Minimum Spanning Trees

Application to Clustering

Algorithms: Design and Analysis, Part II

Clustering

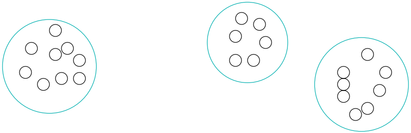
[aka "unsupervised learning"]

Informal goal: Given n "points" [Web pages, images, genome fragments, etc.] classify into "coherent groups".

Assumptions: (1) As input, given a (dis)similarity measure — a distance $d(p, q)$ between each point pair.
(2) Symmetric [i.e., $d(p, q) = d(q, p)$]

Examples: Euclidean distance, genome similarity, etc.

Goal: Same cluster $\iff$ "nearby"



Max-Spacing k-Clusterings

Assume: We know k:= # of clusters desired. [In practice, can experiment with a range of values]

Call points p & q separated if they're assigned to different clusters.

Definition: The spacing of a k-clustering is $\min_{\text{separated } p,q} d(p,q)$. (The bigger the better)

Problem statement: Given a distance measure d and k, compute the k-clustering with maximum spacing.

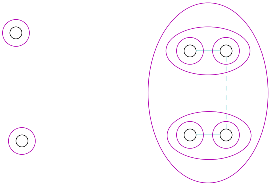
A Greedy Algorithm

- Initially, each point in a separate cluster
- Repeat until only k clusters:
  - Let $p, q =$ closest pair of separated points (determines the current spacing)
  - Merge the clusters containing p & q into a single cluster.

Note: Just like Kruskal's MST algorithm, but stopped early.

- Points $\leftrightarrow$ vertices, distances $\leftrightarrow$ edge costs, point pairs $\leftrightarrow$ edges.

$\Rightarrow$ Called single-link clustering



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Algorithms: Design and Analysis, Part II

Correctness of Greedy Clustering

Correctness Claim

Theorem: Single-link clustering finds the max-spacing k-clustering.

Proof: Let $C_1, \ldots, C_k$ = greedy clustering with spacing S.

Let $\hat{C}_1, \ldots, \hat{C}_k$ = arbitrary other clustering.

Need to show: Spacing of $\hat{C}_1, \ldots, \hat{C}_k$ is $\leq S$.

Correctness Proof

Case 1: $\hat{C}_i$'s are the same as the C_i's [maybe after renaming] $\Rightarrow$ has the same spacing S.

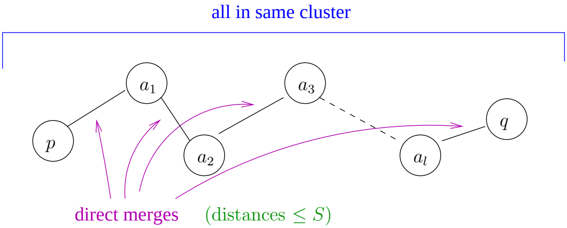
Case 2: Otherwise, can find a point pair p, q such that
(A) p, q in the same greedy cluster C_i
(B) p, q in different clusters $\hat{C}_i, \hat{C}_j$

Property of greedy algorithm: If two points x, y "directly merged at some point", then $d(x, y) \leq S$. [Distance between merged point pairs only goes up.]

Easy case: If p, q directly merged at some point, $S \geq d(p, q) \geq$ spacing of $\hat{C}_1, \ldots, \hat{C}_k$.

Correctness Proof (con'd)

Tricky case: p, q "indirectly merged" through multiple direct merges.



Let $p, a_1, \ldots, a_l, q$ be the path of direct greedy merges connecting p & q.

Key point: Since $p \in \hat{C}_i$ and $q \notin \hat{C}_i$, $\exists$ consecutive pair a_j, a_{j+1} with $a_j \in \hat{C}_i, a_{j+1} \notin \hat{C}_i \Rightarrow S \geq d(a_j, a_{j+1}) \geq$ Spacing of $\hat{C}_1, \ldots, \hat{C}_k$ QED!

since a_j, a_{j+1} directly merged

since a_j, a_{j+1} separated