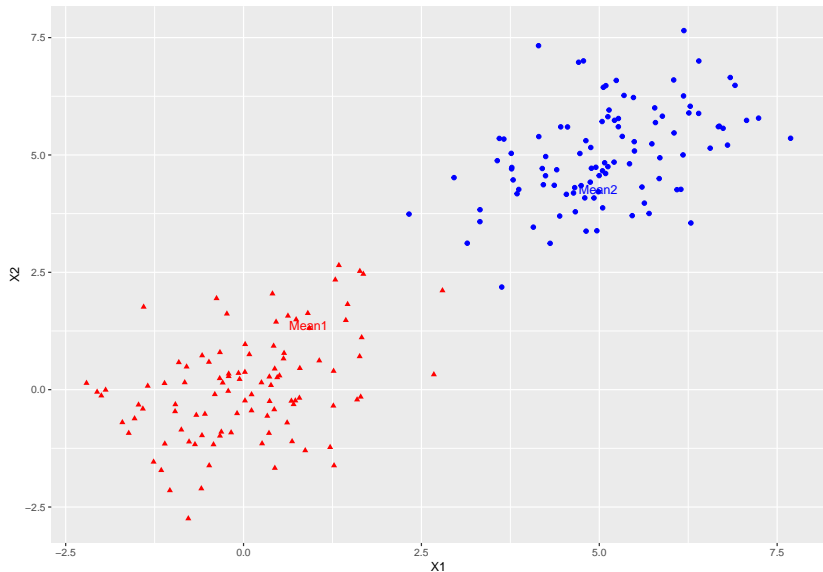
3. Find (Euclidean) distance between each point and the centroids; assign each point to closer centroid:



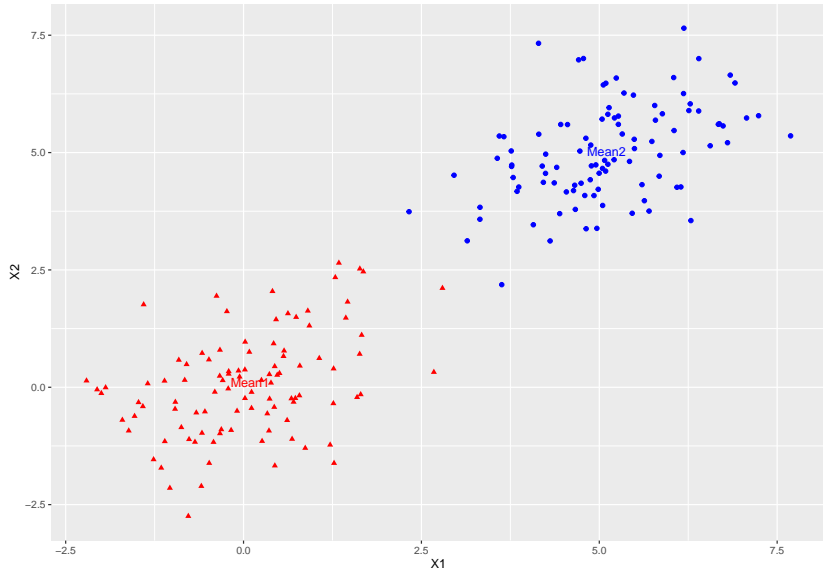
4. Relocate centroids to the mean (X_1 , X_2) value for each cluster:



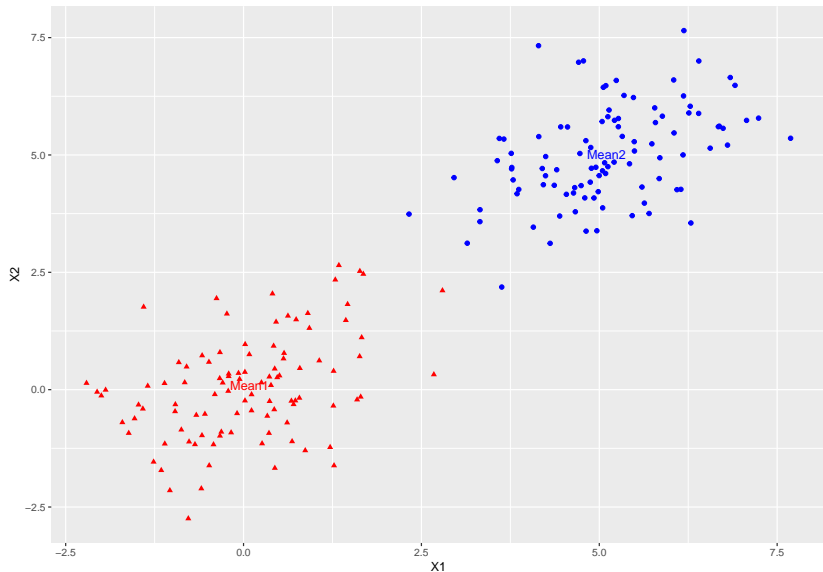
3. Reassign each observation to the closer centroid:



4. Recalculate the centroid locations ...

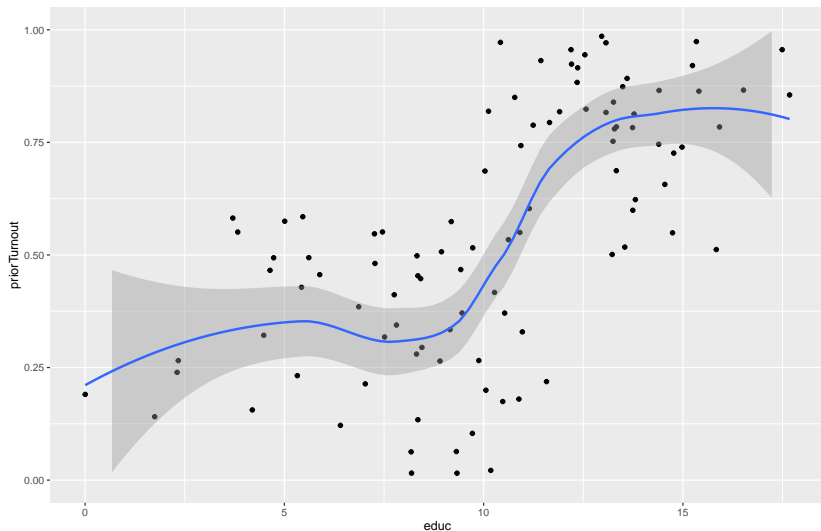


3. Reassign points to clusters ...



Standardization: Why, before clustering?

Suppose we have prior turnout $[0, 1]$ and education (yrs):



```
k2 <- kmeans(df2, centers = 2)
names(k2)
```

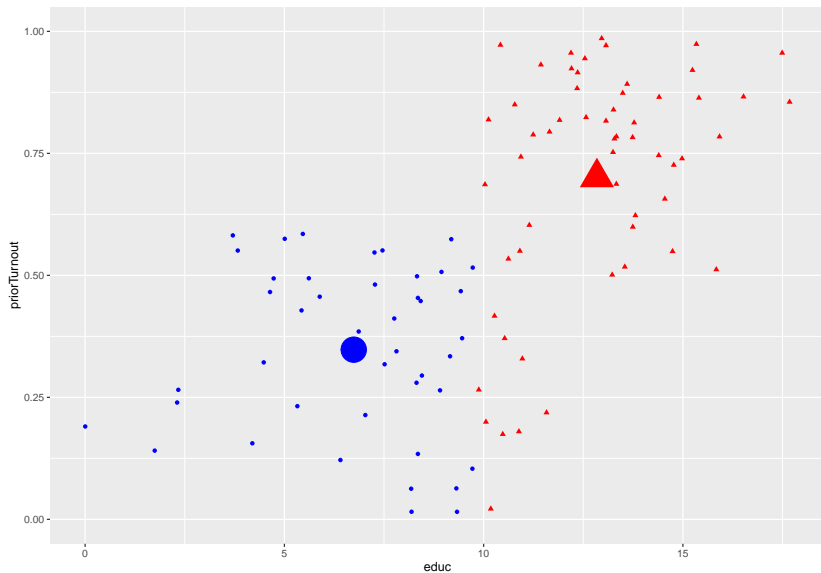
```
## [1] "cluster"      "centers"      "totss"      "within"
## [6] "betweenss"    "size"        "iter"      "ifault"
```

```
table(k2$cluster)
```

```
##
##  1  2
## 57 43
```

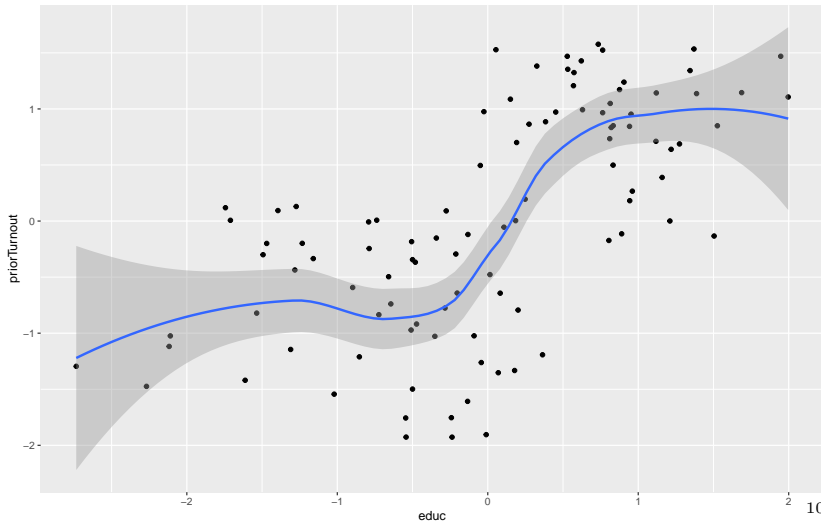
```
k2$centers
```

```
##      educ priorTurnout
## 1 12.841805    0.7007953
## 2  6.740813    0.3477128
```

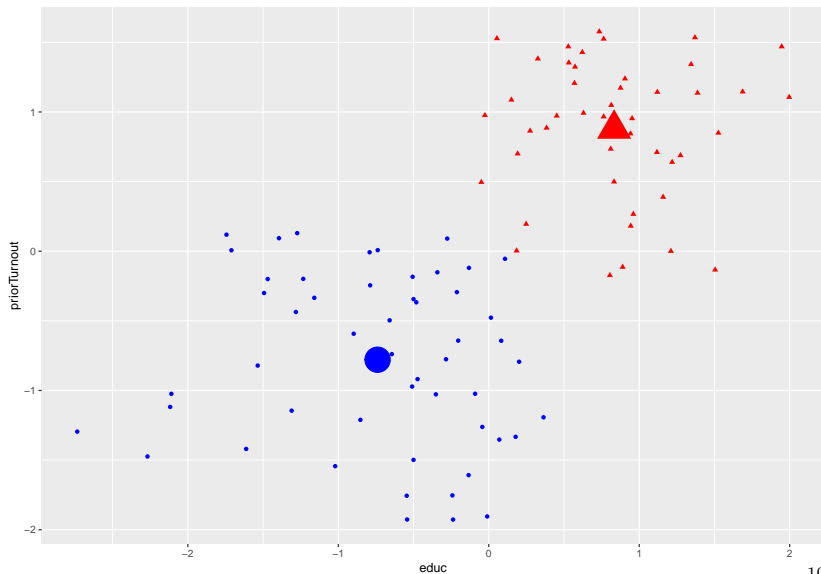


Standardized:

```
df2.standard <- data.frame(scale(df2))  
ggplot(df2.standard, aes(educ, priorTurnout)) +  
  geom_point() + geom_smooth()
```



```
##          educ priorTurnout
## 1 -0.7388515   -0.7791249
## 2  0.8331730    0.8785876
```



Selecting k

How do we select k ?

Quick quiz:

Given $y = (4, 2, 5, 9, 10)$, calculate

$$\sum_{i=3}^4 y_i$$

.

How do we select k ?

Total within-cluster sum of squares:

$$TSS_{\text{Within}} = \sum_{(\text{Clusters})} \sum_{(\text{Obs in Cluster}_i)} (\text{Dist}(\text{Obs to Cluster Mean}))^2$$

How do we select k ?

Total within-cluster sum of squares:

$$\begin{aligned} TSS_{\text{Within}} &= \sum_{(\text{Clusters})} \sum_{(\text{Obs in Cluster}_i)} (\text{Dist}(\text{Obs to Cluster Mean}))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} (\text{Distance}(x_j \text{ to } \mu_i))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} \|x_j - \mu_i\|^2 \end{aligned}$$

How do we select k ?

Total within-cluster sum of squares:

$$\begin{aligned} TSS_{\text{Within}} &= \sum_{(\text{Clusters})} \sum_{(\text{Obs in Cluster}_i)} (\text{Dist}(\text{Obs to Cluster Mean}))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} (\text{Distance}(x_j \text{ to } \mu_i))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} \|x_j - \mu_i\|^2 \end{aligned}$$

► TSS_{Within} should *always* decrease with more clusters

How do we select k ?

Total within-cluster sum of squares:

$$\begin{aligned}TSS_{\text{Within}} &= \sum_{(\text{Clusters})} \sum_{(\text{Obs in Cluster}_i)} (\text{Dist}(\text{Obs to Cluster Mean}))^2 \\&= \sum_{i=1}^k \sum_{x_j \in C_i} (\text{Distance}(x_j \text{ to } \mu_i))^2 \\&= \sum_{i=1}^k \sum_{x_j \in C_i} \|x_j - \mu_i\|^2\end{aligned}$$

- ▶ TSS_{Within} should *always* decrease with more clusters
 - ▶ (But what's the point of 200 obs, 200 clusters?)

How do we select k ?

Total within-cluster sum of squares:

$$\begin{aligned} TSS_{\text{Within}} &= \sum_{(\text{Clusters})} \sum_{(\text{Obs in Cluster}_i)} (\text{Dist}(\text{Obs to Cluster Mean}))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} (\text{Distance}(x_j \text{ to } \mu_i))^2 \\ &= \sum_{i=1}^k \sum_{x_j \in C_i} \|x_j - \mu_i\|^2 \end{aligned}$$

- ▶ TSS_{Within} should *always* decrease with more clusters
 - ▶ (But what's the point of 200 obs, 200 clusters?)
- ▶ Select k s.t. additional cluster yields $\downarrow\downarrow\downarrow$ in TSS_{Within}

How do we select k ?

```
max_k <- 10 # maximum number clusters to test
tot_within_ss <- vector("numeric", length = max_k - 1)

for(idx_k in 2:max_k){

  k_out <- kmeans(df2.standard, centers = idx_k)
  tot_within_ss[idx_k - 1] <- k_out$tot.withinss
}
```

How do we select k ?

```
max_k <- 10 # maximum number clusters to test
tot_within_ss <- vector("numeric", length = max_k - 1)

for(idx_k in 2:max_k){

  k_out <- kmeans(df2.standard, centers = idx_k)
  tot_within_ss[idx_k - 1] <- k_out$tot.withinss

}
```

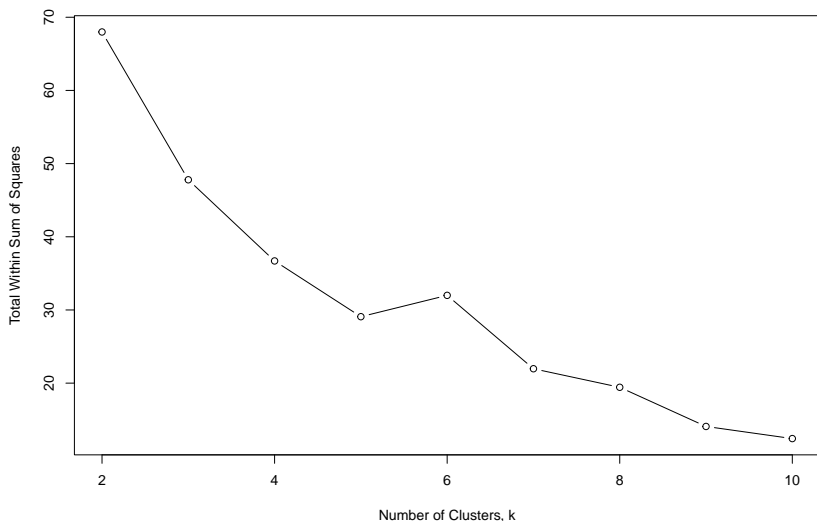
Output:

```
tot_within_ss |> round(1)
```

```
## [1] 68.0 47.8 36.7 29.1 32.0 22.0 19.4 14.1 12.4
```

A Scree Plot

```
plot(2:max_k, tot_within_ss, xlab = "Number of Clusters, k",  
     ylab = "Total Within Sum of Squares", type = "b")
```



How do we select k ?

```
max_k <- 10 # maximum clusters to test
tot_within_ss <- vector("numeric", length = max_k - 1)

for(idx_k in 2:max_k){

  k_out <- kmeans(df2.standard,
                  centers = idx_k,
                  nstart = 10)

  tot_within_ss[idx_k - 1] <- k_out$tot.withinss
}
```

How do we select k ?

```
max_k <- 10 # maximum clusters to test
tot_within_ss <- vector("numeric", length = max_k - 1)

for(idx_k in 2:max_k){

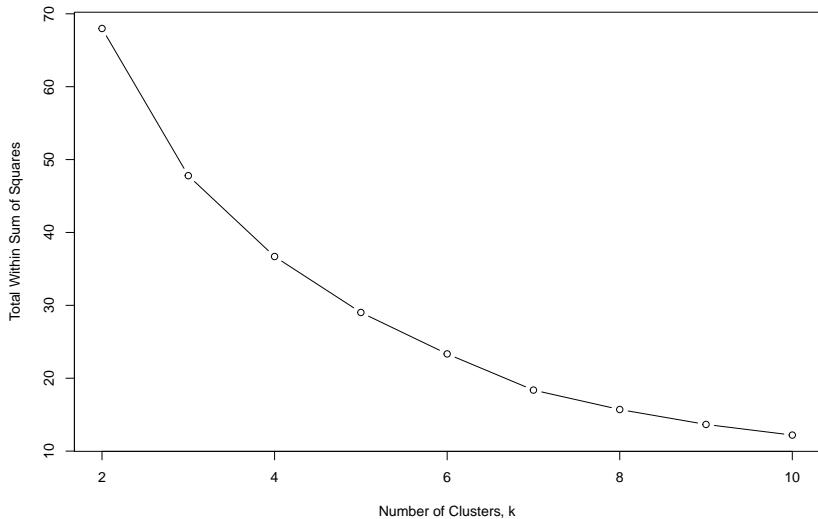
  k_out <- kmeans(df2.standard,
                  centers = idx_k,
                  nstart = 10)

  tot_within_ss[idx_k - 1] <- k_out$tot.withinss
}
```

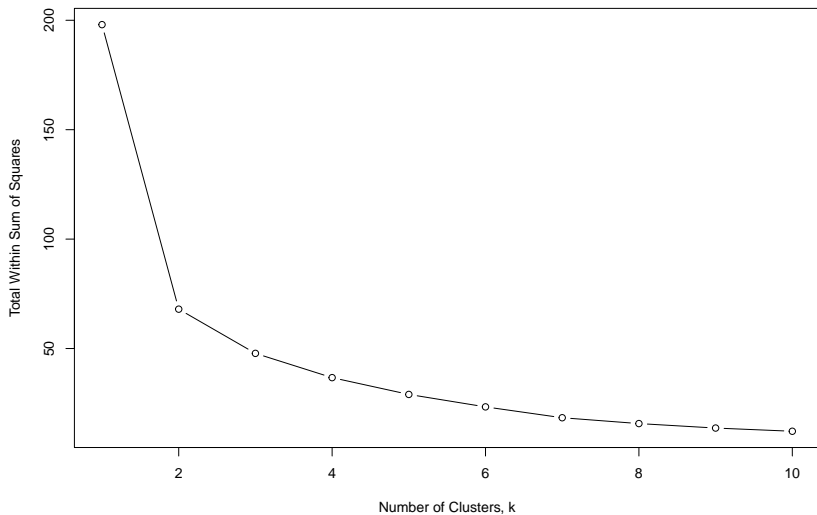
```
tot_within_ss |> round(1)
```

```
## [1] 68.0 47.8 36.7 29.0 23.3 18.4 15.7 13.7 12.2
```

A Better Scree Plot



An Even Better Scree Plot



Other applications: Geolocations

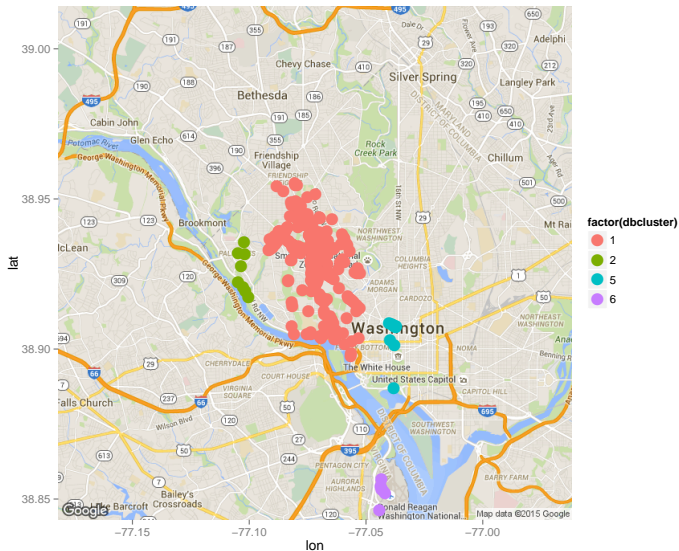


Figure 1: Clusters of Geolocations

Other applications: Regimes

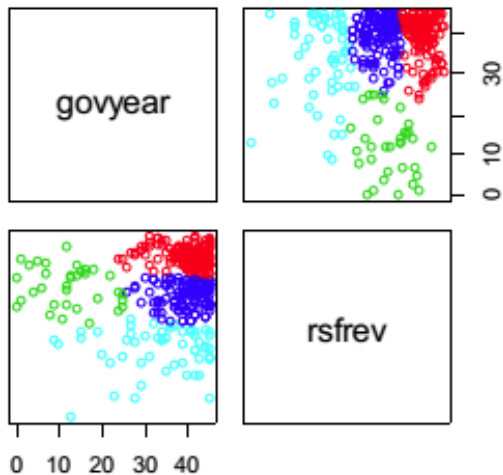


Figure 2: Comparative Regime Types

Other applications: Senate Speeches

Other applications: Senate Speeches

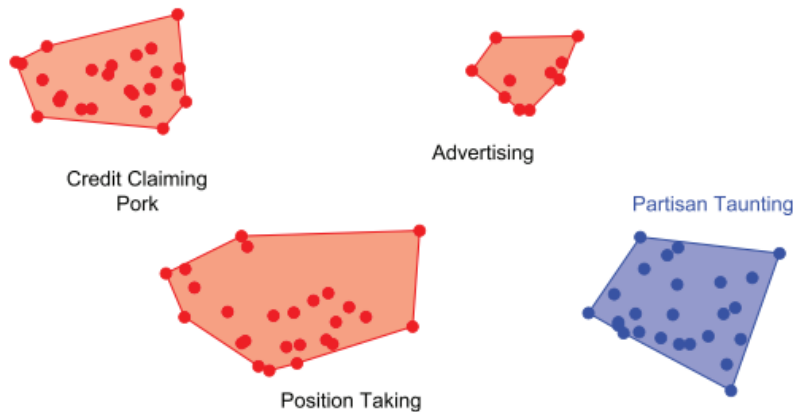


Figure 3: Senate Speeches

DBSCAN (1996)

Density-based clustering

DBSCAN (1996)

Density-based clustering

1. Find each point's neighbors

DBSCAN (1996)

Density-based clustering

1. Find each point's neighbors
2. ID *core* points with enough neighbors

DBSCAN (1996)

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1. Find each point's neighbors
2. ID *core* points with enough neighbors
3. Connect nearby core points

DBSCAN (1996)

Density-based clustering

1. Find each point's neighbors
2. ID *core* points with enough neighbors
3. Connect nearby core points
4. Assign non-core points to near clusters (or noise)

Other applications:

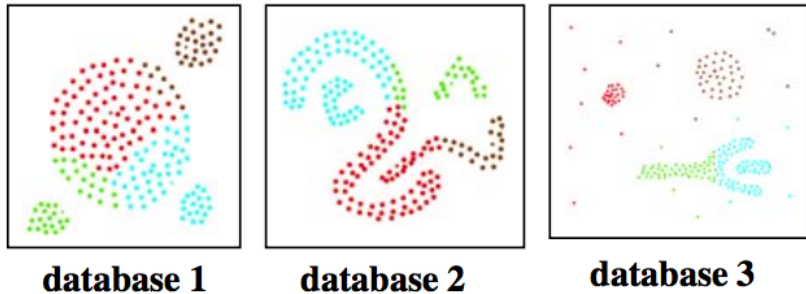
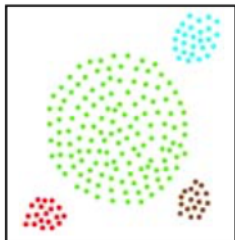


Figure 4: CLARANS: Not Great!

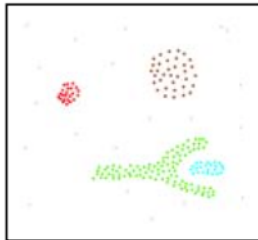
Other applications:



database 1



database 2



database 3

Figure 5: DBSCAN: Great!

Congress Clusters

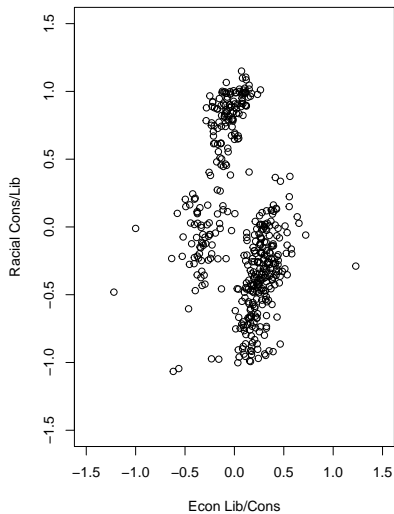
```
congress.url <- "http://j.mp/302nedz"
congress <- read_csv(congress.url)
dwnom80 <- cbind(congress$dwnom1[congress$congress == 80],
                 congress$dwnom2[congress$congress == 80])
dwnom112 <- cbind(congress$dwnom1[congress$congress == 112],
                  congress$dwnom2[congress$congress == 112])

k80two.out <- kmeans(dwnom80, centers = 2)
k112two.out <- kmeans(dwnom112, centers = 2)

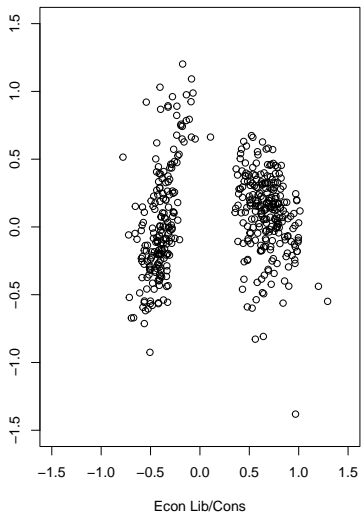
k80four.out <- kmeans(dwnom80, centers = 4)
k112four.out <- kmeans(dwnom112, centers = 4)

lim <- c(-1.5, 1.5)
xlab <- "Econ Lib/Cons"
ylab <- "Racial Cons/Lib"
```

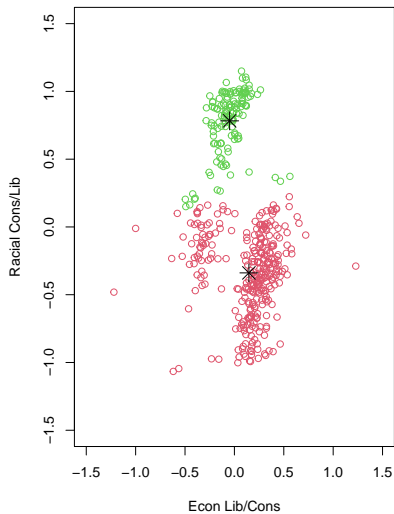
80th Congress



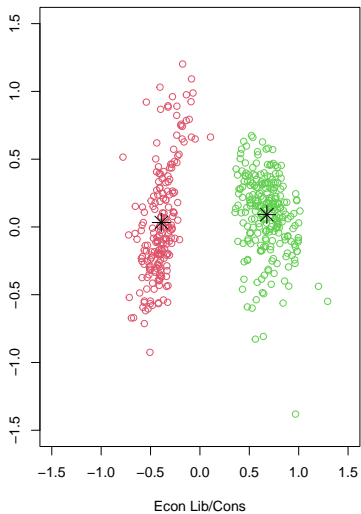
112th Congress



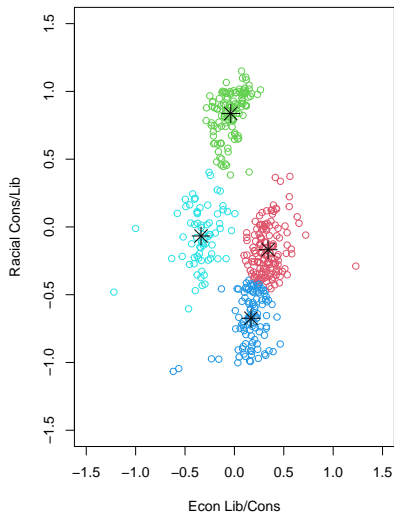
80th Congress



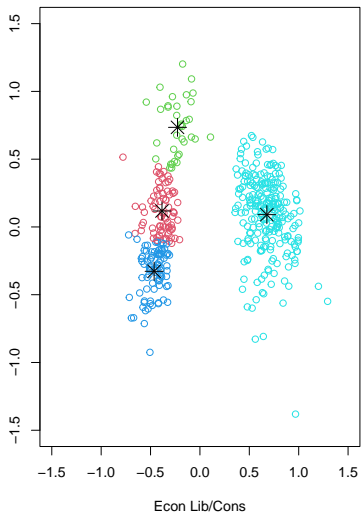
112th Congress



80th Congress



112th Congress



Exercise

Exercise

1. Checkout CRAN Task View for Clustering:

<https://cran.r-project.org/web/views/Cluster.html>

2. Discover clusters in your final project data!

(Use 2 predictors to visualise; more predictors to discover higher-dim clusters.)