Introduction to Unsupervised Learning II

36-600

Fall 2021

The Setting (Reminder From Tuesday)

The setting for *unsupervised learning* is that you have a collection of p measurements (recorded in columns of a data frame) for each of n objects (recorded in rows of a data frame). The term "unsupervised" simply means that none of the variables is a response variable.

One can think of unsupervised learning as being an extension of EDA. In EDA, the goal is to visualize *projected* data to build intuition and to visually assess potential associations between variables. In unsupervised learning, we implement statistical algorithms to uncover potential structure in the data in their native space...e.g., separate clusters of data that represent naturally arising groups that you can identify and describe.

Sounds good. However, the main, overriding issue with unsupervised learning is that *there are no universally accepted mechanisms for model assessment or selection, i.e., there is no unique right answer!*

Hierarchical Clustering

The algorithm for hierarchical clustering is, like that for K-means, straightforward:

Algorithm 10.2 *Hierarchical Clustering*

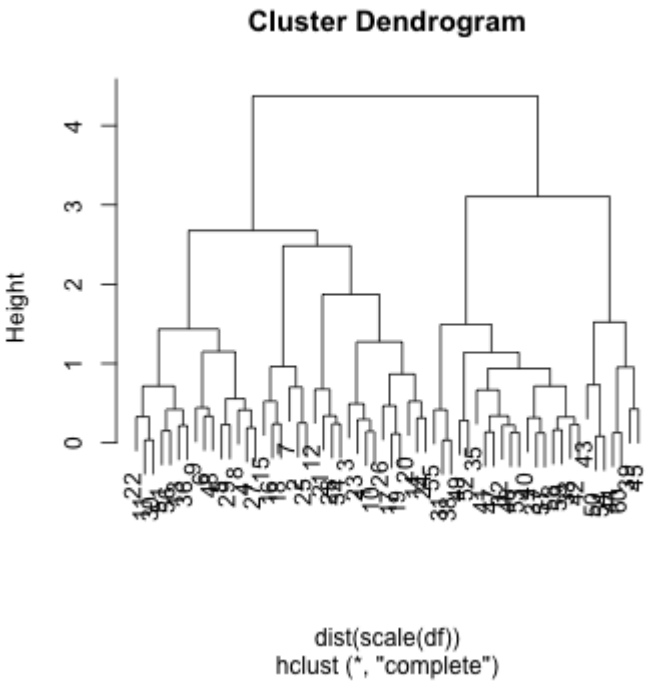
1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.
2. For $i = n, n-1, \ldots, 2$:
   (a) Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.
   (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Note the "[t]reat each observation as its own cluster." This is specifically "bottom-up" or *agglomerative* clustering. A primary limitation of agglomerative clustering is that all clusters lie within other clusters (hence the name "hierarchical").

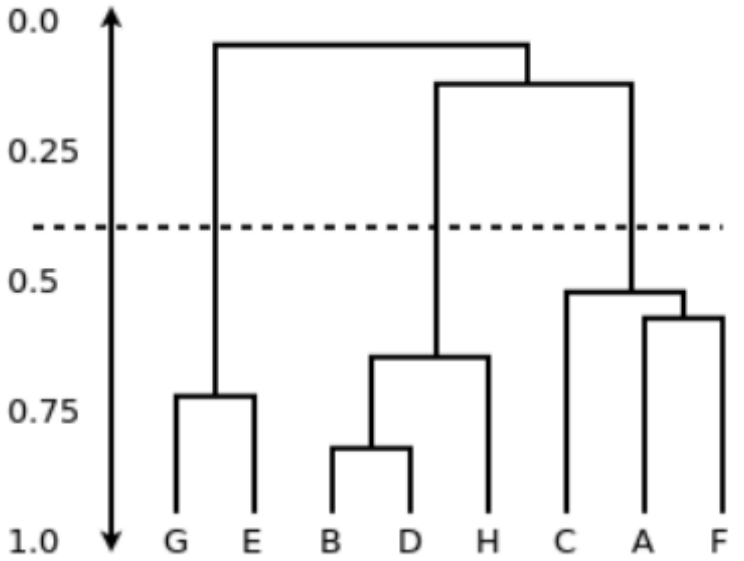
Hierarchical Clustering: Example

Here's an example of a dendrogram for complete-linkage hierarchical clustering. The "height" along the vertical axis at which two clusters fuse indicates dissimilarity...the higher the merge, the greater the dissimilarity between clusters. One extracts cluster members using, e.g., the `cutree()` function and processing its output.

```
hc.out = hclust(dist(scale(df)),method="complete")  # we use the same data as we do for K-means
plot(hc.out)
```



Hierarchical Clustering: Tree Cutting



(Credit goes to Erik Velldal for the above image.)

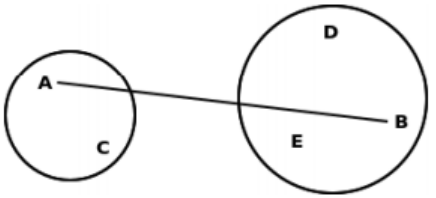
Hierarchical Clustering: Linkage

In agglomerative clustering, clusters are built up piece by piece by linking them together. There is no unique algorithm for how that linking is done! Note the descriptions below, while focusing on *complete linkage* and *average linkage*.

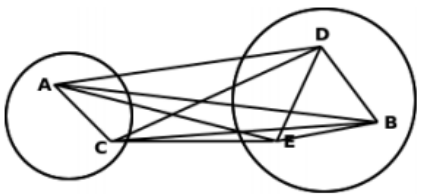
Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.

Hierarchical Clustering: Linkage

Complete linkage:



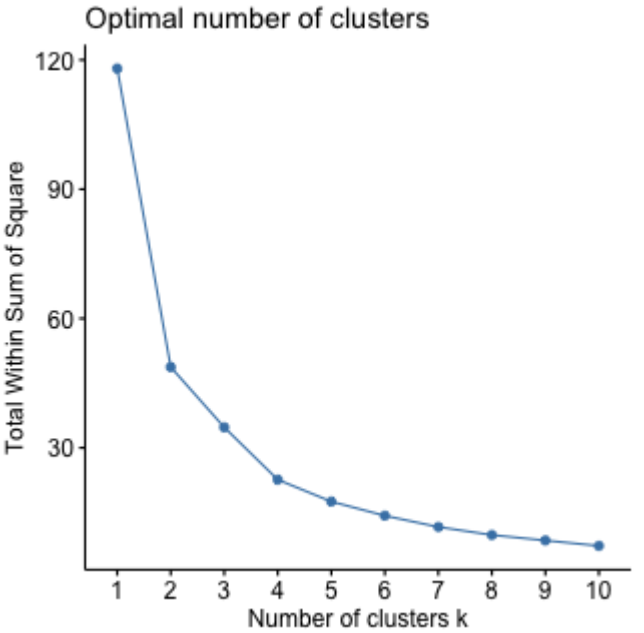
Average linkage:



Hierarchical Clustering: the Elbow Method

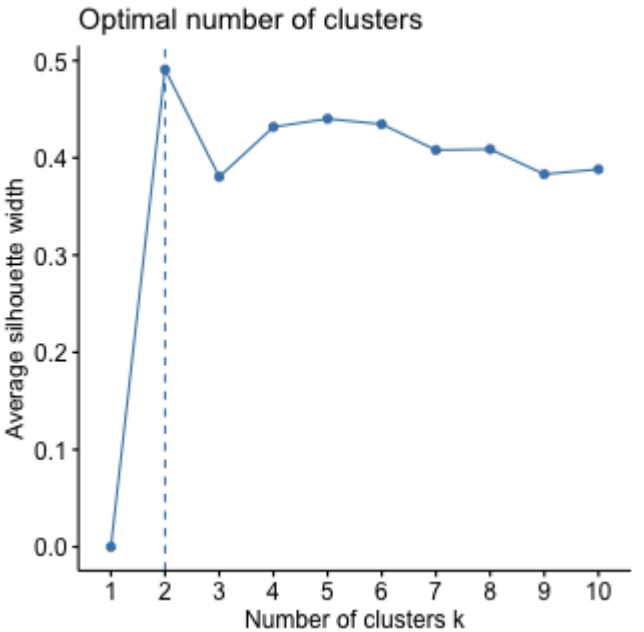
See this web page for a description of techniques you can use to determine the optimal number of clusters. Long-story-short: they are much the same ones as we used with K-means! In the examples we show here, though, you will see that we will utilize `factoextra` package functions exclusively.

```
library(factoextra)
fviz_nbclust(scale(df),FUN=hcut,method="wss")
```



Hierarchical Clustering: the Silhouette Method

```
fviz_nbclust(scale(df),FUN=hcut,method="silhouette")
```



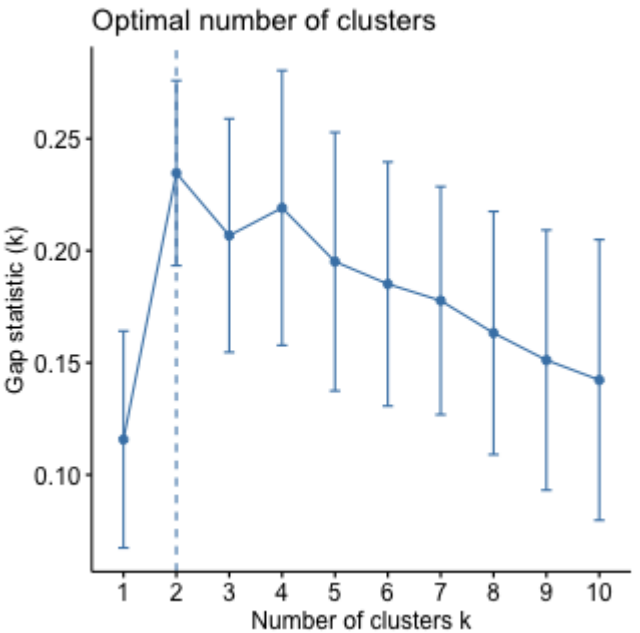
Hierarchical Clustering: the Gap Statistic

We used the gap statistic for K-means...and it can be applied to hierarchical clustering as well:

```
library(cluster)
gs <- clusGap(scale(df),FUN=hcut,nstart=20,K.max=10,B=50)
```

```
## Clustering k = 1,2,..., K.max (= 10): .. done
## Bootstrapping, b = 1,2,..., B (= 50)  [one "." per sample]:
## ................................................. 50
```

```
fviz_gap_stat(gs)
```



K-Means and Hierarchical Clustering: Wrap-Up

So: which of these should you use? Quoting ISLR: "we recommend performing clustering with different choices of [methods and parameters], and looking at the full set of results in order to see what patterns consistently emerge."

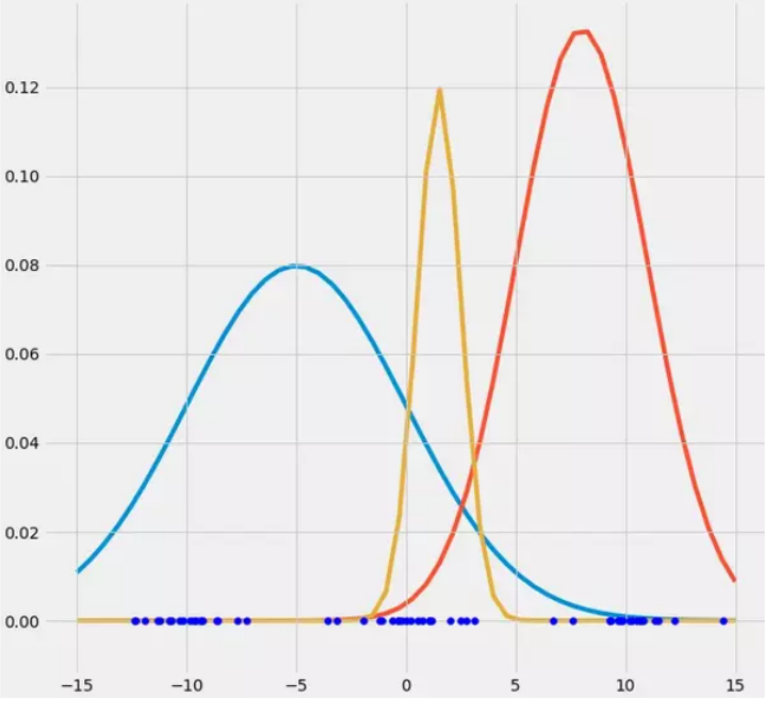
That said:

- In K-means, you specify the number of clusters before running the algorithm, as opposed to hierarchical clustering, where you specify the number of clusters afterwards by cutting across a dendrogram.
- Note that dendrograms can be *really* hard to read when the sample size is large.
- Also note that all data are assigned to clusters in these algorithms.

About That Last Point...

Perhaps we would like to implement an algorithm that does not necessarily force every datum into a cluster.

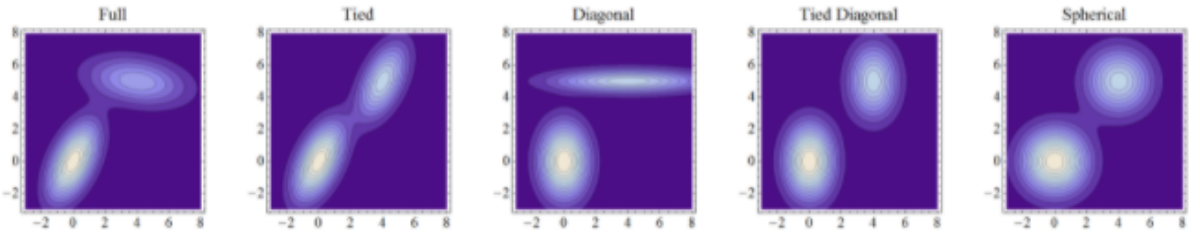
One example of such an algorithm is the *Gaussian Mixture Model* (see, e.g., this paper).



(Courtesy this web page)

GMM: Example

Here we will use the `ClusterR` package to determine the probabilities that data belong to one of a pre-defined number of Gaussian-shaped clusters. Note that a possible limitation of this model is that the Gaussians are *diagonal*: the longest axis lies along the x or y axis, and is not allowed to rotate away from those axes.



That's OK given our current data.

GMM: Example

```
library(ClusterR)
gmm.out <- GMM(df,gaussian_comps=2)
pred    <- predict_GMM(df,gmm.out$centroids,gmm.out$covariance_matrices,gmm.out$weights)
gmm.out$centroids
```

```
##             [,1]       [,2]
## [1,] -0.07563208 0.04640021
## [2,]  2.05763239 2.33456223
```

```
names(pred)
```

```
## [1] "log_likelihood" "cluster_proba"  "cluster_labels"
```

In this output:

- `log_likelihood` is the natural logarithm of the probability density function values at each data point. Higher numbers (meaning less negative, closer to zero) indicate areas where there is a local peak in the mixture model.
- `cluster_proba` is a matrix of probabilities: each row represents a data point, and each column the probability that the data point is in that cluster. You can use this to filter data (i.e., to say that a datum shouldn't be associated with a cluster at all). (Note: the probabilities in each row sum to 1. Axioms!)
- `cluster_labels` is the predicted cluster...basically, it is the number of the column with the highest probability.

GMM: Example

Our data were drawn from two normal distributions, thus we expect that we should see that they map to one of the two normals in the GMM with high probability. The plot below shows the probability of a datum belonging to cluster 1. (When this probability is low, it means it belongs to cluster 2 with high probability. Things get a bit more complicated if we ask for three clusters or more...)

```
hist(pred$cluster_proba,col="turquoise")
```