Clustering

Anil Maheshwari

anil@scs.carleton.ca
School of Computer Science
Carleton University
Canada

Introduction

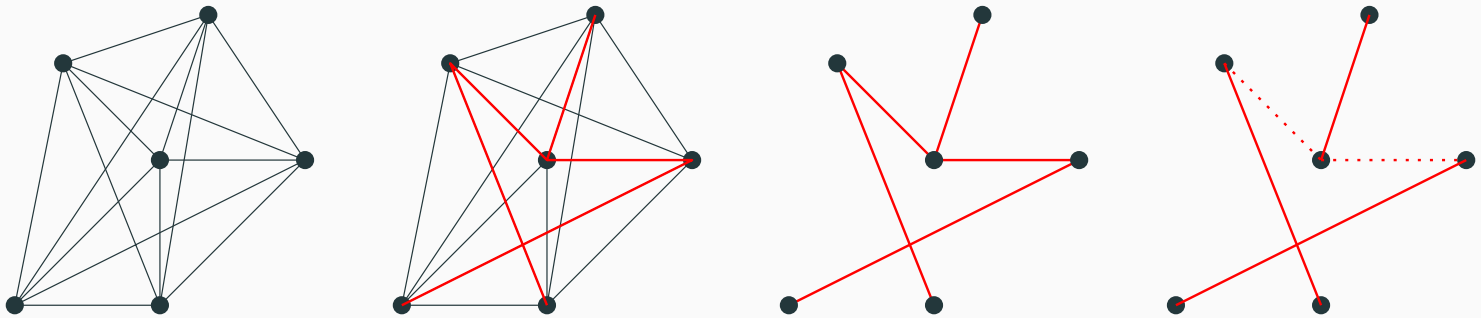
Clustering Problem

Input: A set $X = \{x_1, \ldots, x_n\}$ of n objects. For every pair $x_i, x_j \in X$, we have the distance $d(x_i, x_j) \geq 0$ such that $d(x_i, x_i) = 0$ and $d(x_i, x_j) = d(x_j, x_i)$.

Problem: Divide objects in X into k non-empty groups such that the *gap* between the groups is as large as possible. Distance between two groups is defined as the smallest distance between pair of points, where in the pair points belong to different groups.

Solution

1. Define a complete graph $G = (V = X, E)$, where each edge $e = (x_i, x_j)$ has a weight $d(x_i, x_j)$.
2. Construct a minimum spanning tree T of G
3. Delete $k - 1$ most expensive edges from T
4. Output the resulting k-connected components $C_1, \ldots, C_k$



Claim

The components $C_1, \ldots, C_k$ constitute a k-clustering of X that maximizes the gap.

K-Means Clustering Problem

Input: A set $X = \{x_1, \ldots, x_n\}$ of n-points in $\mathbb{R}^d$. An integer $0 < k \leq n$.

Objective: Partition X into k non-empty clusters $C_1, \ldots, C_k$. Points within a cluster should be *close* to each other compared to points outside the cluster.

Let $C_1, \ldots, C_k$ be a k-clustering of X with centers $\mathcal{C} = \{c_1, \ldots, c_k\}$, where $c_i \in \mathbb{R}^d$.

Define the potential function $\Phi(\mathcal{C}) = \sum_{x \in X} \min_{c \in \mathcal{C}} d(x, c)^2 = \sum_{x \in X} \min_{c \in \mathcal{C}} ||x - c||^2$

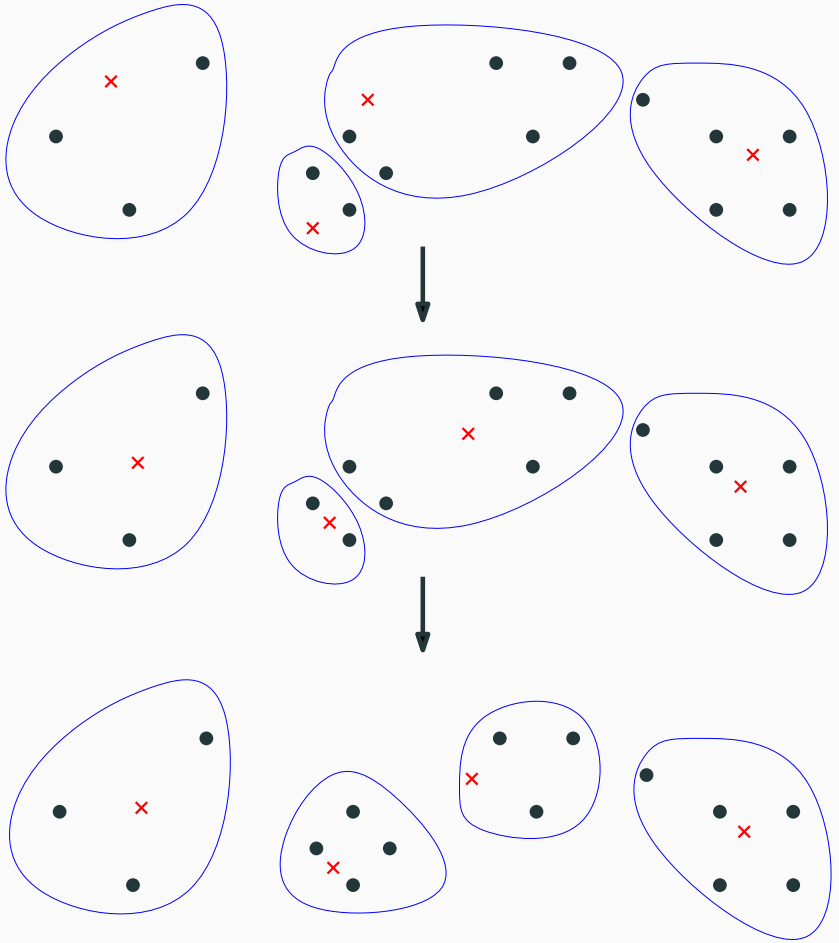
$\Phi(\mathcal{C})$= Sum of the squared distance between each point x in X to its nearest center in $\mathcal{C}$

Problem:
Given X and k, find k-centers $\mathcal{C}$ such that the corresponding clustering $C_1, \ldots, C_k$ minimizes $\Phi(\mathcal{C})$

Llyod's Heuristic

1. Select Initial *Centers*: Arbitrary choose k-centers and initialize $\mathcal{C} = \{c_1, \ldots, c_k\}$
2. Partition X: Compute sets $C_1, \ldots, C_k$ with respect to centers in $\mathcal{C}$. Point $x \in X$ is assigned to the cluster C_i if x's nearest center in $\mathcal{C}$ is c_i.
3. Recompute Centers: For each $i \in \{1, \ldots, k\}$, set c_i (the new cluster center) to be the center of the mass of points in C_i
4. Repeat Steps 2 & 3 till $\mathcal{C}$ no longer changes

An illustration of a Phase of Llyod's Algorithm



Observations

Decrease in Potential

Each execution of Steps 2 & 3 decrease the value of the potential function.

Proof: We will use the following Lemma.

Lemma 1

Consider a set of points S. Let m^* denote the center of mass of S. Let z be an arbitrary point. Define $\Delta(S, z) = \sum_{x \in S} d(x, z)^2$. Then

$\Delta(S, z) = \Delta(S, m^*) + |S| d(m^*, z)^2$

Corollary 1

If S is a single cluster with initial center z, then moving the cluster center to m^* reduces the potential as $\Delta(S, z) - \Delta(S, m^*) = |S| d(m^*, z)^2 \geq 0$

Proof of Lemma

Lemma 1

$\Delta(S, z) = \Delta(S, m^*) + |S|d(m^*, z)^2$, where m^* is center of mass of S and z is an arbitrary point

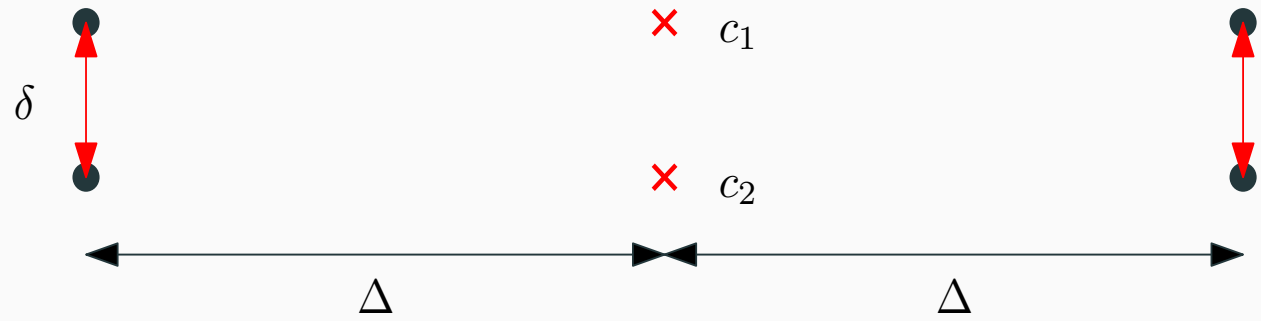
Proof: Assume we are in 2-dimensions. Let $z = (z_x, z_y)$ and $S = \{p_1, \ldots, p_n\}$, where $p_i = (x_i, y_i)$.

1. $m^* = \left(\frac{\sum\limits_i x_i}{n}, \frac{\sum\limits_i y_i}{n} \right)$
2. $\Delta(S, z) = \sum\limits_{p \in S} d(p, z)^2 = \sum\limits_{p=(x_i, y_i) \in S} \left((x_i - z_x)^2 + (y_i - z_y)^2 \right)$
3. $\Delta(S, m^*) = \sum\limits_{p \in S} d(p, m^*)^2 = \sum\limits_i \left(x_i - \frac{\sum x_i}{n} \right)^2 + \sum\limits_i \left(y_i - \frac{\sum y_i}{n} \right)^2$
4. $\Delta(S, z) - \Delta(S, m^*)$
   $= nz_x^2 + nz_y^2 - 2z_x \sum x_i - 2z_y \sum y_i + n \left(\frac{\sum x_i}{n} \right)^2 + n \left(\frac{\sum y_i}{n} \right)^2$
   $= n \left[z_x^2 + z_y^2 - 2z_x \frac{\sum x_i}{n} - 2z_y \frac{\sum y_i}{n} + \left(\frac{\sum x_i}{n} \right)^2 + \left(\frac{\sum y_i}{n} \right)^2 \right]$
   $= |S|d(m^*, z)^2$

□

Is competitive ratio of Llyod's heuristic bounded?

Let $\Phi(\mathcal{C}^*)$ be the potential of an optimal clustering and let $\Phi(\mathcal{C})$ be the potential of the clustering returned by Llyod's heuristic.



Competitive Ratio

Competitive ratio of Llyod's heuristic is unbounded, i.e. $\frac{\Phi(\mathcal{C})}{\Phi(\mathcal{C}^*)} \to \infty$

How to choose initial centers?

Question: How to choose initial centers so that we are guaranteed to have some bounded competitive ratio with respect to optimum?

k-means++ Algorithm

Let $D(x)$= Shortest distance from x to the nearest center among the current set of centers.

k-Means++ Algorithm:

Step 1: Choose an initial cluster center c_1 uniformly at random from X.

Step 2: (**Randomization Step**) Choose the next center c_i by selecting a point $x \in X$ with probability $\frac{D(x)^2}{\sum_{y \in X} D(y)^2}$

Step 3: Repeat Step 2 till k centers are chosen

Step 4: Execute Llyod's Heuristic by choosing $\{c_1, \ldots, c_k\}$ as the initial centers

Observations

1. In the Randomization Step, the points of X that are farther from the currently chosen centers have a higher chance of being selected.
2. The algorithm is $8(\ln k + 2)$-competitive. Let the k-centers returned by k-means++ algorithm be $\mathcal{C}$. Then, $E[\Phi(\mathcal{C})] \leq 8(\ln k + 2)\Phi(\mathcal{C}^*)$.
3. Claim holds for the clustering obtained after Step 3. Step 4 may further improve.
4. Proof is not easy. Consider clusters of an optimal solution $\mathcal{C}^*$. The authors show
   - The algorithm is 2-competitive w.r.t. the points in the optimal cluster, say A, from where the first center c_1 is chosen by the algorithm
   - The algorithm is 8-competitive in all those clusters of optimal from which the algorithm chooses a center.
   - If $\mathcal{C}$ doesn't have centers from some of the clusters of the optimal, then the algorithm is $8(\ln k + 2)$-competitive.

Useful Notations

1. Let $\mathcal{C}$ be the clustering computed by the k++-means algorithm
2. Let $\mathcal{C}^*$ be an optimal clustering
3. $d(x, c) = ||x - c||$ is the Euclidean distance between points x and c
4. Let $D(x) =$ Shortest distance from x to the nearest center in $\mathcal{C}$ (or $\mathcal{C}^*$).
5. $\Phi(\mathcal{C}) = \Phi_{\mathcal{C}}(X)$ refers to potential with respect to the point set X.
   Formally, $\Phi(\mathcal{C}) = \sum_{x \in X} \min_{c \in \mathcal{C}} d(x, c)^2 = \sum_{x \in X} D(x)^2$
   I.e. $\Phi(\mathcal{C})$= Sum of the squared distance between each point in X to its nearest center in $\mathcal{C}$
6. For a subset $A \subseteq X$, define $\Phi_{\mathcal{C}}(A) = \sum_{x \in A} \min_{c \in \mathcal{C}} d(x, c)^2 = \sum_{x \in A} D(x)^2$.

1st Center from an Optimal Cluster

Claim 1

Let A be an arbitrary cluster in optimal $\mathcal{C}^*$. Let $\mathcal{C}$ be the clustering with exactly one center that is chosen from A uniformly at random. Then, $E[\Phi_{\mathcal{C}}(A)] = 2\Phi_{\mathcal{C}^*}(A)$.

Proof: By definition of expected value, $E[\Phi_{\mathcal{C}}(A)] = \sum_{a_0 \in A} \frac{1}{|A|} \sum_{a \in A} ||a - a_0||^2$

From Corollary 1, in $\mathcal{C}^*$, cluster center of A will be its center of mass, say m^*.

$$\begin{aligned} E[\Phi_{\mathcal{C}}(A)] &= \frac{1}{|A|} \sum_{a_0 \in A} \left(\sum_{a \in A} ||a - m^*||^2 + |A|||a_0 - m^*||^2 \right) \text{ (By Lemma 1)} \\ &= 2 \sum_{a \in A} ||a - m^*||^2 \\ &= 2\Phi_{\mathcal{C}^*}(A) \end{aligned}$$

□

Other Centers from Optimal Clusters

Claim 2

Let A be an arbitrary cluster in optimal $\mathcal{C}^*$. Let $\mathcal{C}$ be an arbitrary clustering. Suppose the next center to $\mathcal{C}$ in the k-means++ algorithm is added from A, $E[\Phi_{\mathcal{C}}(A)] \leq 8\Phi_{\mathcal{C}^*}(A)$.

Proof Sketch: By triangle inequality we have for all a and a_0, $D(a_0) \leq D(a) + ||a - a_0||$.

Note that for reals x and y, $\frac{1}{2}(x+y)^2 \leq x^2 + y^2$

Thus, we have $\frac{1}{2}(D(a_0))^2 \leq \frac{1}{2}(D(a_0) + ||a - a_0||)^2 \leq D(a)^2 + ||a - a_0||^2$

Equivalently, $D(a_0)^2 \leq 2D(a)^2 + 2||a - a_0||^2$

Summing over all elements of A, we have

$$\sum_{a \in A} D(a_0)^2 \leq \sum_{a \in A} \left(2D(a)^2 + 2||a - a_0||^2\right)$$

Or, $D(a_0)^2 \leq \frac{2}{|A|} \sum_{a \in A} D(a)^2 + \frac{2}{|A|} \sum_{a \in A} (a - a_0)^2$

Other Centers from Optimal Clusters (contd.)

Probability of choosing $a_0 \in A$ as a center is $\frac{D(a_0)^2}{\sum_{a \in A} D(a)^2}$.

Then, $E[\Phi_{\mathcal{C}}(A)] = \sum_{a_0 \in A} \frac{D(a_0)^2}{\sum_{a \in A} D(a)^2} \sum_{a \in A} \min(D(a), (a - a_0))^2$.

Substituting the expression for $D(a_0)^2$ in $E[\Phi_{\mathcal{C}}(A)]$ we obtain,

$$E[\Phi_{\mathcal{C}}(A)] \leq \frac{2}{|A|} \sum_{a_0 \in A} \frac{\sum_{a \in A} D(a)^2}{\sum_{a \in A} D(a)^2} \sum_{a \in A} \min(D(a), (a - a_0))^2 + \frac{2}{|A|} \sum_{a_0 \in A} \frac{\sum_{a \in A} (a - a_0)^2}{\sum_{a \in A} D(a)^2} \sum_{a \in A} \min(D(a), (a - a_0))^2.$$

Substitute for $\min(D(a), (a - a_0))^2 \leq (a - a_0)^2$ in 1st part and $\min(D(a), (a - a_0))^2 \leq D(a)^2$ in 2nd part and we obtain

$E[\Phi_{\mathcal{C}}(A)] \leq \frac{4}{|A|} \sum_{a_0 \in A} \sum_{a \in A} (a - a_0)^2 = 8\Phi_{\mathcal{C}^*}(A)$ (By Claim 1).

Summary so far

- We analyzed the cases where the algorithm chooses centers from optimal clusters.

- Competitive ratio is within a factor of 8.

- If the selection of centers by the algorithm hits all the clusters of an optimal solution, our algorithm's competitive ratio will be bounded by a constant.

- But, what if the algorithm fails to pick a center from an optimal cluster.

- Let $\mathcal{C} = \{c_1, c_2, \ldots, c_t, \ldots, c_k\}$ be the cluster centers returned by the algorithm.

- It incurs a total cost (potential) of $\Phi_{\mathcal{C}}(X)$.

Strategy: Spread this cost over the k iterations.

Strategy

- Let $\mathcal{C}_t$ be the cluster centers chosen by the algorithm at the end of iteration t, $1 \leq t \leq k$.

- Let us fix an optimal clustering $\mathcal{C}^*$.

- Let H_t be the set of clusters of $\mathcal{C}^*$ that are *hit* by centers in $\mathcal{C}_t$. Let $U_t = [k] \setminus H_t$ be the set of clusters of $\mathcal{C}^*$ that aren't hit (or covered) at the end of iteration $t \in [k]$.

- Define $W_t = t - |H_t|$ as the number of *wasted* iterations, i.e., the iterations where the algorithm fails to hit a new cluster of $\mathcal{C}^*$.

- We will show that the cost incurred by the algorithm at the end of iteration $t \in [k]$ is $\Phi_{\mathcal{C}_t}(H_t) + \frac{W_t \Phi_{\mathcal{C}_t}(U_t)}{|U_t|}$

Strategy (contd.)

Consider $\Phi_{\mathcal{C}_t}(H_t) + \frac{W_t \Phi_{\mathcal{C}_t}(U_t)}{|U_t|}$.

1. At $t = 0$: no clusters of optimal are hit and no iterations are wasted. Thus, $H_0 = \emptyset$, $W_0 = 0$, and $\Phi_{\mathcal{C}_t}(H_t) + \frac{W_t \Phi_{\mathcal{C}_t}(U_t)}{|U_t|} = 0$.
2. At $t = k$: $\Phi_{\mathcal{C}}(H_t) + \Phi_{\mathcal{C}}(U_t) = \Phi_{\mathcal{C}}(X)$, as $W_k = |U_k|$.
3. $\Phi_{\mathcal{C}_t}(H_t)$ captures the cost of clusters hit by the centers chosen in the algorithm for any $t \in [k]$. By Claim 2, the expected cost $E[\Phi_{\mathcal{C}_t}(H_t)] \leq 8\Phi_{\mathcal{C}^*}(X)$.
4. Thus, our task is to evaluate the second term.

Claim 3

Let $\Psi_t = \frac{W_t \Phi_{\mathcal{C}_t}(U_t)}{|U_t|}$, for any $t \in [k]$. For any $t \in [k-1]$, $E[\Psi_{t+1} - \Psi_t] \leq \frac{\Phi_{\mathcal{C}_t}(H_t)}{k-t}$.

First we show that using this claim, we can establish the competitive ratio of the k-Means++ algorithm.

Establishing competitive ratio given Claim 3

Theorem

Let the k-centers returned by k-Means++ algorithm for a point set X be $\mathcal{C}$. Let $\mathcal{C}^*$ be an optimal clustering of X. Then, $E[\Phi_{\mathcal{C}}(X)] \leq 8(2 + \ln k)\Phi_{\mathcal{C}^*}(X)$.

Proof Sketch: $\Phi_{\mathcal{C}}(X) = \Phi_{\mathcal{C}}(H_k) + \Phi_{\mathcal{C}}(U_k)$ as some clusters of $\mathcal{C}^*$ are hit and some aren't hit by the centers in $\mathcal{C}$.

$E[\Phi_{\mathcal{C}}(H_k)] \leq 8\Phi_{\mathcal{C}^*}(X)$ (Claim 2) and $\Phi_{\mathcal{C}}(U_k) = \Psi_k = \sum_{t=0}^{k-1} (\Psi_{t+1} - \Psi_t)$.

$$
\begin{aligned}
E[\Phi_{\mathcal{C}}(X)] &= E[\Phi_{\mathcal{C}}(H_k)] + E[\Phi_{\mathcal{C}}(U_k)] \\
&\leq 8\Phi_{\mathcal{C}^*}(X) + \sum_{t=0}^{k-1} E[\Psi_{t+1} - \Psi_t] \\
&\leq 8\Phi_{\mathcal{C}^*}(X) + \sum_{t=0}^{k-1} \frac{\Phi_{\mathcal{C}_t}(H_t)}{k-t} \\
&\leq 8\Phi_{\mathcal{C}^*}(X) \left(1 + 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{k}\right) \\
&\leq 8(2 + \ln k)\Phi_{\mathcal{C}^*}(X)
\end{aligned}
$$

Proof of Claim 3

Assume that the $(t+1)$-st center c_{t+1} in the k-Means++ algorithm is chosen from the cluster C^*_α of optimal, i.e. $c_{t+1} \in C^*_\alpha$. There are two cases:

Case 1: c_{t+1} hits a previously chosen cluster, i.e., $\alpha \in H_t$.

Case 2: c_{t+1} covers a new cluster, i.e., $\alpha \in U_t$.

Case 1: $\alpha \in H_t$

No new clusters are covered: $H_{t+1} = H_t$ and $U_{t+1} = U_t$.

Number of wasted iterations increases by 1: $W_{t+1} = W_t + 1$.

$$\begin{aligned}
\Psi_{t+1} - \Psi_t &= \frac{W_{t+1}\Phi_{\mathcal{C}_{t+1}}(U_{t+1})}{|U_{t+1}|} - \frac{W_t\Phi_{\mathcal{C}_t}(U_t)}{|U_t|} && (1)\\
&\leq \frac{(W_t+1)\Phi_{\mathcal{C}_t}(U_t)}{|U_t|} - \frac{W_t\Phi_{\mathcal{C}_t}(U_t)}{|U_t|} && (2)\\
&= \frac{\Phi_{\mathcal{C}_t}(U_t)}{|U_t|} && (3)
\end{aligned}$$

The reason that the 2nd inequality holds is that by adding more centers, potential cannot increase. Thus, $\Phi_{\mathcal{C}_{t+1}}(U_t) \leq \Phi_{\mathcal{C}_t}(U_t)$.

Case 2: $\alpha \in U_t$

$$H_{t+1} = H_t \cup \{\alpha\}$$

$$U_{t+1} = U_t \setminus \{\alpha\}$$

$$W_{t+1} = W_t.$$

$$\begin{aligned}
\Psi_{t+1} &= \frac{W_{t+1}\Phi_{\mathcal{C}_{t+1}}(U_{t+1})}{|U_{t+1}|} \\
&= \frac{W_t\Phi_{\mathcal{C}_{t+1}}(U_t \setminus C^*_\alpha)}{|U_t| - 1} \\
&\leq \frac{W_t\left(\Phi_{\mathcal{C}_t}(U_t) - \Phi_{\mathcal{C}_t}(C^*_\alpha)\right)}{|U_t| - 1}
\end{aligned}$$

We need to bound the cost for $\Phi_{\mathcal{C}_t}(C^*_\alpha)$, where C^*_α is a randomly chosen cluster from U_t in $\mathcal{C}^*$.

Bounding $E[\Phi_{\mathcal{C}_t}(C^*_\alpha)]$

$$
\begin{aligned}
E[\Phi_{\mathcal{C}_t}(C^*_\alpha)] &= \sum_{i \in U_t} \frac{\Phi_{\mathcal{C}_t}(C^*_i)}{\Phi_{\mathcal{C}_t}(U_t)} \Phi_{\mathcal{C}_t}(C^*_i) \\
&\geq \frac{\Phi_{\mathcal{C}_t}(U_t)}{|U_t|}
\end{aligned}
$$

The above derivation uses

- Cauchy-Schwarz inequality: for any two vectors a and b in $\Re^d$, $|a \cdot b| \leq |a||b|$, where "$\cdot$" represents the dot product.

- $\sum_{i \in U_t} \Phi_{\mathcal{C}_t}(C^*_i) = \Phi_{\mathcal{C}_t}(U_t)$.

Using $\Psi_{t+1} \leq \frac{W_t\left(\Phi_{\mathcal{C}_t}(U_t) - \Phi_{\mathcal{C}_t}(C^*_\alpha)\right)}{|U_t|-1}$ and $E[\Phi_{\mathcal{C}_t}(C^*_\alpha)] \geq \frac{\Phi_{\mathcal{C}_t}(U_t)}{|U_t|}$, we derive an expression for $E[\Psi_{t+1} - \Psi_t]$ for Case 2.

Bounding $E[\Phi_{\mathcal{C}_t}(C^*_\alpha)]$ (contd.)

Case 2

$E[\Psi_{t+1} - \Psi_t] \leq 0.$

Proof Sketch:

$$
\begin{aligned}
E[\Psi_{t+1}] &\leq E\left[\frac{W_t\left(\Phi_{\mathcal{C}_t}(U_t) - \Phi_{\mathcal{C}_t}(C^*_\alpha)\right)}{|U_t| - 1}\right] \\
&\leq \frac{W_t}{|U_t| - 1}\left(E[\Phi_{\mathcal{C}_t}(U_t)] - E[\Phi_{\mathcal{C}_t}(C^*_\alpha)]\right) \\
&\leq \frac{W_t}{|U_t| - 1}\left(\Phi_{\mathcal{C}_t}(U_t) - \frac{\Phi_{\mathcal{C}_t}(U_t)}{|U_t|}\right) \\
&= \frac{W_t}{|U_t|}\Phi_{\mathcal{C}_t}(U_t) \\
&= \Psi_t
\end{aligned}
$$

Proof of Claim 3

Claim 3

For any $t \in [k-1]$, $E[\Psi_{t+1} - \Psi_t] \leq \frac{\Phi_{\mathcal{C}_t}(H_t)}{k-t}$.

Proof Sketch:

- We need to calculate the probability that we are in Case 1 and Case 2 times the difference in the potential in Case 1 and Case 2, respectively.

- We can ignore Case 2 as $E[\Psi_{t+1} - \Psi_t] \leq 0$.

- The probability that we are in Case 1 is $\frac{\Phi_{\mathcal{C}_t}(H_t)}{\Phi_{\mathcal{C}_t}(X)}$.

$$
\begin{aligned}
E[\Psi_{t+1} - \Psi_t] &\leq \frac{\Phi_{\mathcal{C}_t}(H_t)}{\Phi_{\mathcal{C}_t}(X)} \frac{\Phi_{\mathcal{C}_t}(U_t)}{|U_t|} \text{ (Case 1) } + 0 \text{ (Case 2)} \\
&\leq \frac{\Phi_{\mathcal{C}_t}(H_t)}{|U_t|} \\
&= \frac{\Phi_{\mathcal{C}_t}(H_t)}{k-t}
\end{aligned}
$$

Summary

Implications:

If the centers in k-means++ algorithm are chosen from each cluster of $\mathcal{C}^*$,
$\implies$ Algorithm is 8-competitive.

What if the algorithm doesn't choose centers from some of clusters of $\mathcal{C}^*$?

- This part introduces $8(\ln k + 2)$-factor in the analysis

Theorem (Arthur and Vassilvitskii 2007)

The k-means++ algorithm is $8(\ln k + 2)$-competitive.