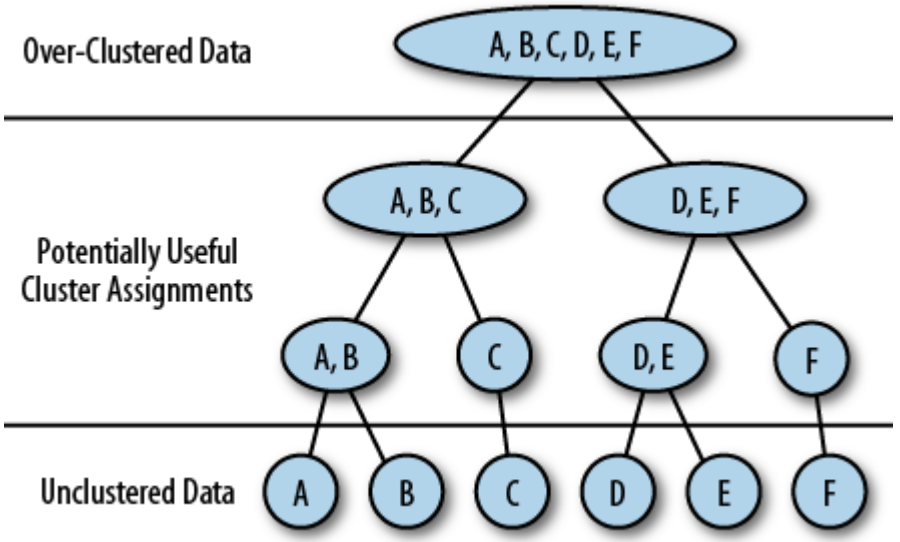
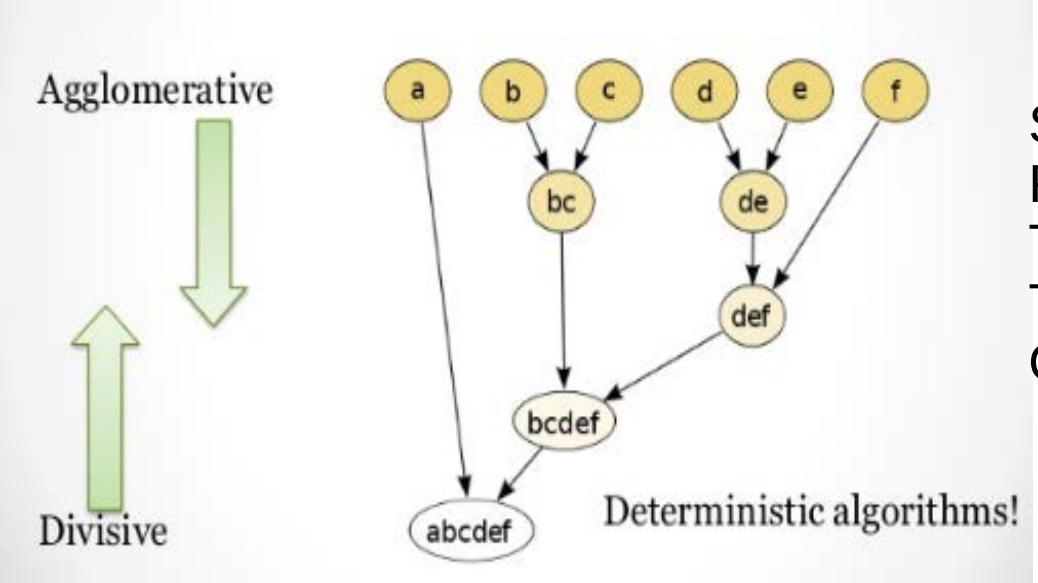
Hierarchical Clustering



Hierarchical Clustering

- **Previously we stated that there are two types of clustering n data points**
  - **Partitioning** such as k-means which we have already presented
  - **Hierarchical** which consists of two methods
    - **Agglomerative methods**: In this method, we begin with each data point being a cluster. We combine clusters based on some distance function until we have a single cluster
    - **Divisive methods**: We begin with all data in a *single cluste*r and divide until each data point is in a single cluster
  - On the next slide, an image from Wikipedia shows the difference.
  - ***We have not specified the decision process for forming clusters! That will come later.***

Agglomerative versus Divisive



Steps in Agglomerative

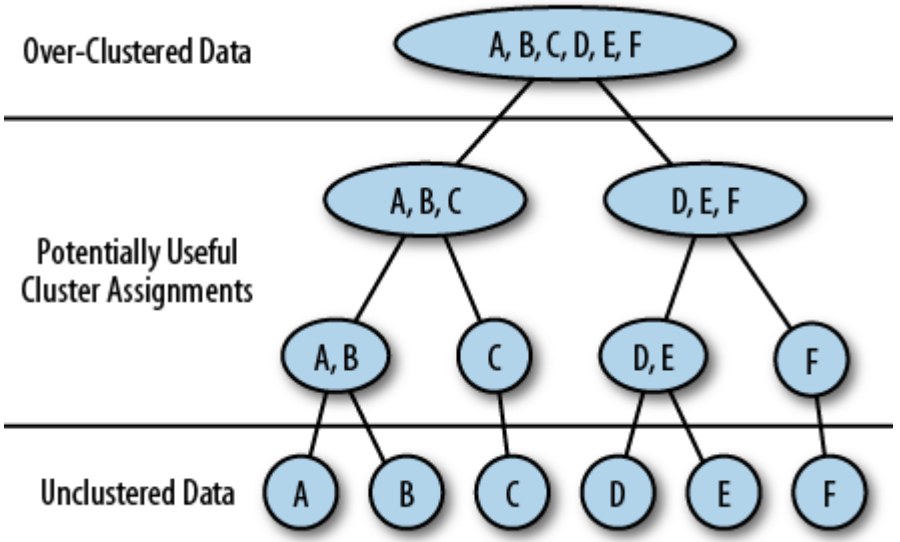
Six clusters = {a}, {b}, {c}, {d}, {e}. {f}
Four clusters = {a}, {bc}, {de}, {f}
Three clusters = {a},{b,c}, {d,e,f}
Two clusters = {a}, {b,c,d,e,f}
One cluster = {a,b,c,d,e,f}

Steps in Divisive

One cluster = {a,b,c,d,e,f}
Two clusters = {a}, {b,c,d,e,f}
Three clusters = {a},{b,c}, {d,e,f}
Four clusters = {a}, {bc}, {de}, {f}
Six clusters = {a}, {b}, {c}, {d}, {e}. {f}

Usable Clusters

- **As we have stated, having one cluster or n clusters is not informative**
- **The diagram below shows how a subject matter expert could determine meaningful clusters**



Determining “distance” between clusters

Before we can start forming clusters we need to define the distance between two clusters

There are several ways to do this

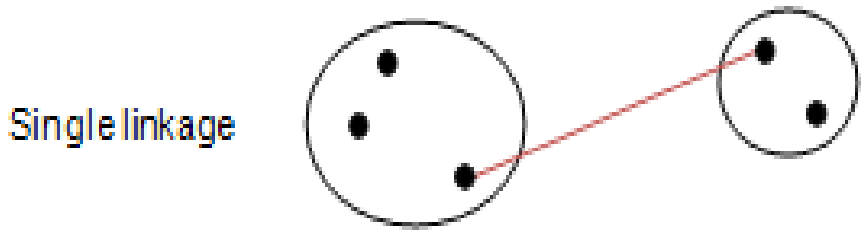
- Some actually involve a distance such as Euclidean distance
- Others involve similarity of clusters

Those that involve notions of distance include

- Single link clustering
- Complete link clustering
- Average link clustering

http://www.analytictech.com/networks/hiclus.htm

Single Linkage



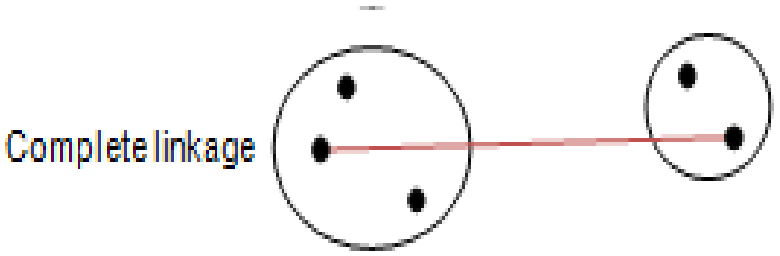
In **single linkage** (SL), the distance between two clusters A and B is defined to be the minimum of all the distances between any element in A and any element in B.

In symbols, D(A,B) = min{d(x,y) where min is over all x in A and all y in B

If A has n elements and B has m elements, how many distances would we have to compute? There is actually a way to reduce the number of such calculations

When we cluster using SL, we join clusters with the the smallest SL distance.

Complete Linkage



In **complete linkage** (CL) the distance between two clusters A and B is defined to be the maximum distance between any element in A and any element in B.

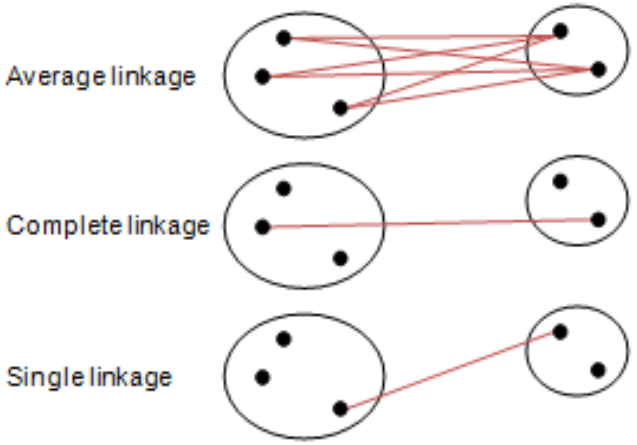
D(A,B) = max{d(x,y) where max is over all x in A and all y in B.

When we cluster using complete linkage, we join clusters with the smallest CL distance.

Average Linkage

In Average Linkage (AL), the distance between clusters A and B is defined to be the average distance between all elements x of A and y of B.

Below, we see all methods side by side.



Algorithm for Agglomerative Clustering

Algorithmic steps for Agglomerative Hierarchical clustering

Let $X = \{x_1, x_2, x_3, ..., x_n\}$ be the set of data points.

1) Begin with the disjoint clustering having level $L(0) = 0$ and sequence number $m = 0$.

2) Find the least distance pair of clusters in the current clustering, say pair (r), (s), according to $d[(r),(s)] = \min d[(i),(j)]$ where the minimum is over all pairs of clusters in the current clustering.

3) Increment the sequence number: $m = m + 1$. Merge clusters (r) and (s) into a single cluster to form the next clustering m. Set the level of this clustering to $L(m) = d[(r),(s)]$.

4) Update the distance matrix, D, by deleting the rows and columns corresponding to clusters (r) and (s) and adding a row and column corresponding to the newly formed cluster. The distance between the new cluster, denoted (r,s) and old cluster(k) is defined in this way: $d[(k), (r,s)] = \min (d[(k),(r)], d[(k),(s)])$.

5) If all the data points are in one cluster then stop, else repeat from step 2).

https://sites.google.com/site/dataclusteringalgorithms/hierarchical-clustering-algorithm

Questions for previous slide

- **On the previous slide, there are variables m and L. How could these be used to assist in Cluster Analysis?**

- **On the next slide, we begin an example. The data items are US Cities. The distance between any two cities is the distance in air miles between them.**
- **We will use these distances to cluster the cities**
- **We will attempt to determine a "usable" number of clusters and give names to each cluster.**

Clustering Air Flights

	BOS	NY	DC	MIA	CHI	SEA	SF	LA	DEN
BOS	0	206	429	1504	963	2976	3095	2979	1949
NY	206	0	233	1308	802	2815	2934	2786	1771
DC	429	233	0	1075	671	2684	2799	2631	1616
MIA	1504	1308	1075	0	1329	3273	3053	2687	2037
CHI	963	802	671	1329	0	2013	2142	2054	996
SEA	2976	2815	2684	3273	2013	0	808	1131	1307
SF	3095	2934	2799	3053	2142	808	0	379	1235
LA	2979	2786	2631	2687	2054	1131	379	0	1059
DEN	1949	1771	1616	2037	996	1307	1235	1059	0

Using SL, we see that the nearest pair of cities is Boston and NY. On the next slide, we will merge them into a single cluster and update the distances.
http://www.analytictech.com/networks/hiclus.htm

One merger m=1

After merging BOS with NY: Why were NY and Boston chosen for merger?

	BOS/NY	DC	MIA	CHI	SEA	SF	LA	DEN
BOS/NY	0	223	1308	802	2815	2934	2786	1771
DC	223	0	1075	671	2684	2799	2631	1616
MIA	1308	1075	0	1329	3273	3053	2687	2037
CHI	802	671	1329	0	2013	2142	2054	996
SEA	2815	2684	3273	2013	0	808	1131	1307
SF	2934	2799	3053	2142	808	0	379	1235
LA	2786	2631	2687	2054	1131	379	0	1059
DEN	1771	1616	2037	996	1307	1235	1059	0

Which entries in the matrix needed to be updated if we use Single Linkage? How were they calculated? For example, why is the distance from {Bos, NY} to {MIA} = 1308?

Which clusters will be merged next?

m=2

After merging DC with BOS-NY:

	BOS/NY/DC	MIA	CHI	SEA	SF	LA	DEN
BOS/NY/DC	0	1075	671	2684	2799	2631	1616
MIA	1075	0	1329	3273	3053	2687	2037
CHI	671	1329	0	2013	2142	2054	996
SEA	2684	3273	2013	0	808	1131	1307
SF	2799	3053	2142	808	0	379	1235
LA	2631	2687	2054	1131	379	0	1059
DEN	1616	2037	996	1307	1235	1059	0

Which clusters will be merged next? Why?

m=3

After merging SF with LA:

	BOS/ NY/DC	MIA	CHI	SEA	SF/LA	DEN
BOS/NY/DC	0	1075	671	2684	2631	1616
MIA	1075	0	1329	3273	2687	2037
CHI	671	1329	0	2013	2054	996
SEA	2684	3273	2013	0	808	1307
SF/LA	2631	2687	2054	808	0	1059
DEN	1616	2037	996	1307	1059	0

m=4

After merging CHI with BOS/NY/DC:

	BOS/NY/DC/ CHI	MIA	SEA	SF/LA	DEN
BOS/NY/DC/CHI	0	1075	2013	2054	996
MIA	1075	0	3273	2687	2037
SEA	2013	3273	0	808	1307
SF/LA	2054	2687	808	0	1059
DEN	996	2037	1307	1059	0

What is the next step? Why?

m=5 and m=6

After merging SEA with SF/LA:

	BOS/NY/DC/CHI	MIA	SF/LA/SEA	DEN
BOS/NY/DC/CHI	0	1075	2013	996
MIA	1075	0	2687	2037
SF/LA/SEA	2054	2687	0	1059
DEN	996	2037	1059	0

After merging DEN with BOS/NY/DC/CHI:

	BOS/NY/DC/CHI/DEN	MIA	SF/LA/SEA
BOS/NY/DC/CHI/DEN	0	1075	1059
MIA	1075	0	2687
SF/LA/SEA	1059	2687	0

m=7

After merging SF/LA/SEA with BOS/NY/DC/CHI/DEN:

	BOS/NY/DC/CHI/DEN/SF/LA/SEA	MIA
BOS/NY/DC/CHI/DEN/SF/LA/SEA	0	1075
MIA	1075	0

When m = 8, we will have constructed a single cluster BOS/NY/DC/CHI/DEN/SF/LA/SEA/MIA

m=7

After merging SF/LA/SEA with BOS/NY/DC/CHI/DEN:

	BOS/NY/DC/CHI/DEN/SF/LA/SEA	MIA
BOS/NY/DC/CHI/DEN/SF/LA/SEA	0	1075
MIA	1075	0

When m = 8, we will have constructed a single cluster BOS/NY/DC/CHI/DEN/SF/LA/SEA/MIA

Analyzing the Clusters

As we have seen, one cluster and n clusters are not usable

At which level do you (as a subject matter expert) think the clusters are useful

Give names to the clusters and defend your answer.