CS 474/574 Machine Learning
7. Clustering

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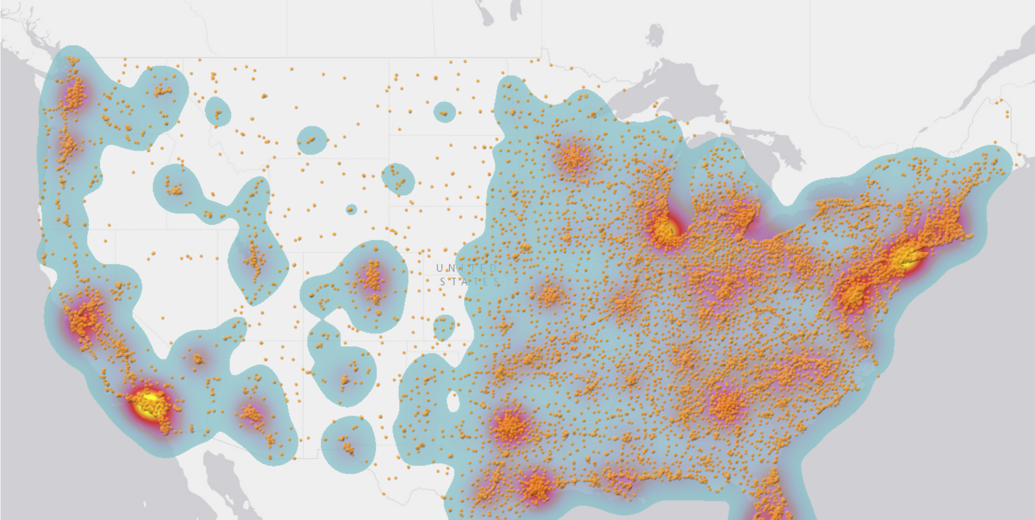
April 5, 2021

It's our nature to see clustering patterns

Distribution of Subway restuarants (Source: https://i.insider.com/58337a73ba6eb6b1018b5a71)



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- The algorithm stops after the centroids no longer changes or change is small enough.

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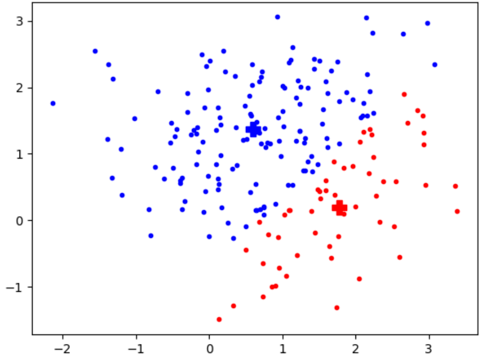
- The method just described above is called Naive k-means. There are many variants of it.

Demo

- Let's see a demo `kmeans.py`



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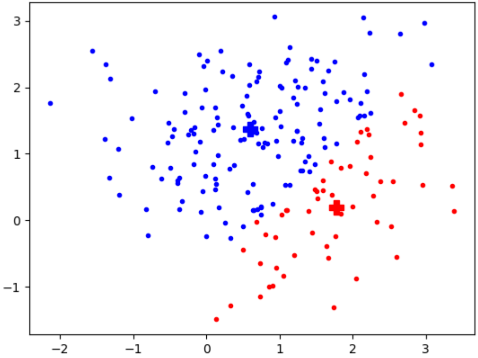
- A centroid (big crosses in the figure below) is NOT necessarily a sample, although it is initialized to a sample.



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- Note that the inter-cluster distance is re-evaluated at each iteration.

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- Let's go over the example on Wikipedia.
  https://en.wikipedia.org/wiki/Single-linkage_clustering#Working_example

Single-linkage clustering III

Algorithm 1: Single-linkage clustering

```
Initialize the distance matrix/dictionary D, and the distance dictionary δ ;
while D has more than one row or column do
    i, j ← arg min_{i,j}(D);
    d = min({D(x, y)|x ∈ i, y ∈ j});
    δ(i, j) = d/2;
    Remove columns and rows for i and j from D;
    Create a new column and new row for a new cluster k = i ∪ j;
    Populate the column and row for k in D;
return δ
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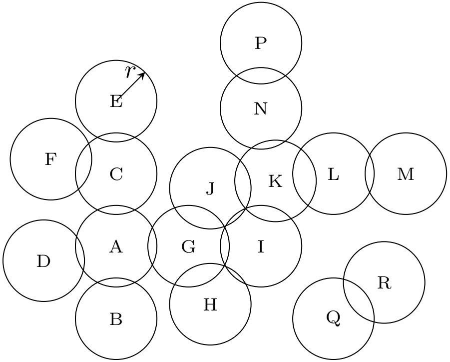
An example. Two samples are neighbors if their distance $< \epsilon$. For each sample, we draw a circle of radius $r = \epsilon/2$.



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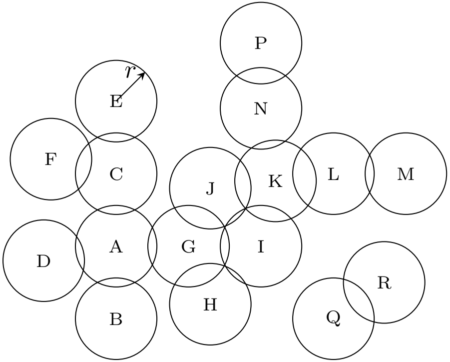

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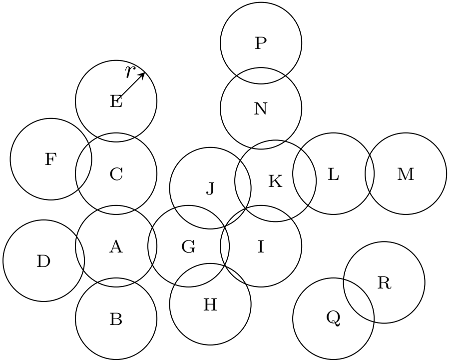

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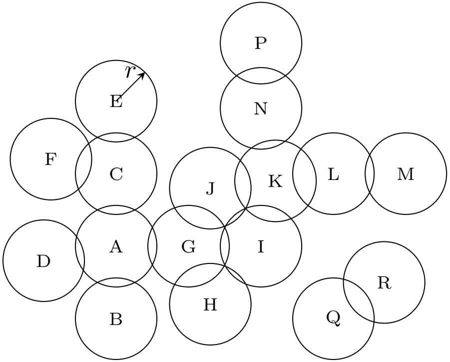
- How to measure "similar enough": distance (e.g., Euclidean) between samples below a threshold ϵ.

An example. Two samples are neighbors if their distance $< \epsilon$. For each sample, we draw a circle of radius $r = \epsilon/2$.



DBSCAN: a density-based clustering algorithm I

- Recall the Subway map earlier. A cluster has a higher density of samples than other parts.
- Density means enough similar samples over an area.
- How to measure density: Given a sample, count the number of samples similar enough to it.
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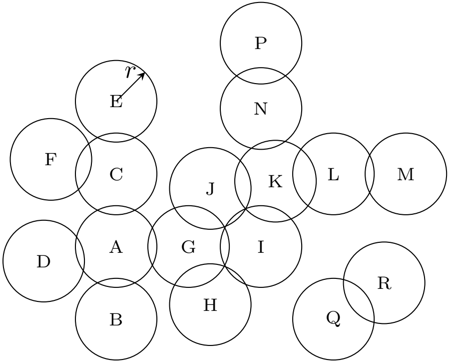

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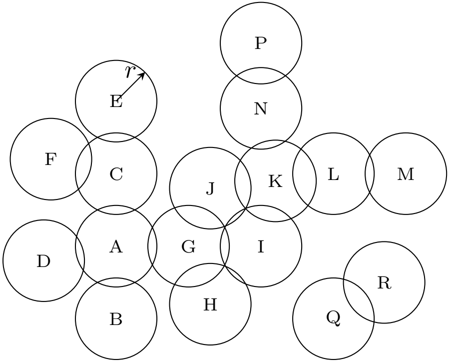

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- Idea 1: Neighbors of samples already in a cluster should be included in the cluster as well.
- Idea 2: But the expansion stops at a neighbor if it doesn't have enough neighbors – density not high enough.

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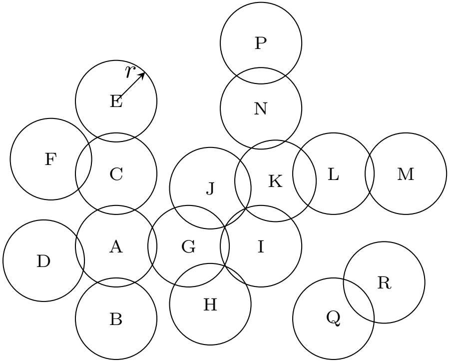
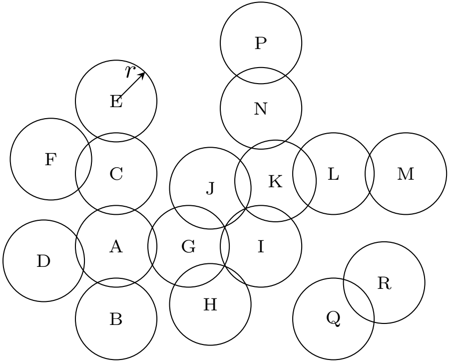


DBSCAN II: an example

1. Let $T = 2$. Denote a set S to hold cluster members to be examined. Initially $S = \{A\}$.

Two samples are neighbors if their distance $< \epsilon$. For each sample, we draw a circle of radius $r = \epsilon/2$.



DBSCAN II: an example

1. Let $T = 2$. Denote a set S to hold cluster members to be examined. Initially $S = \{A\}$.
2. Since A has more than T neighbors, create a cluster with A. And add A's neighbors, B, C, D, G into the cluster. Let $S = \{B, C, D, G\}$.

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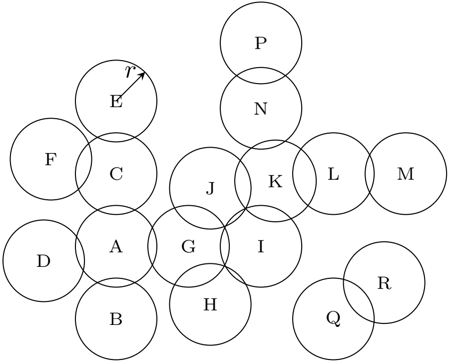

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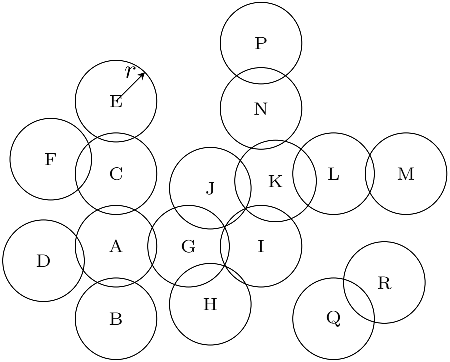

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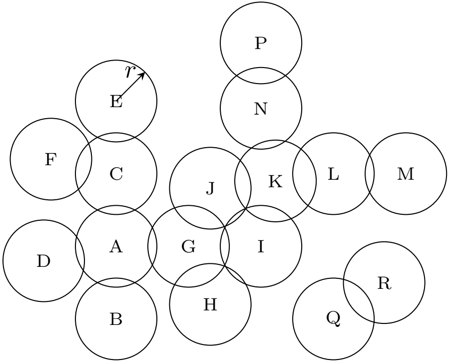

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5. Check whether each element of S has more than T neighbors. K passes the test, so add K's neighbor N, L (J, I already in the cluster) into the cluster. Let $S = \{N, L\}$.

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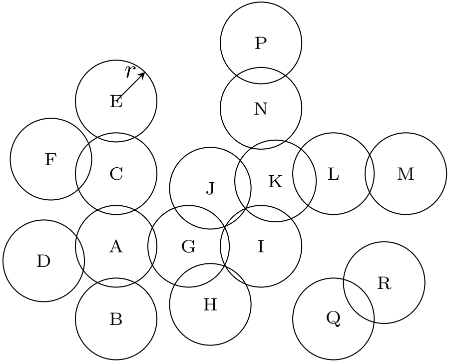

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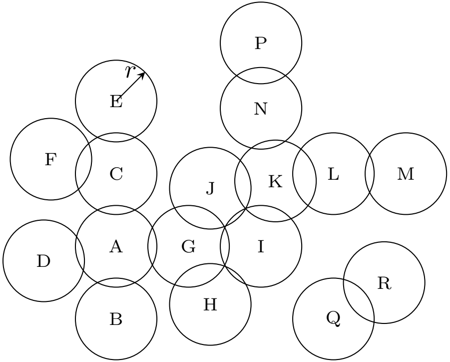
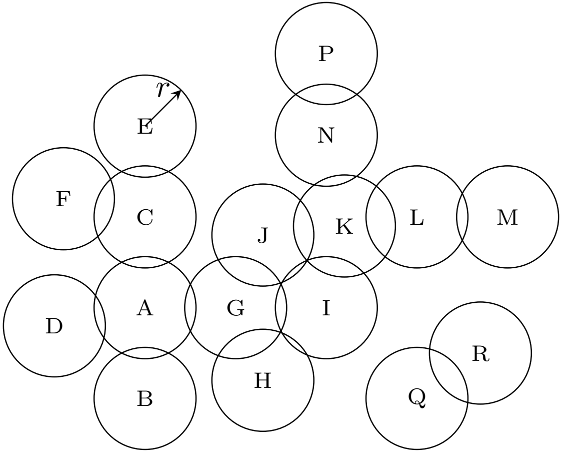
5. Check whether each element of S has more than T neighbors. K passes the test, so add K's neighbor N, L (J, I already in the cluster) into the cluster. Let $S = \{N, L\}$.
6. Check whether each element of S has more than T neighbors. N, L both fail the test. No more expansions.

Two samples are neighbors if their distance $< \epsilon$. For each sample, we draw a circle of radius $r = \epsilon/2$.

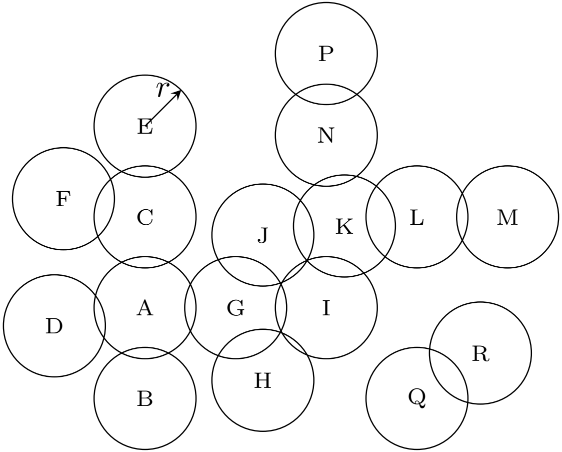


DBSCAN III : an example



- What if we start from Q?

DBSCAN III : an example



- What if we start from Q?
- Because it has less than $T = 2$ neighbors, no cluster will be created from it.

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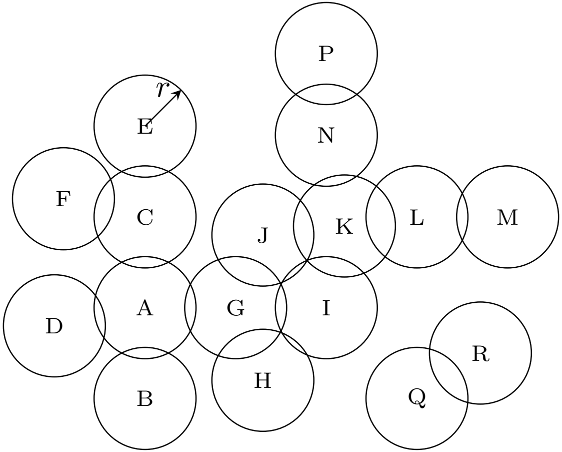

- What if we start from Q?
- Because it has less than $T = 2$ neighbors, no cluster will be created from it.
- Unlike in k-means or hierarchical clustering, not every sample becomes part of a cluster.

DBSCAN IV

Algorithm 2: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
    if x *are NOT assigned to a cluster* **then**
        $N(x) \leftarrow$ neighbors of x ;
        if $|N(x)| > T$ **then**
            Assign x to cluster i;
            Seed set of cluster i: $S \leftarrow N(x)$;
            while $S \neq \emptyset$ **do**
                $y \leftarrow$ one element of S;
                Assign y to cluster i;
                Remove y from S;
                if $|N(y)| > T$ **then**
                    $S \leftarrow S \cup N(y)$;
        i++;

- $N(\cdot)$: a function to compute a sample's neighbors

DBSCAN IV

Algorithm 3: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;

foreach *sample* $x \in X$ **do**

- **if** x *are NOT assigned to a cluster* **then**
  - $N(x) \leftarrow$ neighbors of x ;
  - **if** $|N(x)| > T$ **then**
    - Assign x to cluster i;
    - Seed set of cluster i: $S \leftarrow N(x)$;
    - **while** $S \neq \emptyset$ **do**
      - $y \leftarrow$ one element of S;
      - Assign y to cluster i;
      - Remove y from S;
      - **if** $|N(y)| > T$ **then**
        - $S \leftarrow S \cup N(y)$;
  - i++;

- $N(\cdot)$: a function to compute a sample's neighbors
- Neighbors to a sample are those in close proximity, e.g., in Euclidean distance.

DBSCAN IV

Algorithm 4: Slightly varied DBSCAN

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Initialize cluster index $i \leftarrow 1$;
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- $N(\cdot)$: a function to compute a sample's neighbors
- Neighbors to a sample are those in close proximity, e.g., in Euclidean distance.
- The While-loop is basically a BFS or a DFS, which exhaustively expands a cluster from a sample x.

DBSCAN IV

Algorithm 5: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
  if x *are NOT assigned to a cluster* **then**
    $N(x) \leftarrow$ neighbors of x ;
    if $|N(x)| > T$ **then**
      Assign x to cluster i;
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      while $S \neq \emptyset$ **do**
        $y \leftarrow$ one element of S;
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- Neighbors to a sample are those in close proximity, e.g., in Euclidean distance.
- The While-loop is basically a BFS or a DFS, which exhaustively expands a cluster from a sample x.
- The expansion stops when all samples in the cluster either have all their neighbors visited, or few enough ($< T$) neighbors.

DBSCAN IV

Algorithm 6: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
    if x *are NOT assigned to a cluster* **then**
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        if $|N(x)| > T$ **then**
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- $N(\cdot)$: a function to compute a sample's neighbors
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- The expansion stops when all samples in the cluster either have all their neighbors visited, or few enough ($< T$) neighbors.
- Cluster members with enough neighbors are called **core points** (such as A, G, J, I in the example earlier) while those without enough neighbors are called **non-core points** (such as E, F, D, B, H, N, L).

DBSCAN IV

Algorithm 7: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
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        $N(x) \leftarrow$ neighbors of x ;
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- Originally published in 1996. Won 2014 SIGKDD Time of Test Award. A follow-up paper won 2015 SIGMOD Best Paper Award.

DBSCAN IV

Algorithm 8: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
    if x *are NOT assigned to a cluster* **then**
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- Originally published in 1996. Won 2014 SIGKDD Time of Test Award. A follow-up paper won 2015 SIGMOD Best Paper Award.
- Why you should still use DBSCAN, ACM Trans. on Database Systems, 42(3):21, 2017

DBSCAN V

Algorithm 9: Slightly varied DBSCAN

Data: X: samples, T: a threshold

Initialize cluster index $i \leftarrow 1$;
foreach *sample* $x \in X$ **do**
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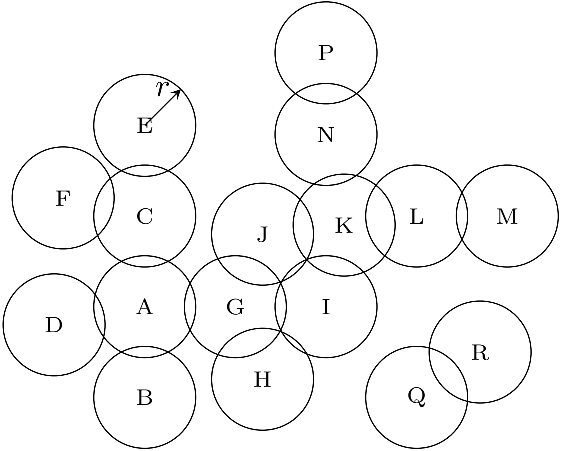
                    $S \leftarrow S \cup N(y)$;
        i++;

An example (radii of circles are half of T)



Other clustering approaches

- Mean-shift

Reading materials

- https://scikit-learn.org/stable/modules/clustering.html