Lecture 2: Classification, Clustering

STATS 202: Data mining and analysis

Rajan Patel

Classification problem

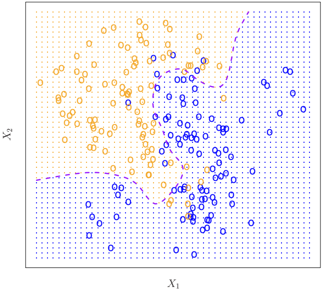

Figure: *

Figure 2.13

Recall:

- $X = (X_1, X_2)$ are inputs.
- Color $Y \in \{$Yellow , Blue$\}$ is the output.
- (X, Y) have a joint distribution.
- Purple line is *Bayes boundary* — the best we could do if we knew the joint distribution of (X, Y)

K-nearest neighbors

To assign a color to the input $\times$, we look at its $K = 3$ nearest neighbors. We predict the color of the majority of the neighbors.

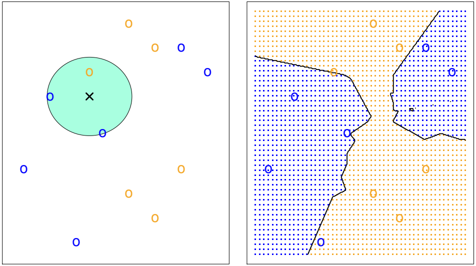

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Figure 2.14

K-nearest neighbors also has a decision boundary

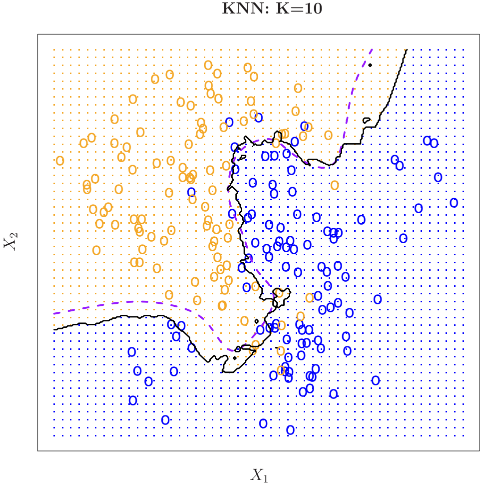

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Figure 2.15

The higher K, the smoother the decision boundary

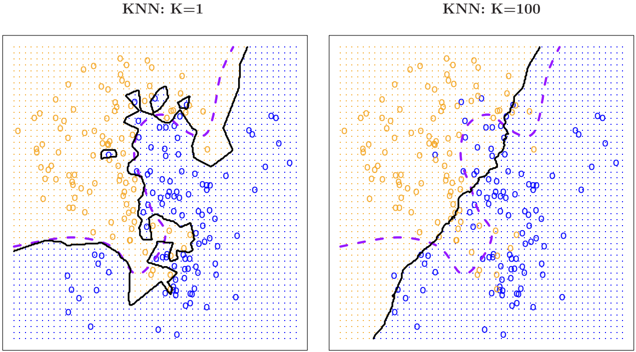

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Figure 2.16

Clustering

As in **classification**, we assign a class to each sample in the data matrix. However, the class *is not an output variable*; we only use input variables.

Clustering is an **unsupervised** procedure, whose goal is to find homogeneous subgroups among the observations.

We will discuss 2 algorithms:

- K-means clustering
- Hierarchical clustering

K-means clustering

- K is the number of clusters and must be fixed in advance.
- The goal of this method is to maximize the similarity of samples within each cluster:

$$\min_{C_1,\dots,C_K} \sum_{\ell=1}^{K} W(C_\ell) \quad ; \quad W(C_\ell) = \frac{1}{|C_\ell|} \sum_{i,j \in C_\ell} \text{Distance}^2(x_{i,:}, x_{j,:}).$$

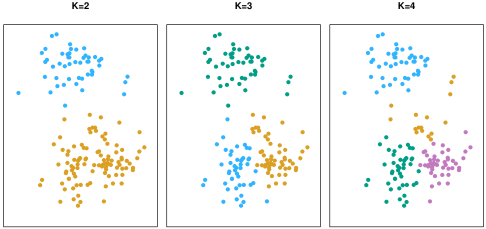

Figure: *

Figure 10.5

K-means clustering algorithm

1. Assign each sample to a cluster from 1 to K arbitrarily, e.g. at random.
2. Iterate these two steps until the clustering is constant:
   - Find the *centroid* of each cluster ℓ; i.e. the average $\overline{x}_{\ell,:}$ of all the samples in the cluster:
     $$x_{\ell,j} = \frac{1}{|C_\ell|} \sum_{i \in C_\ell} x_{i,j} \quad \text{for } j = 1, \ldots, p.$$
   - Reassign each sample to the nearest centroid.

K-means clustering algorithm

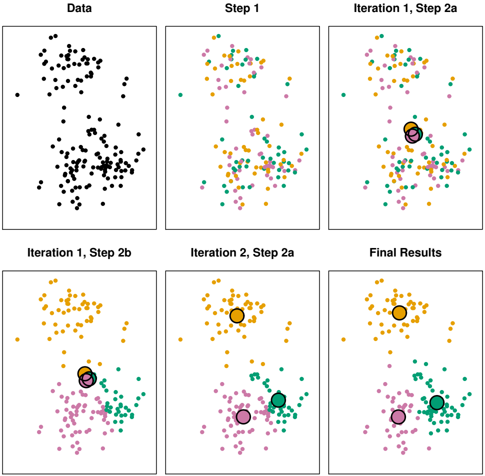

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Figure 10.6

Properties of K-means clustering

- The algorithm always converges to a local minimum of

$$\min_{C_1,\ldots,C_K} \sum_{\ell=1}^{K} W(C_\ell) \quad ; \quad W(C_\ell) = \frac{1}{|C_\ell|} \sum_{i,j \in C_\ell} \mathsf{Distance}^2(x_{i,:}, x_{j,:}).$$

- Each initialization could yield a different minimum.

Example: K-means output with different initializations

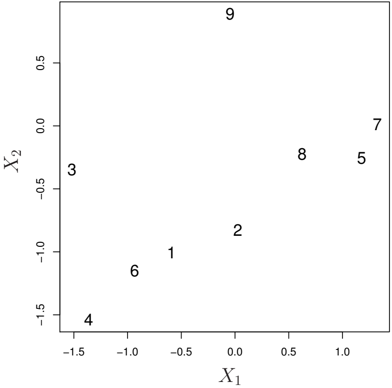
Figure: *

Figure 10.7

In practice, we start from many random initializations and choose the output which minimizes the objective function.

Hierarchical clustering

Most algorithms for hierarchical clustering are *agglomerative*.



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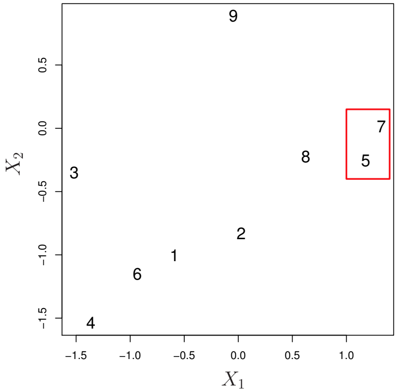

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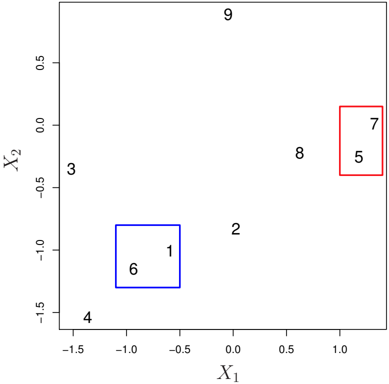

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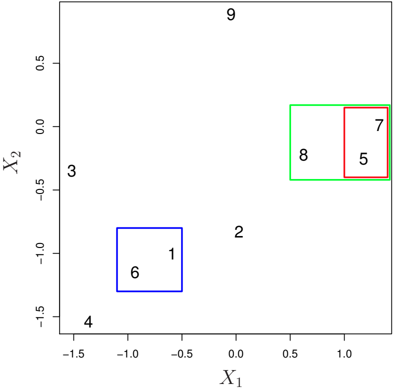

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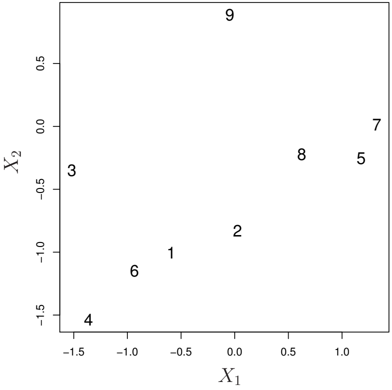

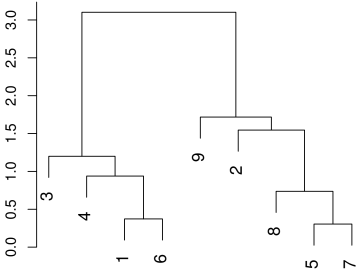

The output of the algorithm is a *dendogram*.

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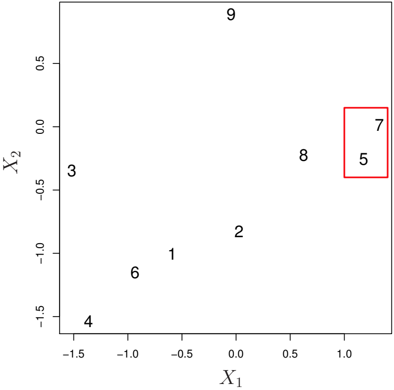

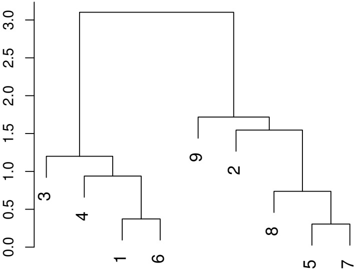

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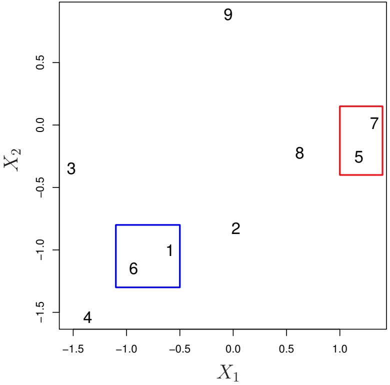

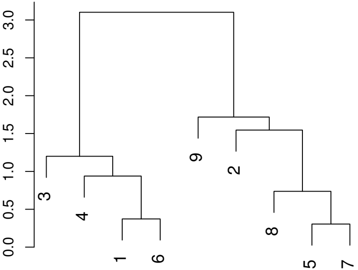

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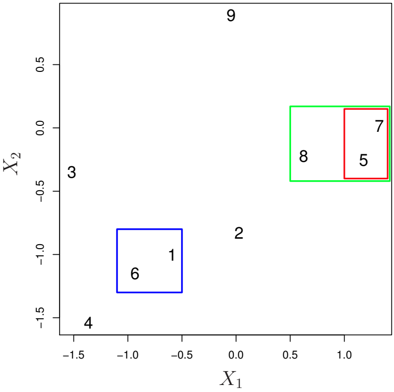

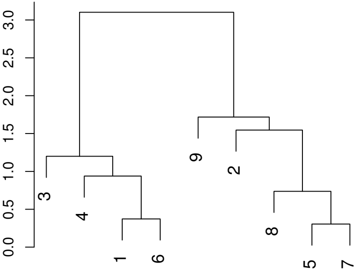

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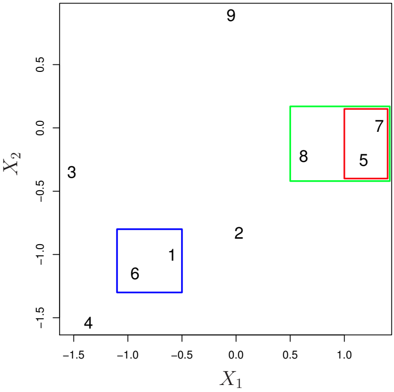

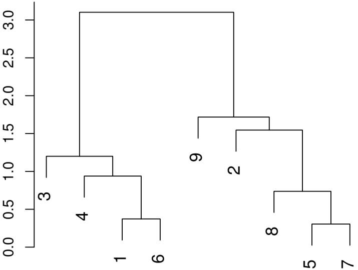

We must be careful about how we interpret the dendogram.

Hierarchical clustering

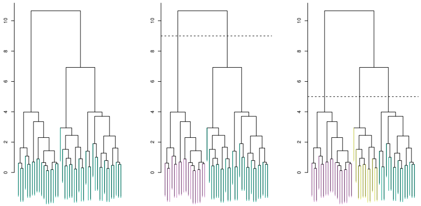

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Figure 10.9

- The number of clusters is not fixed.

Hierarchical clustering

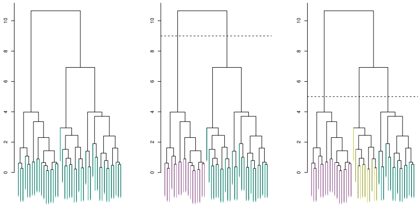

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Figure 10.9

- The number of clusters is not fixed.
- Hierarchical clustering is not always appropriate.

Hierarchical clustering

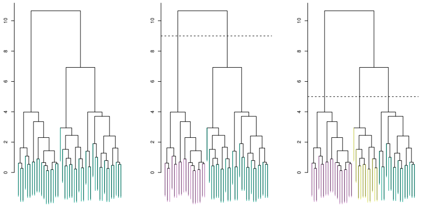

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Figure 10.9

- The number of clusters is not fixed.
- Hierarchical clustering is not always appropriate.

  e.g. Market segmentation for consumers of 3 different nationalities.
  - Natural 2 clusters: gender
  - Natural 3 clusters: nationality

  These clusterings are not nested or hierarchical.

Notion of distance between clusters

At each step, we link the 2 clusters that are “closest” to each other.

Hierarchical clustering algorithms are classified according to the notion of distance between clusters.

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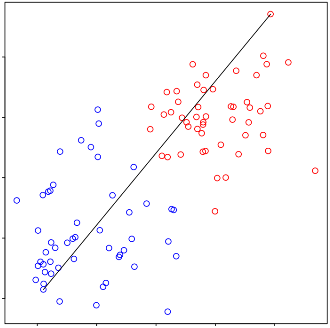

Complete linkage:
The distance between 2 clusters is the *maximum* distance between any pair of samples, one in each cluster.

Notion of distance between clusters

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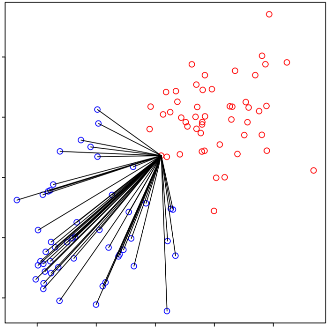

Average linkage:
The distance between 2 clusters is the average of all pairwise distances.

Notion of distance between clusters

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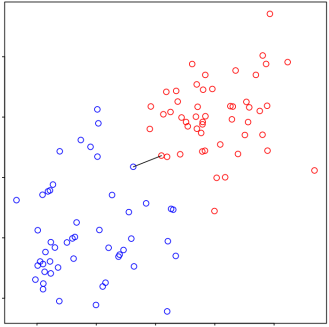

Single linkage:
The distance between 2 clusters is the *minimum* distance between any pair of samples, one in each cluster.

Suffers from the *chaining phenomenon*

Example

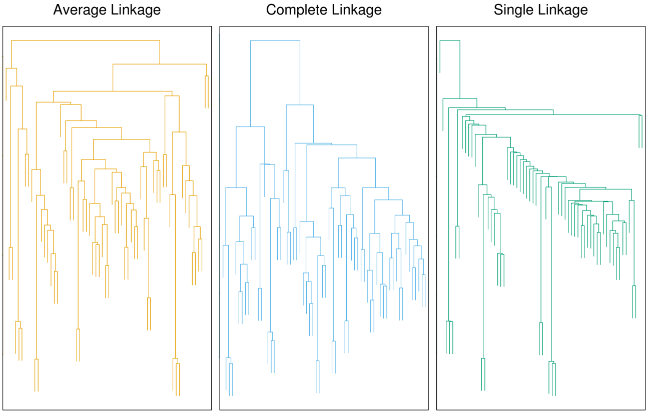

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Figure 10.12

Clustering is riddled with questions and choices

- Is clustering appropriate? i.e. Could a sample belong to more than one cluster?
  - Mixture models, soft clustering, topic models.
- How many clusters are appropriate?
  - Choose subjectively — depends on the inference sought.
  - There are formal methods based on gap statistics, mixture models, etc.
- Are the clusters robust?
  - Run the clustering on different random subsets of the data. Is the structure preserved?
  - Try different clustering algorithms. Are the conclusions consistent?
  - Most important: temper your conclusions.

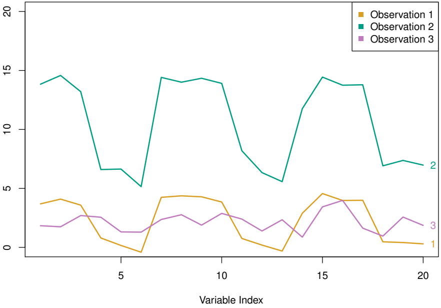
Clustering is riddled with questions and choices

- Should we scale the variables before doing the clustering.
  - Variables with larger variance have a larger effect on the Euclidean distance between two samples.
- Does Euclidean distance capture dissimilarity between samples?

Correlation distance

Example: Suppose that we want to cluster customers at a store for market segmentation.

- Samples are customers
- Each variable corresponds to a specific product and measures the number of items bought by the customer during a year.



Correlation distance

- Euclidean distance would cluster all customers who purchase few things (orange and purple).
- Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.