Data Clustering

and Dimensionality Reduction – PART 2

CS677
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NOTE: used the source below for these slide. You can read the source document instead.

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering videos to watch

- https://www.youtube.com/watch?v=ZueoXMgCd1c >>> Python examples

- https://www.youtube.com/watch?v=b39_vipRkUo
- https://www.youtube.com/watch?v=s5c4dysoWC8
- Check others online

Clustering mixed data

- “Clustering allows us to better understand how a sample might be comprised of distinct subgroups given a set of variables. “
- “While many introductions to cluster analysis typically review a simple application using continuous variables, clustering data of mixed types (e.g., continuous, ordinal, and nominal) **is often of interest**.”

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

Decisions that need to be taken for this approach:

- Calculating distance
- Choosing a clustering algorithm
- Selecting the number of clusters

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

- Publicly available “College” dataset found in the ISLR package will be used, which has various statistics of US Colleges from 1995 (N = 777).
- There are variables that are both categorical and continuous:
- Continuous
  - Acceptance rate
  - Out of school tuition
  - Number of new students enrolled
- Categorical
  - Whether a college is public/private
  - Whether a college is elite, defined as having more than 50% of new students who graduated in the top 10% of their high school class

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

```
set.seed(1680) # for reproducibility

library(dplyr) # for data cleaning
library(ISLR) # for college dataset
library(cluster) # for gower similarity and pam
library(Rtsne) # for t-SNE plot
library(ggplot2) # for visualization
```


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Clustering mixed data

Data cleaning → as a preprocessing step may be needed

- **Acceptance rate** is created by diving the number of acceptances by the number of applications
- **isElite** is created by labeling colleges with more than 50% of their new students who were in the top 10% of their high school class as elite

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Clustering mixed data

```
college_clean <- College %>%
  mutate(name = row.names(.),
         accept_rate = Accept/Apps,
         isElite = cut(Top10perc,
                       breaks = c(0, 50, 100),
                       labels = c("Not Elite", "Elite"),
                       include.lowest = TRUE)) %>%
  mutate(isElite = factor(isElite)) %>%
  select(name, accept_rate, Outstate, Enroll,
         Grad.Rate, Private, isElite)

glimpse(college_clean)
```


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Clustering mixed data

```
## Observations: 777
## Variables: 7
## $ name        (chr) "Abilene Christian University", "Ad...
## $ accept_rate (dbl) 0.7421687, 0.8801464, 0.7682073, 0....
## $ Outstate    (dbl) 7440, 12280, 11250, 12960, 7560, 13...
## $ Enroll      (dbl) 721, 512, 336, 137, 55, 158, 103, 4...
## $ Grad.Rate   (dbl) 60, 56, 54, 59, 15, 55, 63, 73, 80,...
## $ Private     (fctr) Yes, Yes, Yes, Yes, Yes, Yes, Yes,...
## $ isElite     (fctr) Not Elite, Not Elite, Not Elite, E...
```


Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

Calculating Distance

Define notion of (dis)similarity between observations

A popular choice for clustering is Euclidean distance:

- Only valid for continuous variables, and thus is not applicable here.
- To yield sensible results → distance metric that can handle mixed data types.

Gower distance

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

- Gower Distance
- "For each variable type, a particular distance metric that works well for that type is used and scaled to fall between 0 and 1. Then, a linear combination using user-specified weights (most simply an average) is calculated to create the final distance matrix.

The **metrics** used **for each data type** are described below:

- **Quantitative** (interval): range-normalized Manhattan distance
- **Ordinal**: variable is first ranked, then Manhattan distance is used with a special adjustment for ties
- **Nominal**: variables of *k* categories are first converted into *k* binary columns and then the Dice coefficient is used

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

- Gower distance can be calculated in one line using the **daisy** function
- There is a positive skew in the Enroll variable → thus, a log transformation is conducted internally via the *type* argument
- Instructions to perform additional transformations, like for factors that could be considered as asymmetric binary (such as rare events), can be seen in **"daisy"**

```
# Remove college name before clustering

gower_dist <- daisy(college_clean[, -1],
                    metric = "gower",
                    type = list(logratio = 3))

# Check attributes to ensure the correct methods are being used
# (I = interval, N = nominal)
# Note that despite logratio being called,
# the type remains coded as "I"

summary(gower_dist)
```

```
## 301476 dissimilarities, summarized :
##      Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
## 0.0018601 0.1034400 0.2358700 0.2314500 0.3271400 0.7773500
## Metric :  mixed ;  Types = I, I, I, I, N, N
## Number of objects : 777
```


Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Clustering mixed data

As a sanity check, we can print out the most similar and dissimilar pair in the data to see if it makes sense. In this case, University of St. Thomas and John Carroll University are rated to be the most similar given the seven features used in the distance calculation, while University of Science and Arts of Oklahoma and Harvard are rated to be the most dissimilar.

```
gower_mat <- as.matrix(gower_dist)

# Output most similar pair

college_clean[
  which(gower_mat == min(gower_mat[gower_mat != min(gower_mat)]
        arr.ind = TRUE)[1, ], ]
```

```
##                            name accept_rate Outstate Enroll
## 682 University of St. Thomas MN   0.8784638    11712    828
## 284      John Carroll University   0.8711276    11700    820
##     Grad.Rate Private   isElite
## 682        89     Yes Not Elite
## 284        89     Yes Not Elite
```

```
# Output most dissimilar pair

college_clean[
  which(gower_mat == max(gower_mat[gower_mat != max(gower_mat)]
        arr.ind = TRUE)[1, ], ]
```

```
##                                         name accept_rate
## 673 University of Sci. and Arts of Oklahoma   0.9824561
## 251                         Harvard University   0.1561486
##     Outstate Enroll Grad.Rate Private   isElite
## 673     3687    208        43      No Not Elite
## 251    18485   1606       100     Yes     Elite
```


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Choosing a clustering algorithm

The distance matrix has been calculated → now we can select an algorithm for clustering.

While many algorithms that can handle a custom distance matrix exist, **partitioning around medoids (PAM)** will be used here.

- PAM: iterative clustering procedure with the following steps:

1. Choose k random entities to become the medoids
2. Assign every entity to its closest medoid (using our custom distance matrix in this case)
3. For each cluster, identify the observation that would yield the lowest average distance if it were to be re-assigned as the medoid. If so, make this observation the new medoid.
4. If at least one medoid has changed, return to step 2. Otherwise, end the algorithm.

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Choosing a clustering algorithm

- If you know the k-means algorithm, this might look very familiar. In fact, both approaches are identical, except k-means has cluster centers defined by Euclidean distance (i.e., centroids), while cluster centers for PAM are restricted to be the observations themselves (i.e., medoids).
- **pros**: Easy to understand, more robust to noise and outliers when compared to k-means, and has the added benefit of having an observation serve as the exemplar for each cluster
- **cons**: Both run time and memory are quadratic (i.e., $O(n^2)$)

Source: https://dpmartin42.github.io/posts/r/cluster-mixed-types#calculating-distance

Selecting the number of clusters

- A variety of metrics exist to help choose the number of clusters to be extracted in a cluster analysis.
- We will use silhouette width, an internal validation metric which is an aggregated measure of how similar an observation is to its own cluster compared its closest neighboring cluster.
- The metric can range from -1 to 1, where higher values are better.
- After calculating silhouette width for clusters ranging from 2 to 10 for the PAM algorithm, we see that 3 clusters yields the highest value.

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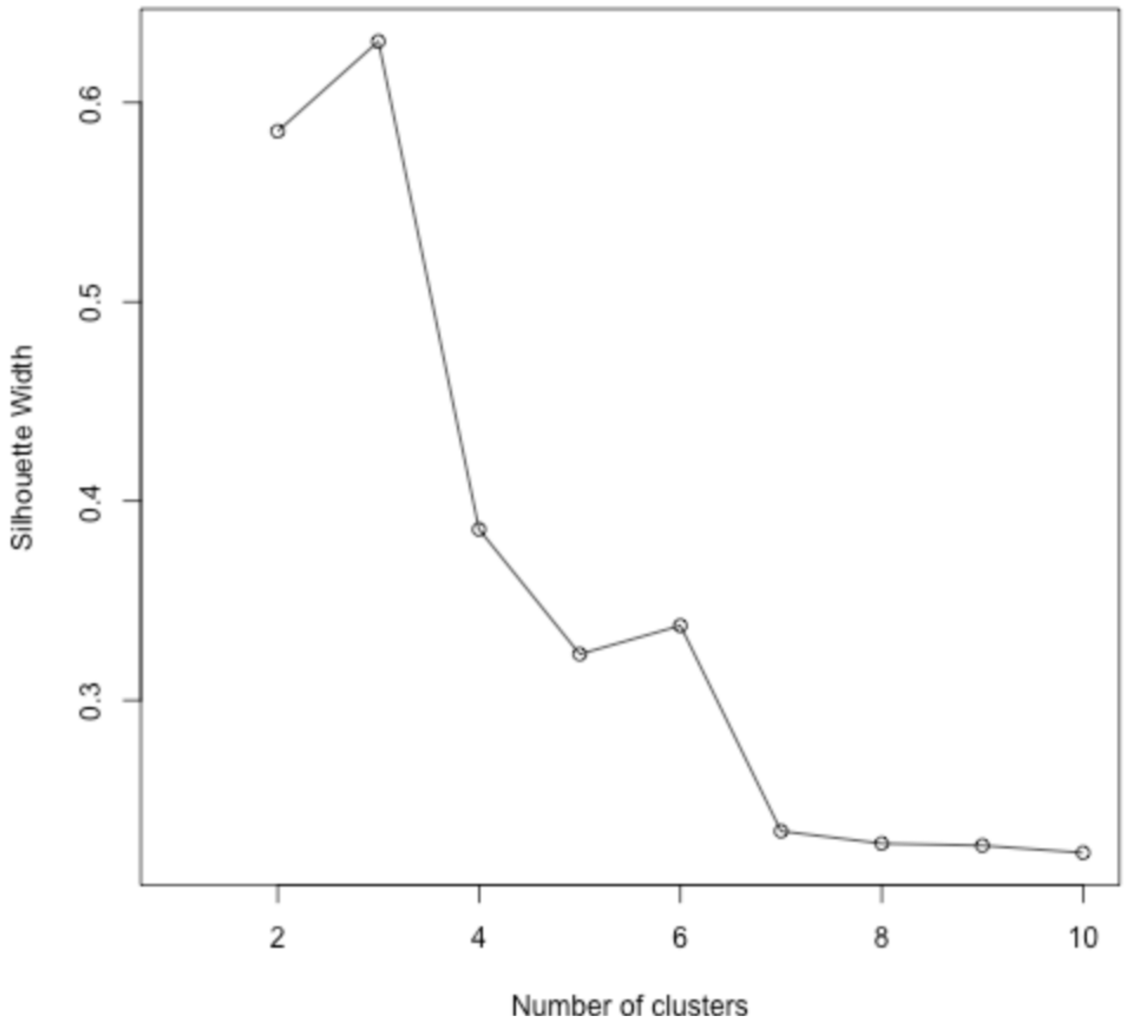
Selecting the number of clusters

```r
# Calculate silhouette width for many k using PAM

sil_width <- c(NA)

for(i in 2:10){

  pam_fit <- pam(gower_dist,
                 diss = TRUE,
                 k = i)

  sil_width[i] <- pam_fit$silinfo$avg.width

}

# Plot sihouette width (higher is better)

plot(1:10, sil_width,
     xlab = "Number of clusters",
     ylab = "Silhouette Width")
lines(1:10, sil_width)
```



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Cluster Interpretation

- **Via Descriptive Statistics**
- **Via Visualization**

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Cluster Interpretation

- **Via Descriptive Statistics**
- After running the algorithm and selecting three clusters, we can interpret the clusters by running **summary** on each cluster. Based on these results, it seems as though Cluster 1 is mainly Private/Not Elite with medium levels of out of state tuition and smaller levels of enrollment. Cluster 2, on the other hand, is mainly Private/Elite with lower levels of acceptance rates, high levels of out of state tuition, and high graduation rates. Finally, cluster 3 is mainly Public/Not Elite with the lowest levels of tuition, largest levels of enrollment, and lowest graduation rate.

```
pam_fit <- pam(gower_dist, diss = TRUE, k = 3)

pam_results <- college_clean %>%
  dplyr::select(-name) %>%
  mutate(cluster = pam_fit$clustering) %>%
  group_by(cluster) %>%
  do(the_summary = summary(.))

pam_results$the_summary
```

```
## [[1]]
##   accept_rate        Outstate        Enroll
##  Min.   :0.3283   Min.   : 2340   Min.   :  35.0
##  1st Qu.:0.7225   1st Qu.: 8842   1st Qu.: 194.8
##  Median :0.8004   Median :10905   Median : 308.0
##  Mean   :0.7820   Mean   :11200   Mean   : 418.6
##  3rd Qu.:0.8581   3rd Qu.:13240   3rd Qu.: 484.8
##  Max.   :1.0000   Max.   :21700   Max.   :4615.0
##    Grad.Rate       Private        isElite        cluster
##  Min.   : 15.00   No :  0    Not Elite:500   Min.   :1
##  1st Qu.: 56.00   Yes:500    Elite    :  0   1st Qu.:1
##  Median : 67.50                              Median :1
##  Mean   : 66.97                              Mean   :1
##  3rd Qu.: 78.25                              3rd Qu.:1
##  Max.   :118.00                              Max.   :1
##
## [[2]]
##   accept_rate        Outstate        Enroll
##  Min.   :0.1545   Min.   : 5224   Min.   : 137.0
##  1st Qu.:0.4135   1st Qu.:13850   1st Qu.: 391.0
##  Median :0.5329   Median :17238   Median : 601.0
```

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Cluster Interpretation – Via Statistics

Another benefit of the PAM algorithm with respect to interpretation is that the medoids serve as exemplars of each cluster. From this, we see that Saint Francis University is the medoid of the Private/Not Elite cluster, Barnard College is the medoid for the Private/Elite cluster, and Grand Valley State University is the medoid for the Public/Not Elite cluster.

```
college_clean[pam_fit$medoids, ]
```

```
##                                name accept_rate Outstate
## 492          Saint Francis College   0.7877629    10880
## 38                 Barnard College   0.5616987    17926
## 234 Grand Valley State University   0.7525653     6108
##     Enroll Grad.Rate Private   isElite
## 492    284        69     Yes Not Elite
## 38     531        91     Yes     Elite
## 234   1561        57      No Not Elite
```

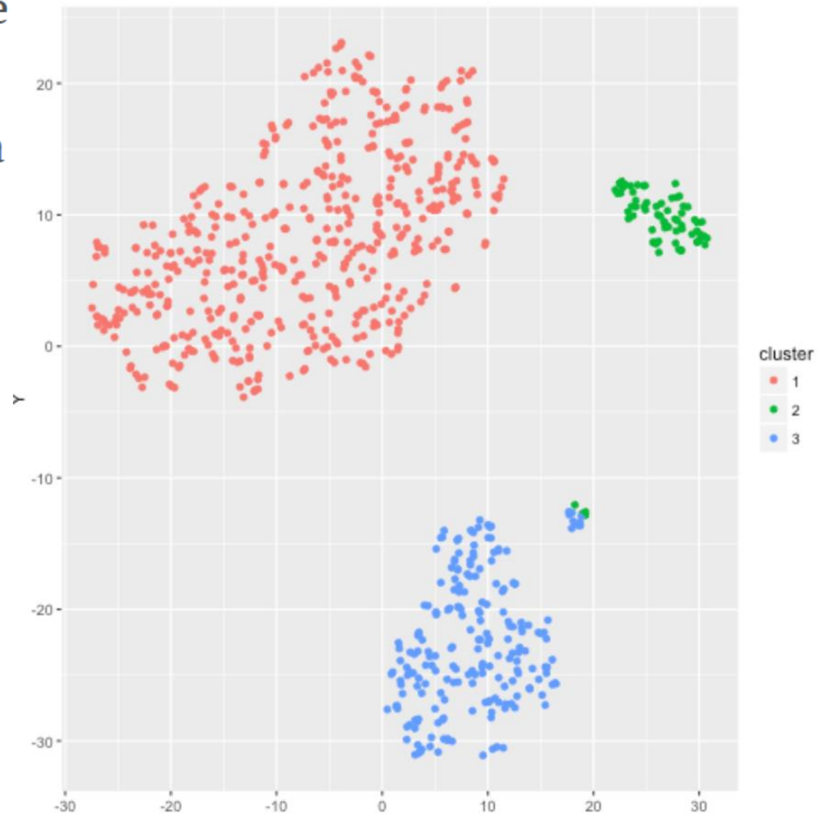
Via Visualization

One way to visualize many variables in a lower dimensional space is with t-distributed stochastic neighborhood embedding, or t-SNE. This method is a dimension reduction technique that tries to preserve local structure so as to make clusters visible in a 2D or 3D visualization. While it typically utilizes Euclidean distance, it has the ability to handle a custom distance metric like the one we created above. In this case, the plot shows the three well-separated clusters that PAM was able to detect. One curious thing to note is that there is a small group that is split between the Private/Elite cluster and the Public/Not Elite cluster.

```
tsne_obj <- Rtsne(gower_dist, is_distance = TRUE)

tsne_data <- tsne_obj$Y %>%
  data.frame() %>%
  setNames(c("X", "Y")) %>%
  mutate(cluster = factor(pam_fit$clustering),
         name = college_clean$name)

ggplot(aes(x = X, y = Y), data = tsne_data) +
  geom_point(aes(color = cluster))
```



Visualization

By investigating further, it looks like this group is made up of the larger, more competitive public schools, like the University of Virginia or the University of California at Berkeley. While not large enough to warrant an additional cluster according to silhouette width, these 13 schools certainly have characteristics distinct from the other three clusters.

```
tsne_data %>%
  filter(X > 15 & X < 25,
         Y > -15 & Y < -10) %>%
  left_join(college_clean, by = "name") %>%
  collect %>%
  .[["name"]]
```

```
##  [1] "College of William and Mary"
##  [2] "Georgia Institute of Technology"
##  [3] "SUNY at Binghamton"
##  [4] "SUNY College at Geneseo"
##  [5] "Trenton State College"
##  [6] "University of California at Berkeley"
##  [7] "University of California at Irvine"
##  [8] "University of Florida"
##  [9] "University of Illinois - Urbana"
## [10] "University of Michigan at Ann Arbor"
## [11] "University of Minnesota at Morris"
## [12] "University of North Carolina at Chapel Hill"
## [13] "University of Virginia"
```

Questions