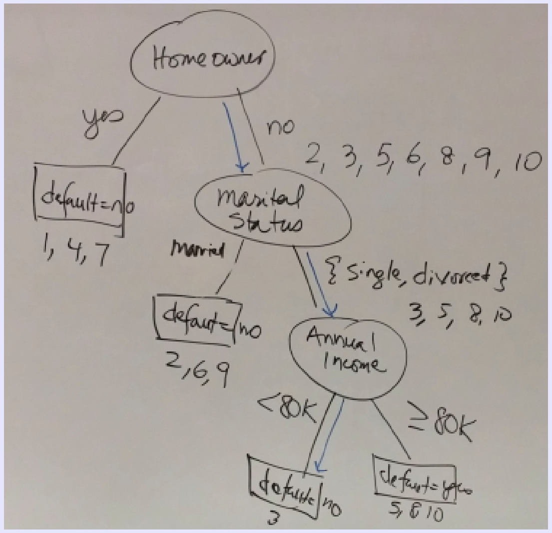

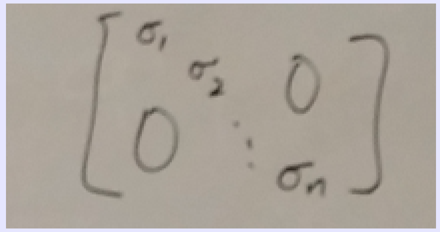

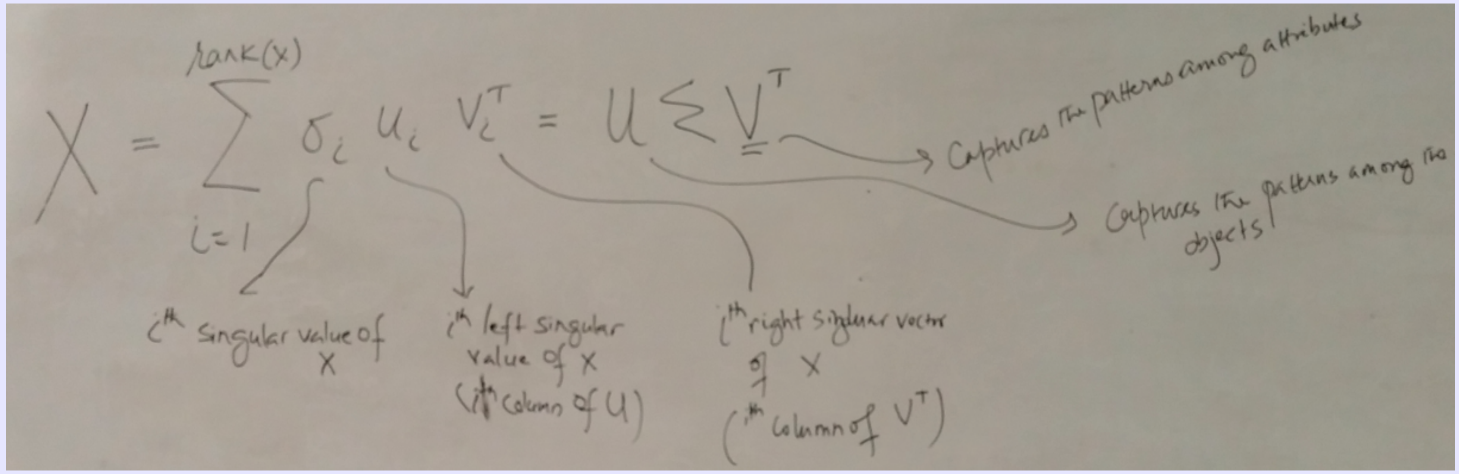

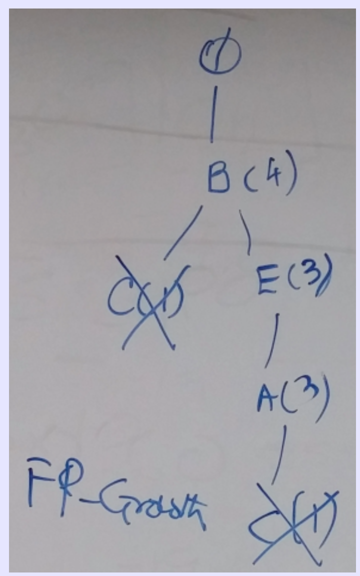

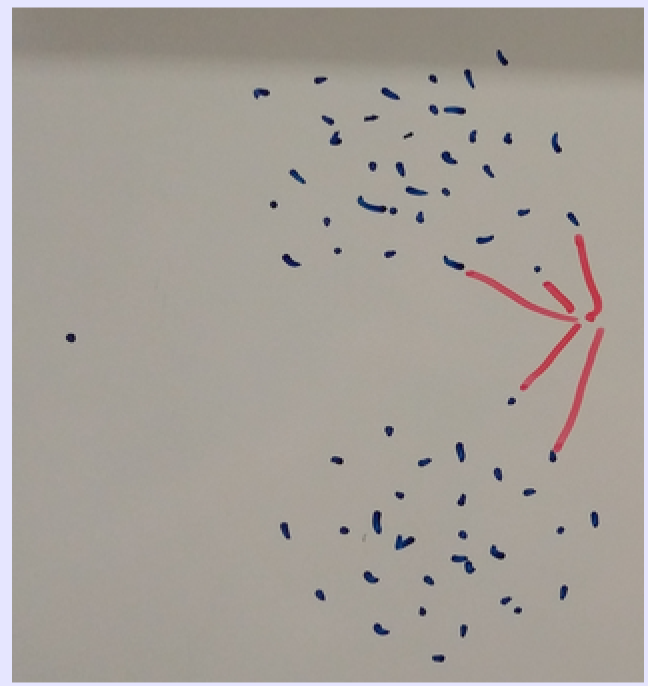

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Vijay K. Gurbani, Ph.D.,
Illinois Institute of Technology

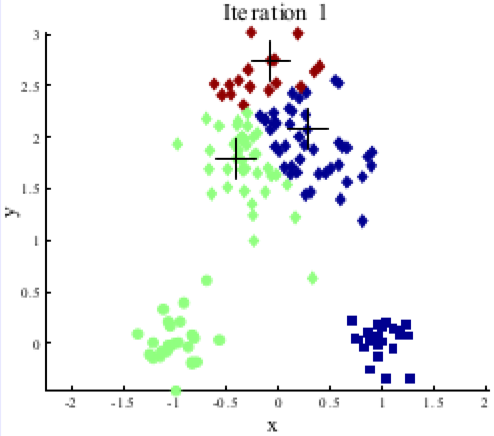
Clustering I

Clustering: K-Means

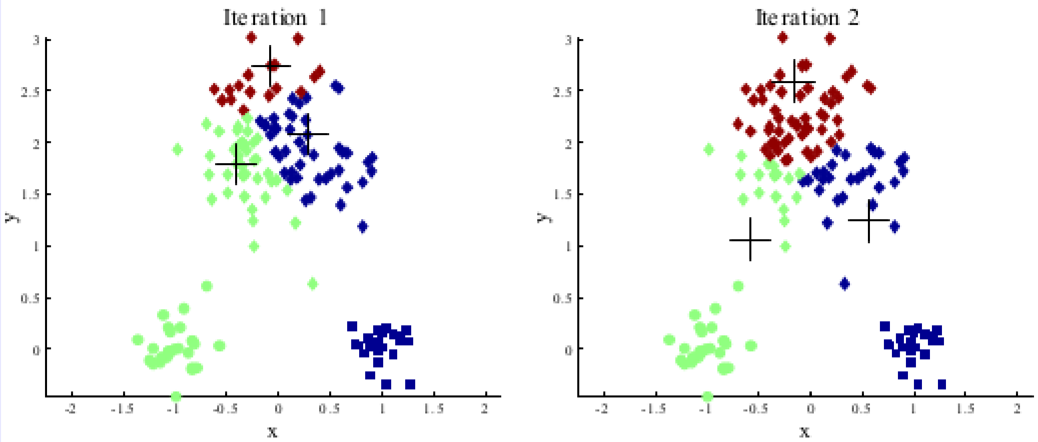
- Computing distances:
  - Euclidean distance (Minkowski, R=2)
  - Manhattan distance (Minkowski, R=1)
  - Jaccard similarity measure
  - Cosine similarity measure
  - …

Used for document data; covered later

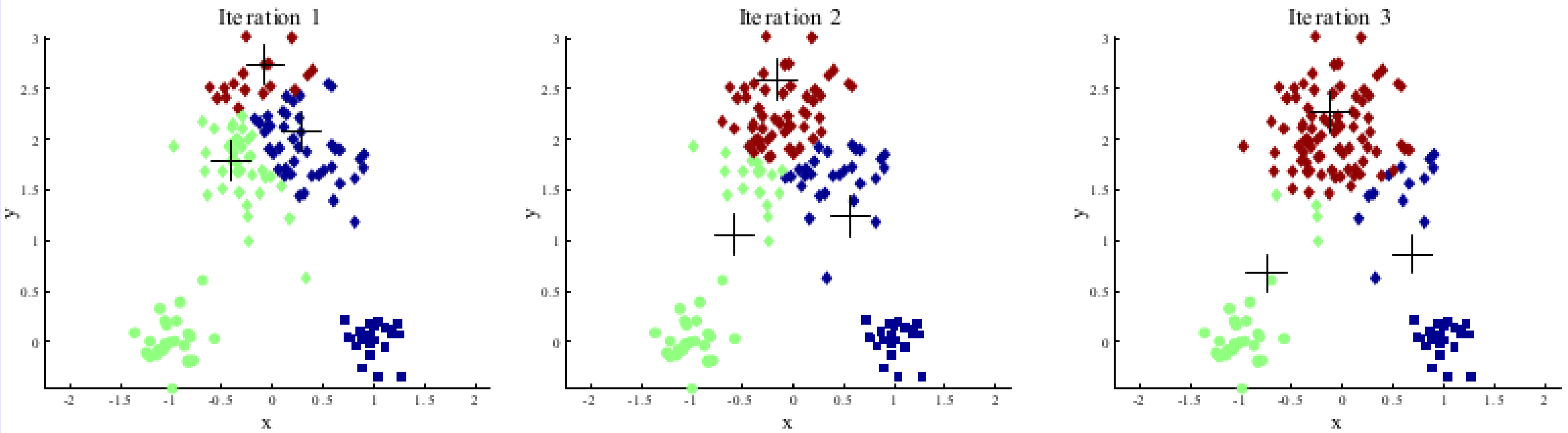
Clustering: K-Means



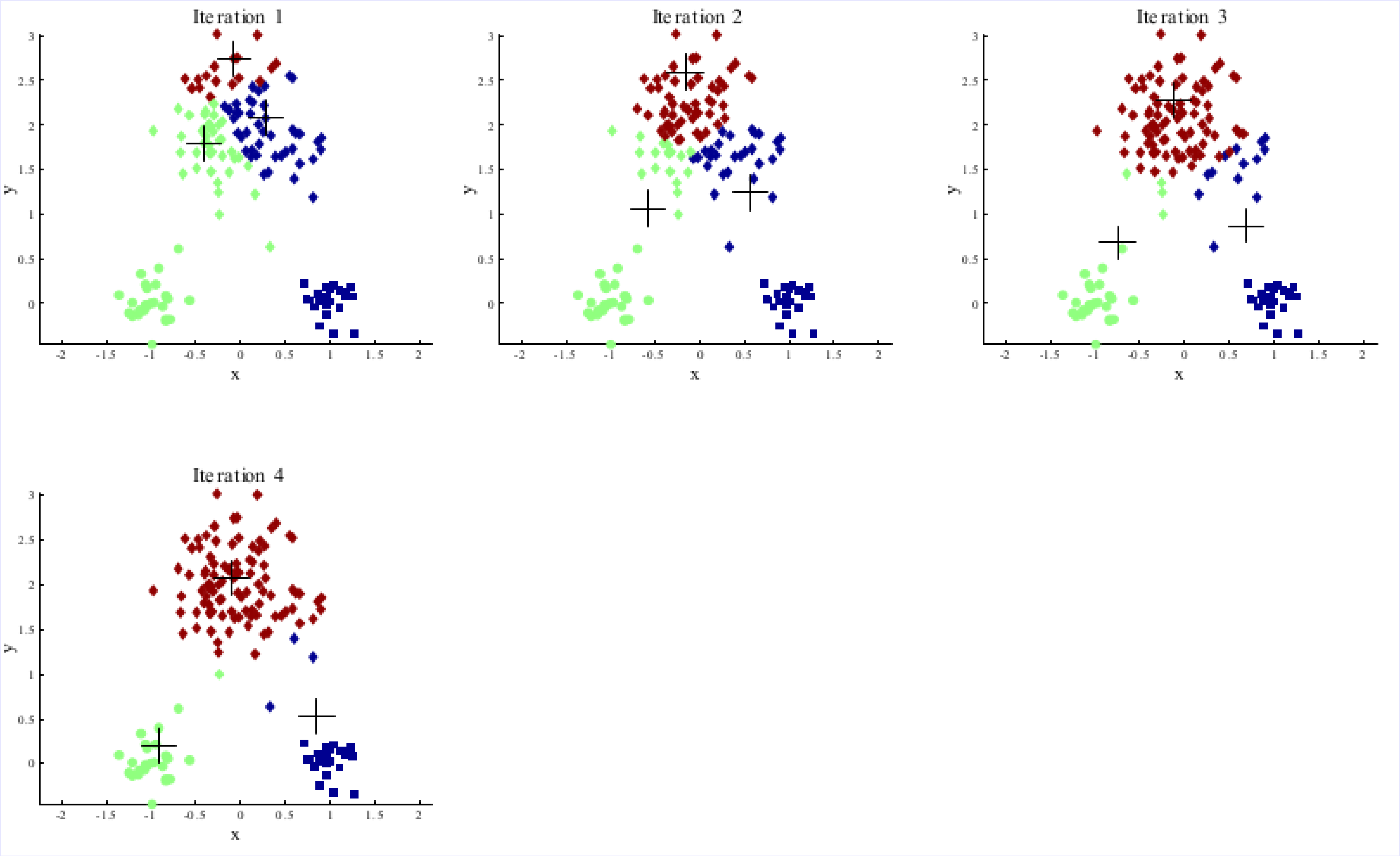
Clustering: K-Means



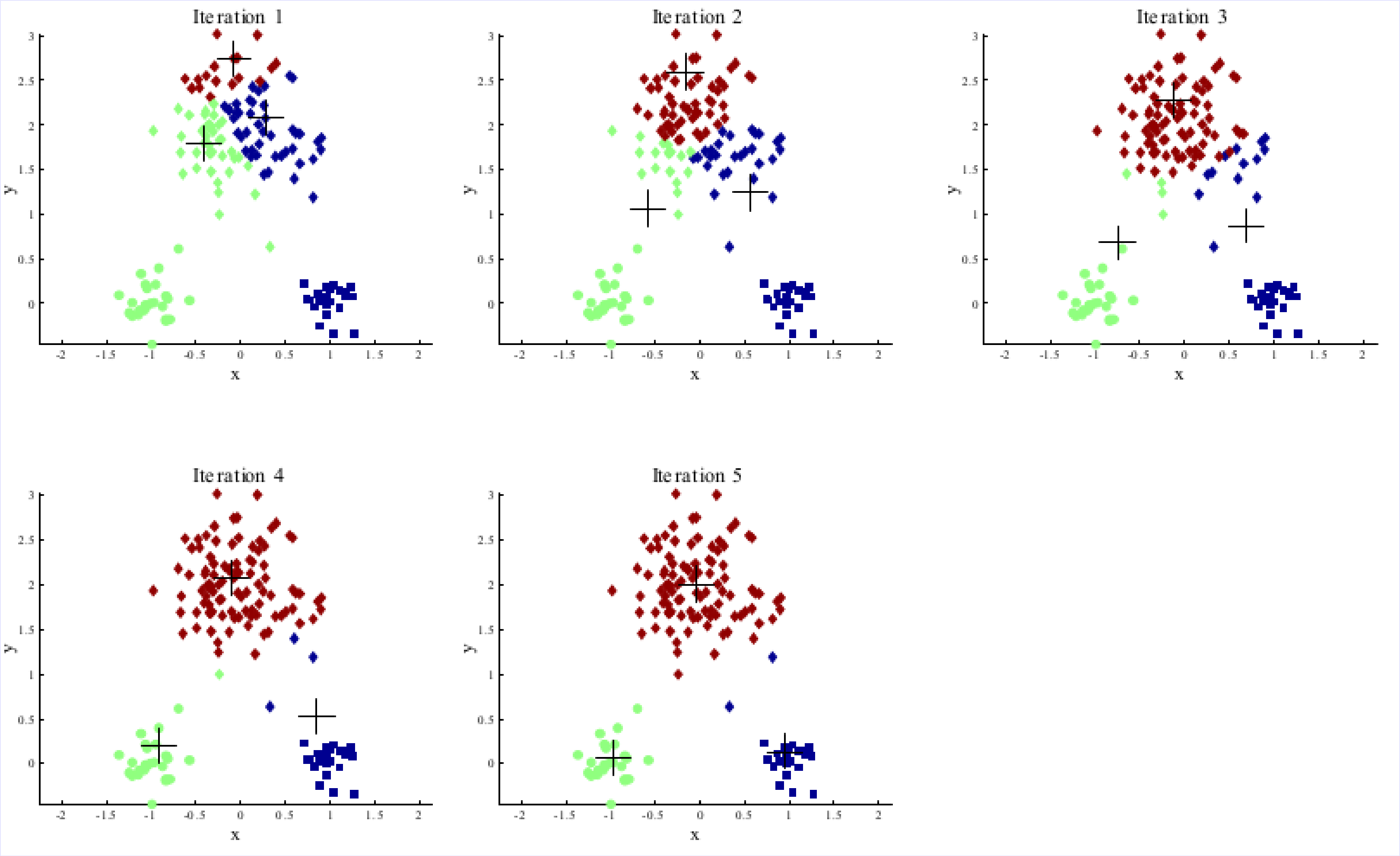
Clustering: K-Means



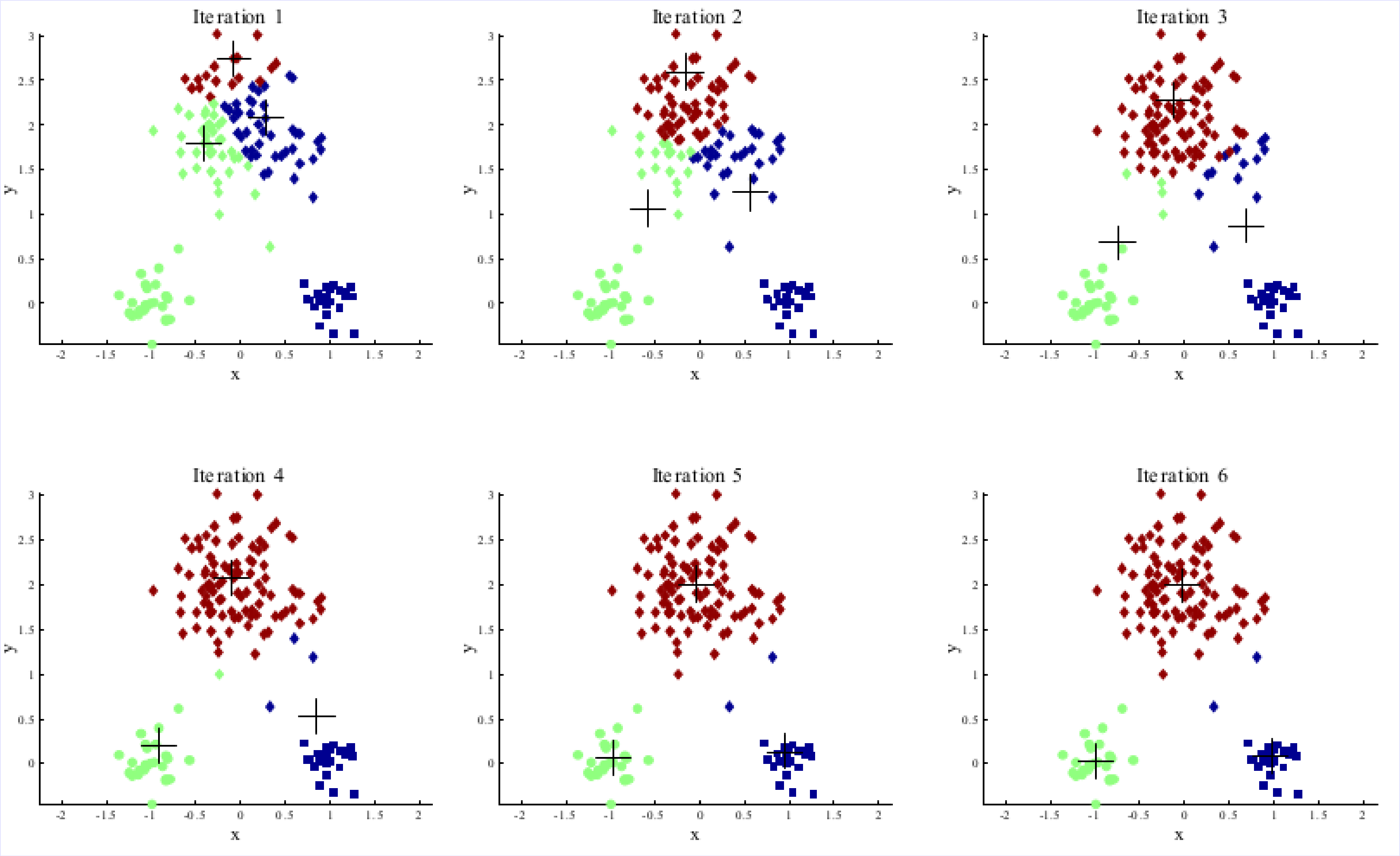
Clustering: K-Means



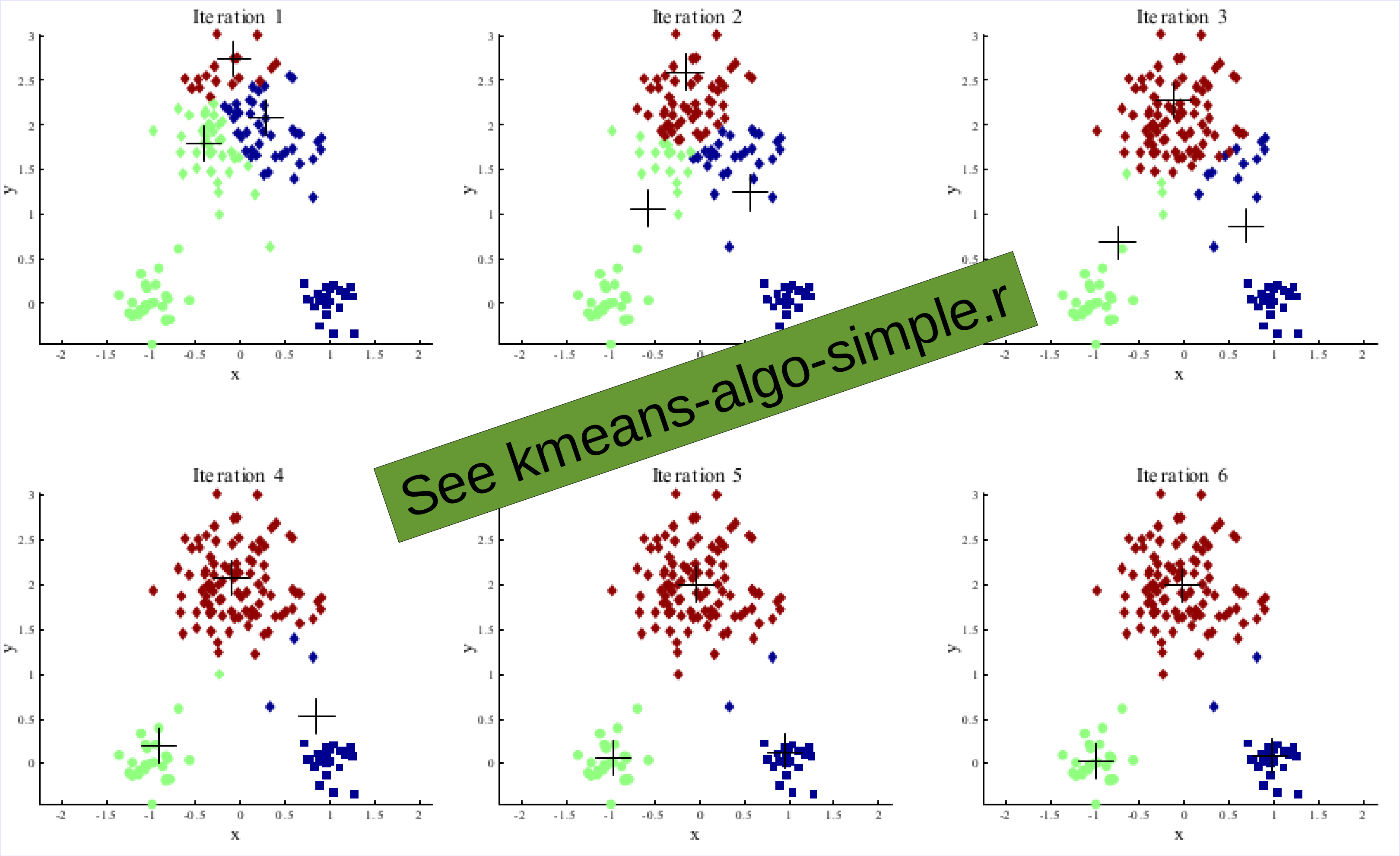
Clustering: K-Means



Clustering: K-Means



Clustering: K-Means



See kmeans-algo-simple.r

Clustering: K-Means

- When do we stop?

Algorithm 8.1 Basic K-means algorithm.

1: Select K points as initial centroids.
2: **repeat**
3: Form K clusters by assigning each point to its closest centroid.
4: Recompute the centroid of each cluster.
5: **until** Centroids do not change.

$$\underset{j}{\operatorname{argmin}}\ Dist(x_i, c_j)\ \forall \text{ observations } i \text{ and clusters } j\ \in\ \{1..K\}$$

$$min(SSE\ =\ \sum_{j=1}^{K} \sum_{x \in c_j} Dist(c_j, x)^2)$$

Clustering: K-Means

- When do we stop?

Algorithm 8.1 Basic K-means algorithm.

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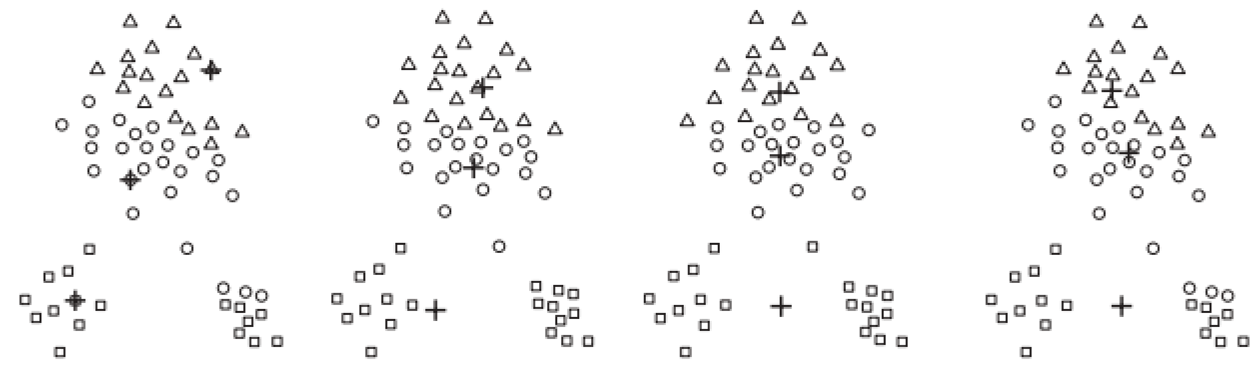
$$min(SSE\ =\ \sum_{j=1}^{K}\sum_{x\in c_j} Dist(c_j, x)^2)$$

- Does K-Means always converge?

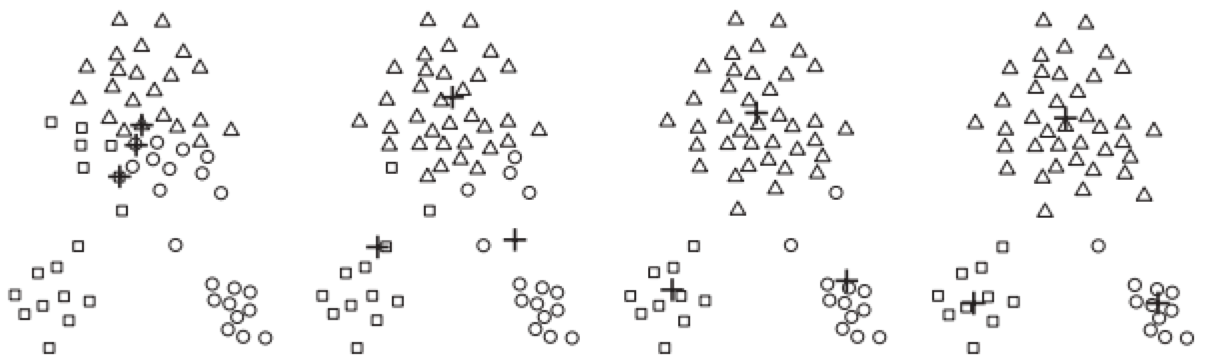
Clustering: K-Means

- How to choose the initial centroids?
  - Random selection of initial centroids may lead to sub-optimal clustering.

All three initial centroids randomly distributed. Leads to suboptimal solution.



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.

All three initial random centroids in one natural cluster. Leads to good solution.

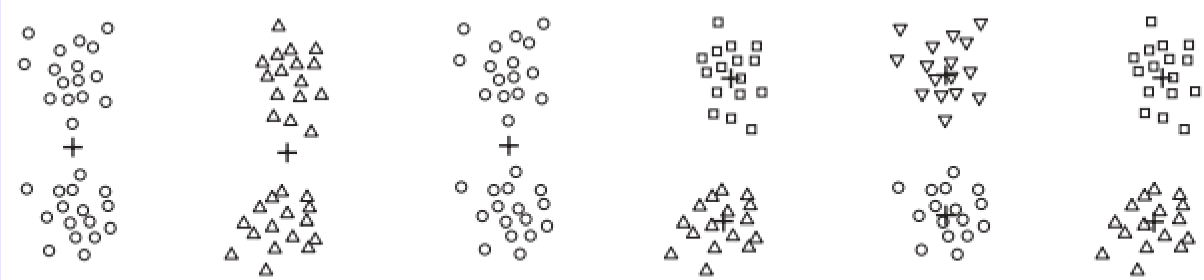
Clustering: Bisecting K-means

- Goal: Form best (optimal) clusters.
- Simple idea: to obtain *K* clusters, split the set of all points into two clusters, select one of the clusters to split, and so on until you have *K* clusters.
  - Which cluster to split?
    - The largest one, or
    - The one with largest error (SSE), or
    - ...

Clustering: Bisecting K-means

Algorithm 8.2 Bisecting K-means algorithm.

```
Initialize the list of clusters to contain the cluster consisting of all points.
repeat
   Remove a cluster from the list of clusters.
   {Perform several "trial" bisections of the chosen cluster.}
   for i = 1 to number of trials do
      Bisect the selected cluster using basic K-means.
   end for
   Select the two clusters from the bisection with the lowest total SSE.
   Add these two clusters to the list of clusters.
until Until the list of clusters contains K clusters.
```

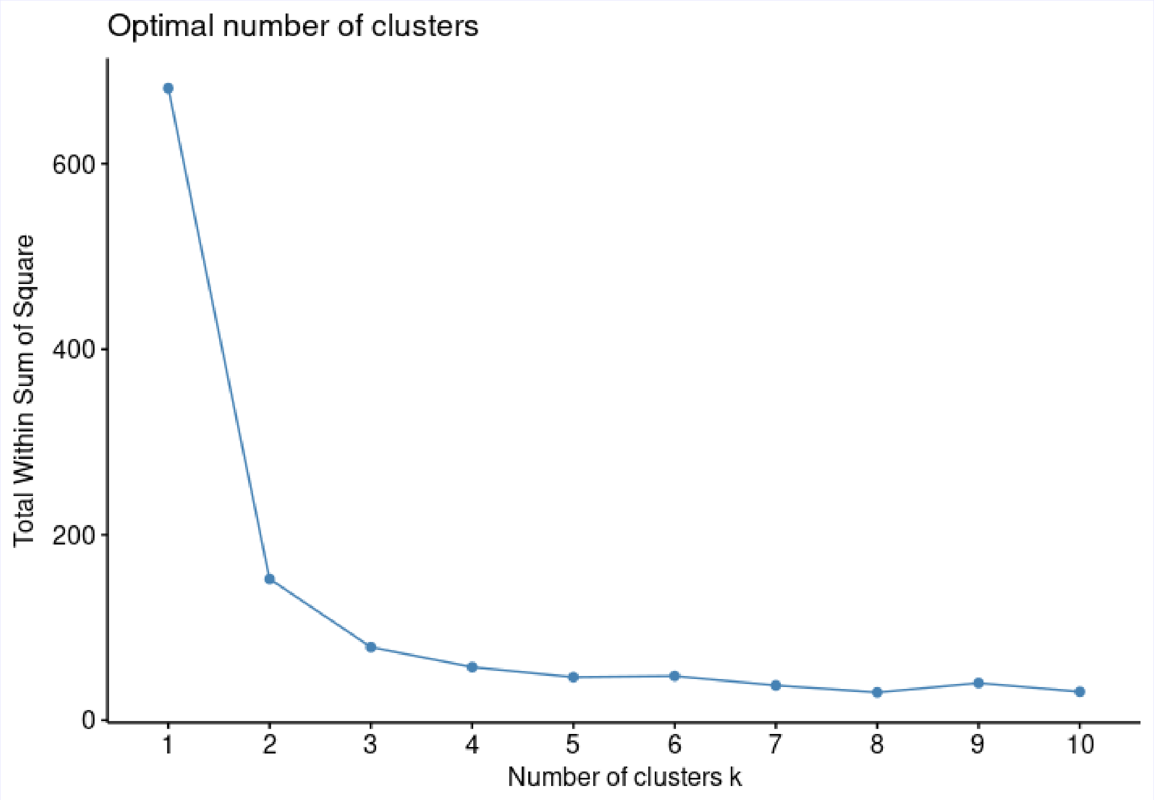


(a) Iteration 1. (b) Iteration 2. (c) Iteration 3.

Figure 8.8. Bisecting K-means on the four clusters example.

Clustering: K-Means

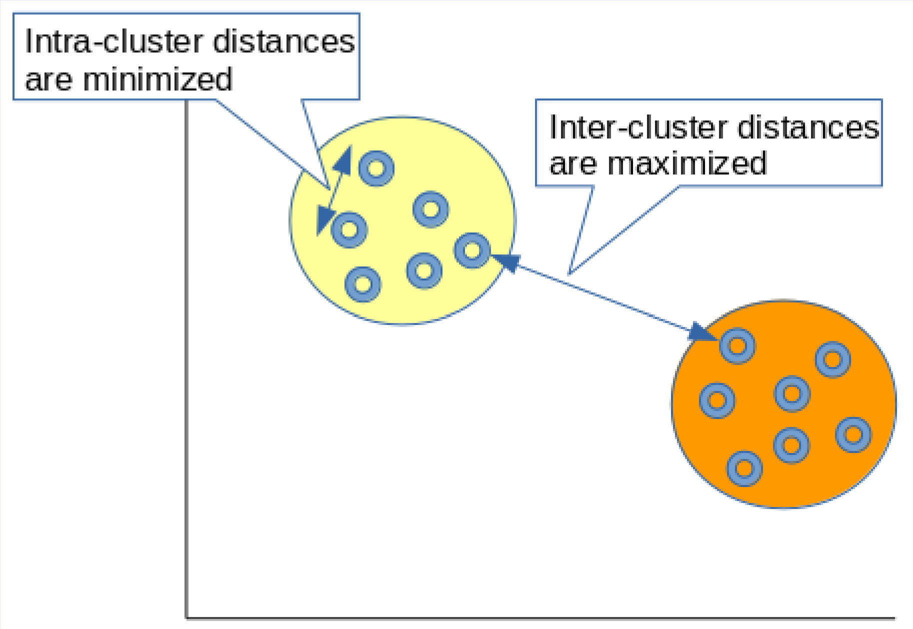
- How to choose the *k* in K-Means?
  - See kmeans-how-many-clusters.r



Within cluster sum of squares is the SSE we saw earlier. We want the total within cluster sum of squares to be minimal.

Cluster analysis

- How do we evaluate the goodness of fit of clustering?
- Clustering should exhibit **low** intra-cluster SS (also called cohesion) and **high** inter-cluster SS (also called separation).
- Metrics of interest:
  - Within cluster SS
  - Total SS
  - Between SS
  - Variance explained



Cluster analysis

- Within cluster SS
  - Sum of squares of each point in the cluster to the cluster centroid: $\sum_{x \in C_i} Dist(c_i, x)^2$, where C_i is cluster i and c_i is centroid of cluster i
- Total SS
  - Sum of squares of each point in the dataset to the **global cluster** mean: $\sum_{x \in D} Dist(C_g, x)^2$, where C_g is global cluster mean, and D is the clustering dataset
- Between SS
  - Total SS - total within cluster SS, where total within cluster SS = $\sum_{j=1}^{k} \sum_{x \in C_j} Dist(c_j, x)^2$, where k is number of clusters, C_j is cluster j, and c_j is centroid of cluster j

Cluster analysis

- Variance
  - Between SS / Total SS (between 0.0 and 1.0)
  - The higher this ratio, the more variance is explained by the clusters.

Clustering: R implementation

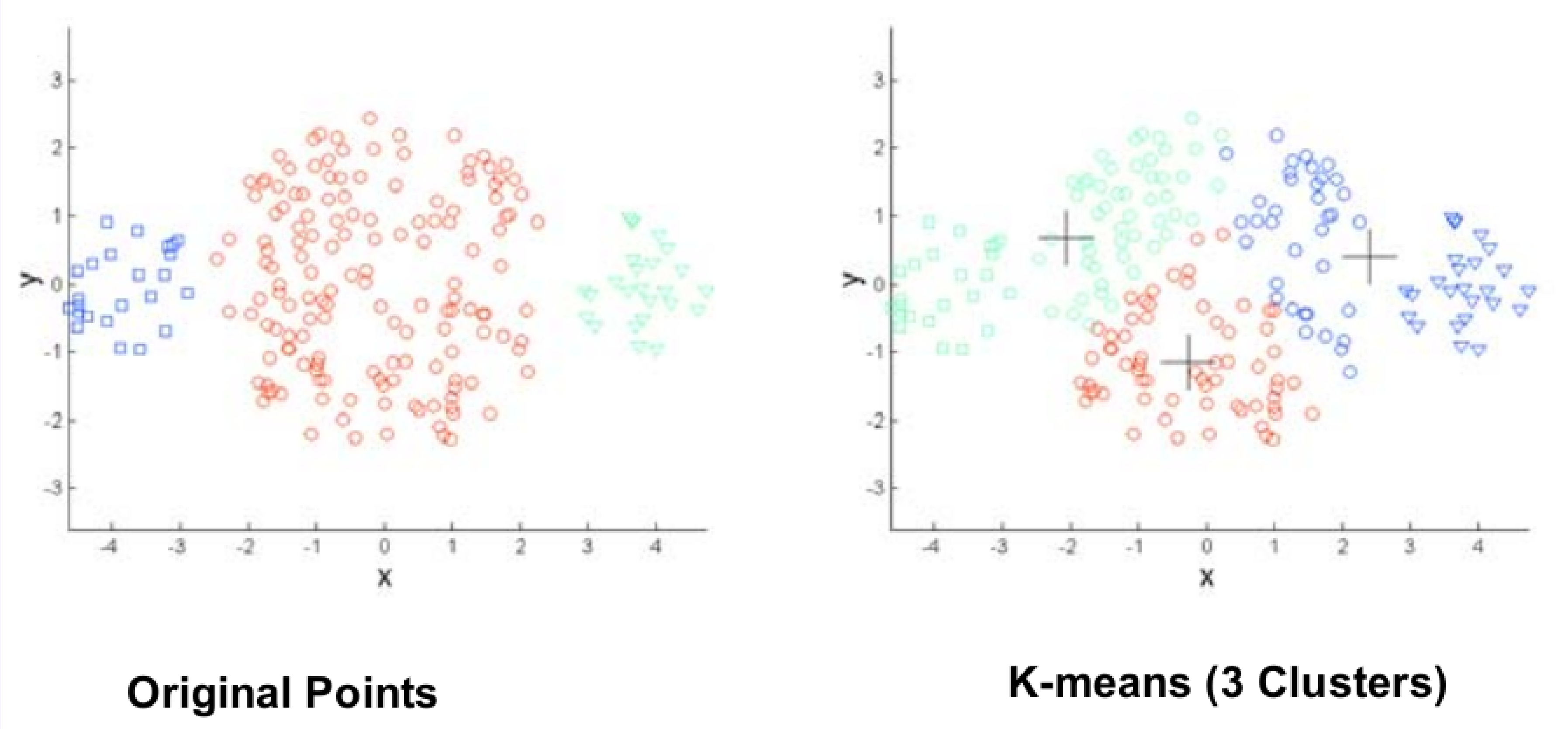
- Clustering in R:
  - Package: cluster, factoextra
  - How to cluster, or using R’s clustering libraries.
  - Visualizing the clusters.
  - Why scale (standardize)?
  - See cluster-and-scaling.r

K-means: Practical issues

- K-means does not handle outliers gracefully; it will try to include these in a cluster.
  – Outlier detection and removal prior to K-means can help.
- What is the right value of *k*?
- K-means has problems when clusters are of differing...

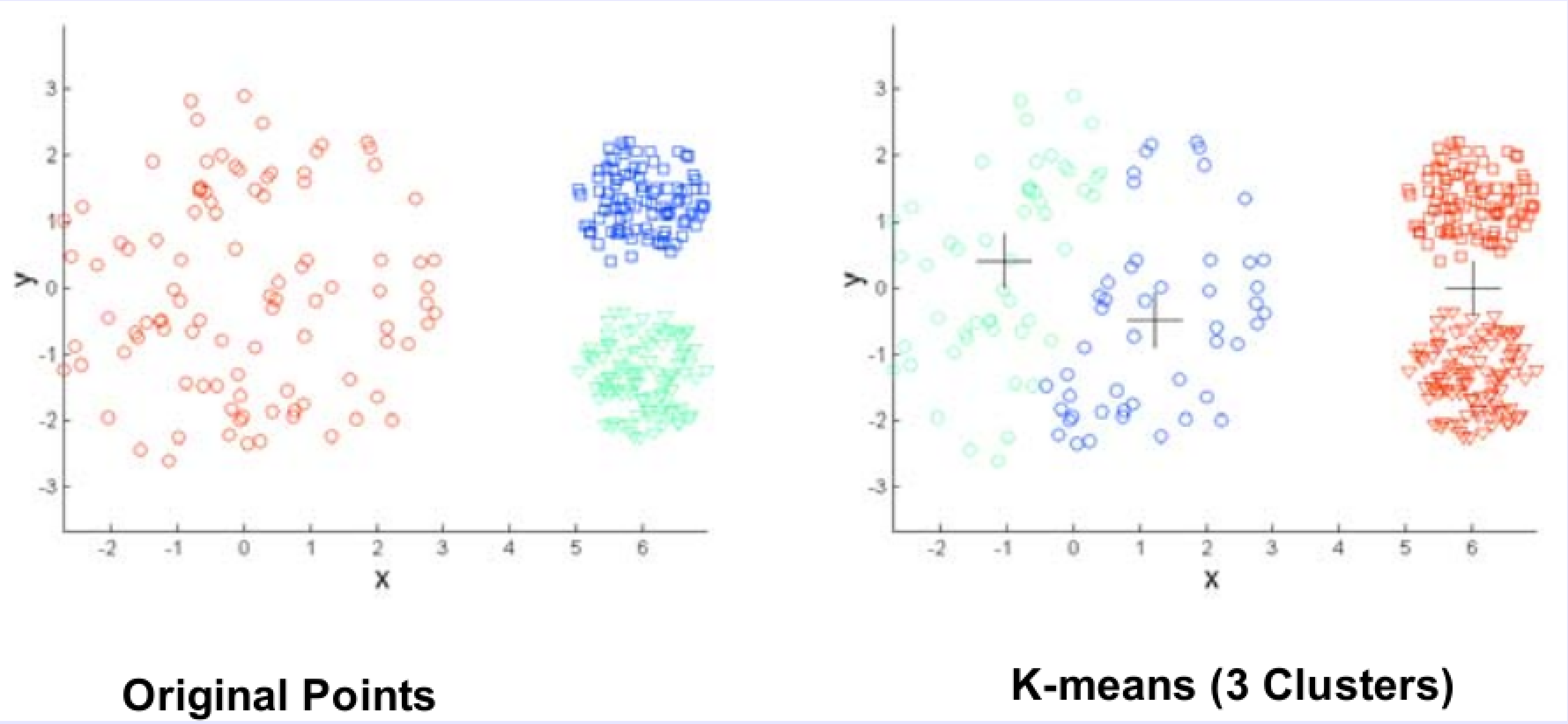
K-means: Practical issues

- K-means: differing sizes.



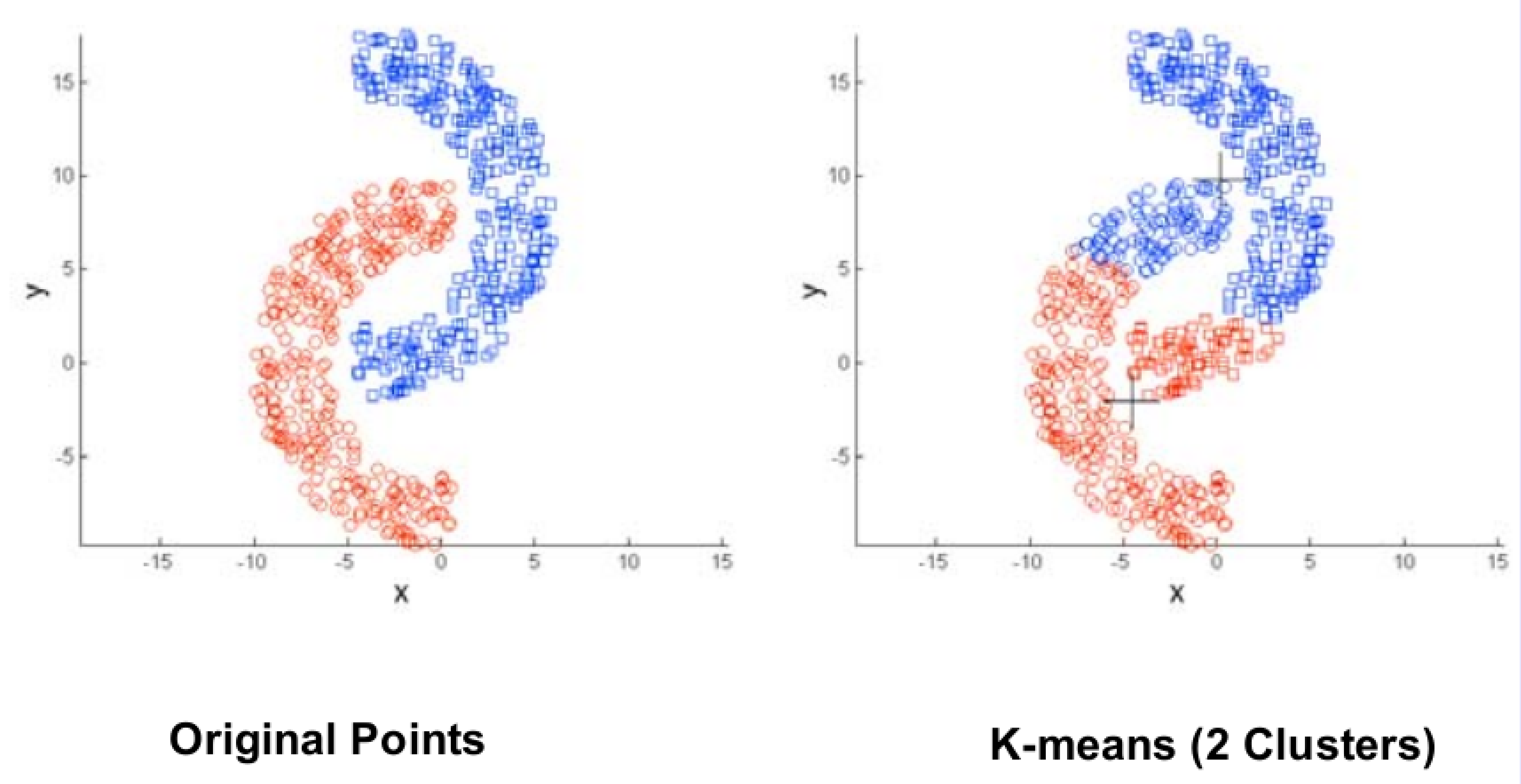
K-means: Practical issues

- K-means: differing densities.



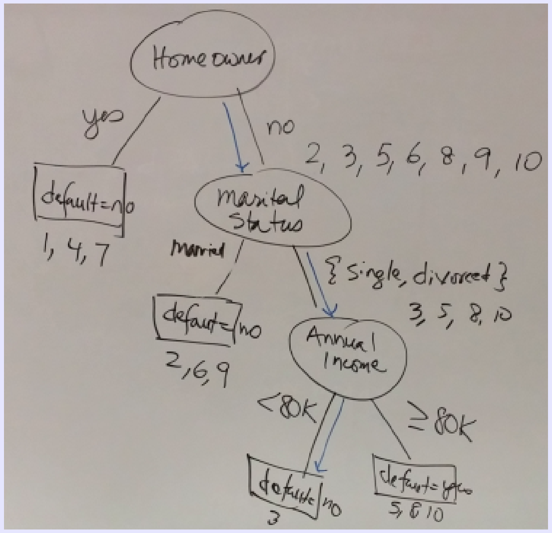
K-means: Practical issues

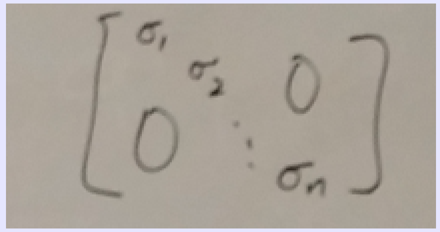
- K-means: problem with non-globular formations.

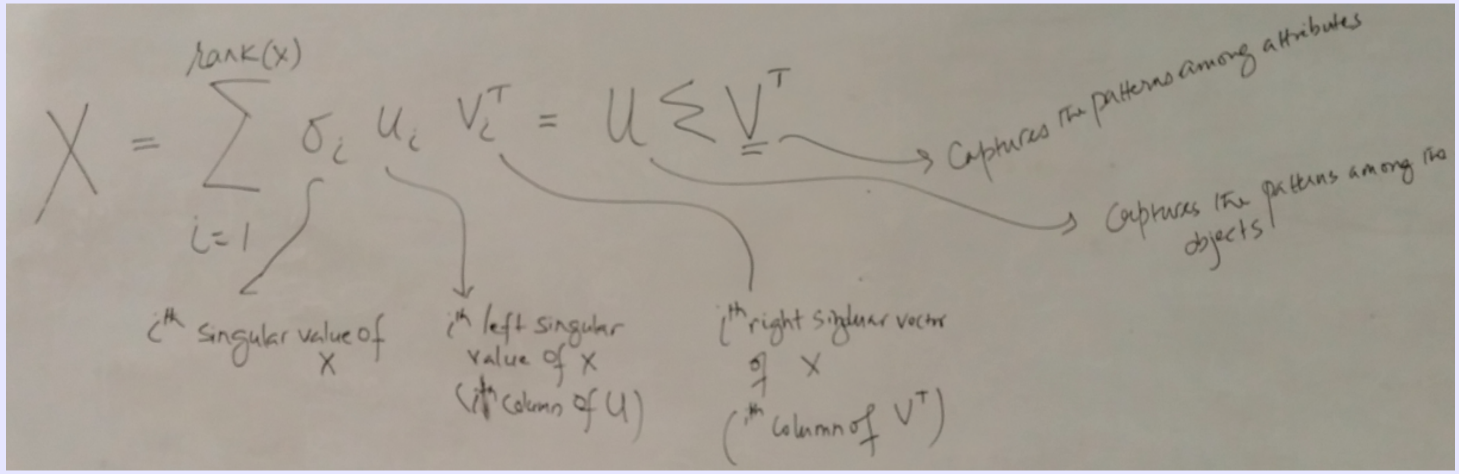


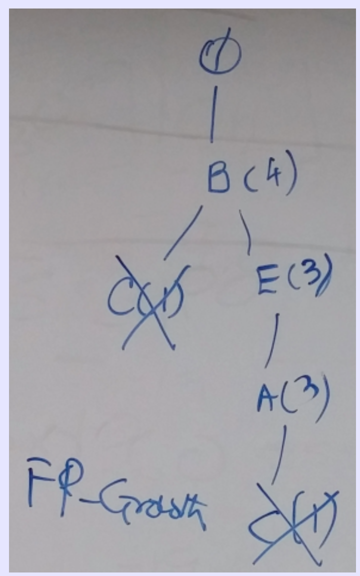
Clustering: K-Means

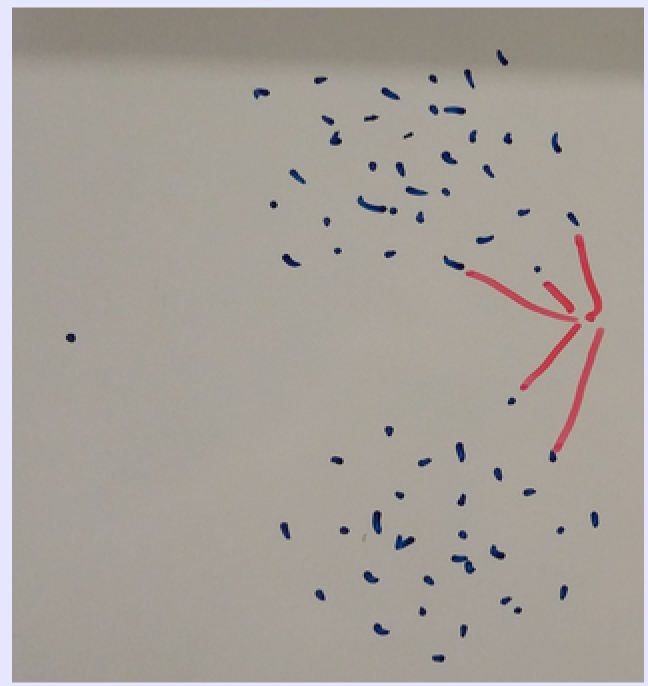
- Complexity
  - Space: $O((m+K)n)$, m = number of observations, and n = number of attributes, K = number of clusters.
  - Time: $O(I*K*m*n)$, I = number of iterations required to converge.
- Additional issues:
  - Empty clusters.
  - Outliers may lead to higher SSE and non-representative cluster centroids.











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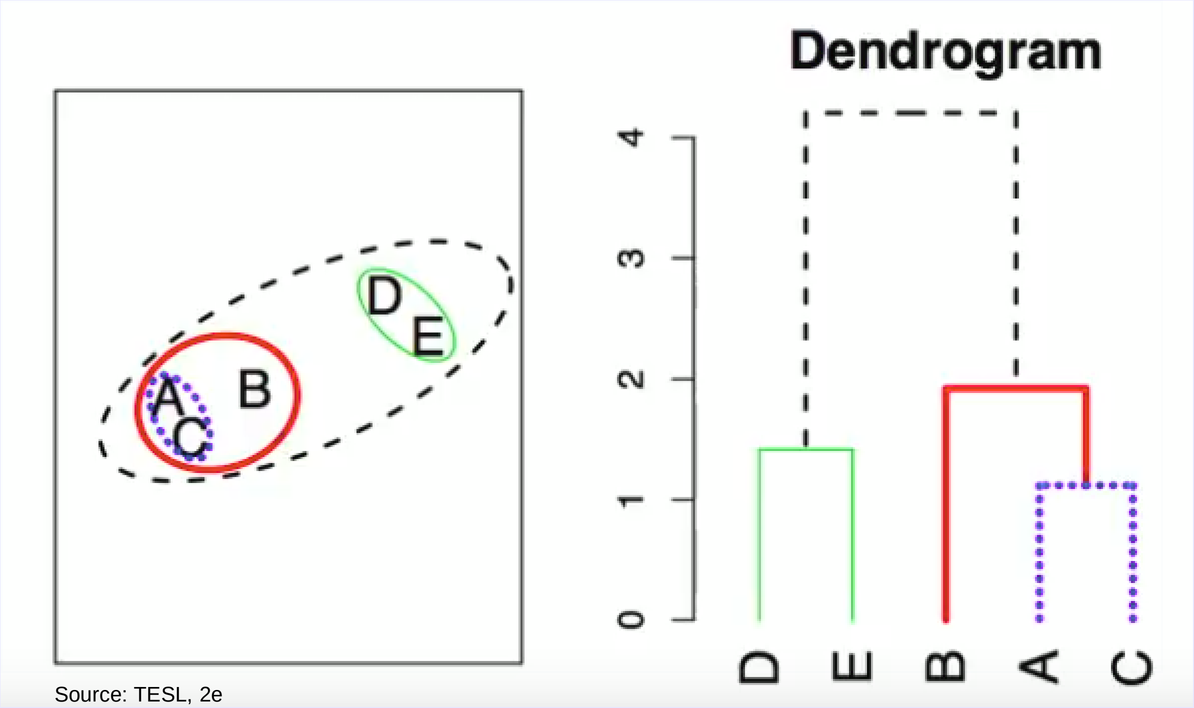
Clustering II

Hierarchical clustering

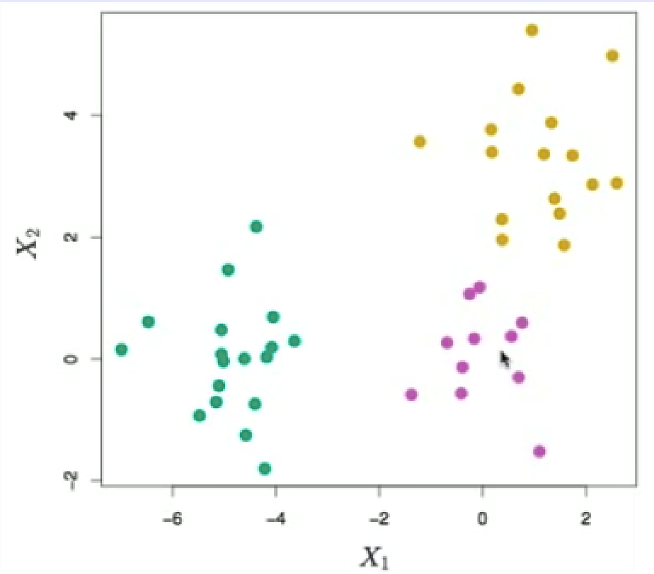
- Inspired by the area of taxonomy, where hierarchical structures are common and elements under the same hierarchy automatically constitute a cluster.
- Unlike K-means, does not require us to choose *k* a-priori. Both an advantage and disadvantage.
- Two approaches:
  - Agglomerative (bottom-up): Each point starts off as an individual cluster, and at each step, merge closest pairs of clusters. (Need cluster proximity metric.)
  - Divisive: All points in one cluster, at each step, split a cluster until singleton clusters of individual points remain. (Which cluster to split and how to do the splitting.)

Hierarchical clustering



- Depicted as tree-like structure called Dendrograms.
- Y-axis labeled with the proximity between clusters.
- Look for closest cluster (in terms, say, squared distance), and join them. And continue until one cluster left.

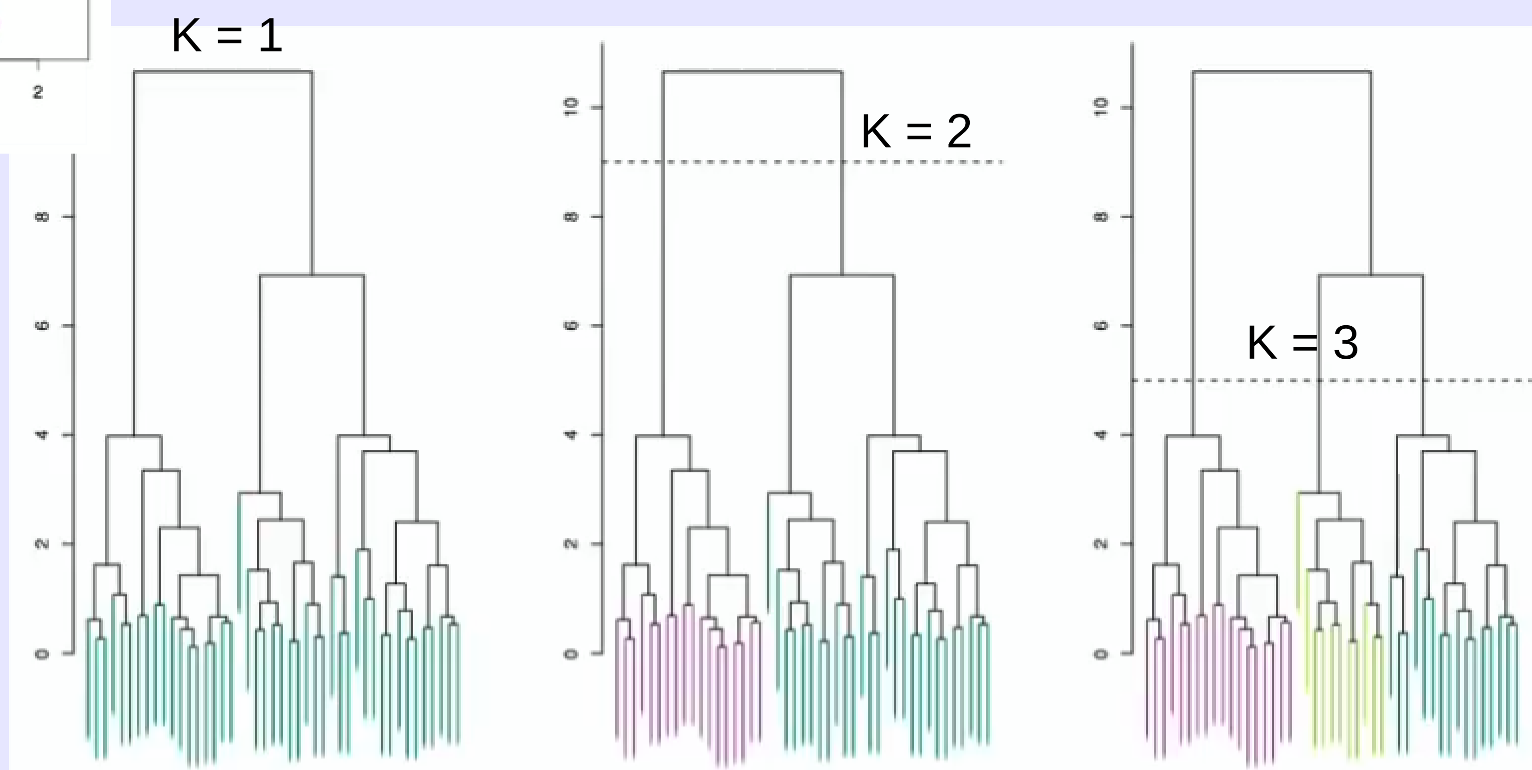
Hierarchical clustering



Source: TESL, 2e

45 data points in 2-D. 3 distinct classes, shown in separate colors. However, we treat the class labels as unknown and seek to cluster the observations to discover classes from the data.

Note: We can play around with K to get required clustering. K can vary from 1 to 45, in which case each point is a cluster.



Hierarchical clustering

Algorithm 8.3 Basic agglomerative hierarchical clustering algorithm.

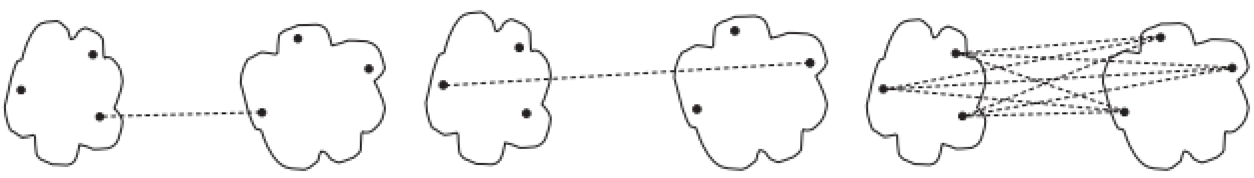
1: Compute the proximity matrix, if necessary.
2: **repeat**
3: Merge the closest two clusters.
4: Update the proximity matrix to reflect the proximity between the new cluster and the original clusters.
5: **until** Only one cluster remains.

Hierarchical clustering

Algorithm 8.3 Basic agglomerative hierarchical clustering algorithm.

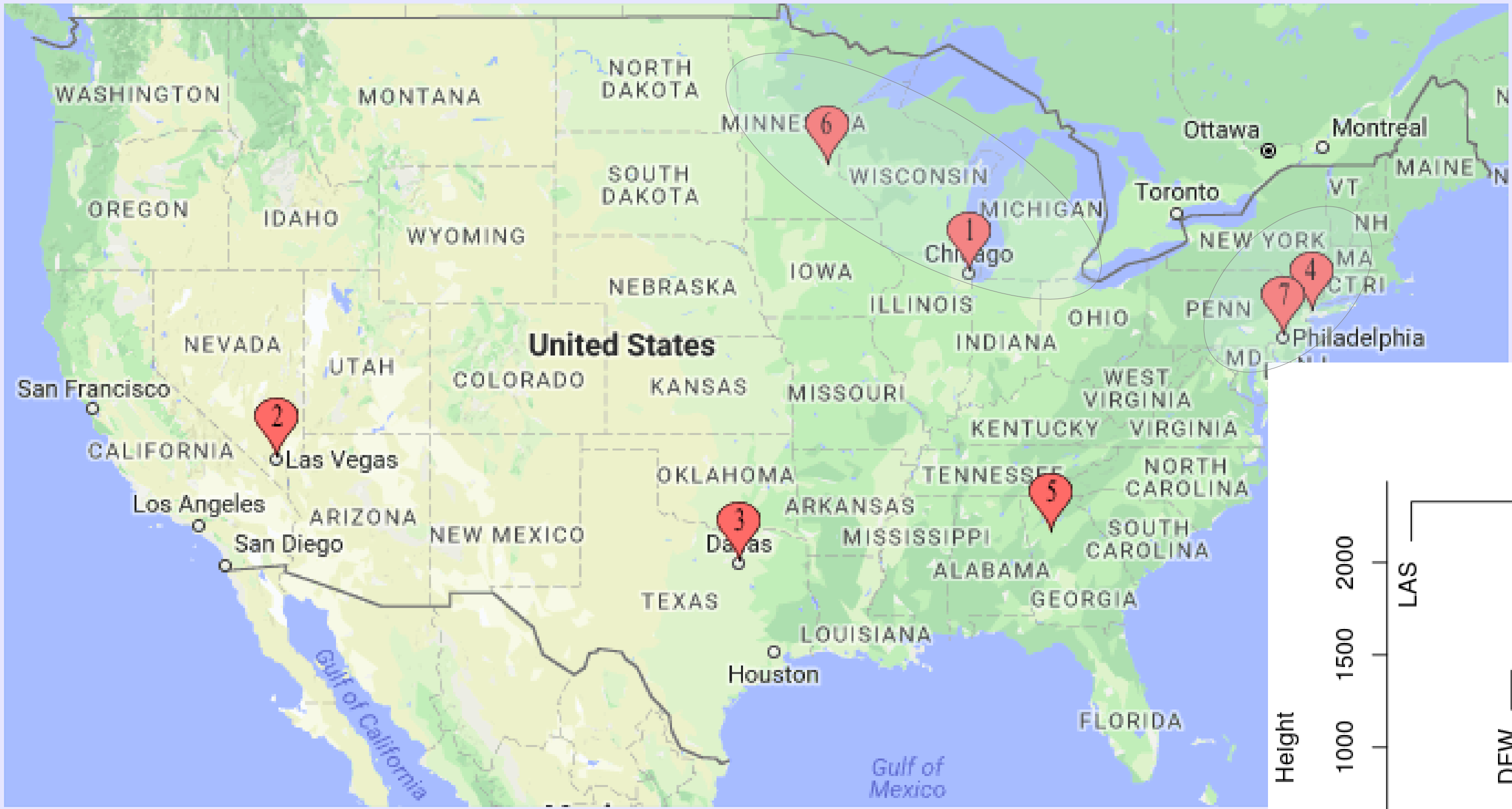
1: Compute the proximity matrix, if necessary.
2: **repeat**
3: Merge the closest two clusters.
4: Update the proximity matrix to reflect the proximity between the new cluster and the original clusters.
5: **until** Only one cluster remains.

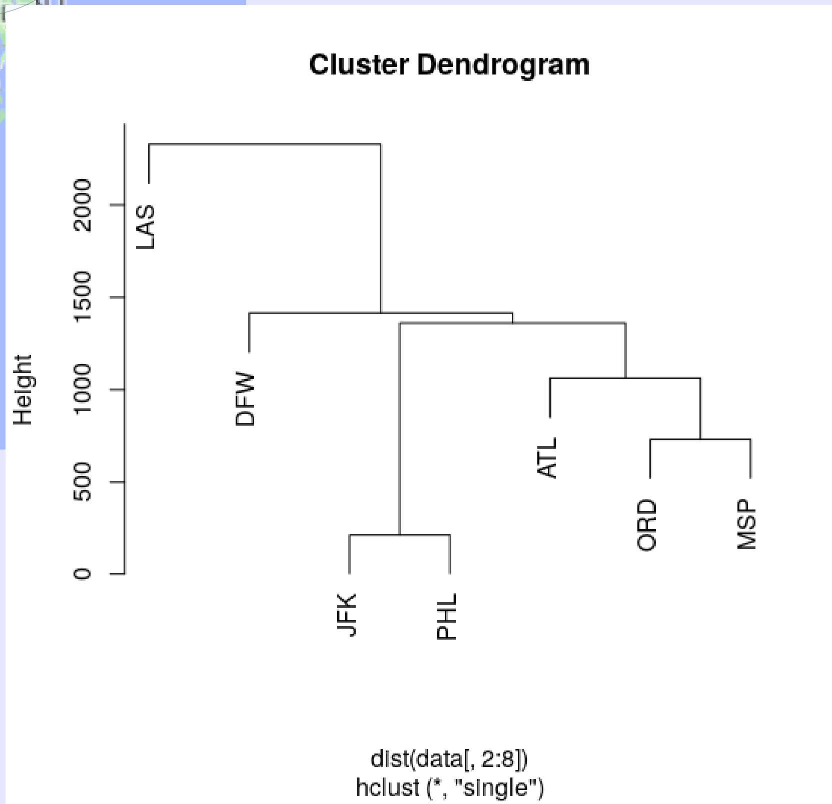
How should this *merge* be done? In other words, how do we define proximity between clusters so that the two closest ones are merged?



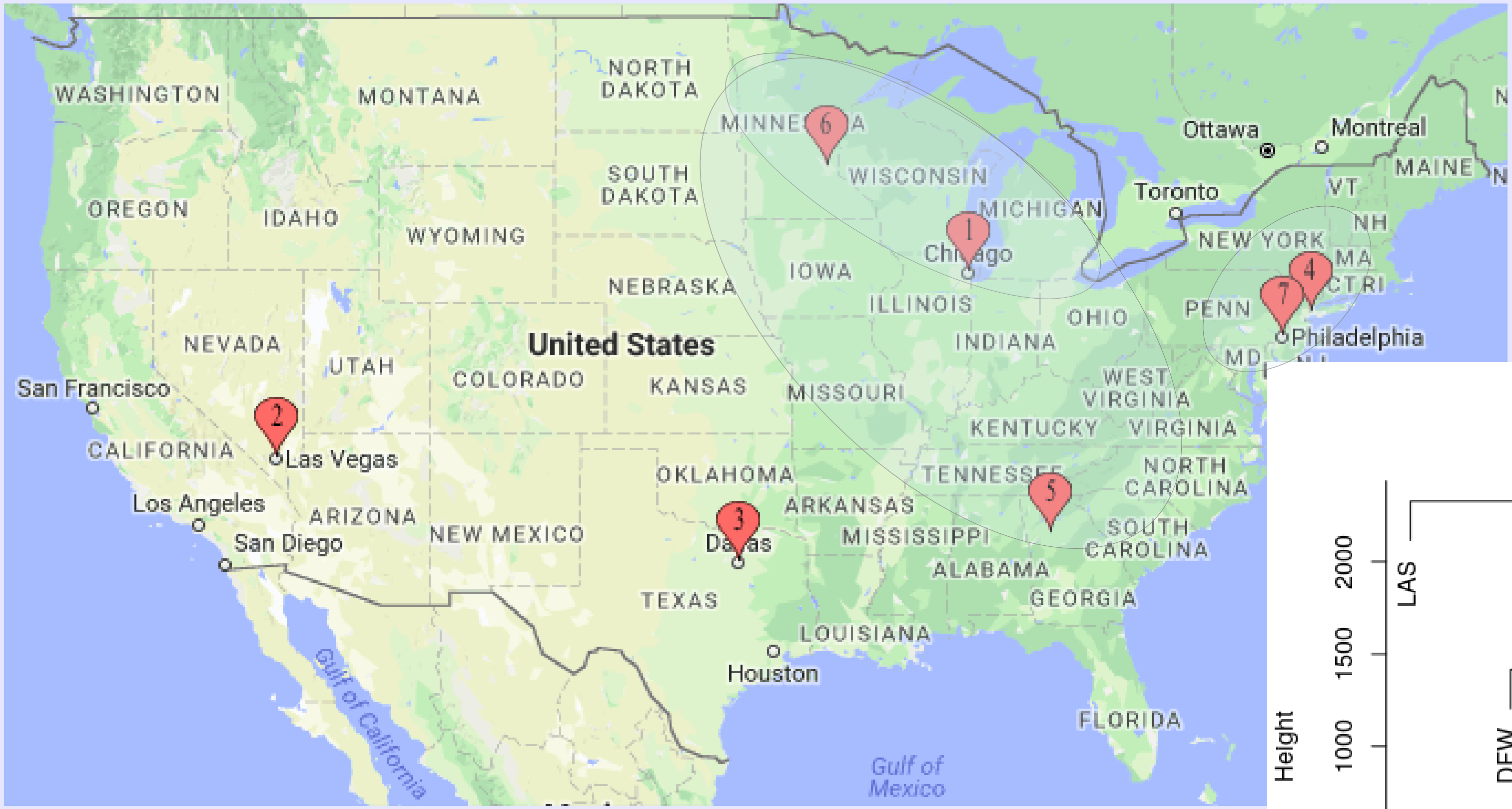
(a) MIN (single link.) (b) MAX (complete link.) (c) Group average.

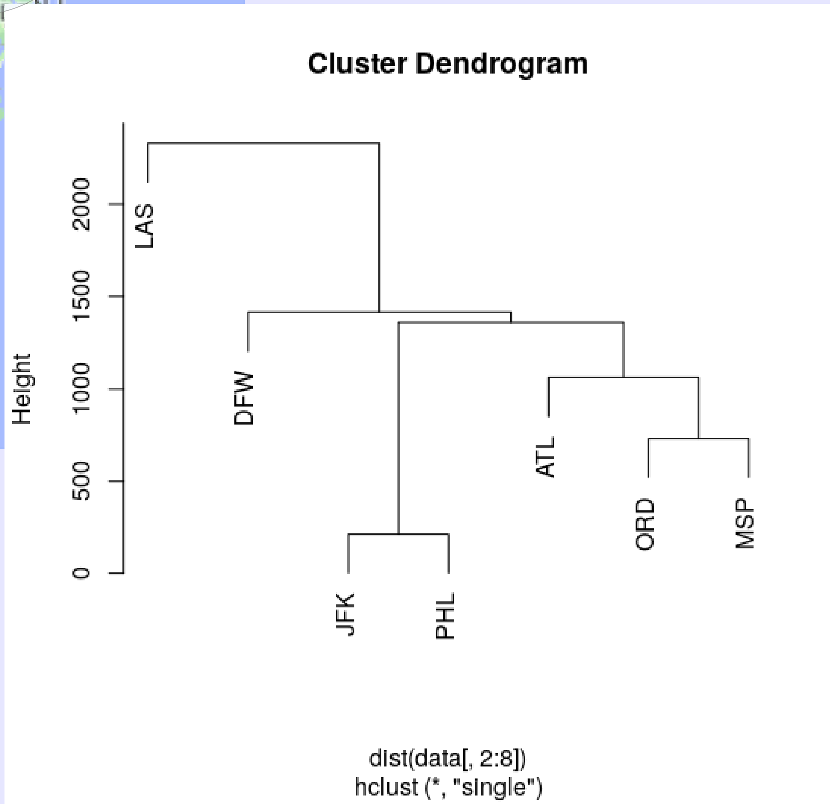
Hierarchical clustering



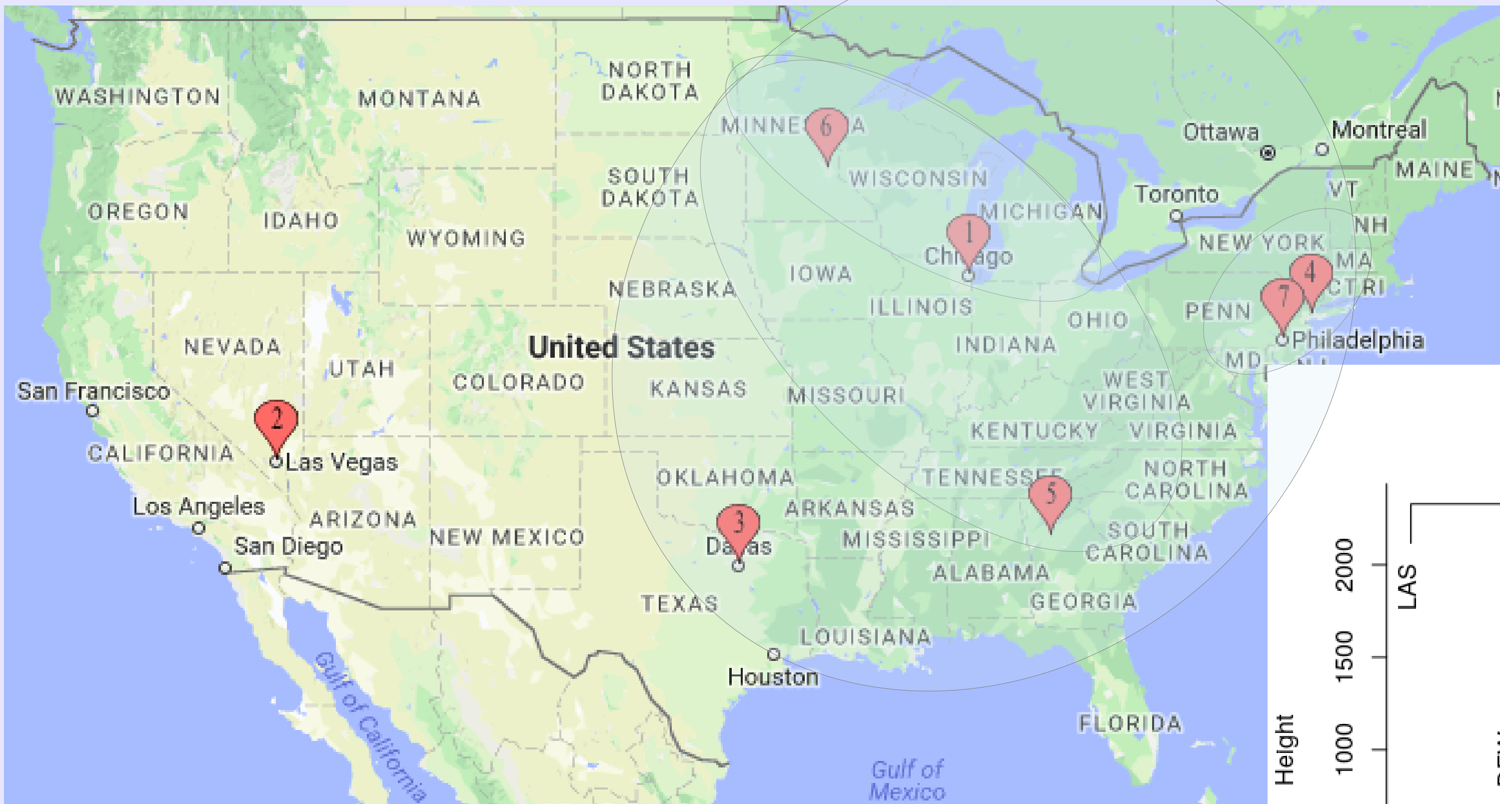


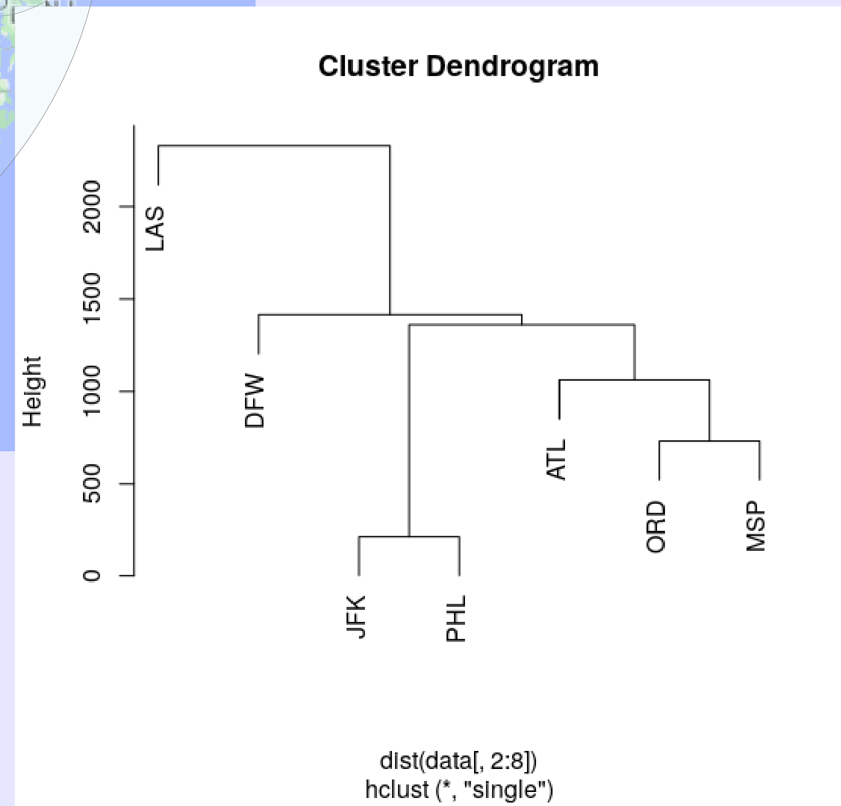
Hierarchical clustering



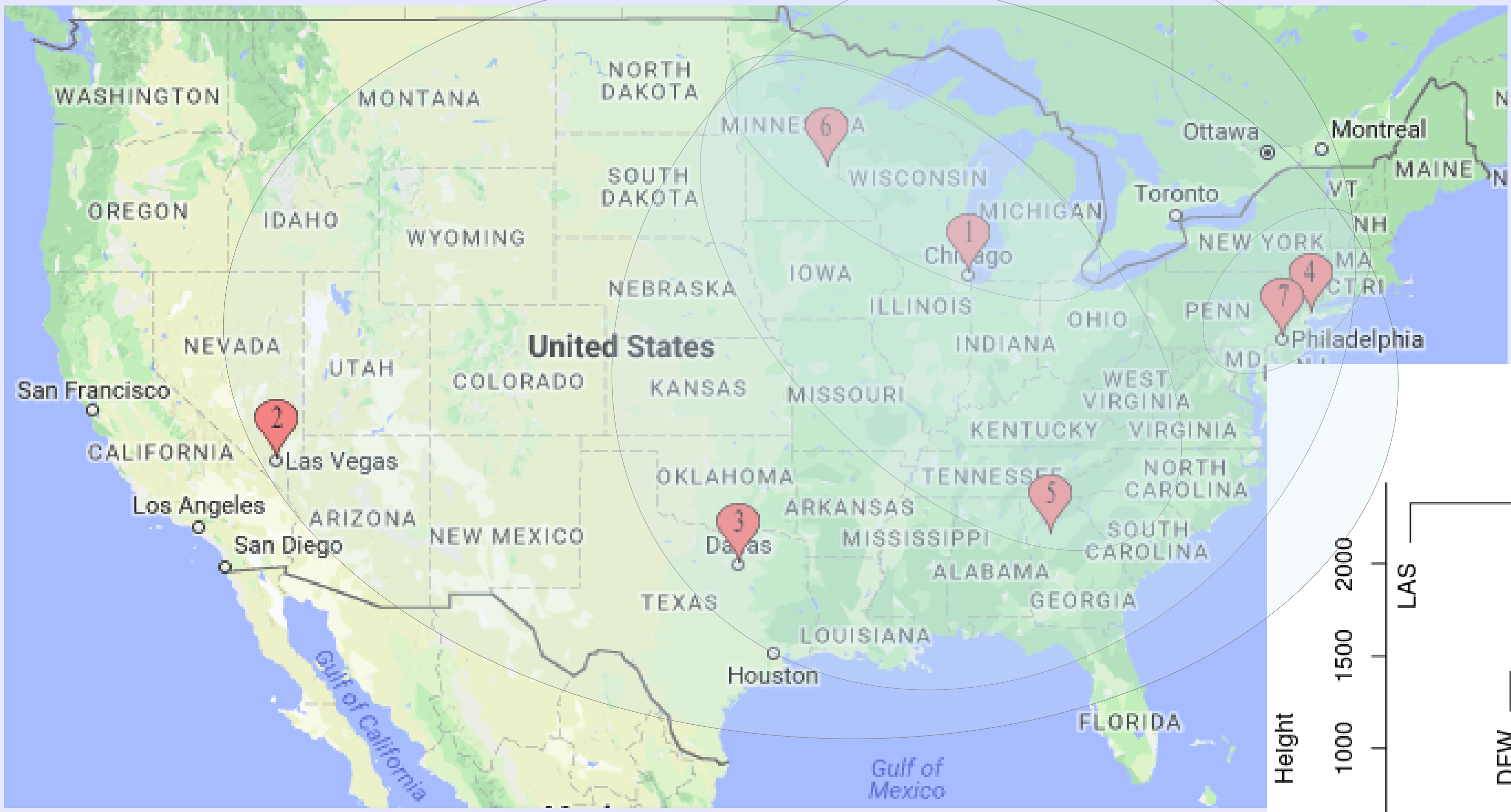


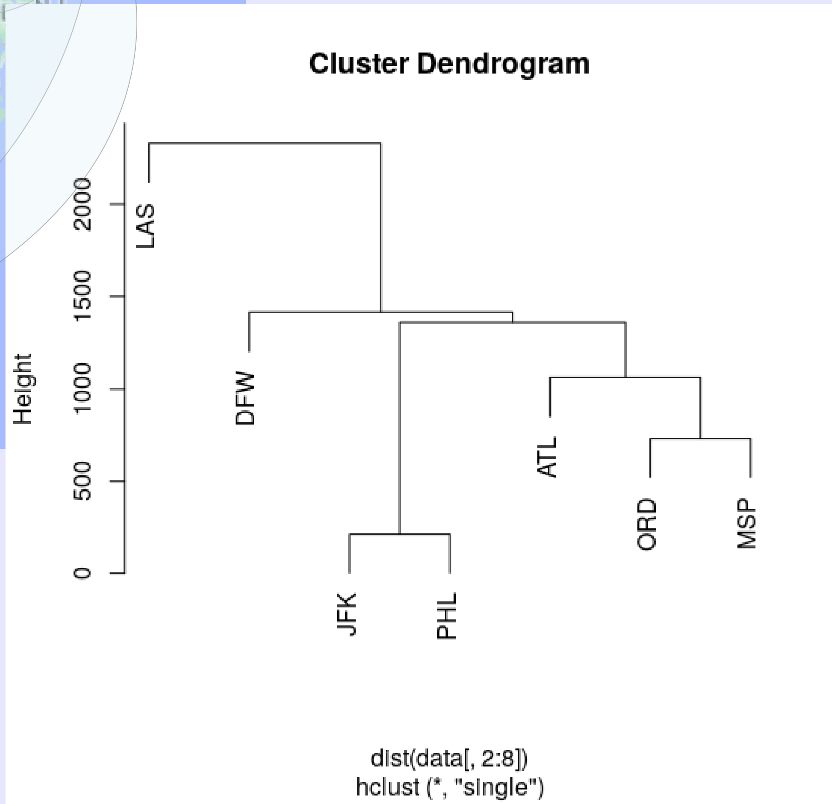
Hierarchical clustering





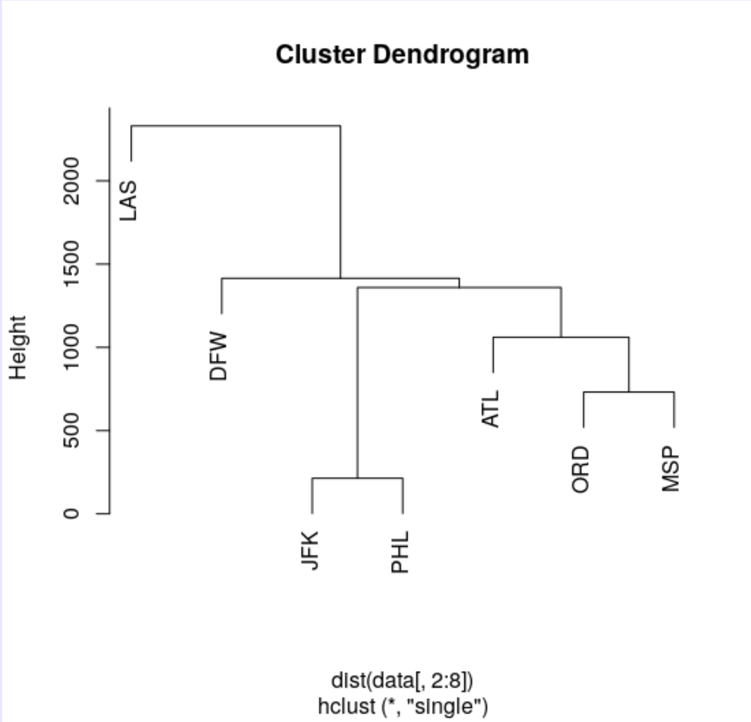
Hierarchical clustering





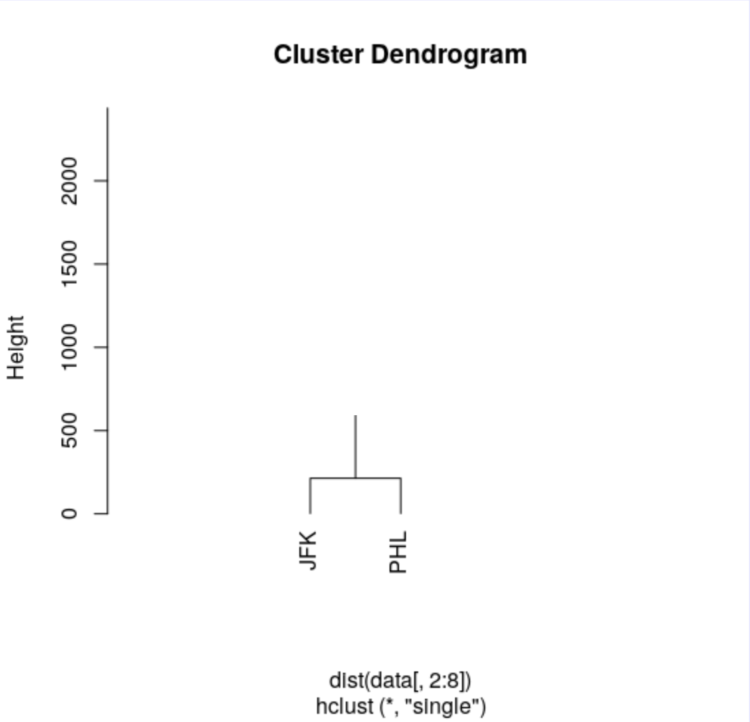
Code: hclust.r

Hierarchical clustering: Updating the proximity matrix



	1	2	3	4	5	6	7
1	0						
2	3367	0					
3	1610	2330	0				
4	1678	4016	2601	0			
5	1061	3408	1543	1482	0		
6	731	2897	1414	2063	1450	0	
7	1560	4008	2518	214	1359	1980	0

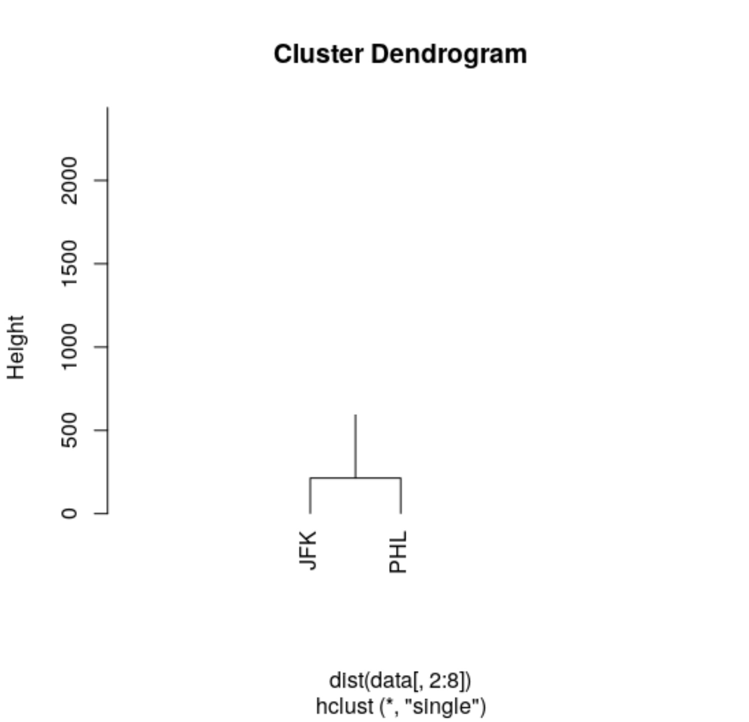
Hierarchical clustering: Updating the proximity matrix



	1	2	3	4	5	6	7
1	0						
2	3367	0					
3	1610	2330	0				
4	1678	4016	2601	0			
5	1061	3408	1543	1482	0		
6	731	2897	1414	2063	1450	0	
7	1560	4008	2518	214	1359	1980	0

Merge closest two clusters.
Merging strategy: MIN (single link)

Hierarchical clustering: Updating the proximity matrix

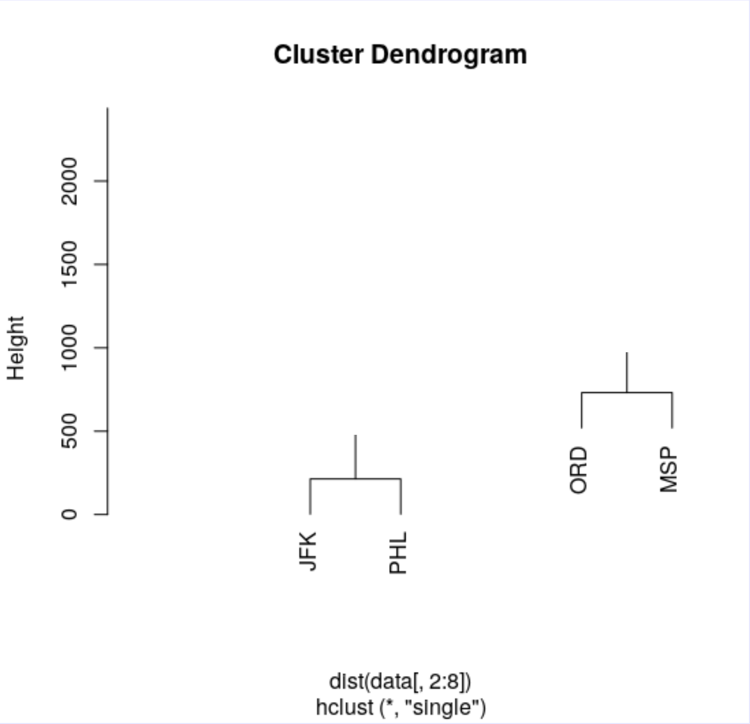


	1	2	3	4,7	5	6
1	0					
2	3367	0				
3	1610	2330	0			
4,7	1560	4008	2518	0		
5	1061	3408	1543	1359	0	
6	731	2897	1414	1980	1450	0

D({4,7}→{1}) = min(D({4}→{1}), D({7}→{1}))
= min(1678, 1560) = 1560
…
D({4,7}→{5}) = min(D({4}→{5}), D({7}→{5}))
= min(1482, 1359) = 1359

D({4,7}→{6}) = min(D({4}→{6}), D({7}→{6}))
= min(2063, 1980) = 1980

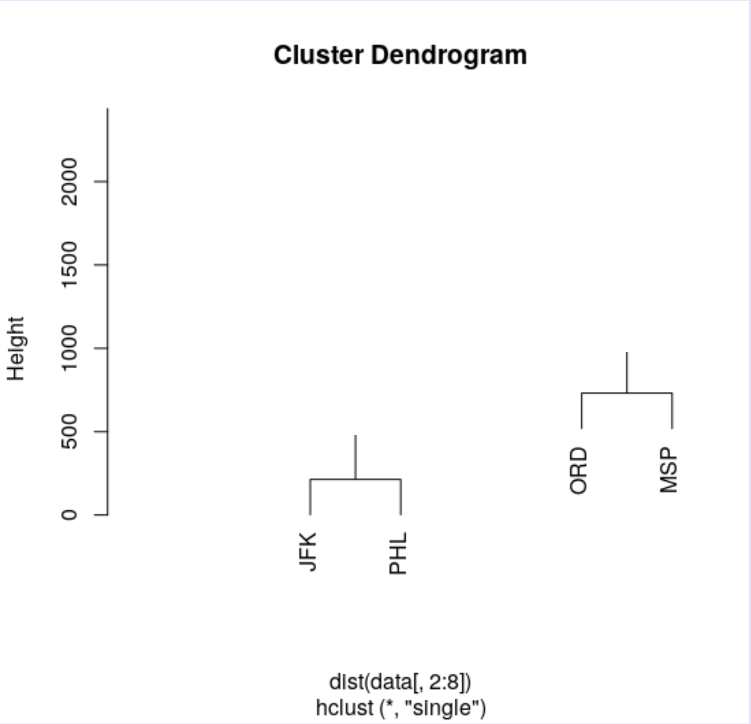
Hierarchical clustering: Updating the proximity matrix



Merge closest two clusters.

	1	2	3	4,7	5	6
1	0					
2	3367	0				
3	1610	2330	0			
4,7	1560	4008	2518	0		
5	1061	3408	1543	1359	0	
6	731	2897	1414	1980	1450	0

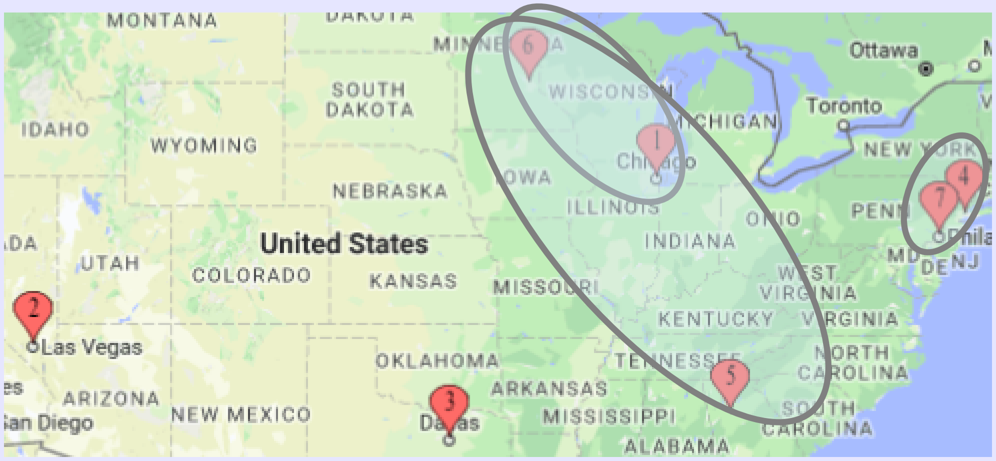
Hierarchical clustering: Updating the proximity matrix

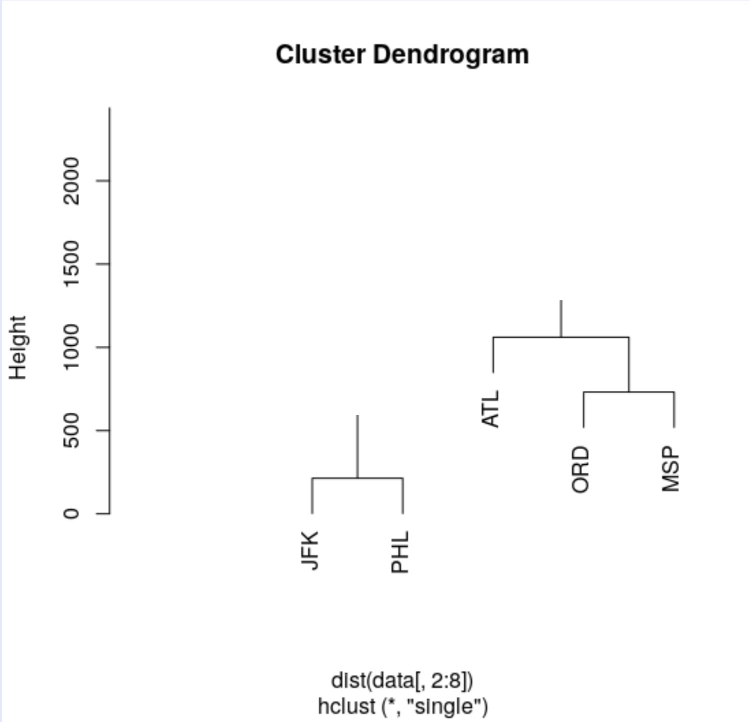


	1,6	2	3	4,7	5
1,6	0				
2	2897	0			
3	1414	2330	0		
4,7	1560	4008	2518	0	
5	1061	3408	1543	1359	0

D({1,6}→{2}) = min(D({1}→{2}), D({6}→{2}))
= min(3367, 2897) = 2897
…
D({1,6}→{5}) = min(D({1}→{5}), D({6}→{5}))
= min(1061, 1450) = 1061
…
D({1,6}→{4,7}) = min(D({1}→{4}), D({1}→{7}),
D({6}→{4}, D({6}→{7}))
= min(1678, 1560, 2063, 1980) = 1560
...

Hierarchical clustering: Updating the proximity matrix

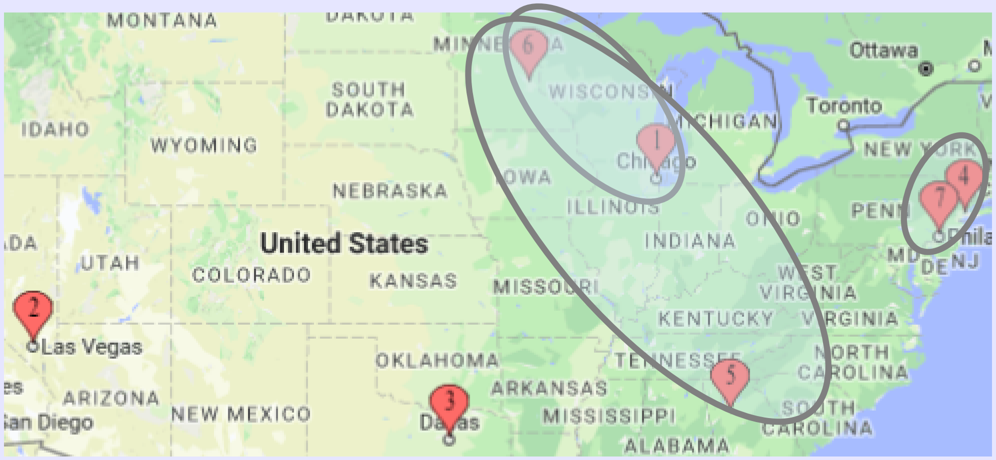


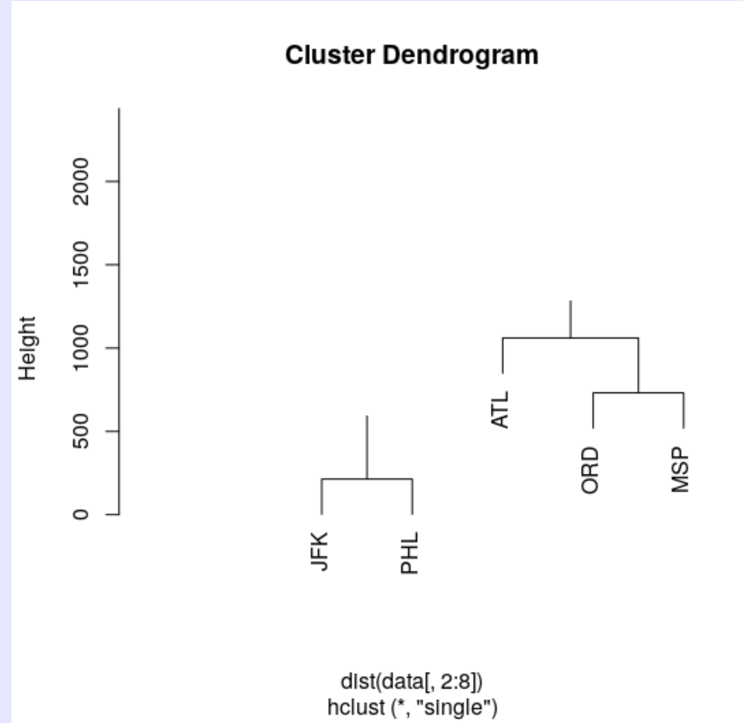


	1,6	2	3	4,7	5
1,6	0				
2	2897	0			
3	1414	2330	0		
4,7	1560	4008	2518	0	
5	1061	3408	1543	1359	0

Merge closest two clusters.

Hierarchical clustering: Updating the proximity matrix

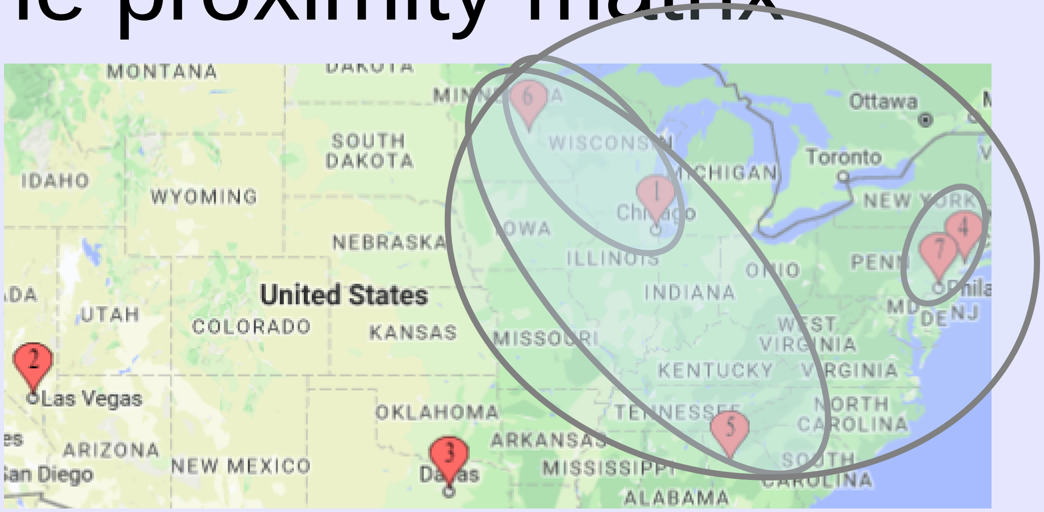


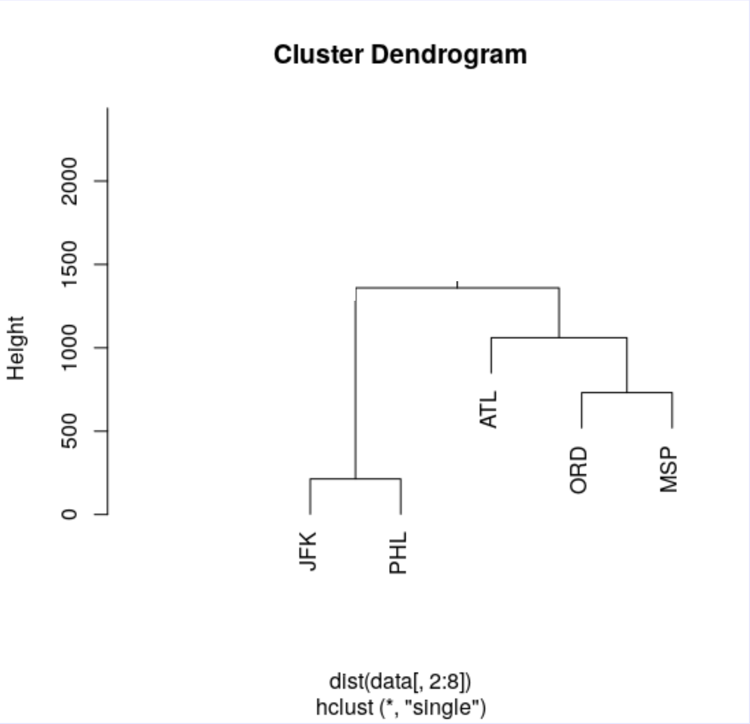


	1,6,5	2	3	4,7
1,6,5	0			
2	2897	0		
3	1414	2330	0	
4,7	1359	4008	2518	0

D({1,6,5}→{2}) = min(D({1}→{2}), D({6}→{2}), D({5}→{2}))
= min(3367, 2897, 3408) = 2897
…
D({1,6,5}→{4,7}) = min(D({1}→{4}), D({6}→{4}), D({5}→{4}),
D({1}→{7}), D({6}→{7}), D({5}→{7}))
= min(1678, 2063, 1482, 1560, 1980, 1359) = 1359
…

Hierarchical clustering: Updating the proximity matrix

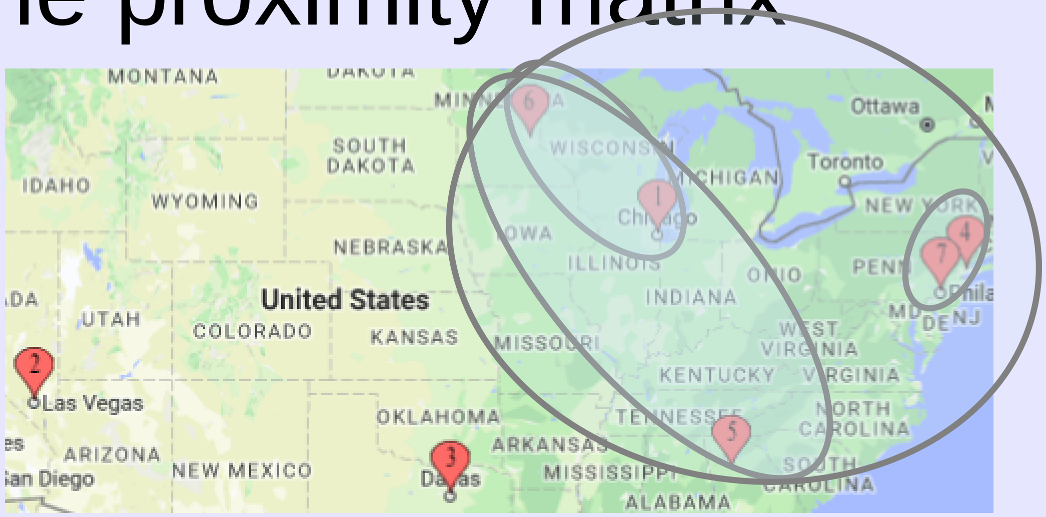


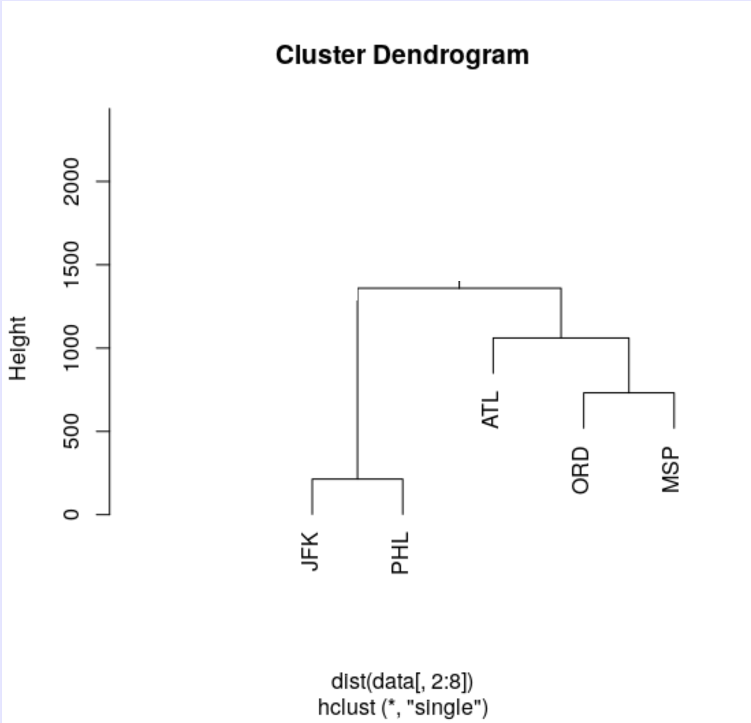


	1,6,5	2	3	4,7
1,6,5	0			
2	2897	0		
3	1414	2330	0	
4,7	1359	4008	2518	0

Merge closest two clusters.

Hierarchical clustering: Updating the proximity matrix



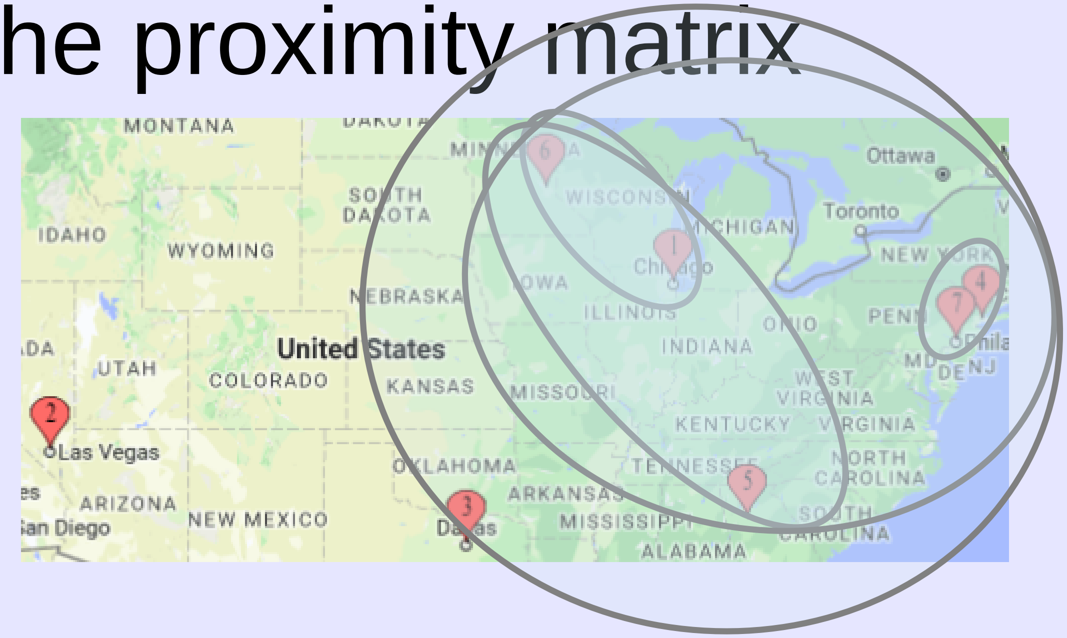


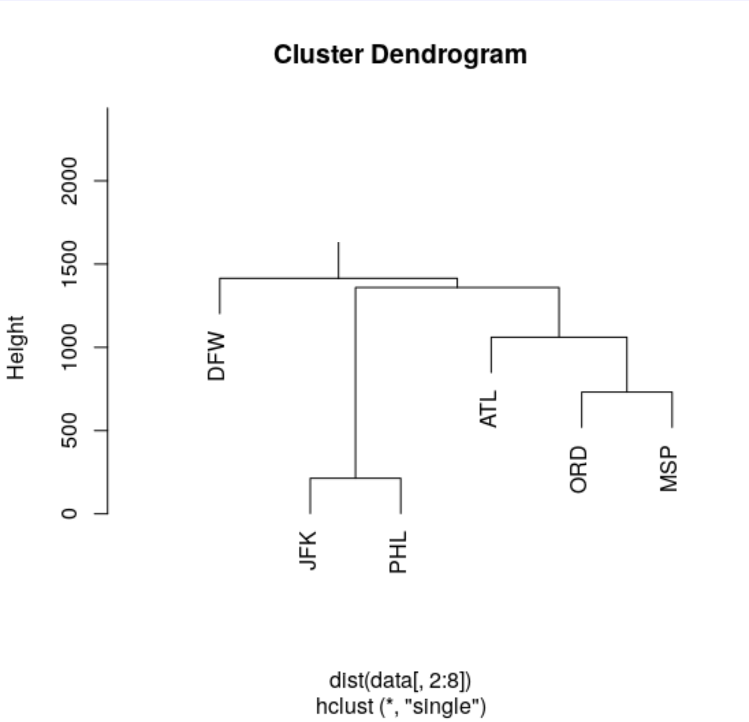
	1,6,5,4,7	2	3
1,6,5,4,7	0		
2	2897	0	
3	1414	2330	0

D({1,6,5,4,7}→{2}) = min(D({1}→{2}), D({6}→{2}), D({5}→{2}), D({4}→{2}), D({7}→{2}))
= min(3367, 2897, 3408, 4016, 4008) = 2897

D({1,6,5,4,7}→{3}) = min(D({1}→{3}), D({6}→{3}), D({5}→{3}), D({4}→{3}), D({7}→{3}))
= min(1610, 1414, 1543, 2601, 2518) = 1414

Hierarchical clustering: Updating the proximity matrix



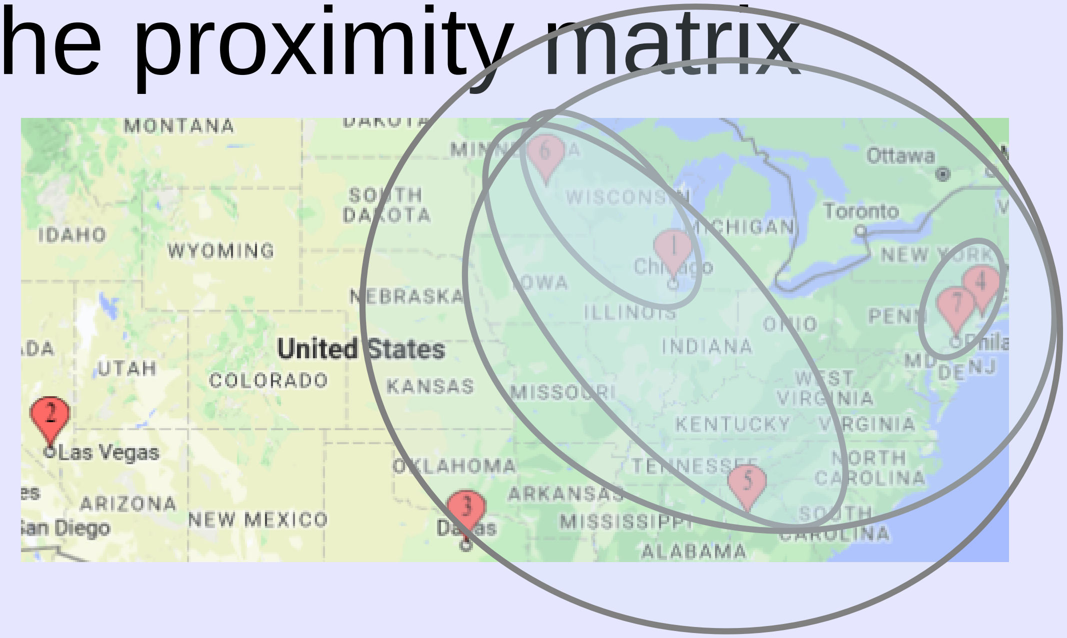


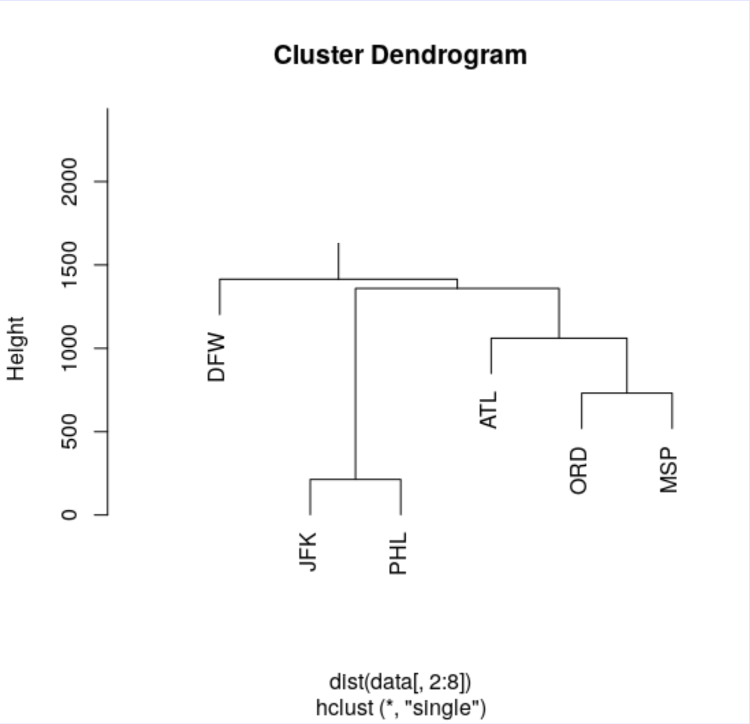
	1,6,5,4,7	2	3
1,6,5,4,7	0		
2	2897	0	
3	1414	2330	0

D({1,6,5,4,7}→{2}) = min(D({1}→{2}), D({6}→{2}), D({5}→{2}), D({4}→{2}), D({7}→{2}))
= min(3367, 2897, 3408, 4016, 4008) = 2897

D({1,6,5,4,7}→{3}) = min(D({1}→{3}), D({6}→{3}), D({5}→{3}), D({4}→{3}), D({7}→{3}))
= min(1610, 1414, 1543, 2601, 2518) = 1414

Hierarchical clustering: Updating the proximity matrix

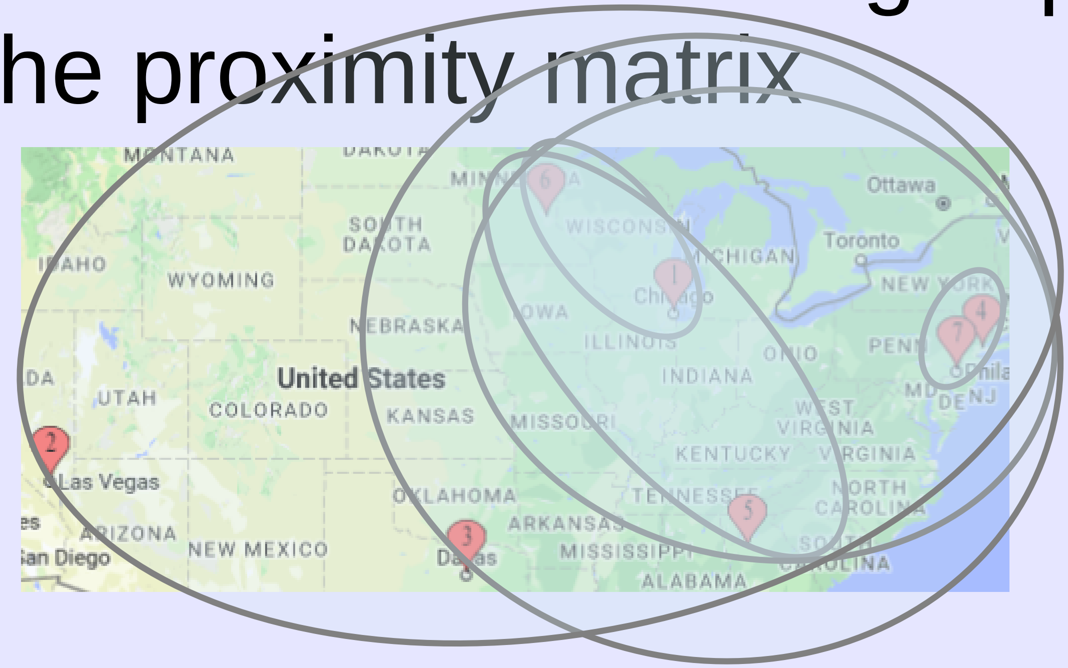


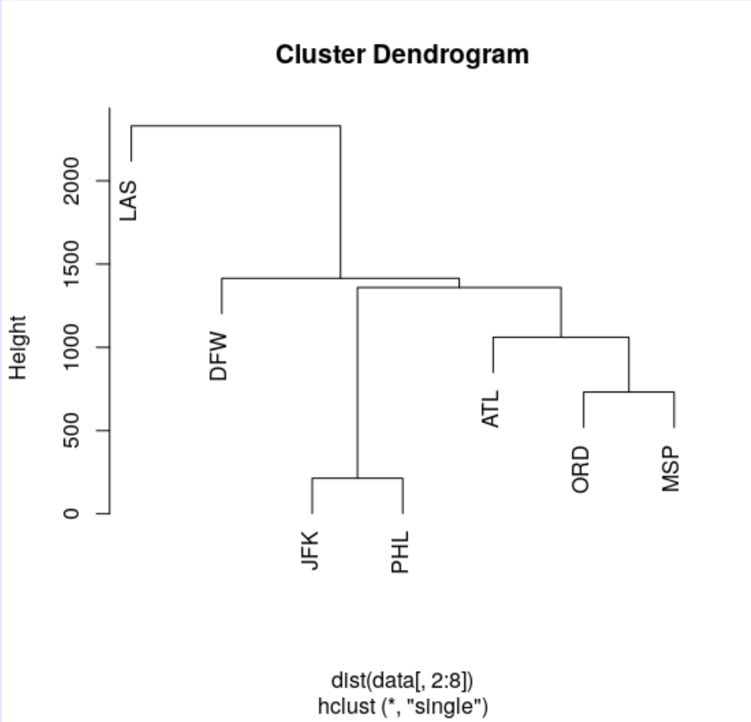


	1,6,5,4,7,3	2
1,6,5,4,7,3	0	
2	2897	0

Merge closest two clusters.

Hierarchical clustering: Updating the proximity matrix





	1,6,5,4,7,3,2
1,6,5,4,7,3,2	0

Merge closest two clusters...until only one cluster remains.

Hierarchical clustering: Updating the proximity matrix

- For complete linkage and group average, proceed as before except update the proximity matrix using **MAX** and **AVG**, respectively.

Hierarchical clustering: Complexity

- Space complexity:
  - *m* is number of data points; storage required: $1/2m^2$ => $O(m^2)$.
- Time complexity:
  - *m* is the number of data points; $O(m^2)$ required for computing the proximity matrix.
  - If distances from each cluster to all other clusters are stored in a heap, overall time required for hierarchical clustering is $O(m^2 \log m)$.

Hierarchical clustering: Practical issues

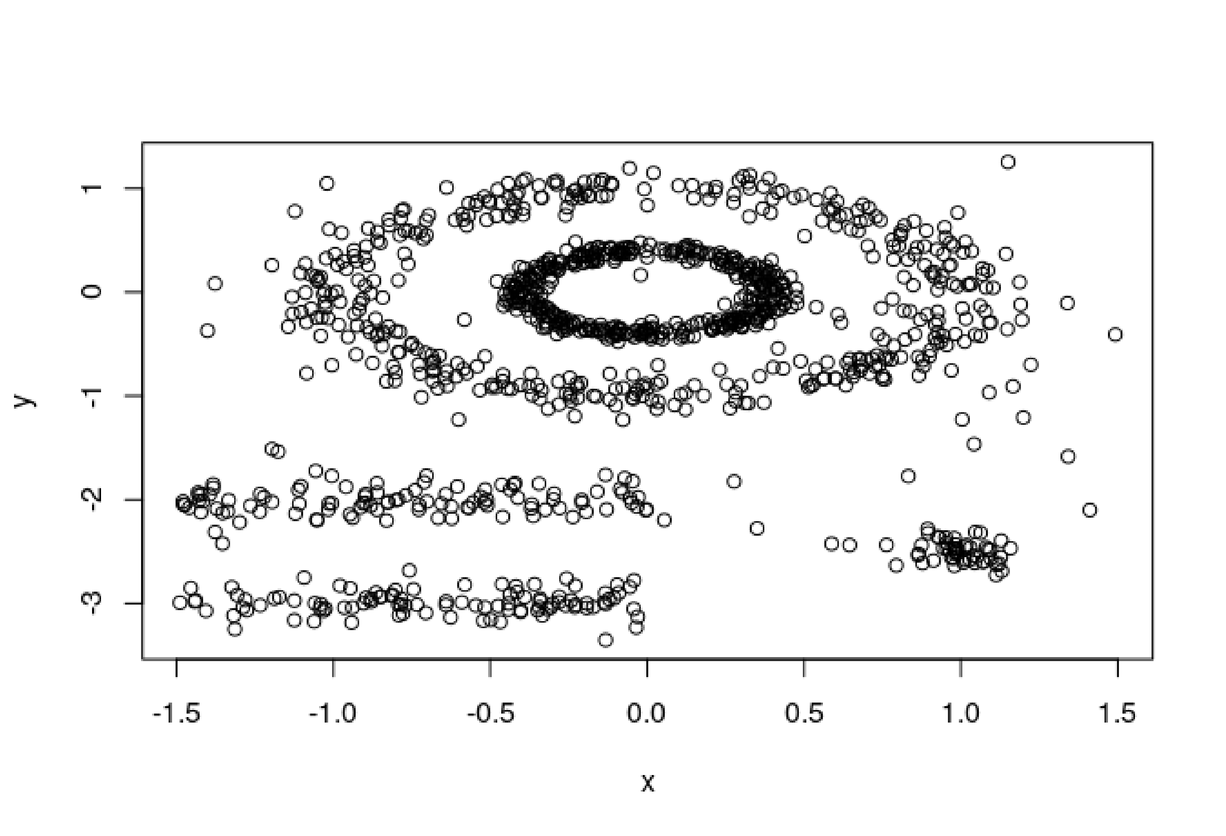
- Scaling matters if attributes are wide ranges.
- What dissimilarity measure should be used?
  - Minkowski with different values for R (Euclidean, ...)
  - Correlation-based
- What type of linkage to use?
- How many clusters to choose? Difficult problem as there is no agreed upon method. Sometimes the domain expert helps, other times study the data.
- Merging decisions are final (unlike k-means where observations may belong to different centroids over time).

Hierarchical clustering: Using as a supervised learning method

- Even though clustering in general is considered an unsupervised learning method, it can be used in supervised learning mode.
- Cluster indicate a class label and each object in a certain cluster belongs to that class.
- Error measures for supervised clustering are the same as classification.
- Code: hclust-iris.r

Density-based clustering: dbscan

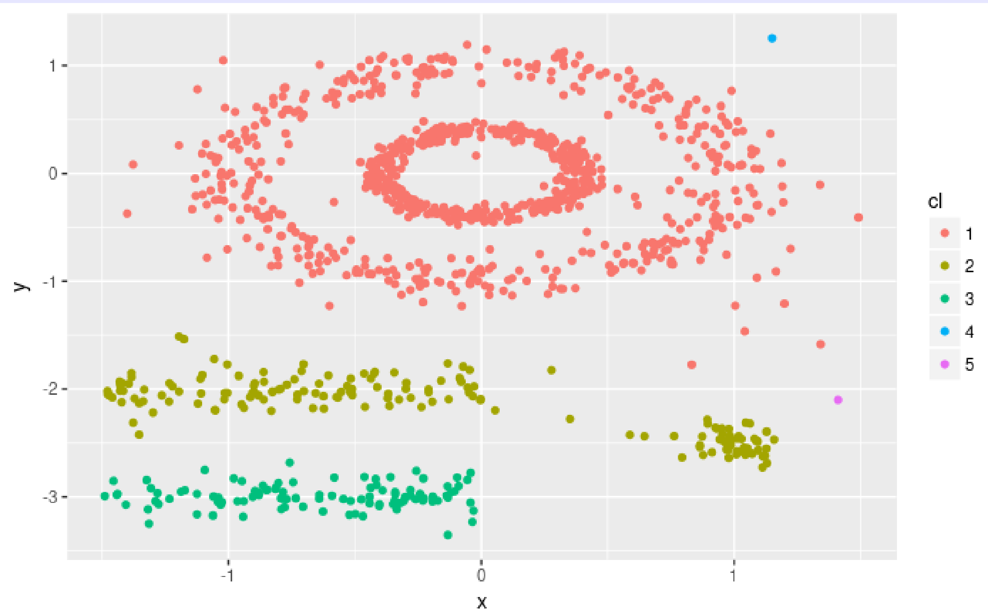
- K-means and hierarchical clustering do not gracefully handle non-globular clusters as shown on the left.

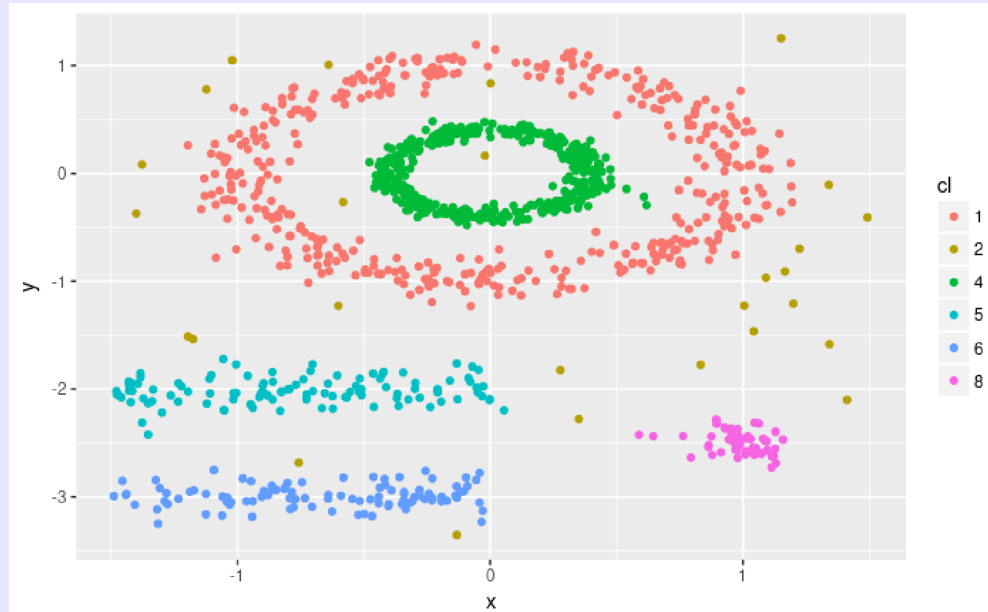


  - They will **find** clusters, but the resulting clusters may not be what we need.

Density-based clustering: Miscellaneous

- Hierarchical clustering do on globular data:





- Observations:
  - Hierarchical clustering is not able to eliminate what would be called "noise" points in DBSCAN. So these become part of a cluster.
  - With 5 clusters hierarchical clustering is unable to discern the two nested clusters. It considers them as one.

Code:
hierarchical-clustering-globular-data.Rmd