$k$-means, $k$-means++

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$k$-Means: The Most Popular Clustering Algorithm

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Llyod’s Local Search Algorithm

1. Begin with $k$ arbitrary centers, typically chosen uniformly at random from the data points.

$$\phi$$ is monotonically decreasing, which ensures no configuration is repeated.
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- Convergence could be slow: $k^n$ possible clusterings.
- Lloyd’s k-means algorithm has polynomial \textbf{smoothed} running time.
Illustration of k-means clustering

Figure: Convergence to Local Optimum

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https://commons.wikimedia.org/w/index.php?curid=19403547
Drawbacks of $k$-means algorithm

- Euclidean distance is used as a metric and variance is used as a measure of cluster scatter.
- The number of clusters $k$ is an input parameter: an inappropriate choice of $k$ may yield poor results. That is why, when performing $k$-means, it is important to run diagnostic checks for determining the number of clusters in the data set.
- Convergence to a local minimum may produce results far away from optimal clustering
$k$-means++

Figure: Reference: https://csci8980bigdataalgo.files.wordpress.com/2013/09/bats-means.pdf
$k$-means++
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- The first fix: *Select centers based on distance.*
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**$k$-means++**

- Interpolate between the two methods:

  Let $D(x)$ be the distance between $x$ and the nearest cluster center. Sample $x$ as a cluster center proportionately to $(D(x))^2$.

  $k$-means++ returns clustering $C$ which is log $k$-competitive.

  In the class we will show that if the cluster centers are chosen from each optimal cluster then $k$-means++ is 8-competitive.
K-Means++
**Theorem**: \( k \)-means++ is \( \Theta(\log k) \) approximate in expectation.

Ostrovsky et al. [06]: Similar method is \( O(1) \) approximate under some data distribution assumptions.
**Proof - 1st cluster**

Fix an optimal clustering $c^*$.

Pick first center uniformly at random.

Bound the total error of that cluster.
Proof - 1st cluster

Let $A$ be the cluster.

Each point $a_0 \in A$ equally likely to be the chosen center.

Expected Error:

$$E[\phi(A)] = \sum_{a_0 \in A} \frac{1}{|A|} \sum_{a \in A} \|a - a_0\|^2$$

$$= 2 \sum_{a \in A} \|a - \bar{A}\|^2 = 2\phi^*(A)$$
Proof - Other Clusters

Suppose next center came from a new cluster in OPT.

Bound the total error of that cluster.
Other CLusters

Let $B$ be this cluster, and $b_0$ the point selected.

Then:
\[
E[\phi(B)] = \sum_{b_0 \in B} \frac{D^2(b_0)}{\sum_{b \in B} D^2(b)} \cdot \sum_{b \in B} \min(D(b), \|b - b_0\|)^2
\]

Key step:
\[
D(b_0) \leq D(b) + \|b - b_0\|
\]
For any $b$: \[ D^2(b_0) \leq 2D^2(b) + 2\|b - b_0\|^2 \]

Avg. over all $b$: \[ D^2(b_0) \leq \frac{2}{|B|} \sum_{b \in B} D^2(b) + \frac{2}{|B|} \sum_{b \in B} \|b - b_0\|^2 \]

Same for all $b_0$  

Cost in uniform sampling
For any $b$: $D^2(b_0) \leq 2D^2(b) + 2\|b - b_0\|^2$

Avg. over all $b$: $D^2(b_0) \leq \frac{2}{|B|} \sum_{b \in B} D^2(b) + \frac{2}{|B|} \sum_{b \in B} \|b - b_0\|^2$

Recall:

$$E[\varphi(B)] = \sum_{b_0 \in B} \frac{D^2(b_0)}{\sum_{b \in B} D^2(b)} \cdot \sum_{b \in B} \min(D(b), \|b - b_0\|)^2$$

$$\leq \frac{4}{|B|} \sum_{b_0 \in B} \sum_{b \in B} \|b - b_0\|^2 = 8\varphi^*(B)$$
Wrap Up

If clusters are well separated, and we always pick a center from a new optimal cluster, the algorithm is $8$-competitive.

Intuition: if no points from a cluster are picked, then it probably does not contribute much to the overall error.

Formally, an inductive proof shows this method is $\Theta(\log k)$ competitive.