k-means, k-means++

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- A 2002 survey of data mining techniques states that it "is by far the most popular clustering algorithm used in scientific and industrial applications."

Llyod's Local Search Algorithm

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- Lloyd's k-means algorithm has polynomial **smoothed** running time.

Illustration of k-means clustering

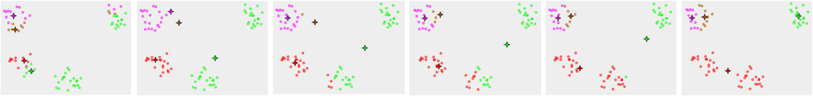
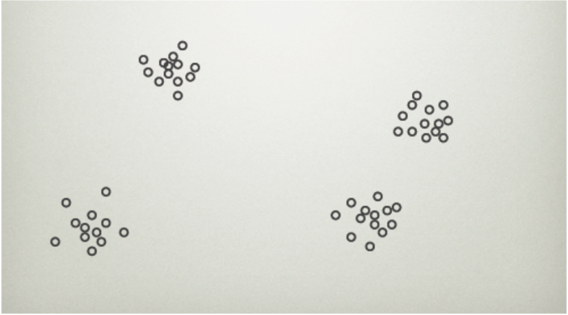


Figure: Convergence to Local Optimum

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++



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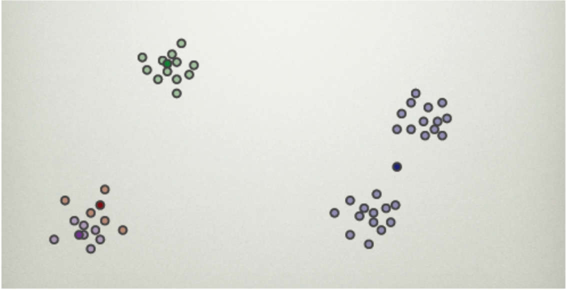
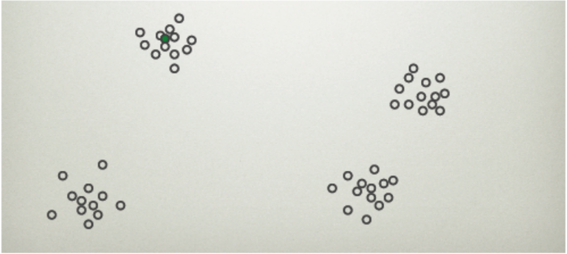


k-means++

- The first fix: *Select centers based on distance.*



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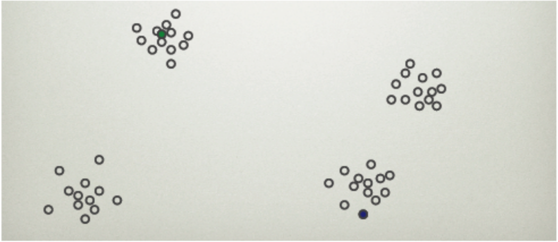

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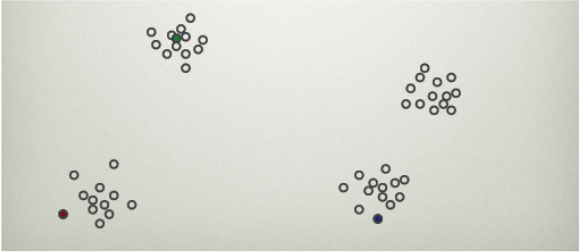

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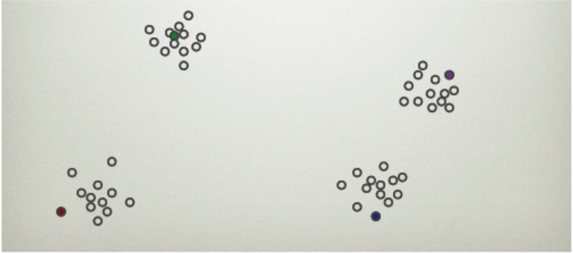

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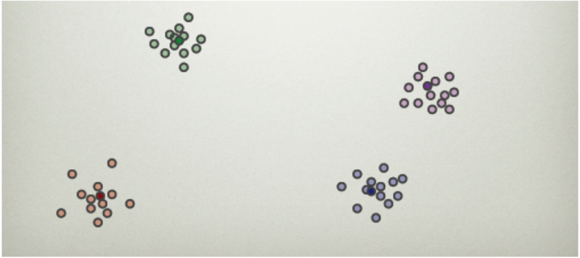
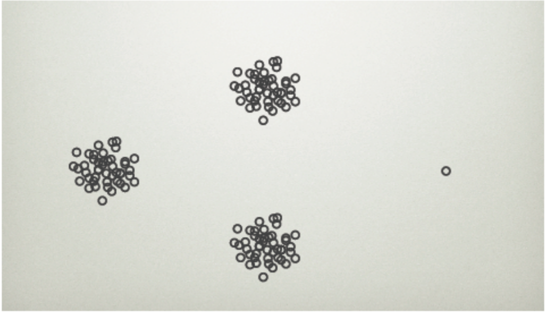


k-means++

- Sensitive to outliers.



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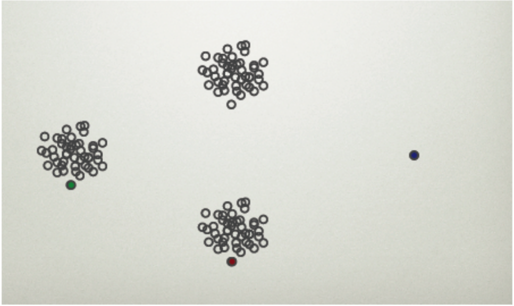

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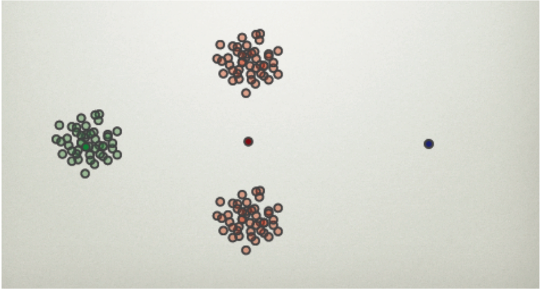


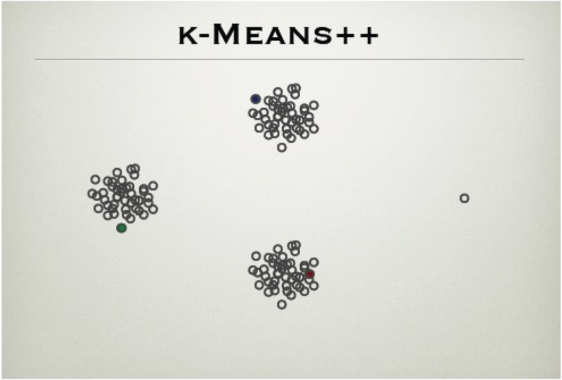
k-means++

- 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 $\mathcal{C}$ 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++

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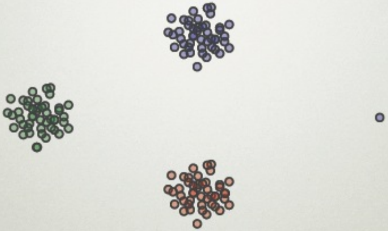
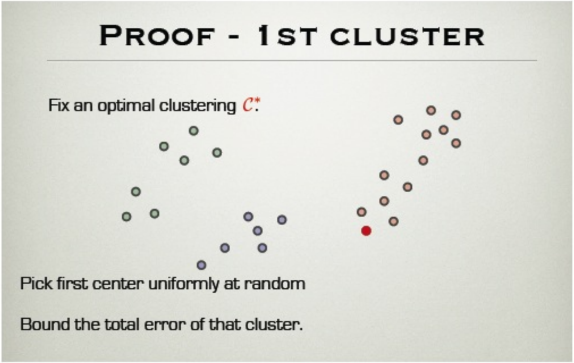


Theorem: k-means++ is $\Theta(\log k)$ approximate in expectation.

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:

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

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

Proof - Other Clusters

Suppose next center came from a new cluster in OPT.

Bound the total error of that cluster.

Other Clusters

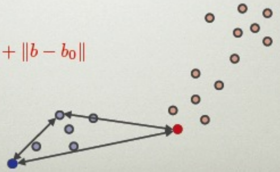
Let B be this cluster, and b_0 the point selected.

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:

$$D(b_0) \leq D(b) + \|b - b_0\|$$



Cont.

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

Cont.

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:

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

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

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.