DATA MINING 1
Hierarchical Clustering

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Revisited slides from Lecture Notes for Chapter 7 “Introduction to Data Mining”, 2nd Edition by Tan, Steinbach, Karpatne, Kumar
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
Dendrograms
Dendrograms
Dendrograms
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 dendrogram 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 an individual 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

- Most 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
Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.
After Merging

• The question is “How do we update the proximity matrix?”
How to Define Inter-Cluster Distance

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

Similarity?

Proximity Matrix
How to Define Inter-Cluster Similarity

- MIN
- MAX
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- Distance Between Centroids
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Proximity Matrix

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Proximity Matrix

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

Distance Between Centroids
MIN or Single Link

- Proximity of two clusters is based on the two closest points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph

- Example:

Distance Matrix:

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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

Original Points

Two Clusters

Three Clusters
MAX or Complete Linkage

• Proximity of two clusters is based on the two 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
Group Average

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

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

- 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

Ward’s Method

Group Average
References

• Clustering. Chapter 7. Introduction to Data Mining.