Cluster Analysis: Discovery Winter Institute in Data Science

Ryan T. Moore

9 January 2020

Supervised and Unsupervised Learning

Hierarchical Clustering

Partitional Clustering

Exercise

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

- ▶ matrix: rectangular array with a few more restrictions than data.frame
- ▶ list: more general type of array that can be rectangular, but need not be. A data.frame is an example of a list

- ▶ matrix: rectangular array with a few more restrictions than data.frame
- ▶ list: more general type of array that can be rectangular, but need not be. A data.frame is an example of a list

- ▶ matrix: rectangular array with a few more restrictions than data.frame
- ▶ list: more general type of array that can be rectangular, but need not be. A data.frame is an example of a list

We can extract variable v1 from data frame df with df\$v1.

Can we extract column c1 from matrix m with m\$c1?

4. Describe list 11 created below:

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

- 5. What is 11\$y?
- 6. What is 11[[1]]?
- 7. What is 11[[3]][2, 2]?

Supervised and Unsupervised Learning

Supervised and Unsupervised Learning

Supervised: Modeling with **known** outcomes

Supervised and Unsupervised Learning

Supervised: Modeling with **known** outcomes

Unsupervised: Discovery w/ unknown outcomes

► Linear regression (LS)

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- ► Bayesian modeling

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- ► Bayesian modeling
- ► LASSO

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- ► Bayesian modeling
- ► LASSO
- ▶ Neural networks (CNNs)

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- Bayesian modeling
- ► LASSO
- ▶ Neural networks (CNNs)
- ▶ Decision trees, forests, etc.

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- Bayesian modeling
- ► LASSO
- ▶ Neural networks (CNNs)
- ▶ Decision trees, forests, etc.

- ► Linear regression (LS)
- ► Generalized linear regression (logistic, probit, Poisson, beta)
- Bayesian modeling
- ► LASSO
- ▶ Neural networks (CNNs)
- ▶ Decision trees, forests, etc.

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

Network analysis

- ► Network analysis
- ▶ Principal components analysis (PCA)

- ► Network analysis
- ▶ Principal components analysis (PCA)
- ▶ (Some neural networks)

- ► Network analysis
- ▶ Principal components analysis (PCA)
- ► (Some neural networks)
- ► Clustering algorithms (most)

▶ Networks: "community detection"

- ▶ Networks: "community detection"
 - ▶ no predefined community labels

- ▶ Networks: "community detection"
 - ▶ no predefined community labels
- ▶ Roll call voting: party/faction detection

- ▶ Networks: "community detection"
 - no predefined community labels
- ▶ Roll call voting: party/faction detection
 - no predefined party/faction labels

- ▶ Networks: "community detection"
 - no predefined community labels
- ▶ Roll call voting: party/faction detection
 - ▶ no predefined party/faction labels
- ▶ Geographic clustering: daily activities

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

▶ Hierarchical clustering

- ▶ Hierarchical clustering
 - ► Find best groups at many levels

- ▶ Hierarchical clustering
 - ▶ Find best groups at many levels
 - ▶ Units in one cluster at each level of hierarchy

- ▶ Hierarchical clustering
 - ▶ Find best groups at many levels
 - ▶ Units in one cluster at each level of hierarchy
- ▶ Partitional clustering

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

- ▶ Hierarchical clustering
 - ► 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

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

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

ightharpoonup Start at $\{a, b, c, d, e\}$

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

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

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

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

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

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

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

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

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

Divisive clustering

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

Divisive clustering is "top-down"

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

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

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

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

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

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

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

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

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

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

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

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

Agglomerative clustering

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

Agglomerative clustering is "bottom-up"

Each unit in different clustering at every level.

Complete linkage clustering: greedily create clusters

Complete linkage clustering: greedily create clusters

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

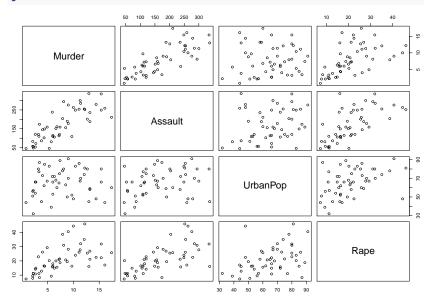
	a	b	c	d
a	0	1	2	3
b	1	0	6	7
\mathbf{c}	2	6	0	8
d	3	7	8	0
_				

Agglomerative Hierarchical Complete Linkage Clusters

	a	b	\mathbf{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

pairs(USArrests)



##

Delaware

Florida

Georgia

Idaho

Illinois

Indiana

Iowa

44 V----

Hawaii

##

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

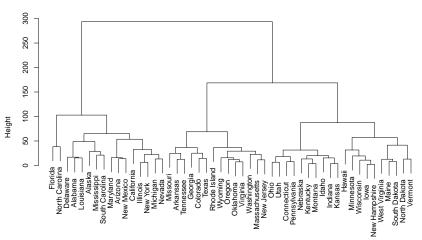
#	## Alaska	37				
#	## Arizona	63	47			
#	## Arkansas	47	77	109		
#	## California	56	45	23	98	
#	## Colorado	42	66	90	37	
#	## Connecticut	128	159	185	85	1

Alabama Alaska Arizona Arkansas Californ

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

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





62 / 94

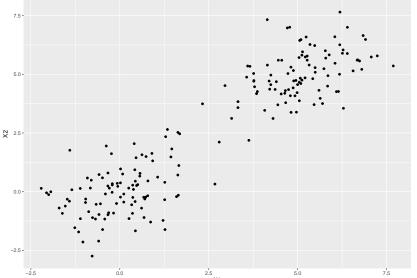
Partitional Clustering

k-means

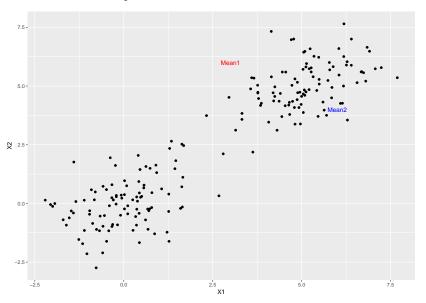
- 0. Standardize variables, or ensure comparable scales. A difference of 1 unit on x should be comparable to a difference of 1 unit on y.
- 1. Choose k, the number of clusters to identify.
- 2. Select the location of a center for each cluster.
- 3. Assign each observation to the cluster defined by the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

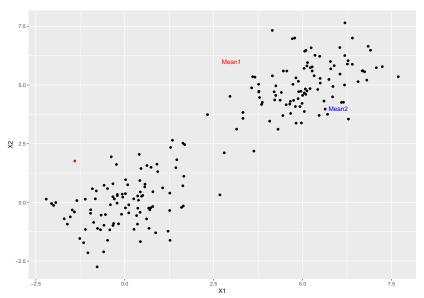
We will find k = 2 clusters. Ideas?



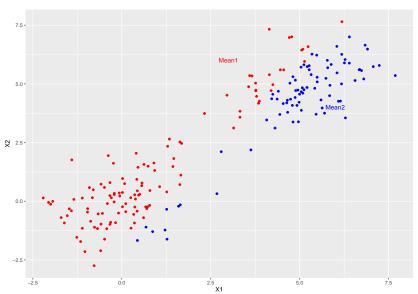
2. Let's randomly select two centroids:



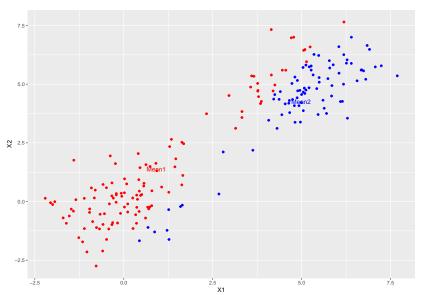
Where "should" this point go?



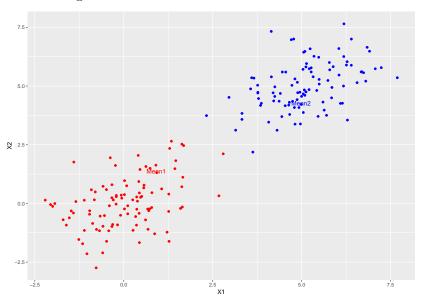
3. Find (Euclidean) distance between each point and the centroids; assign each point to closer centroid:



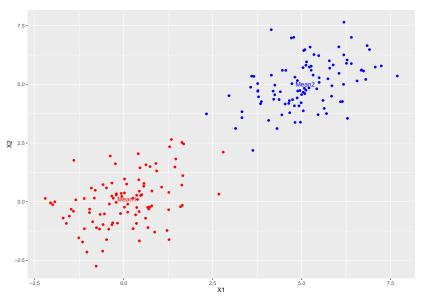
4. Relocate centroids to the mean (X1, X2) value for each cluster:



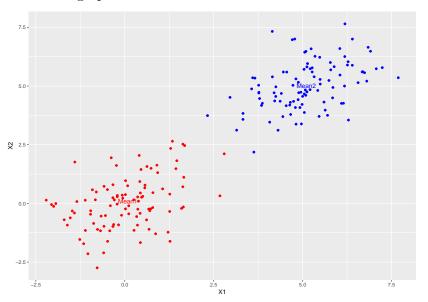
3. Reassign each observation to the closer centroid:



4. Recalculate the centroid locations ...

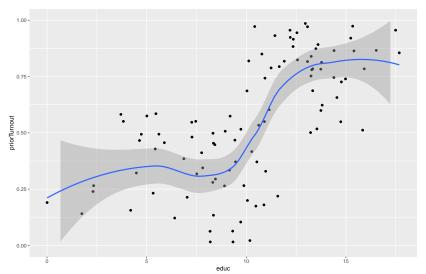


3. Reassign points to clusters ...

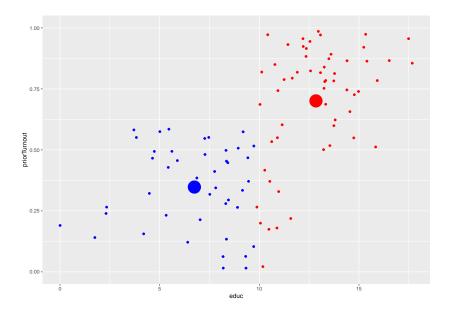


Standardization: Why, before clustering?

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

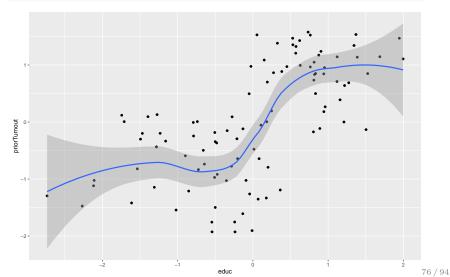


```
k2 <- kmeans(df2, centers = 2)
names(k2)
## [1] "cluster" "centers"
                                   "totss"
                                                  "within
## [5] "tot.withinss" "betweenss" "size"
                                                  "iter"
## [9] "ifault"
table(k2$cluster)
##
## 1 2
## 57 43
k2$centers
         educ priorTurnout
##
## 1 12.841805 0.7007953
## 2 6.740813 0.3477128
```

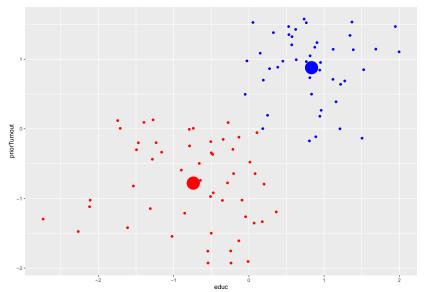


Standardized:

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



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



Other applications: Geolocations

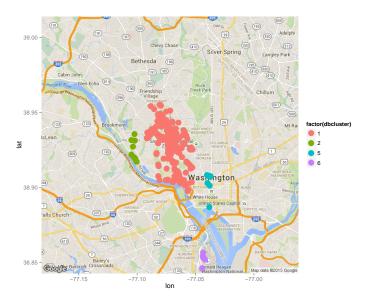


Figure 1: Clusters of Geolocations

Other applications: Regimes

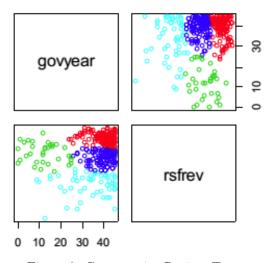


Figure 2: Comparative Regime Types

Other applications: Senate Speeches

Other applications: Senate Speeches

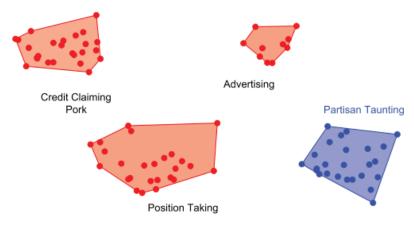


Figure 3: Senate Speeches

Density-based clustering

1. Find each point's neighbors

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

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

- 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:

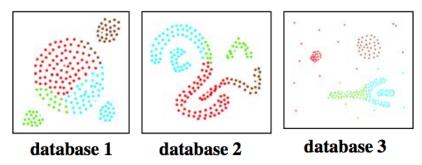


Figure 4: CLARANS: Not Great!

Other applications:

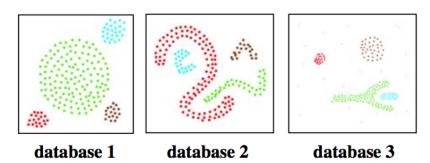
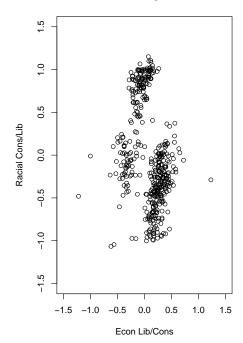


Figure 5: DBSCAN: Great!

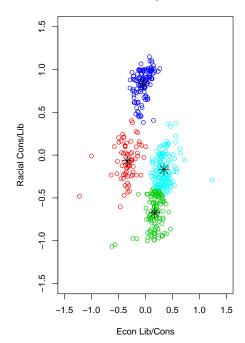
Congress Clusters

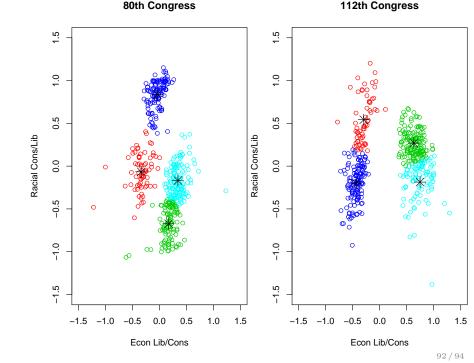
```
congress.url <- "http://j.mp/302nedz"
congress <- read csv(congress.url)</pre>
dwnom80 <- cbind(congress$dwnom1[congress$congress ==</pre>
                                                          80],
                  congress$dwnom2[congress$congress == 80])
dwnom112 <- cbind(congress$dwnom1[congress$congress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

80th Congress



80th 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.)