

# AMAT 583 Lecture 23

Today: Single linkage review

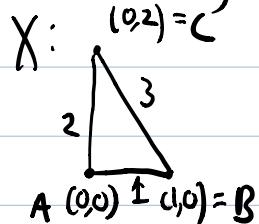
Single linkage for real-valued metrics.

Algorithm for computing single linkage dendograms

Average linkage.

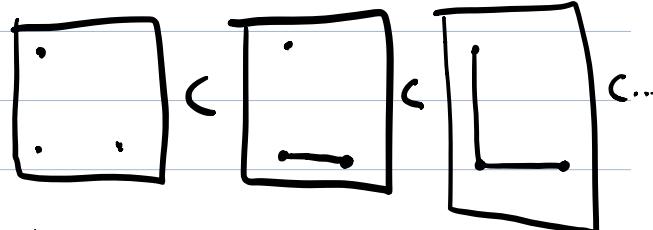
Single linkage ( $\mathbb{N}$ -valued metrics)

Finite Metric Space  $X$



Neighborhood Graphs

$$N_0(x) \subset N_1(x) \subset N_2(x) \subset \dots$$



↓ Consider connected components

Hierarchical Partition  $\{SL(X)_z\}_{z \in \mathbb{N}}$

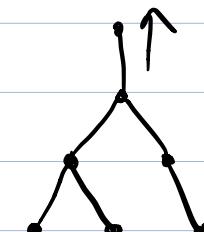
$$SL(X)_0 \quad SL(X)_1 \quad SL(X)_2$$

$$SL_0 = \{\{A\}, \{B\}, \{C\}\}$$

$$SL_1 = \{\{A, B\}, \{C\}\}$$

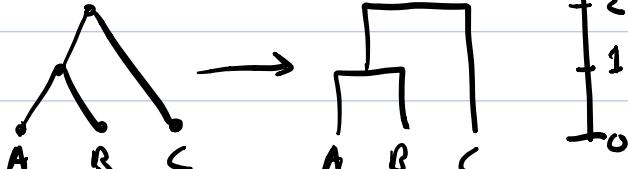
$$SL_2 = \{\{A, B, C\}\}$$

↓ (Untrimmed) Dendrogram



0  
1  
2

↓ Trimmed dendrogram



Algorithm for construction of the (trimmed) single linkage dendrogram.

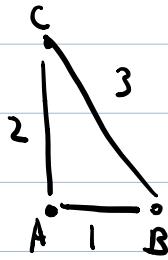
Input: A finite metric space  $(X, d)$

Output: Trimmed single linkage dendrogram  $D$ .

Pseudocode:

- Order pairs of points in  $X$  according to increasing distance.  
[break ties arbitrarily]  $E = ([A, B], [A, C], [B, C])$
- Initially, put each element of  $X$  into its own cluster.  
[As we build we will merge the clusters.]
- Add a vertex to  $D$  at level 0 for each cluster.
- For each edge  $e = [v, w]$  in increasing order:  
If  $v$  and  $w$  belong to different clusters  $S_v$  and  $S_w$ 
  - merge the clusters  $S_v$  and  $S_w$  to form a new cluster  $S$ .
  - Add the vertex  $S$  to  $D$  at level  $d(v, w)$
  - Add the edges  $[S_v, S]$  and  $[S_w, S]$  to  $D$ .

Example:  $X:$



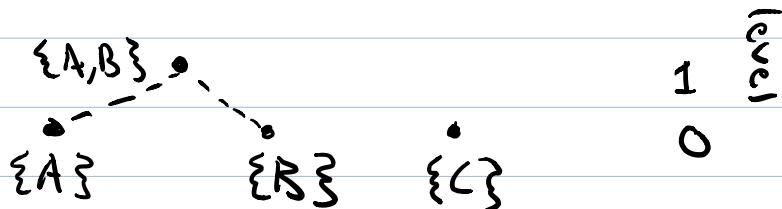
$$E([A,B], [A,C], [B,C])$$

Initial clusters:  $\{A\}, \{B\}, \{C\}$ .

Consider first edge  $[A,B]$ .  $A$  and  $B$  belong to different clusters  $\Rightarrow$  merge these. (Merged cluster is  $\{a,b\}$ .)

now the clusters are  $\{A,B\}, \{C\}$ .

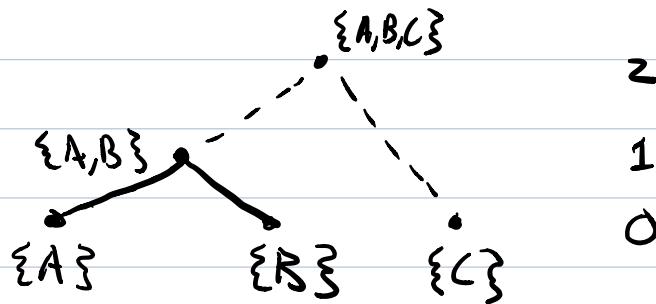
- Add a new vertex labelled  $\{A,B\}$  at level  $d(A,B)=1$ ,
- Add in edges from the unmerged clusters to the merged cluster



Consider next edge  $[A,C]$ .  $A$  and  $C$  belong to different clusters  $\Rightarrow$  merge these. Merged cluster is  $\{A,B,C\}$ .

Now the clusters are  $\{A,B,C\}$  (just one cluster)

- Add a new vertex labelled  $\{A, B, C\}$  at level  $d(A, C) = 1$
- Add in edges from the unmerged clusters to the merged cluster



Consider next edge  $[B, C]$   $B$  and  $C$  already belong to the same cluster so we are done.

Missing details: When implementing this on a computer, how do we store the clusters in a way that allows us to quickly check whether two points belong to the same cluster and quickly merge the clusters?

Answer: Union-find data structure (classical data structure from computer science.)

Reference: Edelsbrunner / Harer Computational Topology, CLRS Chapter 21.