Cluster Analysis: Discovery Winter Institute in Data Science

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2023-01-07

Supervised and Unsupervised Learning

Hierarchical Clustering

Partitional Clustering

Exercise

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

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In base R, can extract variable v1 from data frame df with

▶ df\$v1

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- ▶ df[["v1"]]

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- ▶ df[[6]]

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

1. Describe list 11 created below:

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

- 2. What is 11\$y?
- 3. What is 11[[1]]?
- 4. What is 11[[3]][2, 2]?

Supervised and Unsupervised Learning

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Supervised: Modeling with **known** outcomes

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Unsupervised: Discovery w/ unknown outcomes

► Linear regression (LS)

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If you have y = f(X), it's "supervised".

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- ► (Some neural networks)
- ► Clustering algorithms (most)

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- ▶ Roll call voting: party/faction detection
 - no predefined party/faction labels
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- ► Geographic clustering: daily activities
 - ▶ no "home"/"work"/"leisure" labels

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 - Units in one cluster at each level of hierarchy
- ► Partitional clustering
 - ► Find splits in full set
 - ▶ Units in only one cluster

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

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Divisive clustering

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Divisive clustering is "top-down"

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Agglomerative clustering

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Agglomerative clustering

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

Agglomerative clustering is "bottom-up"

Each unit is in a clustering at every level.

 $Complete\ linkage\ clustering:\ greedily\ create\ clusters$

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

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

b 1 0 6 7 c 2 6 0 8		a	b	c	d
c 2 6 0 8	a	0	1	2	3
	b	1	0	6	7
1 2 7 9 (\mathbf{c}	2	6	0	8
u 3 / 6 (d	3	7	8	0

Agglomerative Hierarchical Complete Linkage Clusters

a 0 1 2 b 1 0 6					
b 1 0 6	3	2	1	0	a
	7	6	0	1	b
c 2 6 0	8	0	6	2	\mathbf{c}
d 3 7 8	0	8	7	3	d

	(a,b)	c	d
(a,b)	0	6	7
\mathbf{c}	6	0	8
d	7	8	0

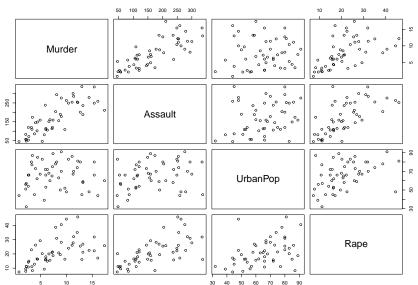
Agglomerative Hierarchical Complete Linkage Clusters

	a	b	c	d
a	0	1	2	3
b	1	0	6	7
\mathbf{c}	2	6	0	8
d	3	7	8	0

	(a,b)	c	d
(a,b)	0	6	7
\mathbf{c}	6	0	8
d	7	8	0

("friends of friends")

pairs(USArrests)



Colorado

Delaware

Florida

Georgia ## Hawaii

Idaho

Illinois

Indiana

Iowa

Connecticut

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

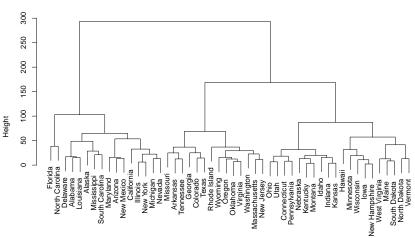
d %>% round(0)					
##	Alabama	Alaska	Arizona	Arkansas	Californ
## Alaska	37				
## Arizona	63	47			
## Arkansas	47	77	109		
## California	56	45	23	98	

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

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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))</pre>
  q <- as.matrix(q)
  for(i in 1:nrow(q)){
    storage[row(q), i] \leftarrow mahalanobis(x = q,
                                          center=q[i, ],
                                          cov = vc)
  }
  return(sqrt(storage))
```

Recluster w/ Alternative Distance Metric: Mahalanobis d mah <- mahal(USArrests, cov(USArrests))</pre> row.names(d_mah) <- colnames(d_mah) <- row.names(USArrests)

d mah <- as.dist(d mah)</pre> d mah %>% round(1) ## Alabama Alaska Arizona Arkansas Californ ## Alaska 4.4

3.2 ## Arizona 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

Connecticut 2.8 5.4 2.9 2.6

1.7 3.0 5.0 2.6 ## Delaware

Florida 1.8 4.6 2.3 2.5

Georgia 2.2 5.4 5.0 3.3

5.6 3.5 4.5 3.8 3 ## Hawaii

4.9

2.1

2.4

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Idaho 2.7 3.8 2.5 1.5

2.0

Illinois

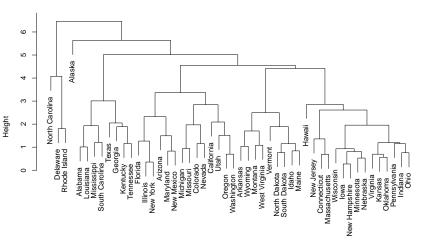
Recluster w/ Alternative Distance Metric: Mahalanobis

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plot(hag)</pre>
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Cluster Dendrogram



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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

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- ► (Assault has large variance, and cor w/ UrbanPop)
- ► Mahalanobis dist allows vars on different scales to all contribute.
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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

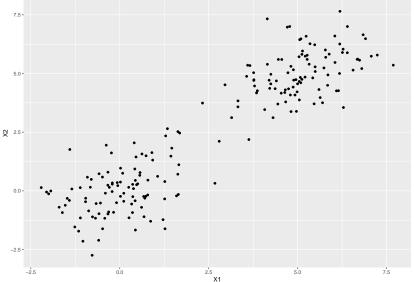
Partitional Clustering

k-means

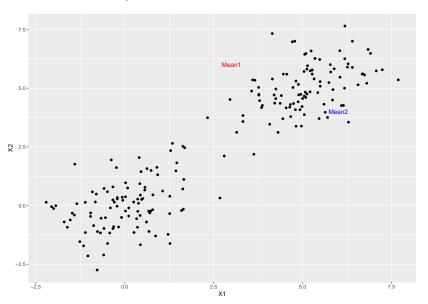
- 0. Standardize variables, or ensure comparable scales. A difference of 1 unit on x should be comparable to a difference of 1 unit on y.
- 1. Choose k, the number of clusters to identify.
- 2. Select the location of a center for each cluster.
- 3. Assign each observation to the cluster defined by the 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 X1 and X2 on comparable scales.

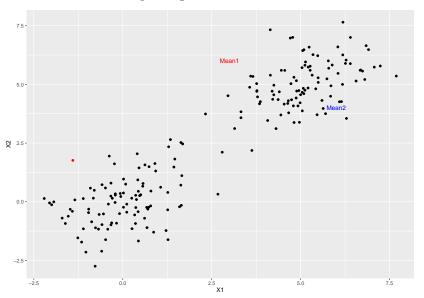
We will find k = 2 clusters. Ideas?



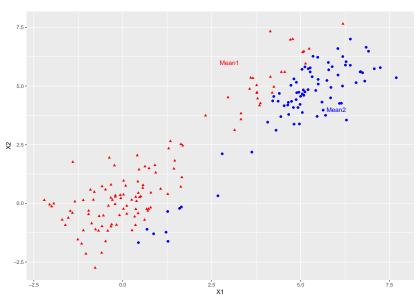
2. Let's randomly select two centroids:



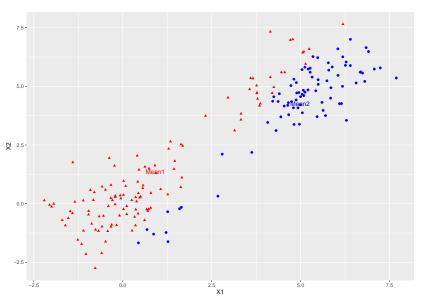
Where "should" this point go?



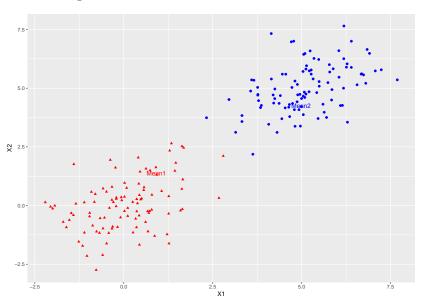
3. Find (Euclidean) distance between each point and the centroids; assign each point to closer centroid:



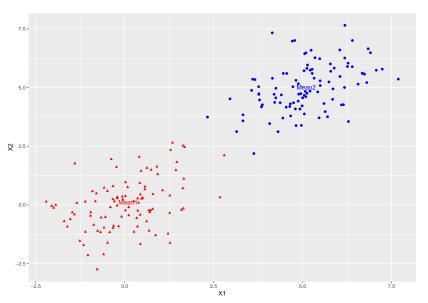
4. Relocate centroids to the mean (X1, X2) value for each cluster:



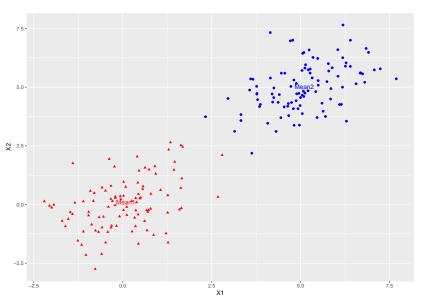
3. Reassign each observation to the closer centroid:



4. Recalculate the centroid locations ...

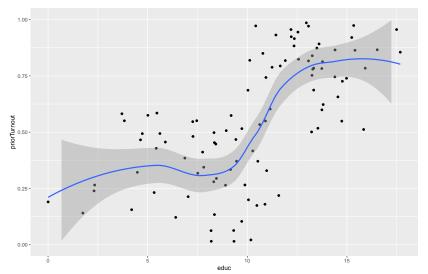


3. Reassign points to clusters ...



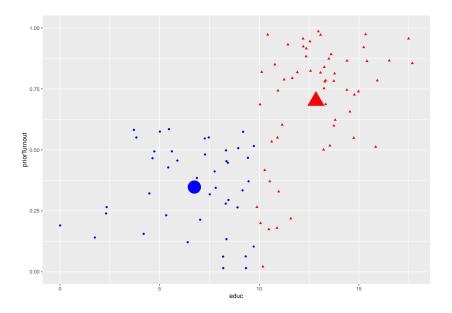
Standardization: Why, before clustering?

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



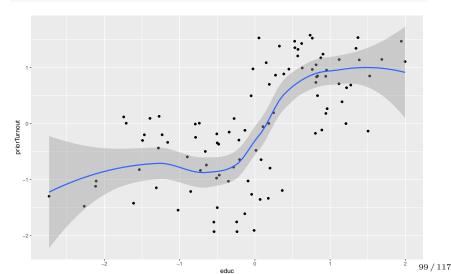
```
k2 <- kmeans(df2, centers = 2)
names(k2)
## [1] "cluster"
                     "centers"
                                   "totss"
                                                   "within
## [6] "betweenss" "size"
                                   "iter"
                                                   "ifaul
table(k2$cluster)
##
## 1 2
## 57 43
k2$centers
```

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

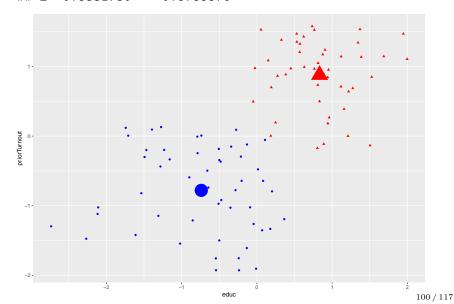


Standardized:

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



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



Other applications: Geolocations

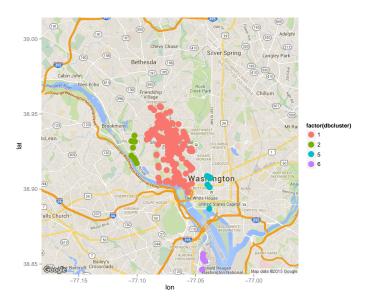


Figure 1: Clusters of Geolocations

Other applications: Regimes

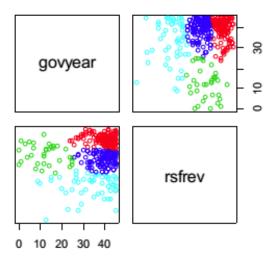


Figure 2: Comparative Regime Types

Other applications: Senate Speeches

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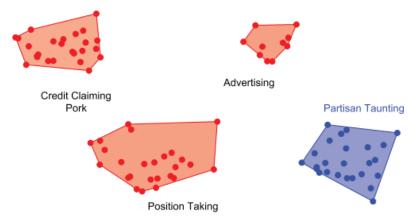


Figure 3: Senate Speeches

Density-based clustering

1. Find each point's neighbors

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- 3. Connect nearby core points
- 4. Assign non-core points to near clusters (or noise)

Other applications:

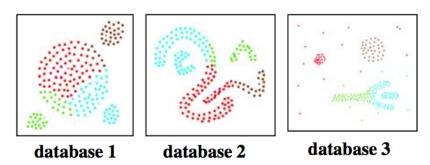


Figure 4: CLARANS: Not Great!

Other applications:

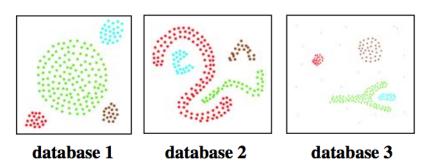
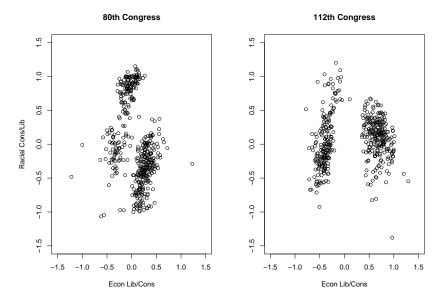
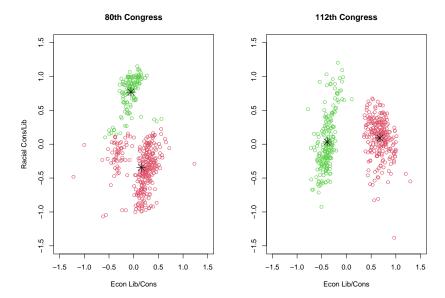


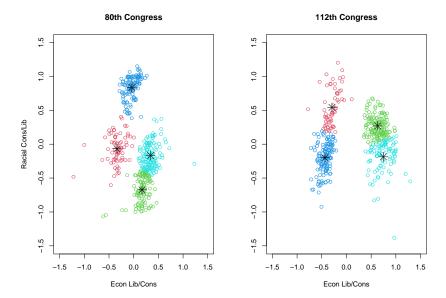
Figure 5: DBSCAN: Great!

Congress Clusters

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







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.)