

Hierarchical Agglomerative Clustering

Density-based Clustering

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What is Clustering

Input

Data set $X = \{x_1, x_2, \dots, x_n\} \in \mathcal{X}$

Distances $D: X \times X \rightarrow \mathbb{R}_{\geq 0}$

often $X \subset \mathbb{R}^d$

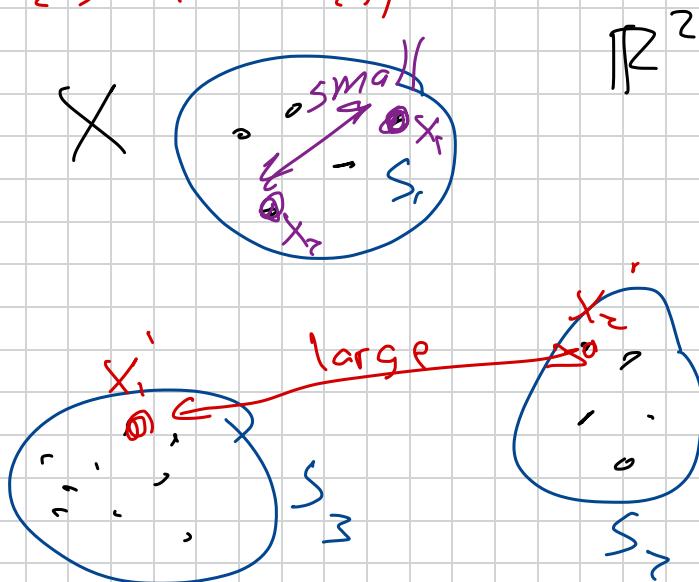
$$D(x_1, x_2) = \|x_1 - x_2\|$$

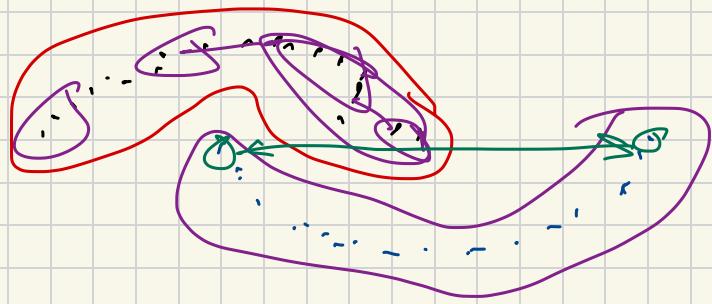
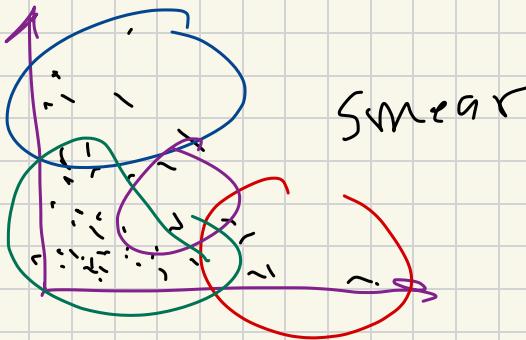
Goal Partition X into

\Rightarrow sets S_1, S_2, \dots, S_K

$$S_i \cap S_j = \emptyset, \quad \bigcup_{j=1}^K S_j = X$$

- Points in cluster $x_i, x_j \in S_j$
close $D(x_i, x_j)$ small
- Points in diff clusters $x_i \in S_i, x_j \in S_j$
 $D(x_i, x_j)$ large





- When data is easily or naturally clusterable, then most clustering algorithms work quickly and well
- When data is **not** easily or naturally clusterable, then no algorithm will find good clusters

Hierarchical Agglomerative Clustering (HAC)

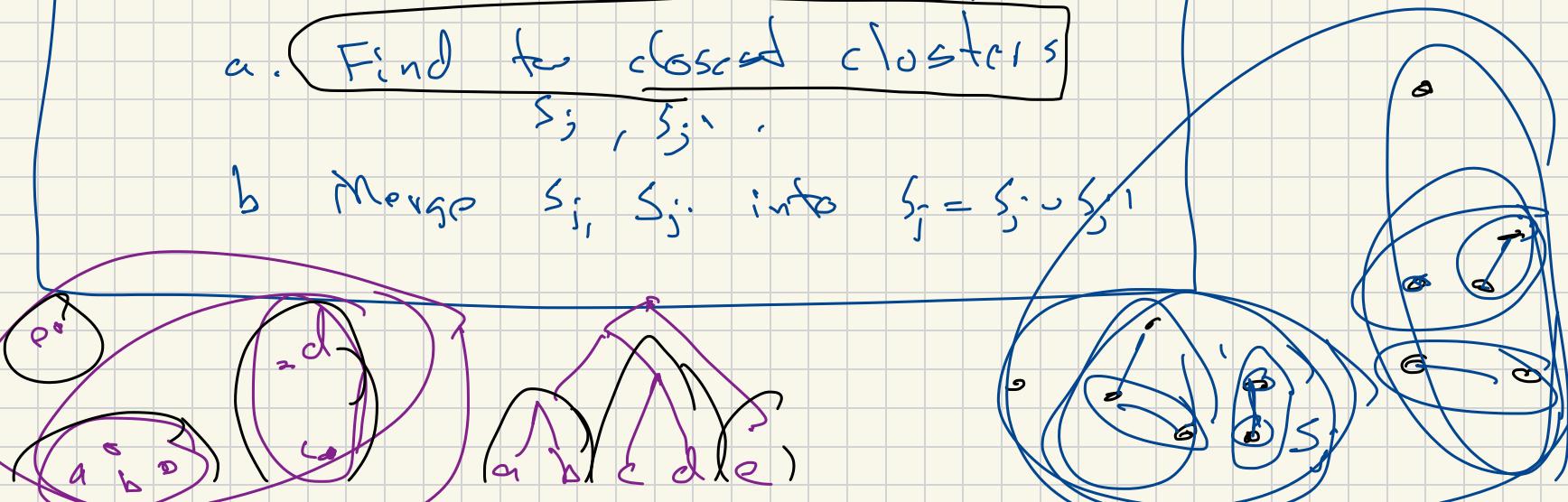
1. Each $x \in X$ is its own cluster

$$S_1 = \{x_1\}, S_2 = \{x_2\}, \dots$$

2. while (more than 1 cluster)

a. Find the closest clusters
 $S_j, S_{j'}$.

b. Merge $S_j, S_{j'}$ into $S_j = S_j \cup S_{j'}$



Find two closest clusters

distance $D(S_1, S_2)$

$$D: X \times X$$

• Distribution Dist w_s, D_k

• $D(c_i, c_j)$

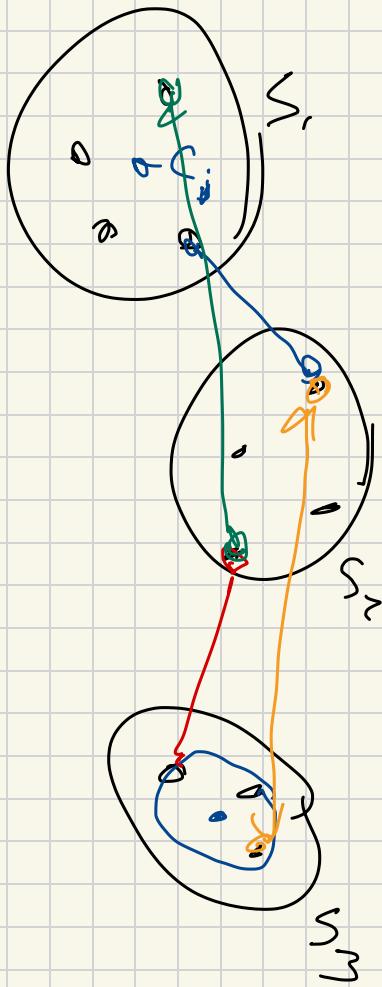
c_i "center" S_i
 \hookrightarrow mean(S_i)
 \hookrightarrow center of MEB

single link

$$\Rightarrow D(S_1, S_2) = \min_{x \in S_1, x_2 \in S_2} D(x_1, x_2)$$

complete Link

$$\Rightarrow D(S_1, S_2) = \max_{x \in S_1, x_2 \in S_2} D(x_1, x_2)$$



Runtimes of HAC Single-Link

- ~ How many merges? $\hookrightarrow O(n)$
- ↳ $n-1 = O(n)$ merges.

Find closest 2 clusters.

Merge $s_j, s_k \Rightarrow s_j''$ update $\{ \text{group distances} \}$

Update $O(n)$ distances
maintain in PQ $O(\log n)$ time
each $O(1)$ time

$\hookrightarrow O(n^2 \log n)$ time. slow

Density-based clustering

DBScan \approx chopped off Single Link HAC

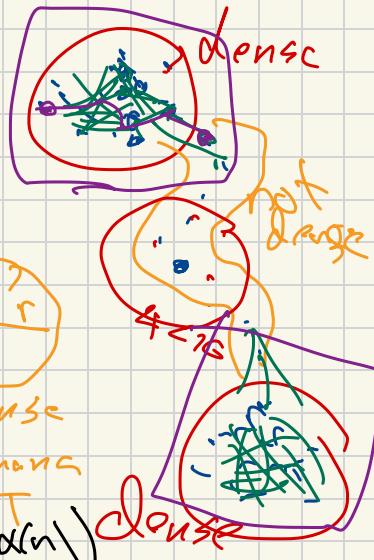
- radius r = clusters to be separated if $D_{SL}(s_1, s_2) > r$.

• threshold $T = \min \# pts$
 $T=10$ in ball radius r

1. For all $x \in X$, find
 $\# pts$ in ball $B_r(x)$ $O(n \log n)$
 if $> T \Rightarrow x$ is core

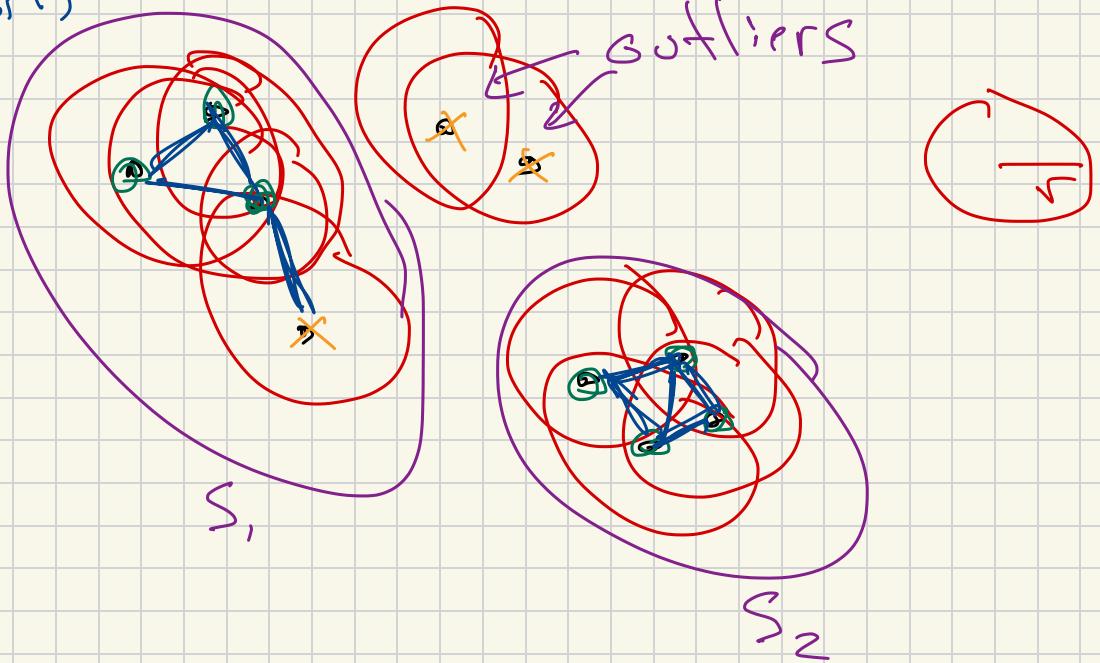
2. Build graph on core pts to $O(n^2)$
 all neighbors (radius r)

3. Clusters are connected components of Graph $O(n \alpha n)$ cluster



threshold
 $T = 3$

Edges



DBScan

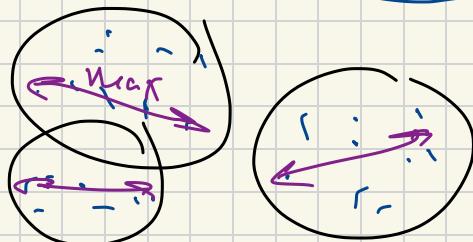
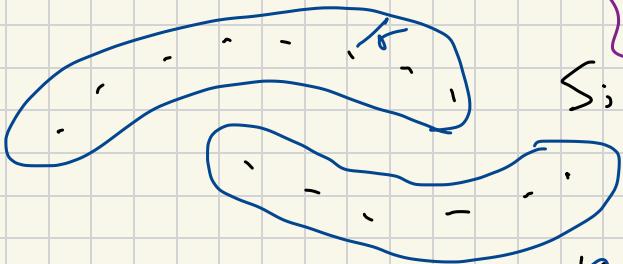
How many clusters?

- DBScan : depending on r , T

- HAC : Singl., Comple. Link

threshold

Singl. = min distance between points in diff clusters



Comple. Link = max dist between pts in cluster

$r \leftarrow$ threshold.

(i)

Plug in values, look at clusters!

- look at sample data

sanity check

