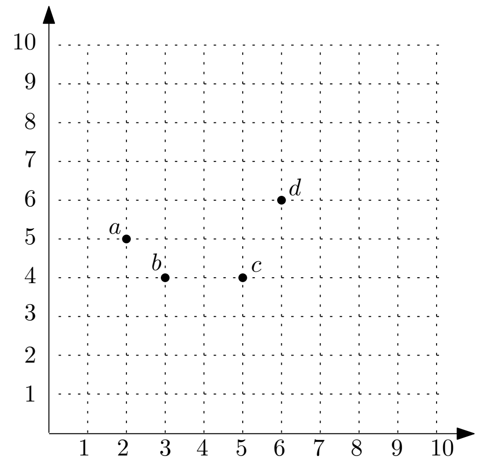
CMSC5724: Exercise List 9

Answer Problems 1-2 based on the following dataset:



Problem 1. Recall that, in discussing hierarchical clustering, we introduced 3 distance metrics on two sets of points: *min*, *max*, and *mean*. Let $S_1 = \{a, c\}$ and $S_2 = \{b, d\}$. What is the distance between S_1 and S_2 under those three metrics, respectively (assuming that the distance of two points is calculated by Euclidean distance)?

Answer.
Min: $\sqrt{2}$, as is the distance between a and b.
Max: $\sqrt{17}$, as is the distance between a and d.
Mean: $(\sqrt{2} + \sqrt{17} + 2 + \sqrt{5})/4$, as is the average of $dist(a, c)$, $dist(a, d)$, $dist(c, b)$ and $dist(c, d)$.

Problem 2. Show the dendrogram returned by the Agglomerative algorithm under the min and max metrics, respectively.

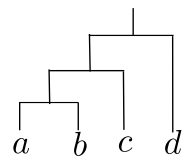
Answer.
Min. At the beginning of the algorithm, each point is regarded as a singleton cluster. In other words, there are 4 clusters, whose mutual distances are given by:

	a	b	c	d
a	-	$\sqrt{2}$	$\sqrt{10}$	$\sqrt{17}$
b	-	-	2	$\sqrt{13}$
c	-	-	-	$\sqrt{5}$

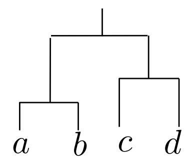
Since a and b have the smallest distance (among all pairs of clusters), the algorithm merges the two points into a cluster which we denote as S_1. Now, there are 3 clusters left, whose mutual distances are:

	S_1	c	d
S_1	-	2	$\sqrt{13}$
c	-	-	$\sqrt{5}$

Hence, the algorithm merges S_1 with c into a cluster which we denote as S_2. Now that there are only two clusters left (i.e., S_2 and d), the last merge is trivial. The following dendrogram illustrates the above process.



Max. Repeating the above algorithm with respect to max results in the following dendrogram:



Problem 3. Suppose that we use d_{min} to define the similarity of two clusters C_1, C_2. Give an algorithm to compute the dendrogram on n points in $O(n^2 \log n)$ time.

Answer. Our algorithm maintains a BST T at any moment that stores the distances of all pairs of the current clusters.

At the beginning, each object forms a cluster by itself. Hence, T contains $\binom{n}{2}$ cluster-pair distances.

Consider, in general, that the current clusters are $C_1, C_2, ..., C_k$. We remove the smallest cluster-pair distance from T. Suppose that this is the distance between C_i and C_j. Then:

- We merge C_i and C_j into a new cluster C_{new}.
- Delete from T the distance between C_i and every other cluster. Do the same for C_j.
- Insert into T the distance between C_{new} and every other existing cluster C (i.e., $C_1, ..., C_k$ except C_i, C_j).

To implement the above, the key is to compute $d(C_{new}, C)$, namely, the distance between C_{new} and C. We achieve the purpose as follows:

$$d_{min}(C_{new}, C) \quad = \quad \min\{d_{min}(C_i, C), d_{min}(C_j, C)\}$$

In summary, when there are $k \geq 2$ clusters left, the next merge requires:

- Removing the minimum distance from T
- Deleting $O(k)$ distances into T
- Inserting $O(k)$ distances into T.

The total time for the above operations is $O(k \log k^2) = O(k \log k)$ (notice that T stores $O(k^2)$ distances).

Therefore, the total running time of our algorithm is

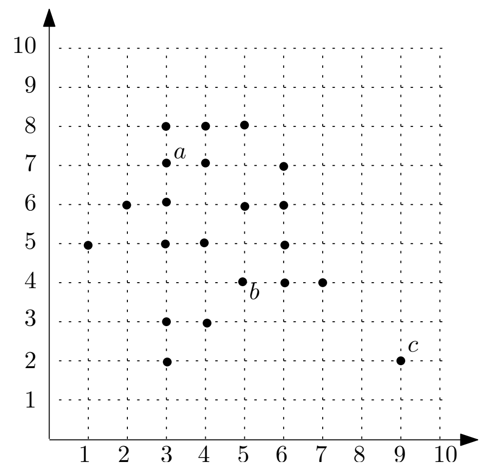
$$\sum_{k=2}^{n} O(k \log k) \quad = \quad O(n^2 \log n).$$

Problem 4. Suppose that we use d_{mean} to define the similarity of two clusters C_1, C_2. As discussed in the lecture, $d_{mean}(C_1, C_2) = \frac{1}{|C_1||C_2|} \sum_{(p_1,p_2) \in C_1 \times C_2} dist(p_1, p_2)$. Give an algorithm to compute the dendrogram on n points in $O(n^2 \log n)$ time.

Answer. The algorithm is precisely the same as the one in Problem 3, but with one change. Recall that the key to ensure $O(n^2 \log n)$ time is to compute $d(C_{new}, C)$ in constant time from $d(C_i, C)$ and $d(C_j, C)$ when we merge together C_i and C_j into C_{new}. When $d = d_{mean}$, we can do so as follows:

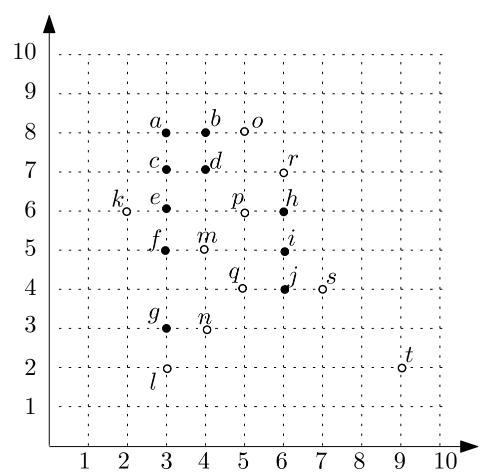
$$d_{mean}(C_{new}, C) \quad = \quad \frac{|C_i| \cdot d_{mean}(C_i, C) + |C_j| \cdot d_{mean}(C_j, C)}{|C_i| + |C_j|}.$$

Problem 5. Consider the set P of points below:

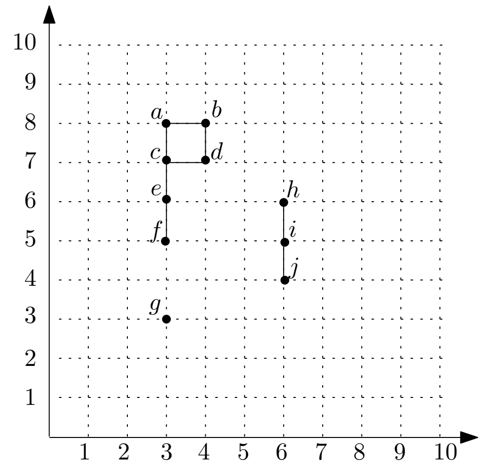


Set $\epsilon = 1$ and $minpts = 3$. Show the clusters output by DBSCAN, assuming that the distance metric is Euclidean distance.

Answer. First, identify the core and non-core points, shown below in black and white, respectively.



Then, the algorithm temporarily ignores the non-core points, and draws an edge between each pair of core points that are within distance $r = 1$. This creates a graph:



It proceeds by computing the connected components of the graph. In the above graph, there are 3 connected components: $C_1 = \{a, b, c, d, e, f\}$, $C_2 = \{g\}$, and $C_3 = \{h, i, j\}$.

C_1, C_2 and C_3 form a cluster, respectively. In the final step, the algorithm assigns each non-core point z to each cluster that contains a core point whose neighborhood covers z. Consider, for example, point m. It is added to P_1 because m is in the neighborhood of f. After assigning all the non-core points, we get $\{a, b, c, d, e, f, k, m, o\}$, $\{g, n, l\}$, $\{h, i, j, p, q, r, s\}$ as the final clusters. Note that point t is regarded as noise.

Problem 6. Given a pair of parameters ϵ and *minpts*, describe an algorithm to compute the DBSCAN clusters in $O(n^2)$ time, assuming that the distance metric is Euclidean distance, and that the dimensionality of the data space is a constant.

Answer. First, compute the distance graph. Then, discard all the edges whose weights are more than ϵ. All these can be done in $O(n^2)$ time. Let G be the graph obtained at this moment.

For each vertex, get its degree in G. It is a core point if its degree is at least $minpts - 1$. Otherwise, it is a non-core point. Remove the non-core points from G and their edges. Let G' be the graph obtained at this moment. All these can be done in $O(n^2)$ time.

Now, compute the connected components of G', which takes $O(n^2)$ time. Treat each connected component as a cluster.

For every non-core point u, look at its neighbors in G. If u has a core-point neighbor v, add u to the cluster of v. Doing so for all the u takes $O(n^2)$ time in total.