Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree like diagram that records the sequences of merges or splits
Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendogram at the proper level

- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)
Hierarchical Clustering

- Two main types of hierarchical clustering
  - Agglomerative:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive:
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a point (or there are k clusters)

- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time
Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. Repeat
     4. Merge the two closest clusters
     5. Update the proximity matrix
     6. Until only a single cluster remains
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms
Starting Situation

- Start with clusters of individual points and a proximity matrix.
Intermediate Situation

- After some merging steps, we have some clusters

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Proximity Matrix
We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.
The question is “How do we update the proximity matrix?”
How to Define Inter-Cluster Similarity

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward’s Method uses squared error

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Proximity Matrix:

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p1  p2  p3  p4  p5  ...
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p3
p4
p5
...```

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|---|----|----|----|----|----|------
| p1|    |    |    |    |    |      
| p2|    |    |    |    |    |      
| p3|    |    |    |    |    |      
| p4|    |    |    |    |    |      
| p5|    |    |    |    |    |      

MIN
MAX
Group Average
Distance Between Centroids
Other methods driven by an objective function
  - Ward’s Method uses squared error
Cluster Similarity: MIN or Single Link

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

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Hierarchical Clustering: MIN

Nested Clusters

Dendrogram
Strength of MIN

- Can handle non-elliptical shapes
Limitations of MIN

- Sensitive to noise and outliers
Cluster Similarity: MAX or Complete Linkage

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

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Hierarchical Clustering: MAX

Nested Clusters

Dendrogram
Strength of MAX

- Less susceptible to noise and outliers
Limitations of MAX

- Tends to break large clusters
- Biased towards globular clusters
Cluster Similarity: Group Average

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

\[
\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum_{p_i \in \text{Cluster}_i} \sum_{p_j \in \text{Cluster}_j} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| \times |\text{Cluster}_j|}
\]

- Need to use average connectivity for scalability since total proximity favors large clusters

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Hierarchical Clustering: Group Average

Nested Clusters

Dendrogram
Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link
- Strengths
  - Less susceptible to noise and outliers
- Limitations
  - Biased towards globular clusters
Cluster Similarity: Ward’s Method

- Similarity of two clusters is based on the increase in squared error when two clusters are merged
  - Similar to group average if distance between points is distance squared

- Less susceptible to noise and outliers

- Biased towards globular clusters

- Hierarchical analogue of K-means
  - Can be used to initialize K-means
Hierarchical Clustering: Comparison

MIN

MAX

Group Average

Ward’s Method
Hierarchical Clustering: Time and Space requirements

- \( O(N^2) \) space since it uses the proximity matrix.
  - \( N \) is the number of points.

- \( O(N^3) \) time in many cases
  - There are \( N \) steps and at each step the size, \( N^2 \), proximity matrix must be updated and searched
  - Complexity can be reduced to \( O(N^2 \log(N)) \) time for some approaches
Hierarchical Clustering: Problems and Limitations

- Once a decision is made to combine two clusters, it cannot be undone
- No objective function is directly minimized
- Different schemes have problems with one or more of the following:
  - Sensitivity to noise and outliers
  - Difficulty handling different sized clusters and convex shapes
  - Breaking large clusters