4.7 Clustering [focusing on single linkage]

Clustering

Clustering. Given a set U of n points labeled $p_1, \ldots, p_n$, classify into coherent groups.

photos, documents. micro-organisms

Distance function. Numeric value specifying "closeness" of two objects.

number of corresponding pixels whose intensities differ by some threshold

Fundamental problem. Divide into clusters so that points in different clusters are far apart.

- Routing in mobile ad hoc networks.
- Identify patterns in gene expression.
- Document categorization for web search.
- Similarity searching in medical image databases
- Skycat: cluster 10^9 sky objects into stars, quasars, galaxies.

Clustering of Maximum Spacing

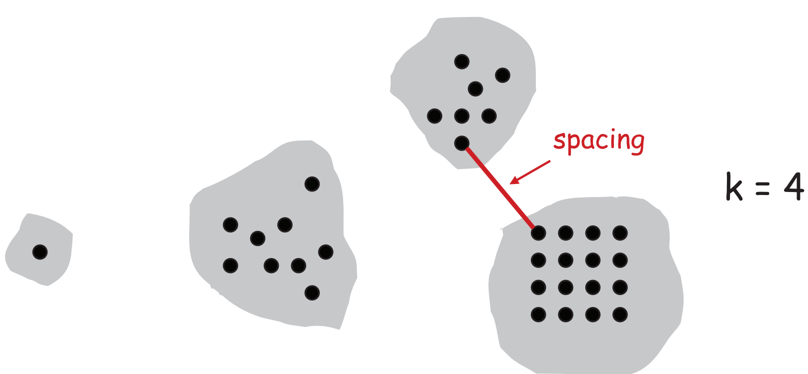
Goal: Divide objects into k non-empty groups (aka clusters): k-clustering

Distance function. Assume it satisfies several natural properties.

- $d(p_i, p_j) = 0$ iff $p_i = p_j$ (identity of indiscernibles)
- $d(p_i, p_j) \geq 0$ (nonnegativity)
- $d(p_i, p_j) = d(p_j, p_i)$ (symmetry)

Spacing. Min distance between any pair of points in different clusters.

Clustering of maximum spacing. Given an integer k, find a k-clustering of maximum spacing.



Greedy Clustering Algorithm

Single-linkage clustering algorithm.

- Form a graph on the vertex set U, corresponding to n clusters.
- Find the closest pair of objects such that each object is in a different cluster, and add an edge between them.
- Repeat n-k times until there are exactly k clusters.

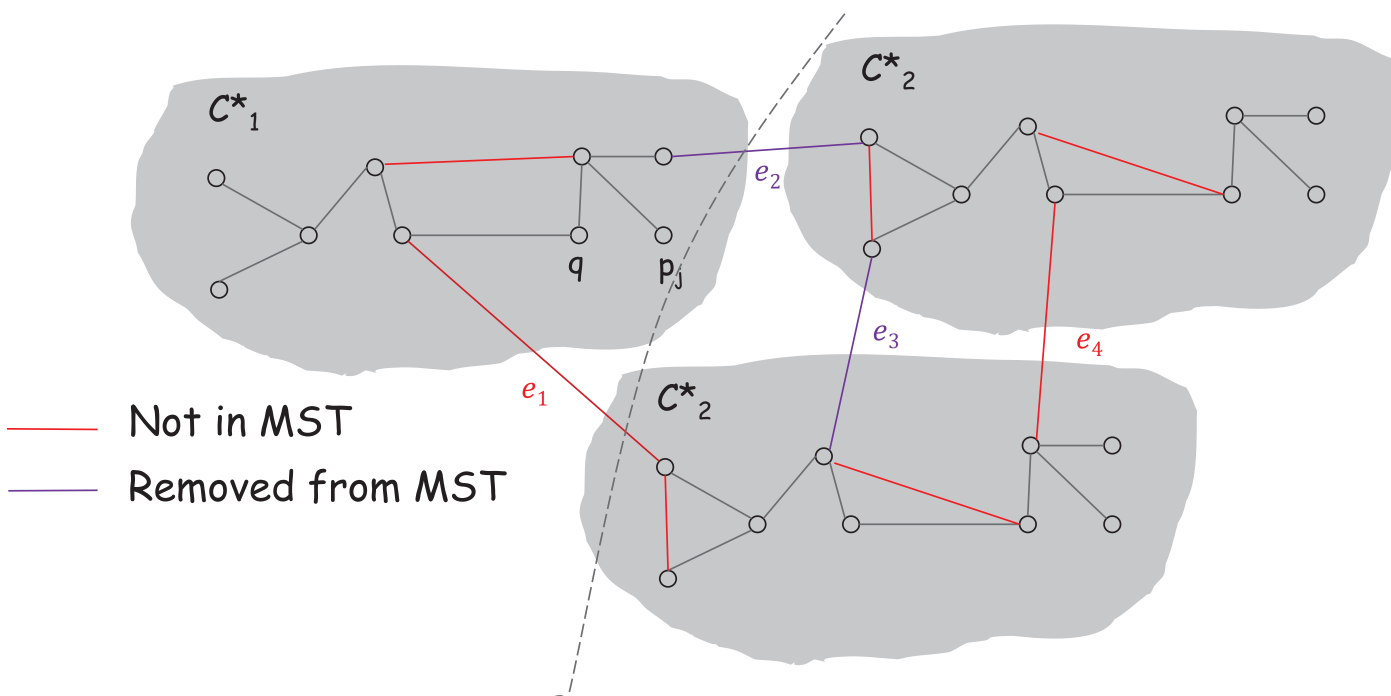
Key observation. This procedure is precisely Kruskal's algorithm (except we stop when there are k connected components).

Remark. Equivalent to finding an MST and deleting the k-1 most expensive edges.

Greedy Clustering Algorithm: Analysis

Theorem. Let C^* denote the clustering $C^*_1, \ldots, C^*_k$ formed by deleting the k-1 most expensive edges of a MST. Then C^* is a k-clustering of max spacing.

Observation: The spacing of C^* is the length d^* of the $(k-1)^{st}$ most expensive edge (in MST).



Cut Property ➔ $d(e_1) \geq d(e_2)$

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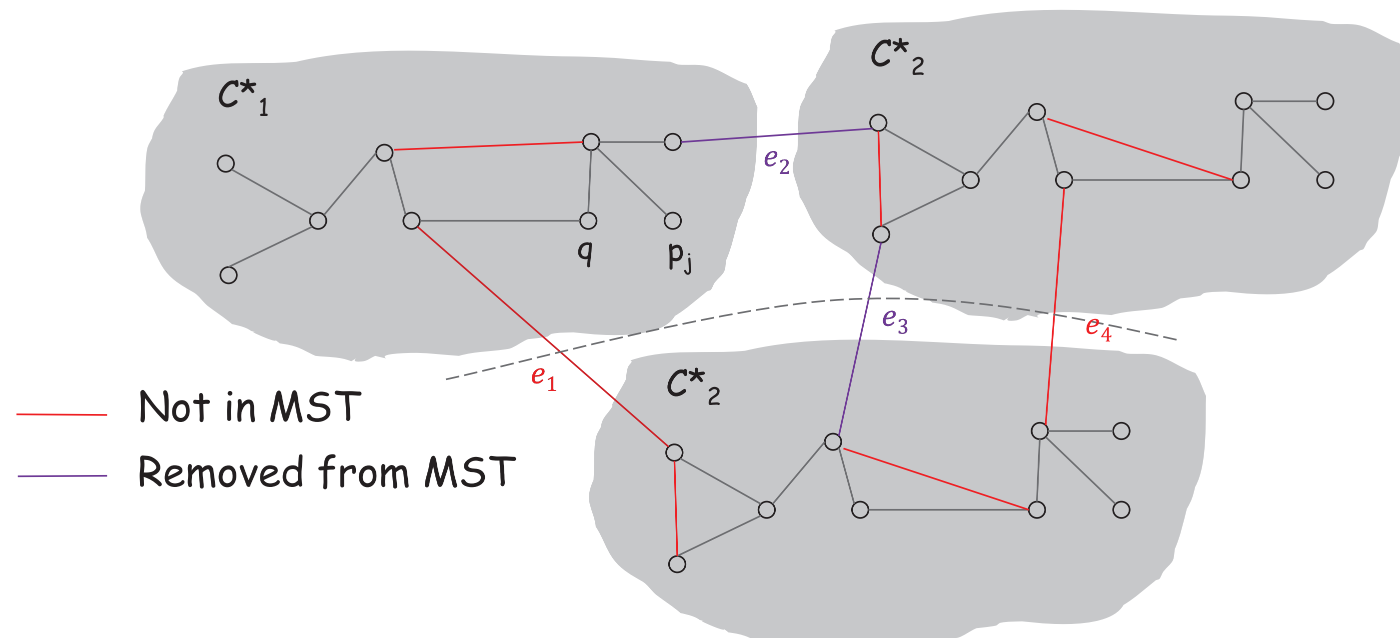

Cut Property ➔ $d(e_1), d(e_4) \geq d(e_2)$

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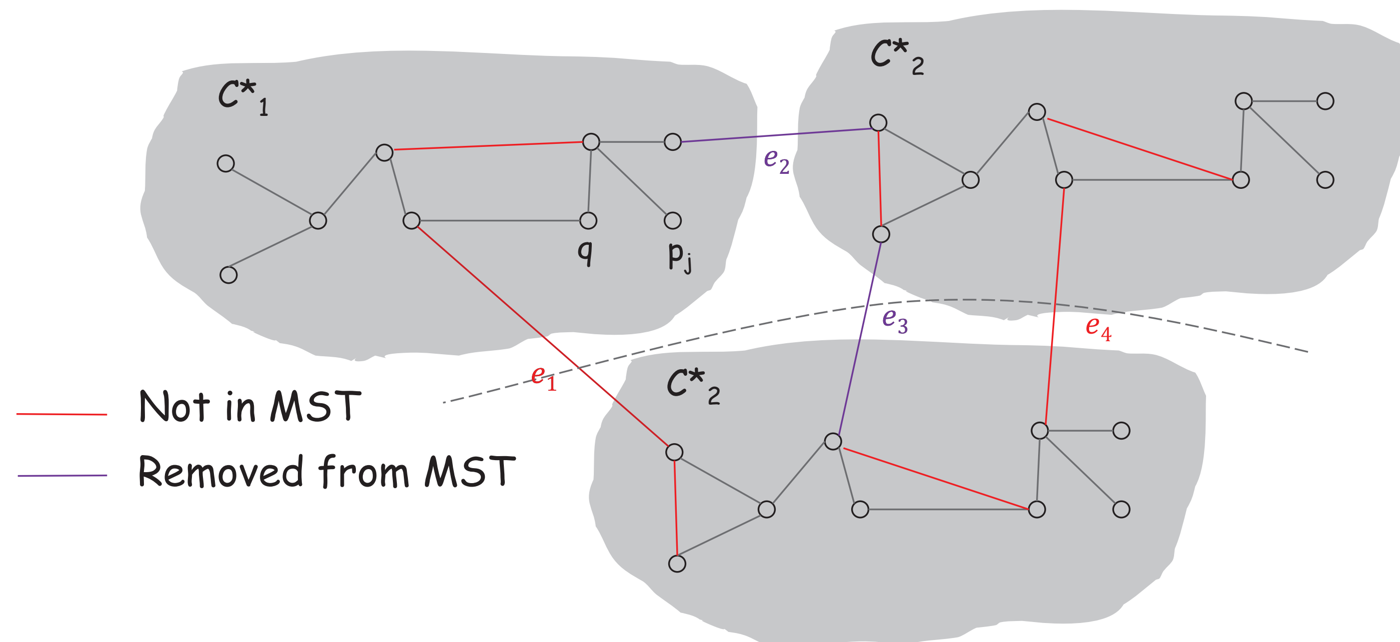

Cut Property ➔ $d(e_1) \geq d(e_3) \rightarrow d(e_1) \geq \max\{d(e_2), d(e_3)\}$

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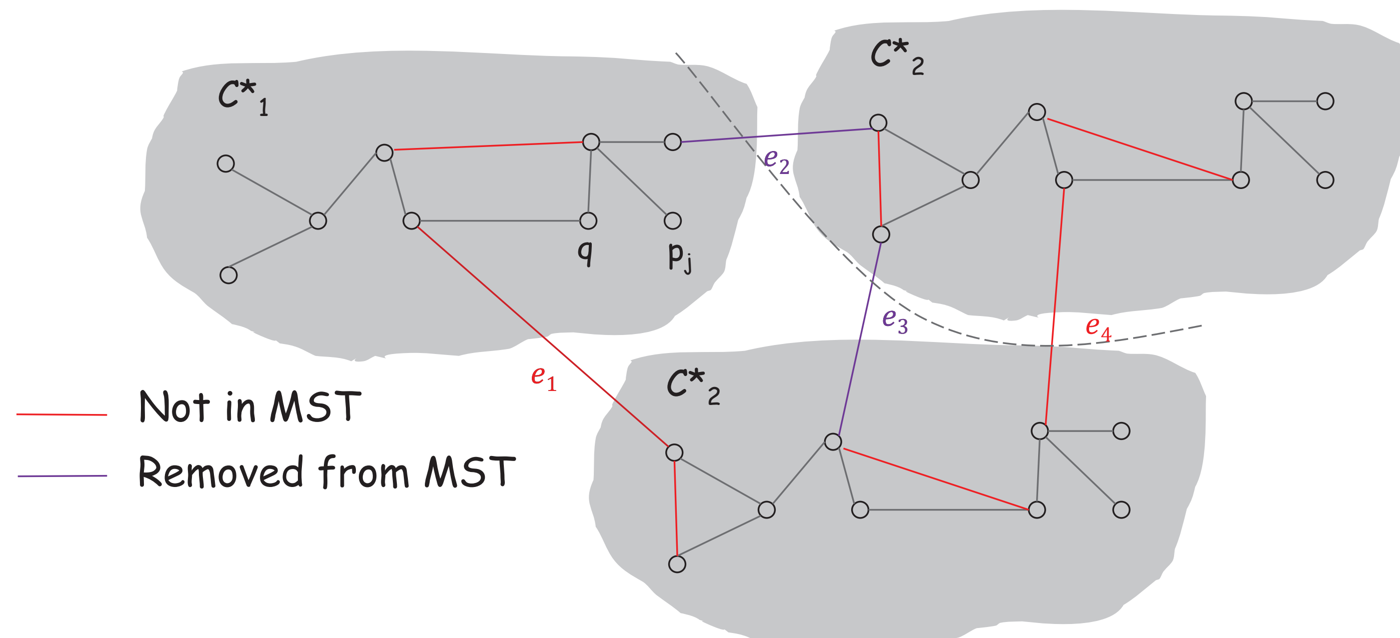

Cut Property ➔ $d(e_4) \geq \max\{d(e_2), d(e_3)\}$

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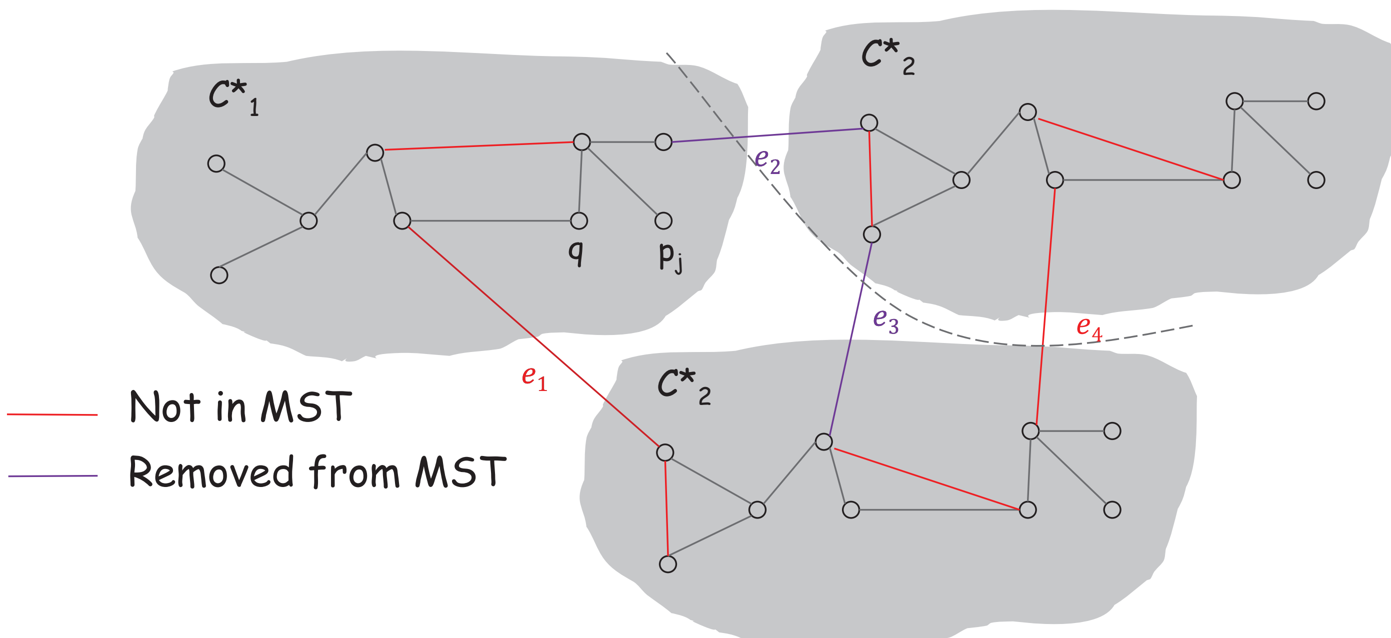

Spacing = $\max\{d(e_2), d(e_3)\}$

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Theorem. Let C^* denote the clustering $C^*_1, \ldots, C^*_k$ formed by deleting the k-1 most expensive edges of a MST. Then C^* is a k-clustering of max spacing.

Proof?

Greedy Clustering Algorithm: Analysis

Theorem. Let C^* denote the clustering $C^*_1, \ldots, C^*_k$ formed by deleting the $k-1$ most expensive edges of a MST. Then C^* is a k-clustering of max spacing.

Pf. Let C denote some other clustering $C_1, \ldots, C_k$.

- The spacing of C^* is the length d^* of the $(k-1)^{st}$ most expensive edge (in MST).

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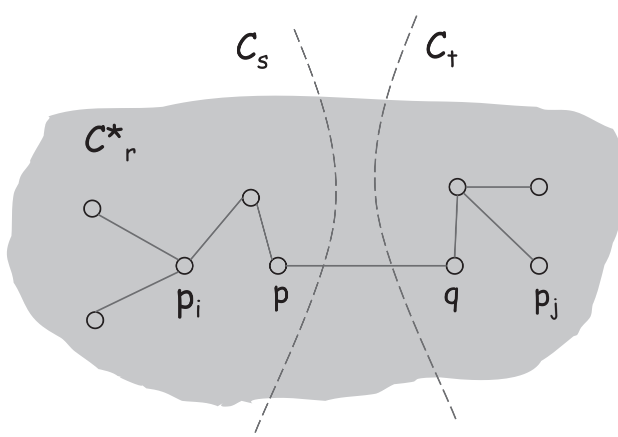
- The spacing of C^* is the length d^* of the $(k-1)^{st}$ most expensive edge (in MST).
- Let p_i, p_j be in the same cluster in C^*, say C^*_r, but different clusters in C, say C_s and C_t.



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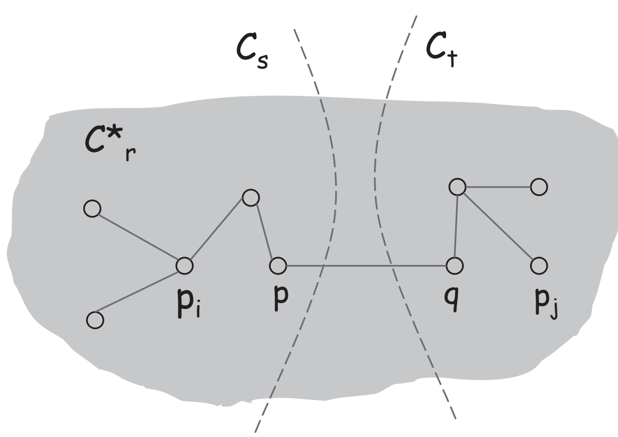
- Let p_i, p_j be in the same cluster in C^*, say C^*_r, but different clusters in C, say C_s and C_t.
- Some edge (p, q) on p_i-p_j path in C^*_r spans two different clusters in C.



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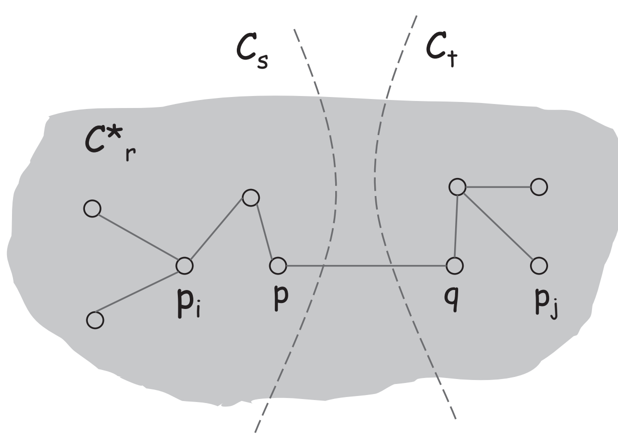
- All edges on p_i-p_j path have length $\leq d^*$ since Kruskal chose them (and we did not delete them from our MST).



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- All edges on p_i-p_j path have length $\leq d^*$ since Kruskal chose them (and we did not delete them from our MST).
- Spacing of C is $\leq d^*$ since p and q are in different clusters. ▪