8 Hierarchical Agglomerative Clustering

This marks the beginning of the *clustering* section. The basic idea is to take a set X of items and somehow partition X into subsets, so each subset has similar items. Obviously, it would be great if we could be more specific, but that would end up omitting some particular form of clustering.

Clustering is an extremely *broad and ill-defined* topic. There are **many many** variants; we will not try to cover all of them. Instead we will focus on three broad classes of algorithms, and try to touch on some new developments.

Shouldn't we be spending *more* emphasis on clustering? Perhaps not. Of all of the studies that have emerged, one theme has rung consistently:

> *When data is easily cluster-able, most clustering algorithms work quickly and well.*
> *When data is not easily cluster-able, then no algorithm will find good clusters.*

8.1 Hard Clustering Formulation

Lets specify our clustering goal a bit more. Start with a set $X \subset \mathcal{M}$ (say $\mathcal{M} = \mathbb{R}^d$), and a metric $\mathbf{d} : \mathcal{M} \times \mathcal{M} \to \mathbb{R}_+$.

A *cluster* S is a subset of X. A *clustering* is a partition $\mathcal{C}(X) = \{S_1, S_2, \ldots, S_k\}$ where

(C1) each $S_i \subset X$,

(C2) each pair $S_i \cap S_j = \emptyset$ (this is relaxed in *soft* clustering), and

(C3) $\bigcup_{i=1}^{k} S_i = P$.

Then the goal is two-fold:

width: For each $S \in \mathcal{C}(X)$ for all $x, x' \in S$ then $\mathbf{d}(x, x')$ is small.

split: For each $S_i, S_j \in \mathcal{C}(X)$, for all (most) $x_i \in S_i$ and $x_j \in S_j$ (and $i \neq j$) then $\mathbf{d}(x_i, x_j)$ is large.

Overall, the goal is for ("split" / "width") or ("split" - "width") to be large.

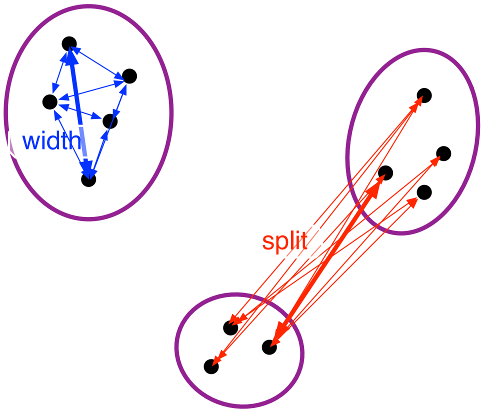


Figure 8.1: Example of clustering $\mathcal{C}(X) = \{S_1, S_2, S_3\}$.

8.2 Hierarchical/Agglomerative Clustering

The first type of clustering we study is *hierarchical*. The basic algorithm is:

> *If two points (clusters) are close (or close enough), put them in the same cluster. Repeat.*

A bit more formally, we can write this as an algorithm.

Algorithm 8.2.1 Hierarchical Clustering

```
Each $x_i \in X$ is a separate cluster $S_i$.
while Two clusters are close enough do
  Find the closest two clusters $S_i, S_j$
  Merge $S_i$ and $S_j$ into a single cluster
```

It remains to define *close enough* and *closest*. These both basically require a distance between clusters. There are several options:

- distance between *center* of clusters. What does *center* mean?
  - the mean (average) point.
  - the center-point (like a high-dimensional median)
  - center of the MEB (minimum enclosing ball)
  - some (random) representative point
- distance between closest pair of points
- distance between furthest pair of points
- average distance between all pairs of points in different clusters
- radius of minimum enclosing ball of joined cluster
- smallest average distance between points in a cluster and center in the other

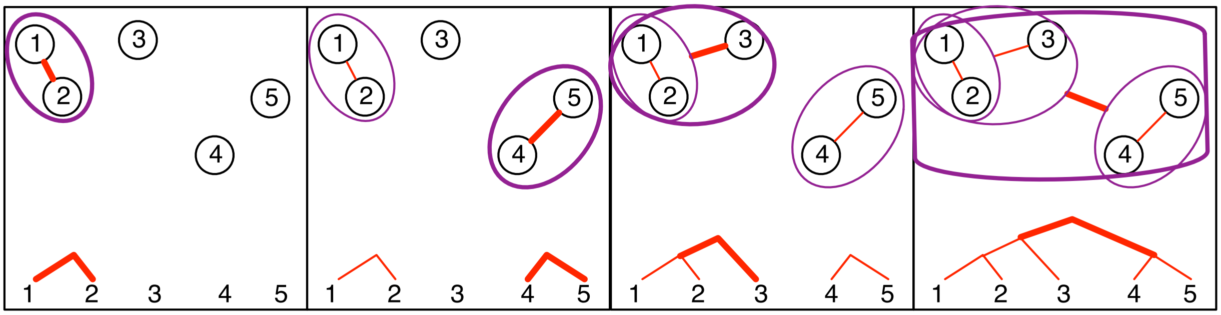
Among all clusters, there are often ties. Often break ties arbitrarily, but these choices can dramatically change the resulting clusters.

Finally we need to define *close enough*; this indicates some sort of threshold. There are again several options:

- If information is known about the data, perhaps some absolute value τ can be given.
- If the { diameter, or radius of MEB, or average distance from center point} is beneath some threshold. This fixes the scale of a cluster, which could be good or bad.
- If the *density* is beneath some threshold; where *density* is # points/volume or # points / radius^d
- If the joined (both clusters) density increases too much from single cluster density.
  Variations of this are called the "elbow" technique.
- When the number of clusters is k (for some magical value k).

8.2.1 Hierarchy

We can keep track of the order clusters are merged and build a *hierarchy* of clusterings. This can be useful structure beyond an opaque single partition of the data. This also means we do not need to (initially) choose when to stop. We can keep merging until there is only 1 cluster remaining. Then we can choose to "chop off the top of the tree" later.



The most famous example of this are phylogenic trees.

8.2.2 Efficiency

Lets use as an example where the distance between clusters is the distance between the centroids, and we stop when there is one cluster. For n points, this takes about n^3 time steps.

In each we make one merge, so there are $n - 1 = O(n)$ rounds. In each round with m clusters, we may need to check $\binom{m}{2}$ pairs, to find the closest pair. When $m < n/2$ (which if half of all rounds), then this takes about $n^2/4 = O(n^2)$ time each round. It then takes only at most n time to recompute the centroid. So the total cost is about $(n-1) \cdot n^2/4 = O(n^3)$.

We can reduce this to $O(n^2 \log n)$. We maintain a *priority queue* of the $\binom{m}{2} = O(n^2)$ distances. Each update takes the closest distance in $O(\log n)$ time, but then affects $O(n)$ distances in the queue. These take $O(n \log n)$ time total to update. Centroids can also be updated in $O(1)$ time (by storing the count and center point - they can be merged by taking the weighted average). So each round takes $O(n \log n)$ time, and the total process takes $O(n^2 \log n)$ time.

But this is still pretty slow (as we will see compared to other techniques).

8.3 Density-Based Clustering

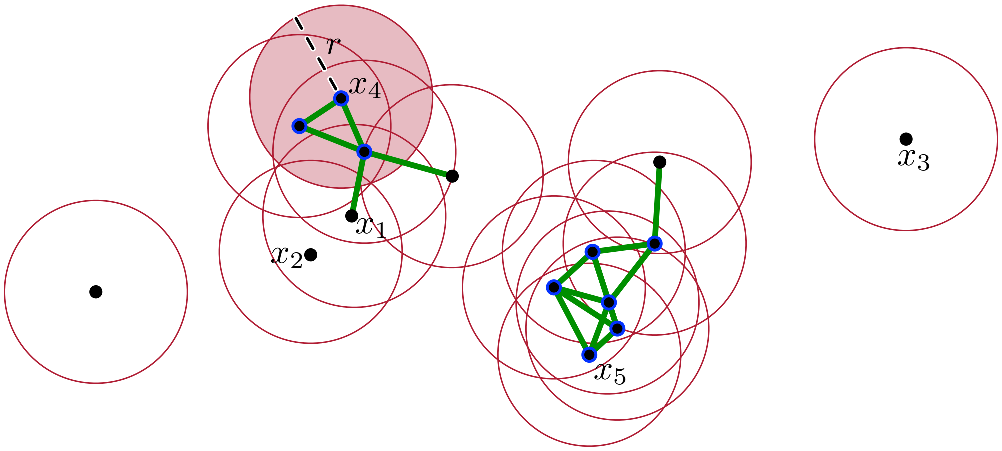
Density-based clustering can be seen as an efficient extension of hierarchical agglomerative clustering. The basic premise is that data points which are sufficiently closed should be assigned into the same cluster; however, at the behest of efficiency, it omits the building of an explicit hierarchy. It also adds a density requirement.

The most widely used variant is called *DBScan*. The algorithm has two parameters r (a radius, the literature usually uses ε) and τ (a density parameter, the literature usually uses minPts). Now given a data set X and a distance $\mathbf{d} : X \times X \to \mathbb{R}$, a point $x \in X$ is designated a *core point* if at least τ points from X are within a distance r from x. That is, x is a core point if $|\{x' \in X \mid \mathbf{d}(x, x') \leq r\}| \geq \tau$. These points are all in clusters.

Next we consider a *graph* $G = (X, E)$, where all data points are edges, and the edge set E has the following property. An edge $e_{i,j} \in E$ between points $x_i, x_j \in X$ if and only if (1) $\mathbf{d}(x_i, x_j) \leq \tau$ and (2) at least one of x_i or x_j is a core point.

Now each connected component of G is a cluster. Recall a *connected component* involving a point $x \in X$ includes all points $x' \in X$ that are *reachable* from x. And a point x' is reachable if there is a sequence $x_0, x_1, \ldots, x_k$ where $x_0 = x$, $x_k = x'$ and each consecutive pair x_j, x_{j+1} has an edge $e_{j,j+1} \in E$.

Example. An example data set X of $n = 15$ points. They are clustered using DBScan using a density parameters of $\tau = 3$, and radius r as illustrated in the balls. For instance x_4 is a core point, since there 3 points in the highlighted ball of radius r around it. All core points are marked, and the induced graph is shown.



Note that even though x_1 and x_2 are within a distance r, they are not connected since neither is a core point. The points with no edges, like x_2 and x_3, are not in any clusters. And there are two distinct clusters from the two connected components of the graph: point x_5 is in a different cluster than x_1 and x_4, which are in the same cluster.

Interpretation. So all core points (the points which are in dense enough regions) are in clusters, as well as any points close enough to those points. And points are connected in the same clusters if they are connected by a path through dense regions. This allows the clusters to adapt to the shape of the data.

However, there is no automated way to choose the parameters r and τ. This choice will greatly affect the shape, size, and meaning of the clusters. Also, this model also assumes that the notion of density is consistent throughout the dataset.

A major advantage of DBScan is that it can usually be computed efficiently. For each $x \in X$ we need to determine if it is a core points, and find neighbors, but these can usually quickly be accomplished with fast nearest neighbor search algorithms (e.g., LSH in Chapter 4.6). Then usually the connected components (the clusters) can be recovered without building the entire graph. However, in the worst case, the algorithm will have runtime quadratic in the n, the size of the data set.