Clustering: Centroid-Based Partitioning

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In this lecture, we will discuss another fundamental topic in data mining: **clustering**.

At a high level, the objective of clustering can be stated as follows. Let \( P \) be a set of objects. We want to divide \( P \) into several groups—each of which is called a **cluster**—satisfying the following conditions:

- **(Homogeneity)** Objects in the same cluster should be similar to each other.
- **(Heterogeneity)** Objects in different clusters should be dissimilar.
Typically, the similarity between two objects $o_1, o_2$ is measured by a distance function $dist(o_1, o_2)$: the larger $dist(o_1, o_2)$, the less similar they are.

We will consider only distance functions satisfying the triangle inequality, namely, for any objects $o_1, o_2, o_3$, it holds that:

$$\text{dist}(o_1, o_2) + \text{dist}(o_2, o_3) \geq \text{dist}(o_1, o_3)$$
Today we will focus on **centroid-based partitioning**, which works as follows. Let \( k \) be the number of clusters desired. It first identifies \( k \) objects \( c_1, ..., c_k \) (which are not necessarily in \( P \)) called **centroids**. Then, it forms clusters \( P_1, P_2, ..., P_k \) where \( P_i \) includes all the objects in \( P \) that have \( c_i \) as their nearest centroid. Formally:

\[
P_i = \{ o \in P \mid \text{dist}(o, c_i) \leq \text{dist}(o, c_j) \ \forall j \in [1, k] \}\]

If an object \( o \) happens to be equi-distance from two centroids \( c_i, c_j \), it can be assigned to either \( P_i \) or \( P_j \) arbitrarily.
We will discuss two classic algorithms of centroid-based partitioning:

1. *k*-center
2. *k*-means
$k$-center
Problem

Let $P$ be a set of $n$ objects in $\mathbb{R}^d$, and $k$ be an integer at most $n$. Let $C$ be a set of objects in $\mathbb{R}^d$; we refer to $C$ as a centroid set. Define for each object $o \in P$, its centroid distance as

$$d_C(o) = \min_{c \in C} \text{dist}(o, c).$$

The radius of $C$ is defined to be

$$r(C) = \max_{o \in P} d_C(o).$$

The goal of the $k$-center problem is to find a centroid set $C$ of size $k$ with the minimum radius.
This problem is **NP-hard**, namely, no algorithm can solve the problem in time polynomial to both $n$ and $k$ (unless $P = NP$). Hence, we will aim to find approximate answers with precision guarantees.

Let $C^*$ be an optimal centroid set for the $k$-center problem. A set $C$ of $k$ objects is $\rho$-approximate if $r(C) \leq \rho \cdot r(C^*)$. We will give an algorithm that guarantees to return a 2-approximate solution.
A 2-Approximate Algorithm

**algorithm** \( k \)-center \((P)\)

/* this algorithm returns a 2-approximate subset \( C \) */

1. \( C \leftarrow \emptyset \)
2. add to \( C \) an arbitrary object in \( P \)
3. for \( i = 2 \) to \( k \)
4. \( o \leftarrow \) an object in \( P \) with the maximum \( d_C(o) \)
5. add \( o \) to \( C \)
6. return \( C \)

The algorithm can be easily implemented in \( O(nk) \) time.
Example

Example: $k = 3$

Initially, $C = \{c_1\}$
Example

Example: \( k = 3 \)

After a round, \( C = \{ c_1, c_2 \} \)
Example

Example: $k = 3$

After another round, $C = \{c_1, c_2, c_3\}$
Example

Example: $k = 3$

$r(C)$ is the radius of the largest circle.
Theorem

The $k$-center algorithm is 2-approximate.

Proof

Let $C^* = \{c_1^*, c_2^*, ..., c_k^*\}$ be an optimal centroid set, i.e., it has the smallest radius $r(C^*)$. Let $P_1^*, P_2^*, ..., P_k^*$ be the optimal clusters, namely, $P_i^* \ (1 \leq i \leq k)$ contains all the objects that find $c_i^*$ as the closest centroid among all the centroids in $C^*$.

Let $C = \{c_1, c_2, ..., c_k\}$ be the output of our algorithm. We want to prove $r(C) \leq 2r(C^*)$. 
Case 1: \( C \) has an object in each of \( P_1^*, P_2^*, ..., P_k^* \).

Take any object \( o \in P \). We will prove that \( d_C(o) \leq 2r(C^*) \), which in turn will establish the fact that \( r(C) \leq 2r(C^*) \).

Suppose that \( o \in P_i^* \) (for some \( i \in [1, k] \)), and \( c \) is an object in \( C \cap P_i^* \). It holds that:

\[
\begin{align*}
    d_C(o) & \leq dist(c, o) \\
           & \leq dist(c, c^*) + dist(c^*, o) \\
           & \leq 2r(C^*).
\end{align*}
\]
Proof (cont.).

Case 2: At least one of $P_1^*, ..., P_k^*$ covers no object in $C$. By the pigeon hole principle, one of $P_1^*, ..., P_k^*$ must cover at least two objects $c_1, c_2 \in C$. It thus follows that

$$dist(c_1, c_2) \leq 2r(C^*).$$

Next we will prove $r(C) \leq dist(c_1, c_2)$ which will complete the whole proof.

Without loss of generality, assume that $c_2$ was picked after $c_1$ by our algorithm. Hence, $c_2$ has the largest centroid distance at this moment (by how our algorithm runs). Therefore, any object $o \in P$ has a centroid distance at most $dist(c_1, c_2)$ at this moment. Its centroid distance can only decrease in the rest of the algorithm. It thus follows that $r(C) \leq dist(c_1, c_2)$. $\square$
$k$-means
The $k$-means problem is defined only on point objects.

**Problem**

Let $P$ be a set of $n$ points (a.k.a. objects), and $k$ be an integer at most $n$. Let $C$ be a set of points in $\mathbb{R}^d$; we refer to $C$ as a **centroid set**. Define for each object $o \in P$ its **centroid distance** as

$$d_C(o) = \min_{c \in C} \text{dist}(o, c)$$

where $\text{dist}(o, c)$ is the straight line distance between $p$ and $c$. The **cost** of $C$ is defined to be

$$\phi(C) = \sum_{o \in P} d_C^2(o).$$

The goal of the $k$-means problem is to find a centroid set $C$ of size $k$ with the minimum cost.

The problem is once again NP-hard.
**algorithm** $k$-means ($P$)

1. $C \leftarrow$ an arbitrary subset of $P$ with size $k$
2. repeat
3. $C_{old} \leftarrow C$
   /* assume $C_{old} = \{c_1, ..., c_k\}$ */
4. partition $P$ into $P_1, ..., P_k$ such that $P_i$ ($1 \leq i \leq k$) is the set of objects that find $c_i$ as the nearest centroid (among the centroids in $C_{old}$). if an object $o$ is equi-distant from two centroids $c_i$ and $c_j$, it is assigned to $P_i$ or $P_j$ arbitrarily
5. for $i = 1$ to $k$
6. $c_i \leftarrow$ the geometric center of $P_i$
7. $C = \{c_1, ..., c_k\}$
8. until $C_{old} = C$
9. return $C$

Remark: The **geometric center** of a point set $P$ is the point whose $i$-th coordinate is the average of all the $i$-th coordinates of the points in $P$. 
Example

Suppose $k = 2$. Points $c'_1$ and $c'_2$ are the initial two centroids which are chosen arbitrarily.

Round 1.

$P_1$ includes all the black points (they are closer to $c'_1$ than $c'_2$), and $P_2$ the red points. $c_1$ and $c_2$ are the new centroids.
Example

Points $c'_1$ and $c'_2$ are the two centroids from the last round.

Round 2.

$P_1$ includes all the black points, and $P_2$ the red points. $c_1$ and $c_2$ are the new centroids.
Example

Points $c'_1$ and $c'_2$ are the two centroids from the last round.

Round 3.

$P_1$ includes all the black points, and $P_2$ the red points. The new centroids $c_1$ and $c_2$ are identical to $c'_1$ and $c'_2$, respectively. The algorithm therefore terminates.
An important question to answer is whether the $k$-means algorithm can run forever. Next we will prove that it will not, namely, it will always terminate.

We will need the lemma below:

**Lemma**

Let $P$ be a set of points in $\mathbb{R}^d$, and $c$ the geometric center of $P$. For any point $q \in \mathbb{R}^d$ such that $q \neq c$, it holds that

$$\sum_{p \in P} (\text{dist}(c, p))^2 < \sum_{p \in P} (\text{dist}(q, p))^2.$$ 

The proof is elementary, and omitted. **Hint:** take the derivative of $\sum_{p \in P} (\text{dist}(q, p))^2$ with respect to each coordinate of $q$. 

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Theorem

The $k$-means algorithm always terminates.

Proof

First observe that there can be only a finite number of centroid sets that can possibly be produced at the end of each round (think: why?). We will show that after each round, the cost of the centroid set is strictly lower than that of the old centroid set, unless the two centroid sets are identical. This implies that the algorithm must terminate eventually.
Proof (Continued.)

Let $C_{\text{old}} = \{c'_1, ..., c'_k\}$ be the old centroid set at the beginning of a round. By definition, its cost equals $\phi(C_{\text{old}}) = \sum_{o \in P}(d_{C_{\text{old}}}(o))^2$. Let $P_1, ..., P_k$ be the partitions obtained at Line 4 of the algorithm in Slide 19. We can thus rewrite $\phi(C_{\text{old}})$ as:

$$\phi(C_{\text{old}}) = \sum_{i=1}^{k} \sum_{o \in P_i}(\text{dist}(o, c'_i))^2$$

Let $C = \{c_1, ..., c_k\}$ be the new centroid set obtained at Line 7. By the lemma of the previous slide, we know

$$\sum_{o \in P_i}(\text{dist}(o, c'_i))^2 \geq \sum_{o \in P_i}(\text{dist}(o, c_i))^2$$

where the equality holds only if $c'_i = c_i$. In other words, if $C_{\text{old}} \neq C$, then $\phi(C_{\text{old}}) > \sum_{i=1}^{k} \sum_{o \in P_i}(\text{dist}(o, c_i))^2$. 
Proof (Continued.)

By definition, \( d_C(o) \leq \text{dist}(o, c_i) \) where \( o \) is an object in \( P_i \). Hence,

\[
\sum_{i=1}^{k} \sum_{o \in P_i} (\text{dist}(o, c_i))^2 \geq \sum_{i=1}^{k} \sum_{o \in P_i} (d_C(o))^2
\]

\[
= \phi(C)
\]

We thus have shown \( \phi(C_{old}) > \phi(C) \), which completes the whole proof.
The rest of the slides will be tested in the quizzes and final exam.
Let $C^*$ be an optimal centroid set for the $k$-means problem. A centroid set $C$ is said to be $\rho$-approximate if $\phi(C) \leq \rho \cdot \phi(C^*)$.

The $k$-means algorithm on Slide 28 does not have a bounded approximation ratio. In other words, the centroid set $C$ it returns can have a cost that is greater than $\phi(C^*)$ by an arbitrarily large ratio (i.e., $\rho = \infty$).

Next, we describe a technique to choose the initial centroid set carefully, which will lead to a good approximation ratio.
In the algorithm of Slide 19, replace the centroid set $C$ at Line 1 with the centroid set returned by the following algorithm.

**algorithm** $k$-seeding ($P$)

1. $c \leftarrow$ a random point chosen uniformly from $P$
2. $C = \{c\}$
3. **for** $i = 2$ **to** $k$
4. $c \leftarrow$ a point from $P$ chosen as follows: each $p \in P$ is chosen as $c$
   with probability $\frac{(d_c(p))^2}{\sum_{p' \in P}(d_c(p'))^2}$
5. **if** $c \notin C$ **then**
6.    add $c$ to $C$
7. **else** go to Line 4
8. **return** $C$
It is known that a centroid set chosen as in the previous slide already guarantees an $O(\log k)$ approximation ratio in expectation.

The proof falls out of the scope of this course, but can be found in: David Arthur, Sergei Vassilvitskii: k-means++: the advantages of careful seeding. SODA 2007: 1027-1035.

In practice, one can run $k$-means by using the above centroid set as the initial centroid set. Remember $k$-means strictly improves the quality of the centroid set after every single round.