Hierarchical Clustering

Hierarchical Clustering

- It is time to explore another clustering method!
- Hierarchical clustering is very common in biology and lends itself nicely to visualizing clusters.
- It can also help the user decide on an appropriate number of clusters.

Hierarchical Clustering

- Section Overview:
    - Theory and Intuition of Hierarchical Clustering
    - Coding Example of Hierarchical Clustering

Hierarchical Clustering

Theory and Intuition

Hierarchical Clustering

- Like most clustering algorithms, Hierarchical Clustering simply relies on measuring which data points are most "similar" to other data points.
- "Similarity" is defined by choosing a distance metric.

Hierarchical Clustering

- ***So why use Hierarchical Clustering?***
  - Easy to understand and visualize.
  - Helps users decide how many clusters to choose.
  - Not necessary to choose cluster amount **before** running the algorithm.

Hierarchical Clustering

- ***So why use Hierarchical Clustering?***
  - Divides points into ***potential*** clusters:
    - Agglomerative Approach:
      - Each point begins as its own cluster, then clusters are joined.
    - Divisive Approach:
      - All points begin in the same cluster, then clusters are split.

Hierarchical Clustering

- Hierarchical Clustering
  - Divides points into ***potential*** clusters:

N1 **N2** **N3** **N4** **N5** **N6**

Hierarchical Clustering

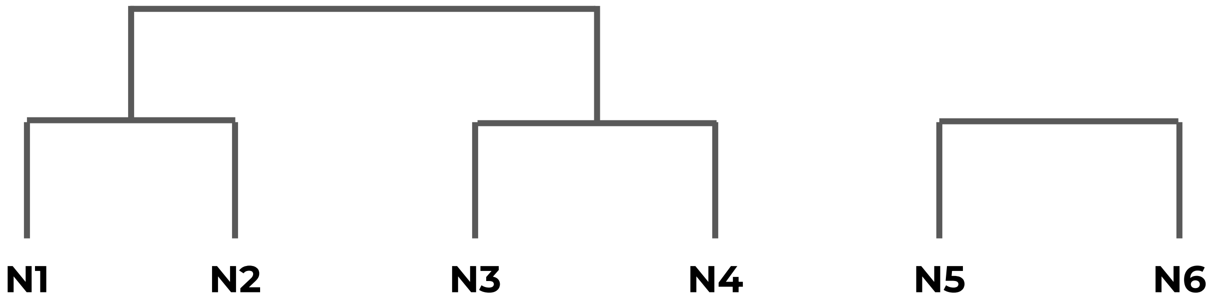
- Hierarchical Clustering
    - Agglomerative:

Hierarchical Clustering

- Hierarchical Clustering
    - Agglomerative:

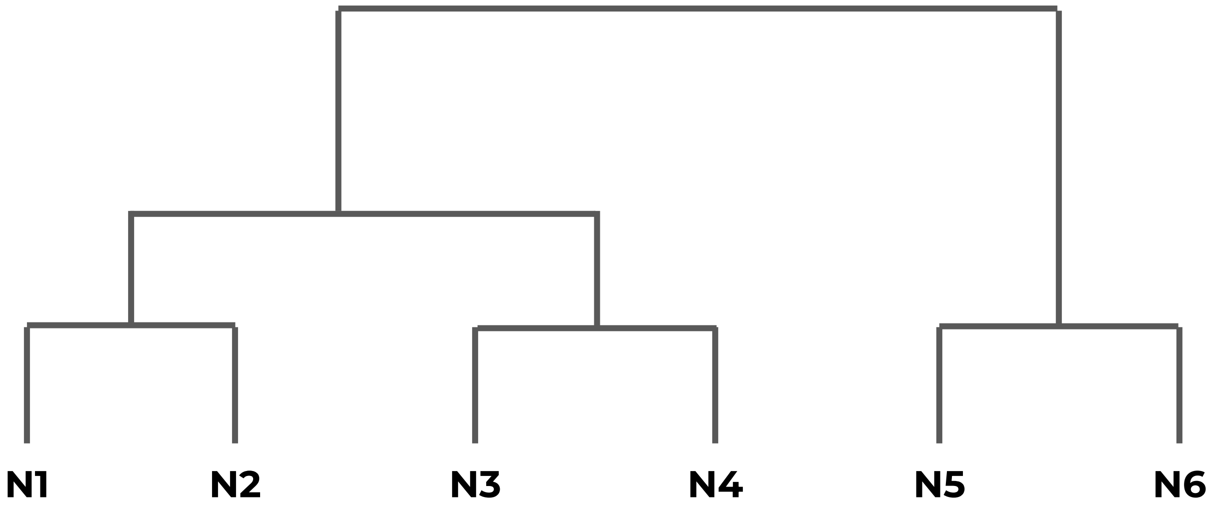
Hierarchical Clustering

- Hierarchical Clustering
  - Agglomerative:



Hierarchical Clustering

- Hierarchical Clustering
  - Agglomerative:



Hierarchical Clustering

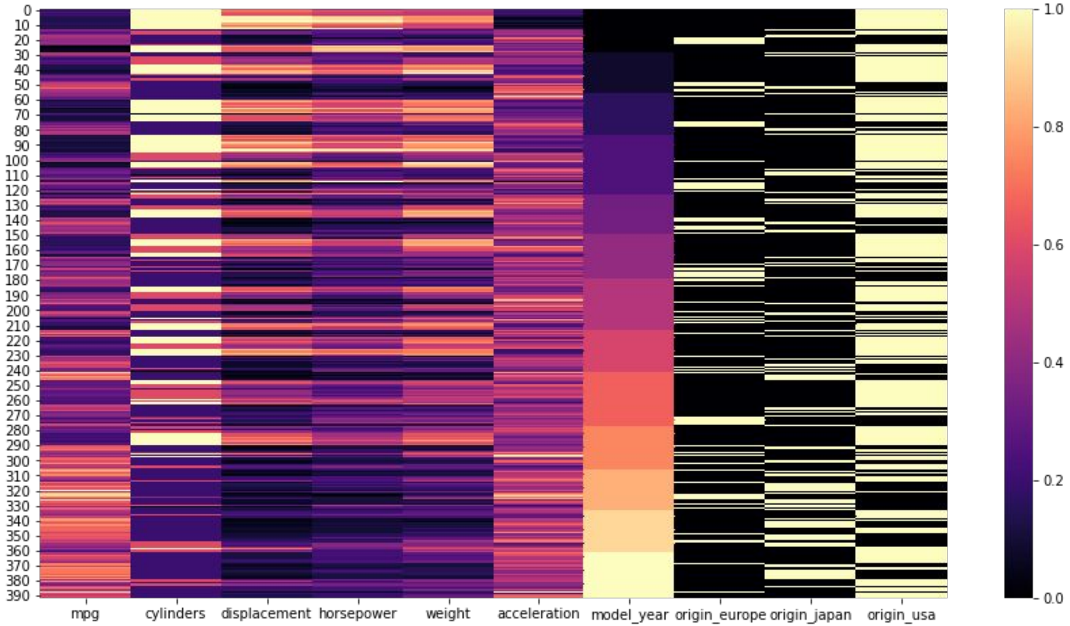
- Opposite of the Agglomerative approach is a **Divisive** approach, which starts with all points belonging to the same cluster, and the begins divisions to separate out clusters.

Hierarchical Clustering

- ***Hierarchical Clustering Process***
  - Compare data points to find most similar data points to each other.
  - Merge these to create a cluster.
  - Compare clusters to find most similar clusters and merge again.
  - Repeat until all points in a single cluster.

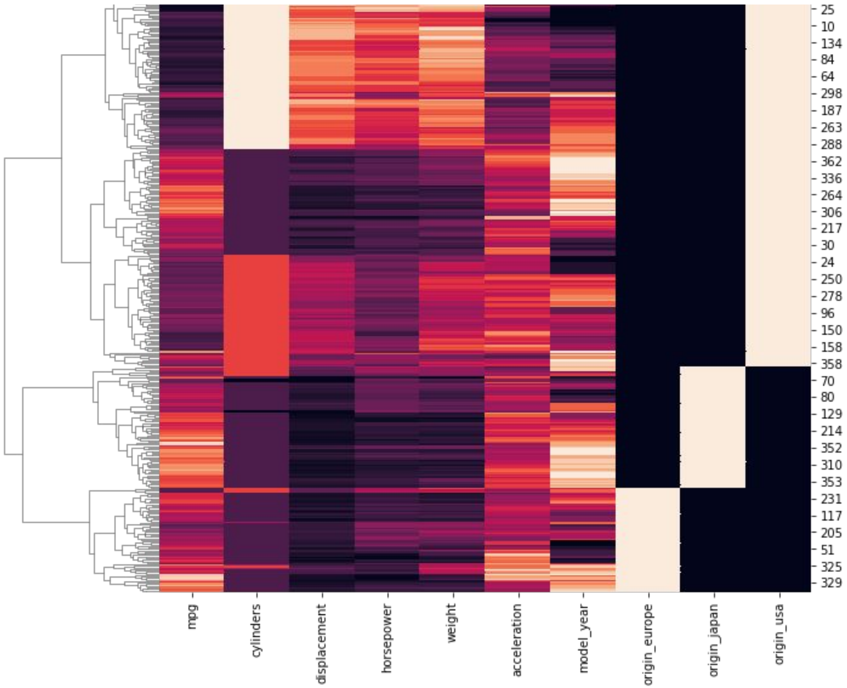
Hierarchical Clustering

- ***Hierarchical Clustering Process***



Hierarchical Clustering

- ***Hierarchical Clustering Process***



Hierarchical Clustering

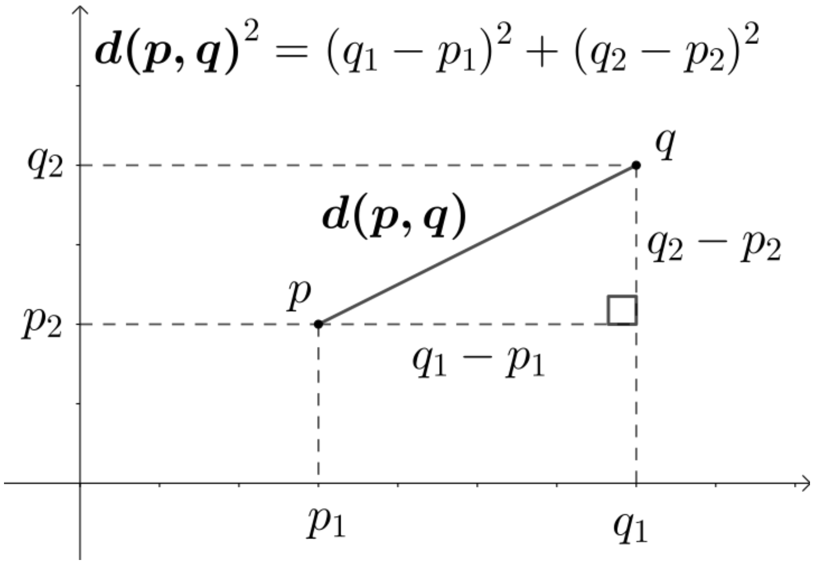
- There are a few key topics we still need to understand for Hierarchical Clustering:
  - Similarity Metric
  - Dendrogram
  - Linkage Matrix

Hierarchical Clustering

- Similarity Metric
  - Measures distance between two points.
  - Many options:
    - Euclidean Distance
    - Manhattan
    - Cosine
    - and many more...

Hierarchical Clustering

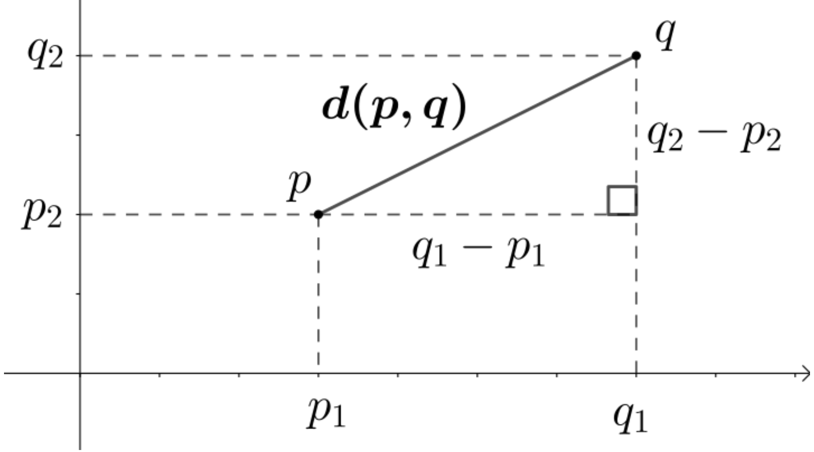
- Similarity Metric
    - Default choice is Euclidean



Hierarchical Clustering

- Similarity Metric
    - Default choice is Euclidean

$$\boxed{\boldsymbol{d}(\boldsymbol{p},\boldsymbol{q})^2 = (q_1 - p_1)^2 + (q_2 - p_2)^2}$$



Hierarchical Clustering

- Similarity Metric
  - Each dimension would be a feature
  - For **n** data points and **p** features:
    - $D^2 = (x_{11} - x_{12})^2 + \ldots + (x_{n-1p-1} - x_{np})^2$

Hierarchical Clustering

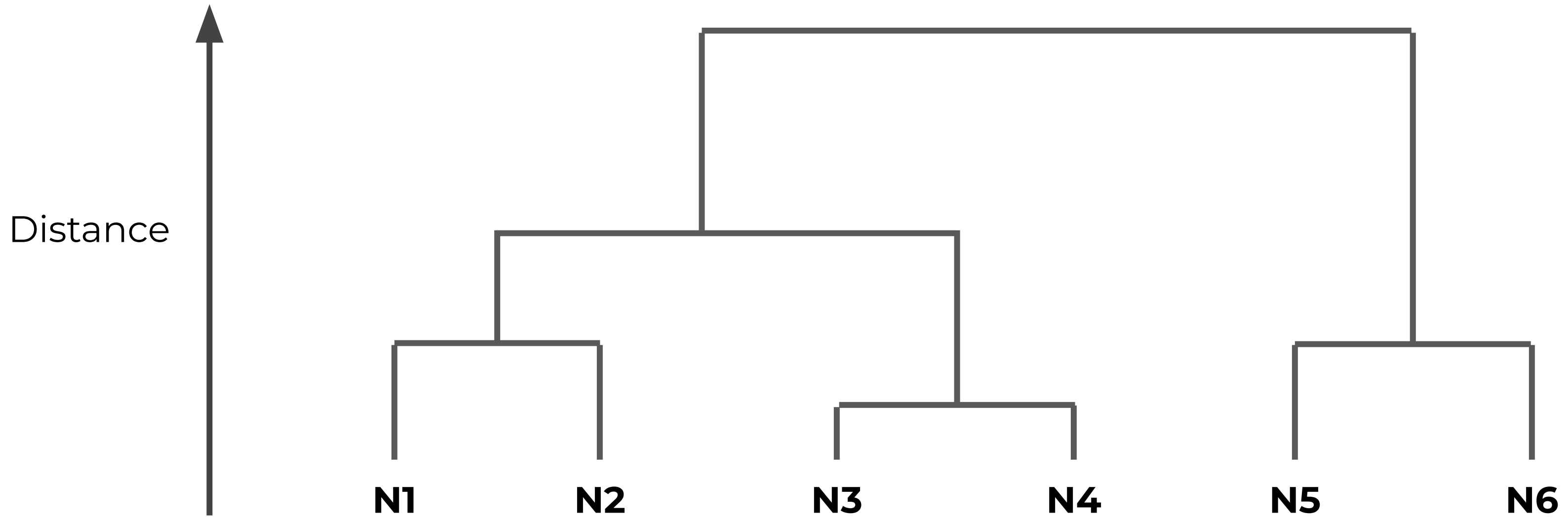
- Similarity Metric
  - Each dimension would be a feature
  - For **n** data points and **p** features:
    - $D^2 = (x_{11} - x_{12})^2 + \ldots + (x_{n-1p-1} - x_{np})^2$
  - Using MinMaxScaler we can scale all features to be between 0 and 1.
  - This allows for maximum distance between a feature to be 1.

Hierarchical Clustering

- Dendrogram:
  - Plot displaying all potential clusters.
  - Very computationally expensive to compute and display for larger data sets.
  - Very useful for deciding on number of clusters.

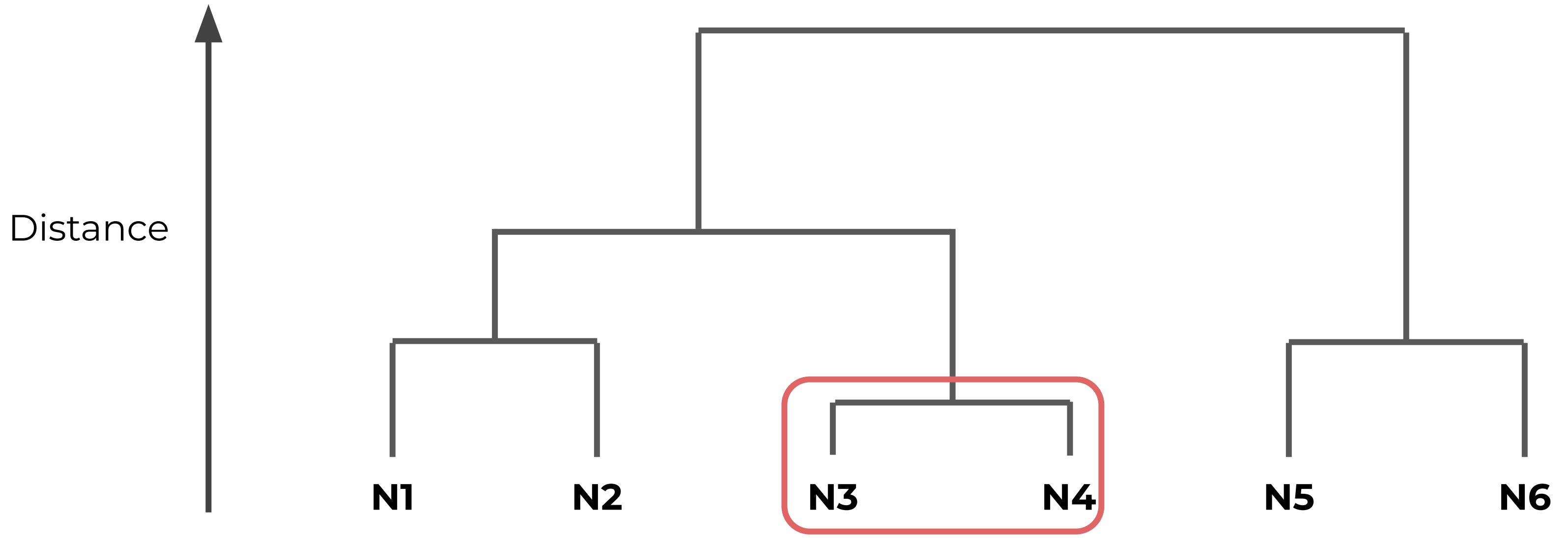
Hierarchical Clustering

- Dendrogram:



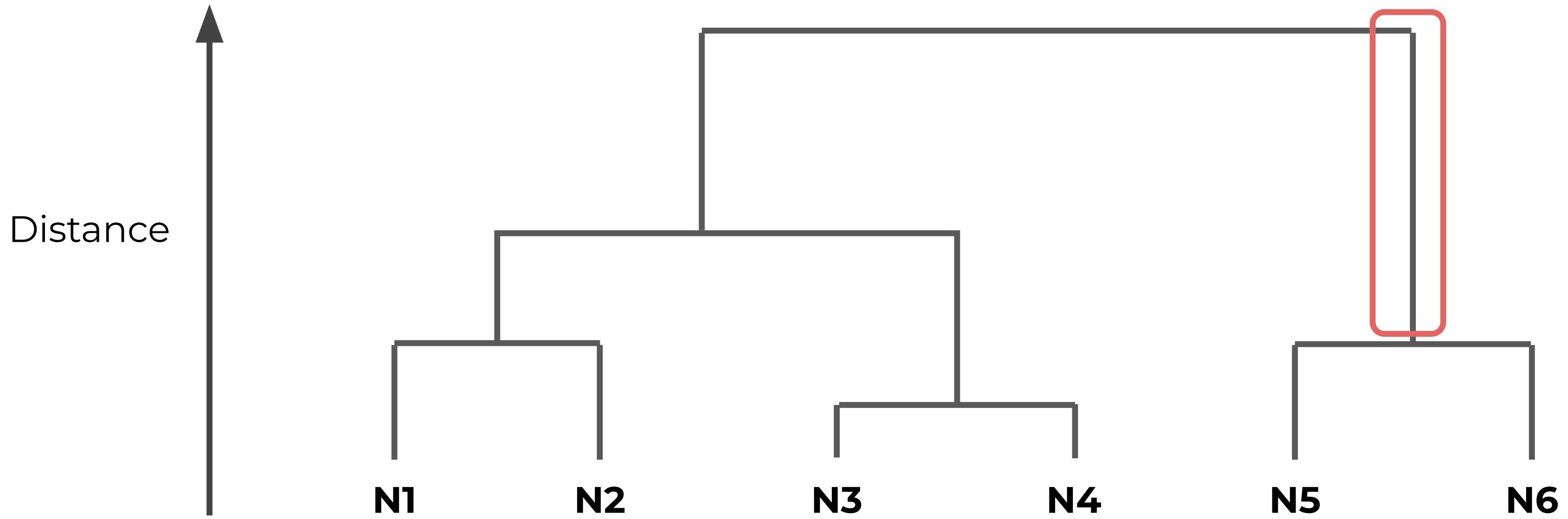
Hierarchical Clustering

- Dendrogram:



Hierarchical Clustering

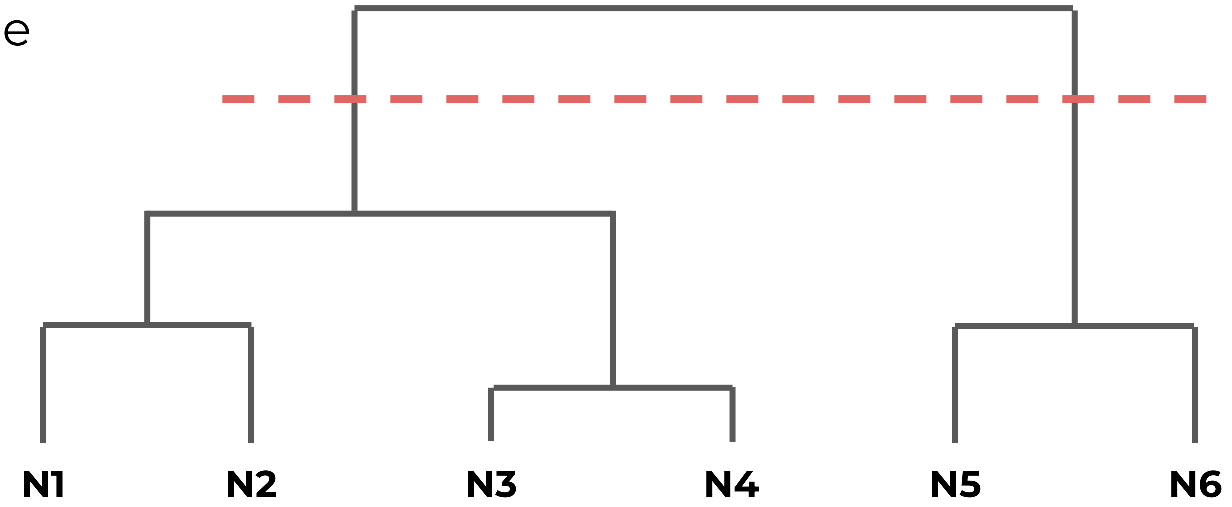
- Dendrogram:



Hierarchical Clustering

- Dendrogram:

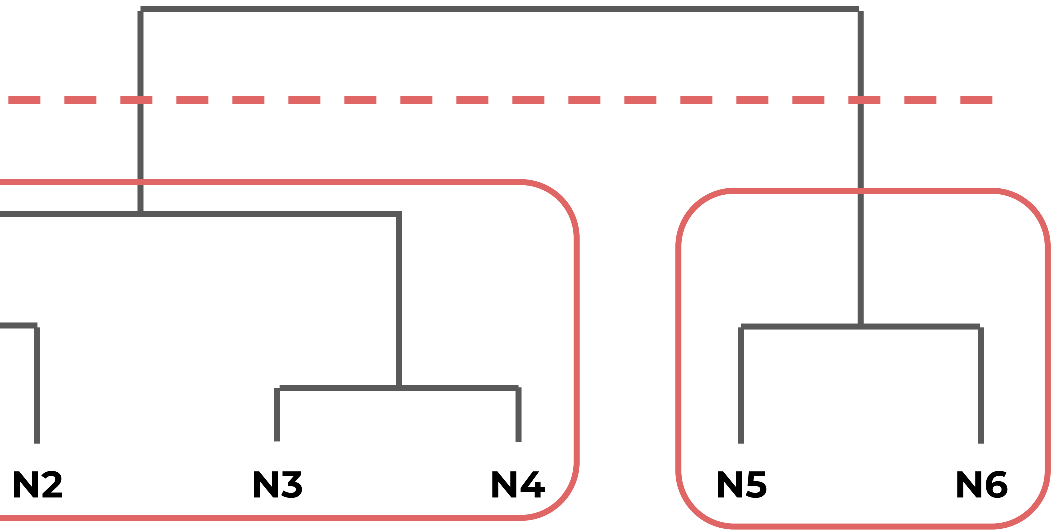
“Slice” to decide cluster count



Hierarchical Clustering

- Dendrogram:

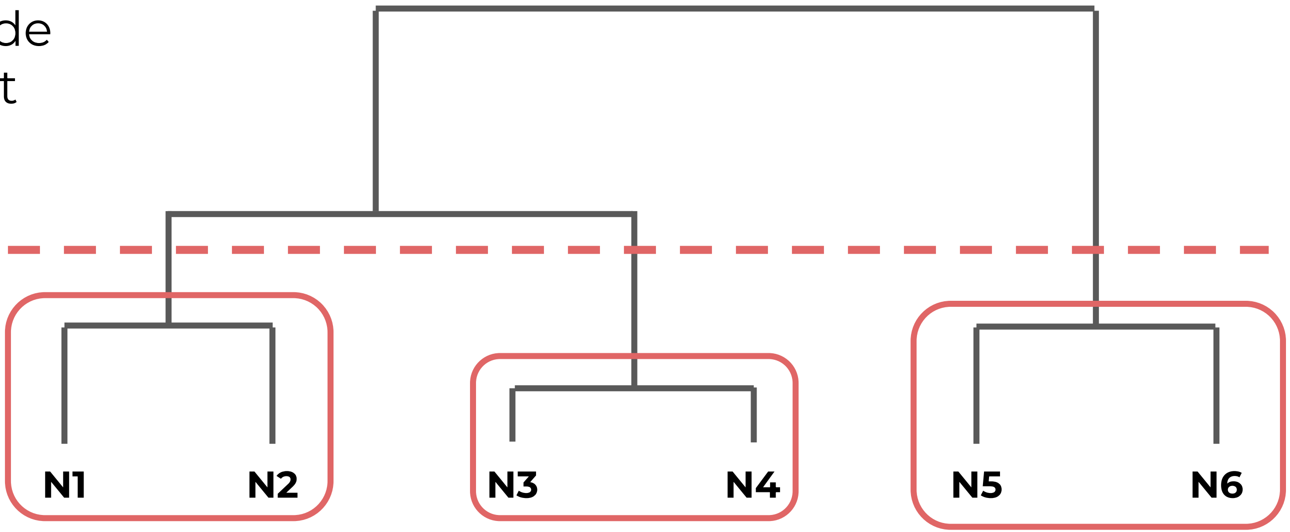
“Slice” to decide cluster count



Hierarchical Clustering

- Dendrogram:

“Slice” to decide cluster count



Hierarchical Clustering

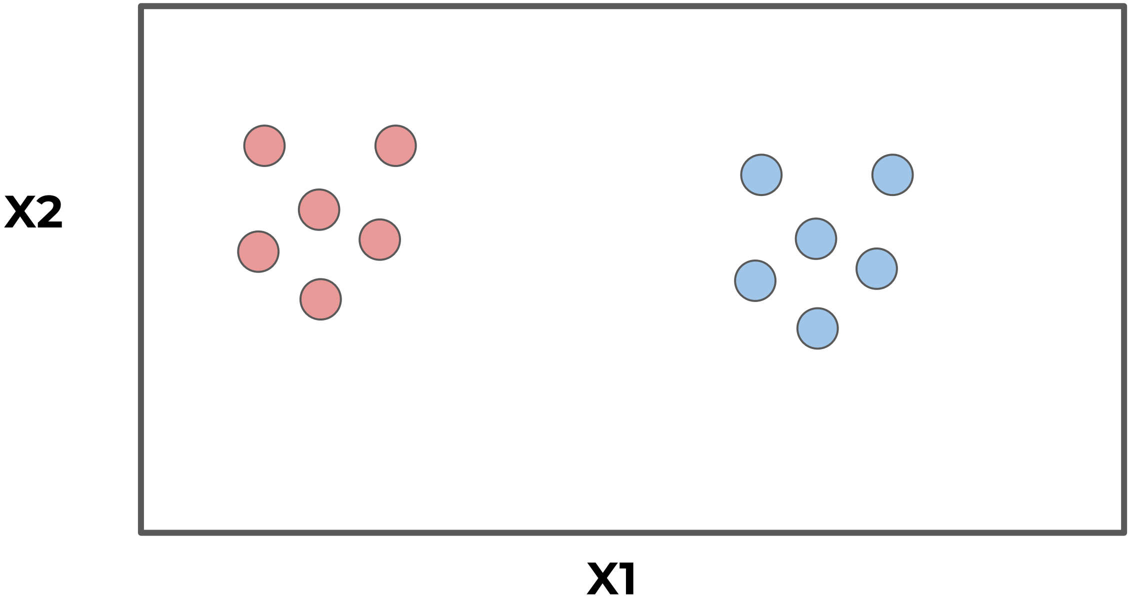
- Linkage
  - How do we measure distance from a point to an entire cluster?
  - How do we measure distance from a cluster to another cluster?

Hierarchical Clustering

- Linkage
  - Once two or more points are together and we want to continue agglomerative clustering to join clusters, we need to decide on a **linkage** parameter.

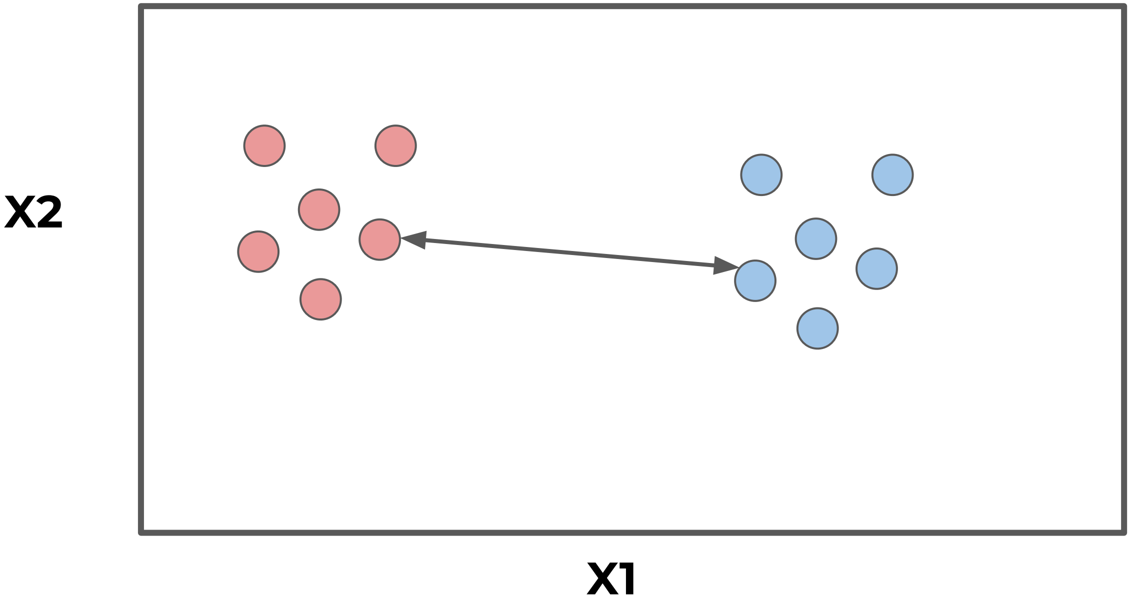
Hierarchical Clustering

- Linkage



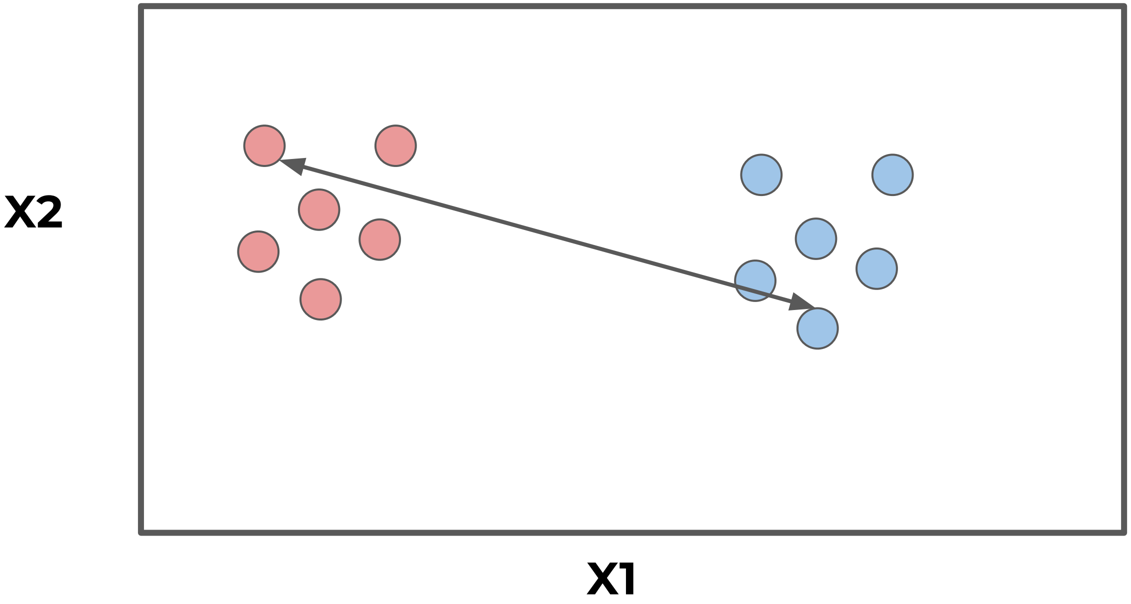
Hierarchical Clustering

- Linkage



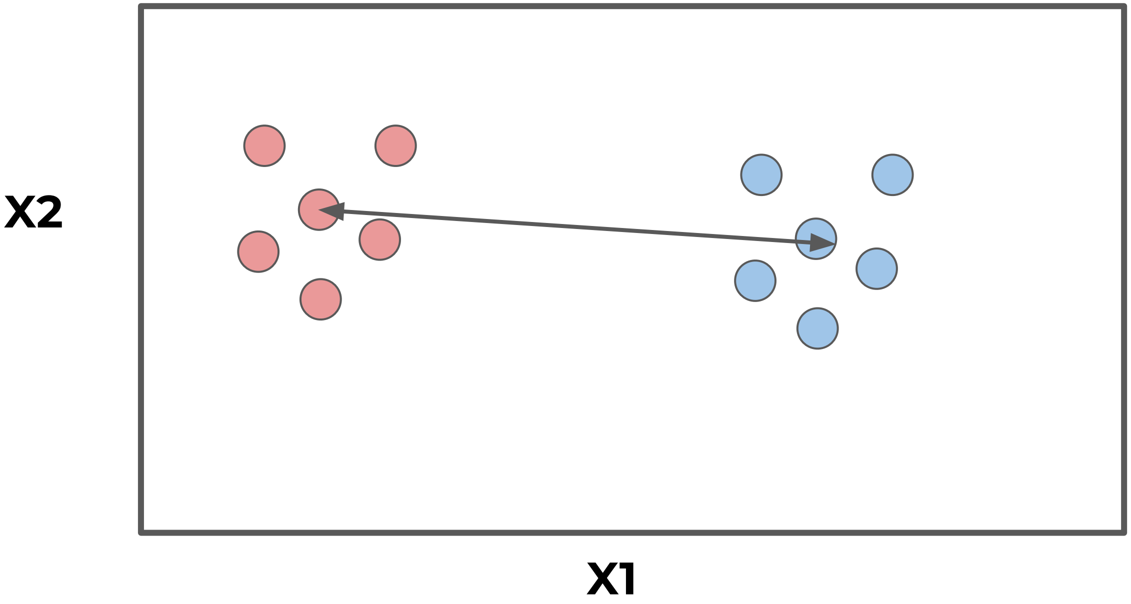
Hierarchical Clustering

- Linkage



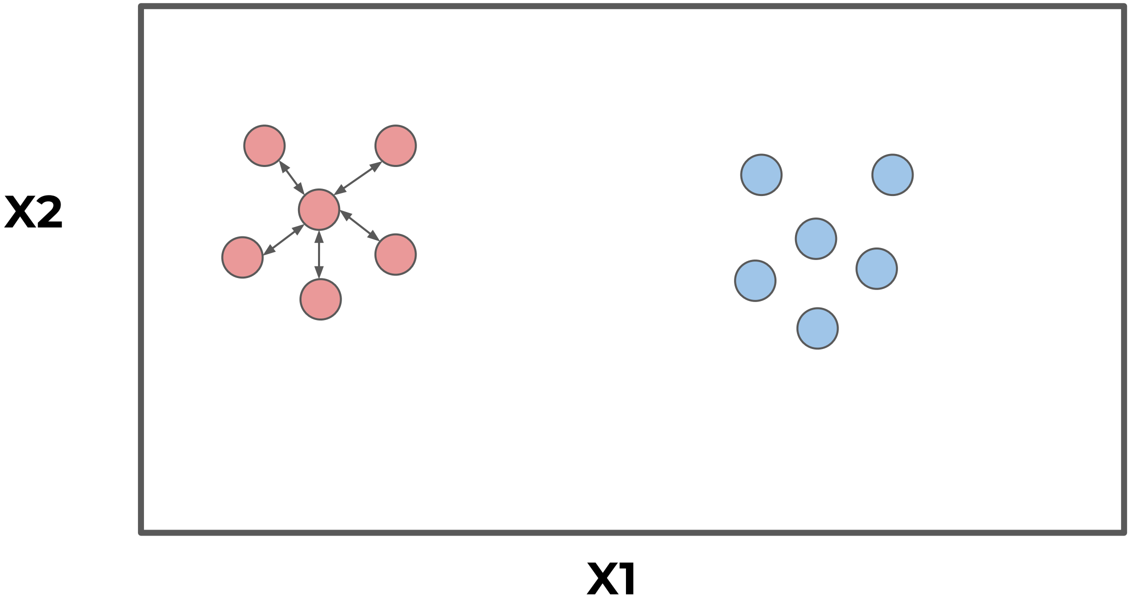
Hierarchical Clustering

- Linkage



Hierarchical Clustering

- Linkage



Hierarchical Clustering

- Linkage
  - Criterion determining which distance to use between sets of observation.
  - Algorithm will merge pairs of clusters that minimizes the criterion.

Hierarchical Clustering

- Linkage:
  - **Ward:** minimizes variance of clusters being merged.
  - **Average:** uses average distances between two sets.
  - **Minimum** or **Maximum** distances between all observations of the two sets.