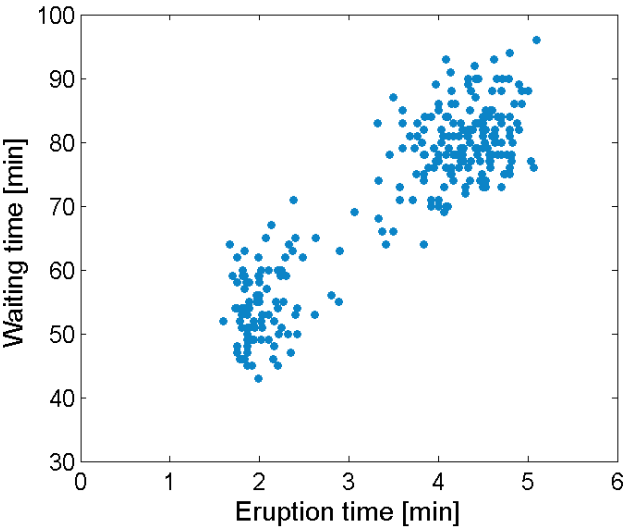
Clustering

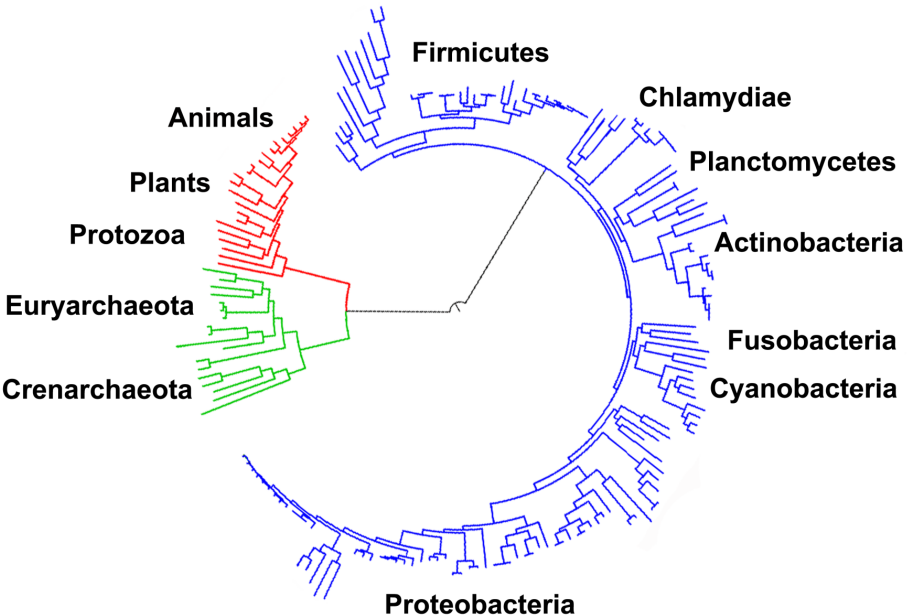
Basic and advanced Concepts

Old Faithful Geyser Data

Old Faithful, Wyoming



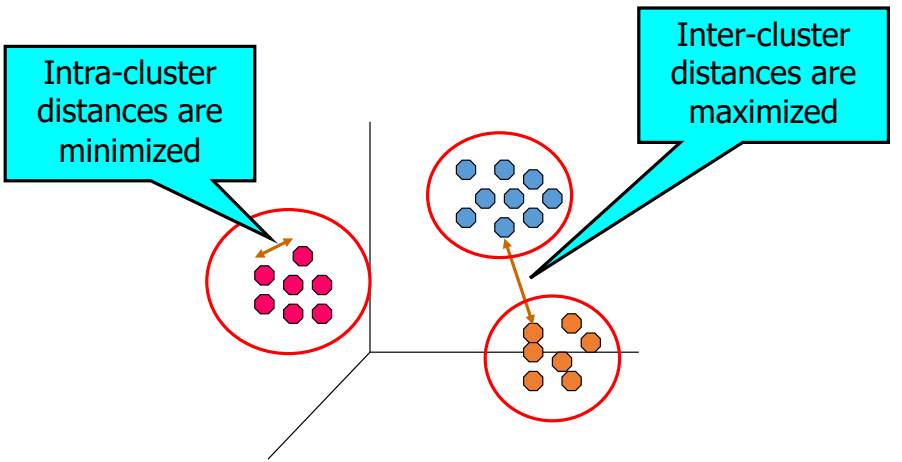
Evolutionary Tree



From Wikipedia

What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups

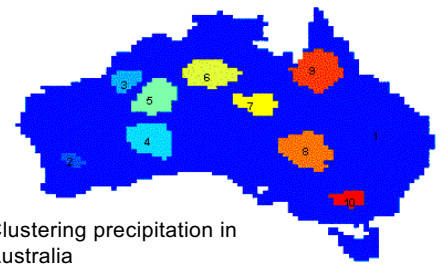


Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations, group celestial objects galaxy, nearby stars, quasars (Sloan Digital Sky Survey).

- **Summarization**
  - Reduce the size of large data sets.

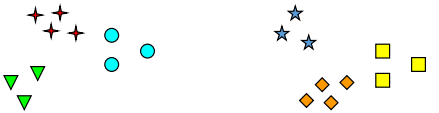
	Discovered Clusters	*Industry Group*
1	Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP



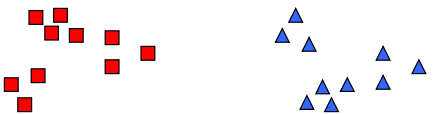
Clustering precipitation in Australia

Notion of a Cluster can be Ambiguous

How many clusters?



Six Clusters

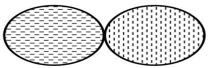


Two Clusters

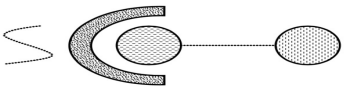
Four Clusters

Different types of clusters

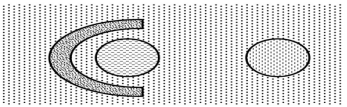
(a) Well-separated clusters. Each point is closer to all of the points in its cluster than to any point in another cluster.



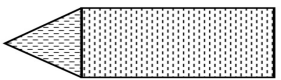
(b) Center-based clusters. Each point is closer to the center of its cluster than to the center of any other cluster.

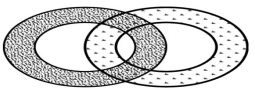


(c) Contiguity-based clusters. Each point is closer to at least one point in its cluster than to any point in another cluster.



(d) Density-based clusters. Clusters are regions of high density separated by regions of low density.





Overlapping cluster

(e) Conceptual clusters. Points in a cluster share some general property that derives from the entire set of points. (Points in the intersection of the circles belong to both.)

Figure 8.2. Different types of clusters as illustrated by sets of two-dimensional points.

Terminology

- X: A set of objects or data points that we want to cluster
- $C \subseteq X$: any subset of X can be a cluster, but not necessarily a meaningful cluster.
- $\{C_i \subseteq X\}_{i=1}^{K}$: K-clustering.
- $C_i \cap C_j = \emptyset$ for all $i \neq j$: If no two clusters have points in common the clustering is non-overlapping.
- $C_i \cap C_j \neq \emptyset$ for some $i \neq j$: If any two clusters have points in common the clustering is overlapping.
- $\bigcup_{i=1}^{K} C_i = X$: complete clustering.
- $\bigcup_{i=1}^{K} C_i \subset X$: partial clustering.
- $\{C_i\}_{i=1}^{K}$ partitions X: complete and non-overlapping clustering.
- c_i: cluster center

Two ways to specify a clustering

Directly provide the clustering as set of subsets $\{C_i\}_{i=1}^{K}$ of X.

Give the class memberships instead as a vector M containing cluster label for each data point

SSE Criterion

- Most common clustering criterion is Sum of Squared Error (SSE) (also called potential)
  - For each point, the error is the **distance** to its cluster **center**
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(c_i, x) \qquad c_i = argmin_c \sum_{x \in C_i} dist^2(c, x)$$

  - *x* is a data point in cluster C_i and c_i is the representative point for cluster C_i
  - Given two clusterings, we can choose the one with the smallest SSE.
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a larger SSE than a poor clustering with bigger K.

Distances and Similarities

Clustering criterion (potential) can similarly be defined in terms of Similarity function.

- While using similarity the goal is to maximize, instead of minimize.

$$\text{Total Cohesion} = \sum_{i=1}^{K} \sum_{\mathbf{x} \in C_i} cosine(\mathbf{x}, \mathbf{c}_i)$$

Table 8.2. K-means: Common choices for proximity, centroids, and objective functions.

Proximity Function	Centroid	Objective Function
Manhattan (L_1)	median	Minimize sum of the L_1 distance of an object to its cluster centroid
Squared Euclidean (L_2^2)	mean	Minimize sum of the squared L_2 distance of an object to its cluster centroid
cosine	mean	Maximize sum of the cosine similarity of an object to its cluster centroid
Bregman divergence	mean	Minimize sum of the Bregman divergence of an object to its cluster centroid

K-means Clustering

- Input: K (the number of clusters)

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

Centroid for Euclidean distance, Bregman divergence and Cosine similarity is the **mean**

$$\mathbf{c}_i = \frac{1}{m_i} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$

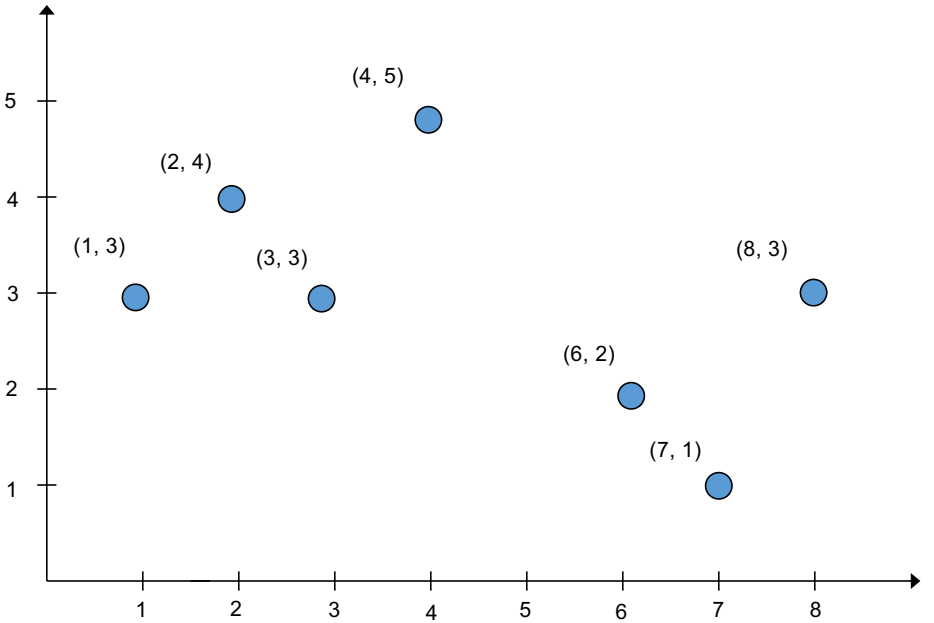
Centroid for Manhattan distance is the **median**

Proof why mean minimizes the SSE with Euclidean Distance

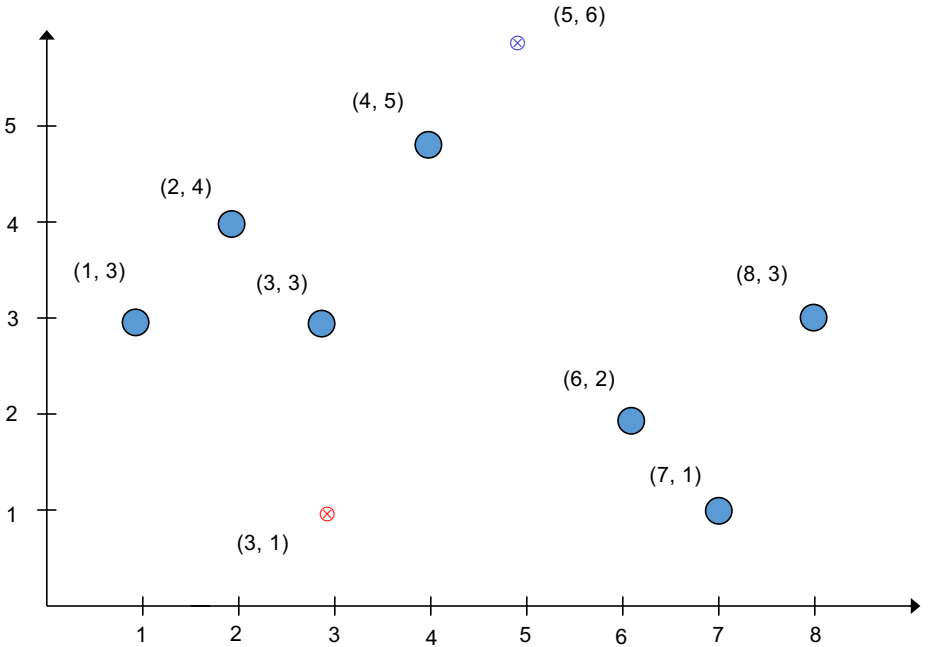
$$\begin{aligned}
\frac{\partial}{\partial c_k}\text{SSE} &= \frac{\partial}{\partial c_k}\sum_{i=1}^{K}\sum_{x\in C_i}(c_i - x)^2 \\
&= \sum_{i=1}^{K}\sum_{x\in C_i}\frac{\partial}{\partial c_k}(c_i - x)^2 \\
&= \sum_{x\in C_k} 2 * (c_k - x_k) = 0
\end{aligned}$$

$$\sum_{x\in C_k} 2 * (c_k - x_k) = 0 \Rightarrow m_k c_k = \sum_{x\in C_k} x_k \Rightarrow c_k = \frac{1}{m_k}\sum_{x\in C_k} x_k$$

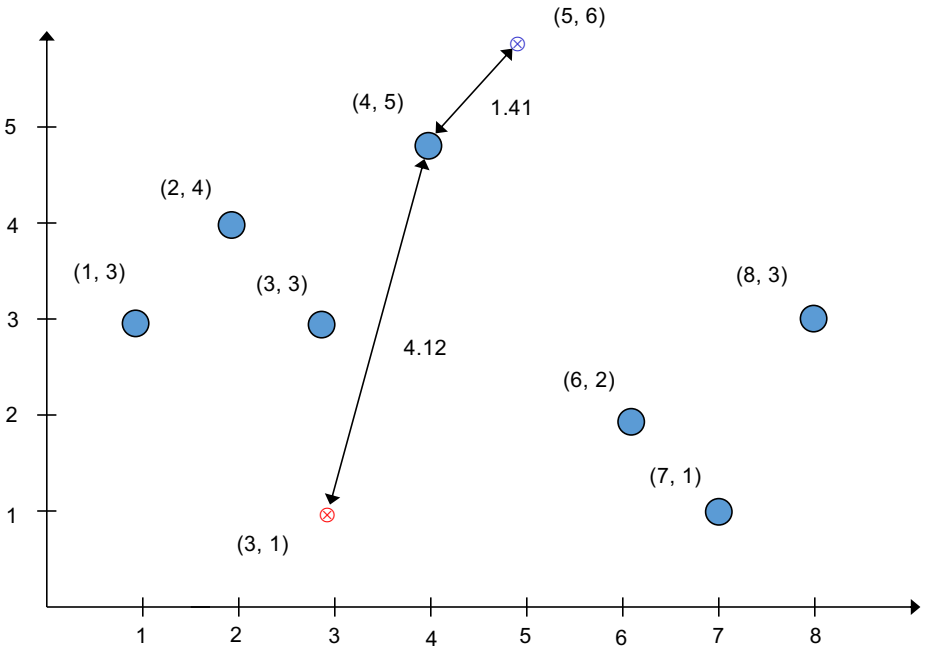
K-means: Example



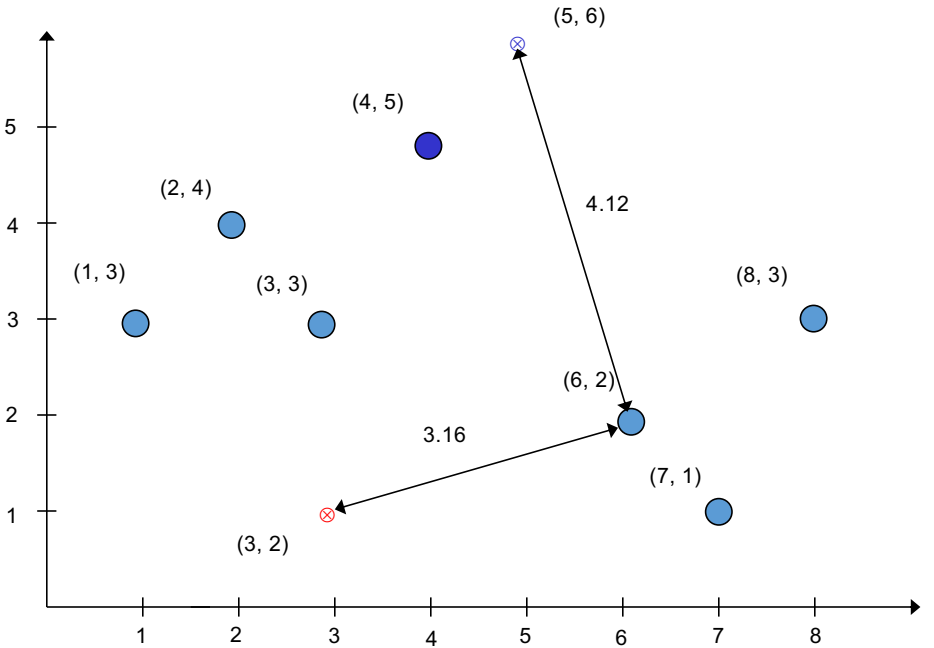
K-means: Example



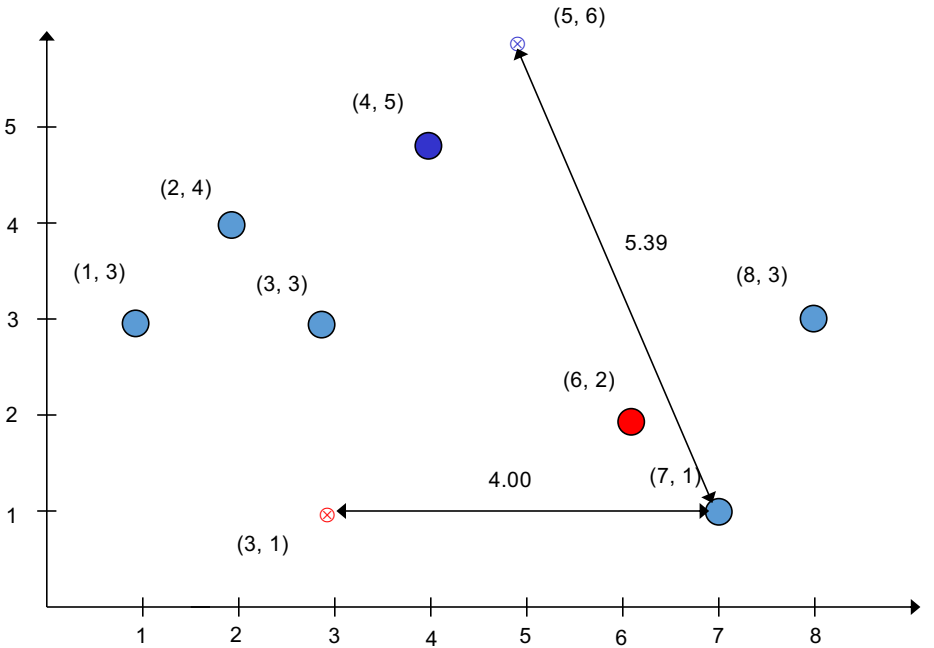
K-means: Example



K-means: Example



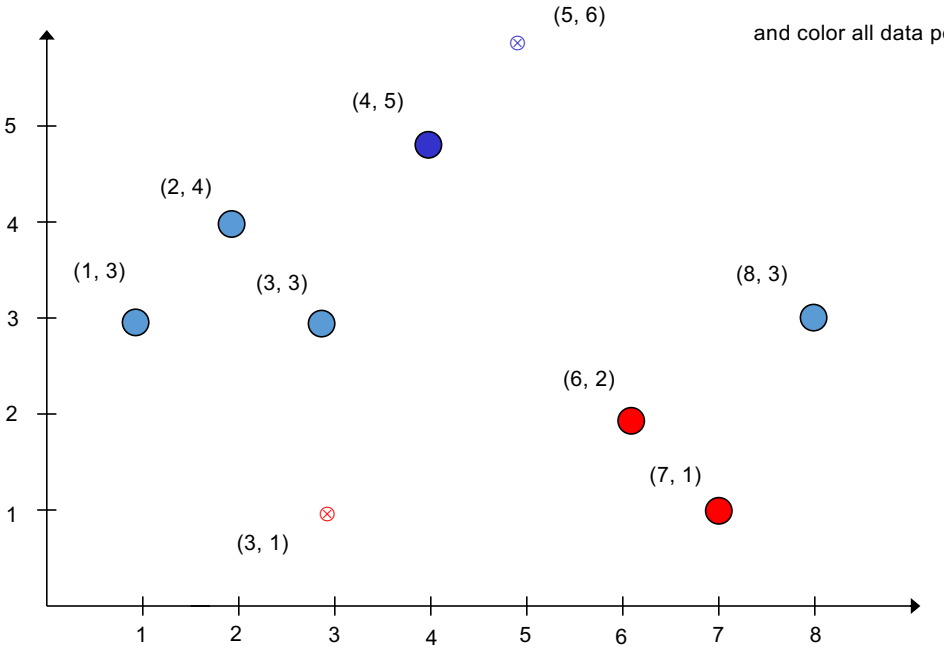
K-means: Example



K-means: Example

Now: calculate all distances...

and color all data points.

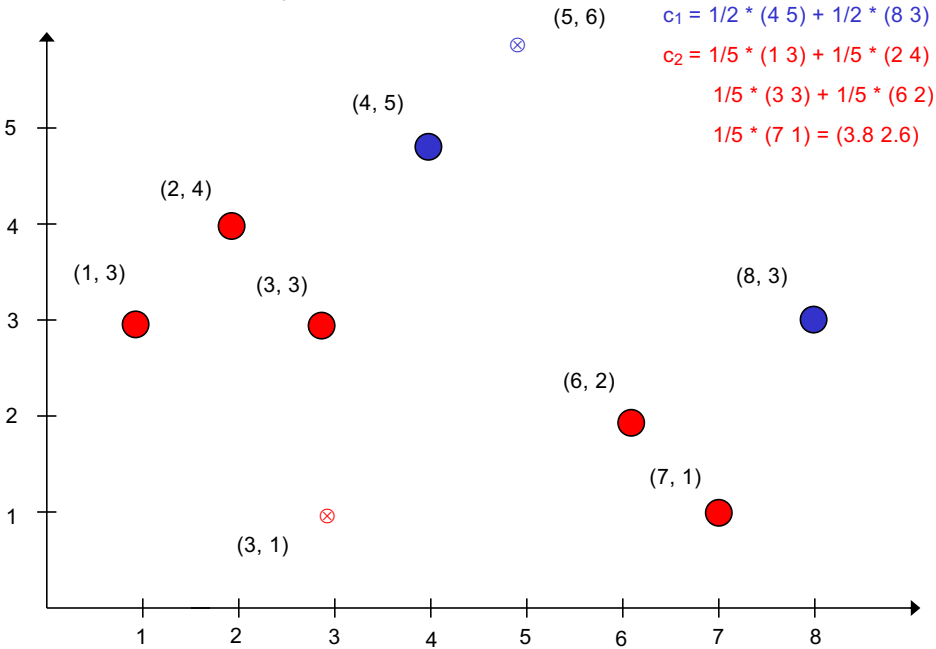


K-means: Example

Now: move cluster centers to be the average of data points.

c_1 = 1/2 * (4 5) + 1/2 * (8 3) = (6 4)

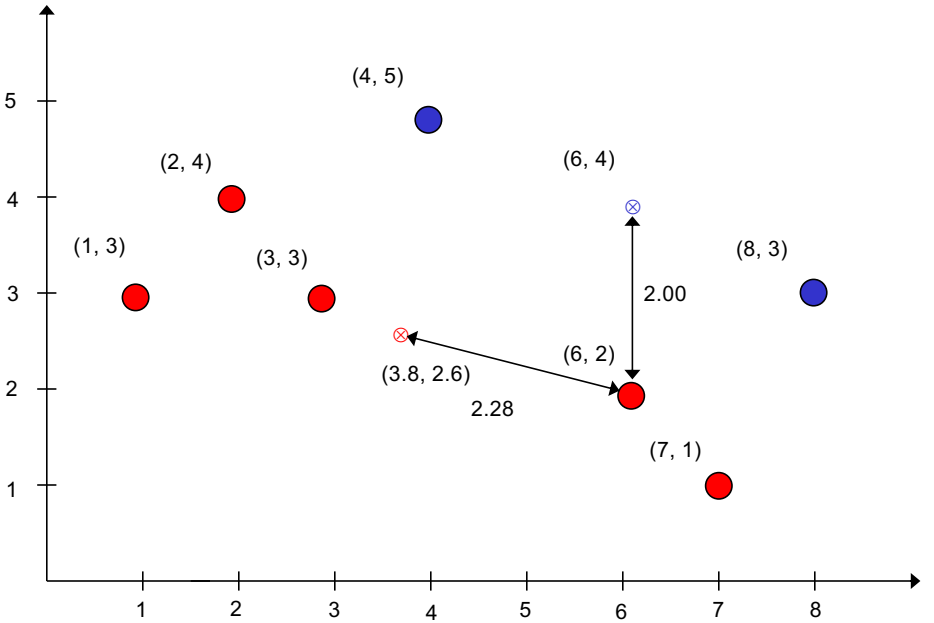
c_2 = 1/5 * (1 3) + 1/5 * (2 4) +
1/5 * (3 3) + 1/5 * (6 2) +
1/5 * (7 1) = (3.8 2.6)



Now: start next iteration

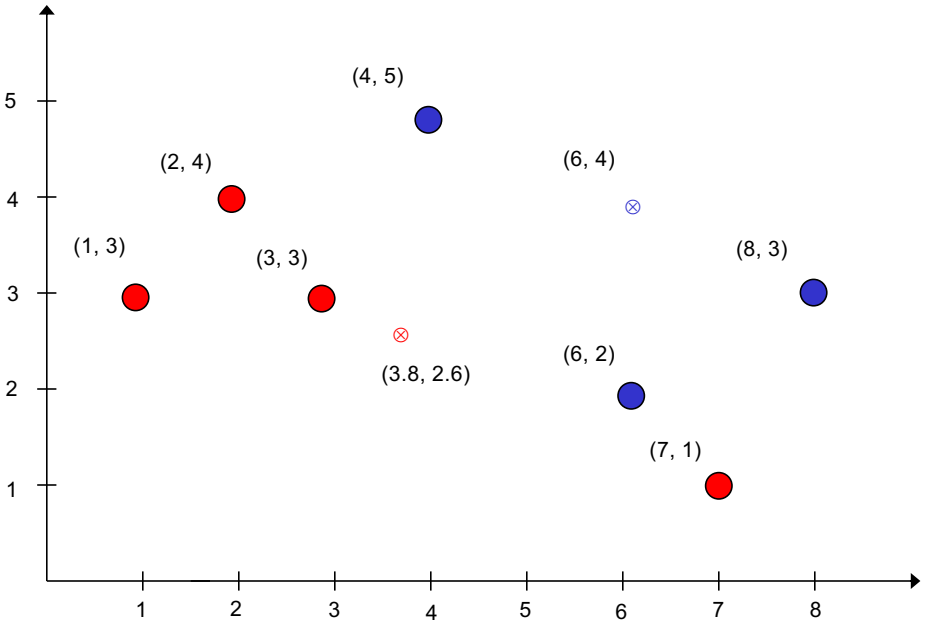
repeat distance calculation.

K-means: Example



Now: calculate all other distances...

K-means: Example

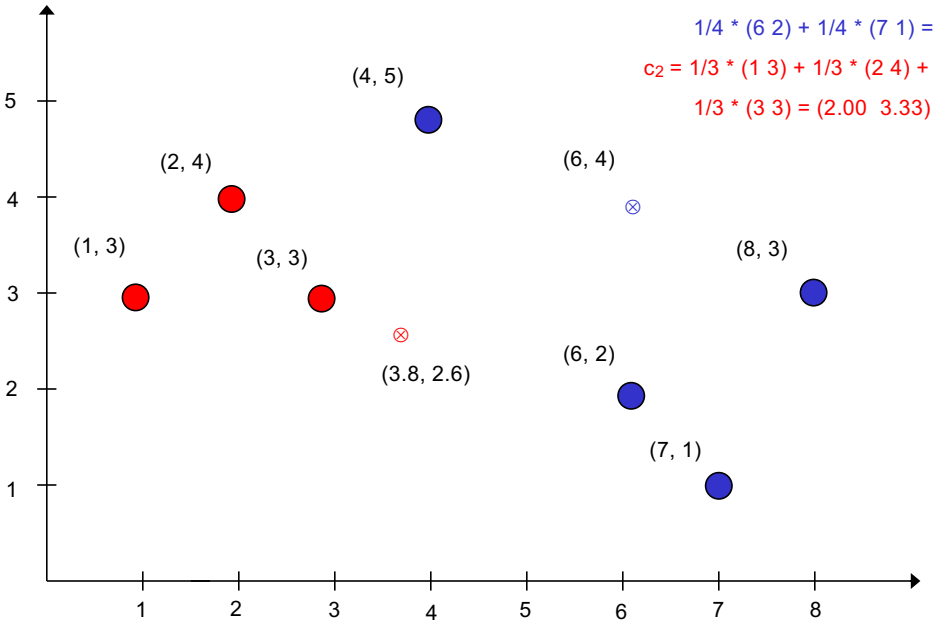


K-means: Example

Now: move cluster centers to be the average of data points.

c_1 = 1/4 * (4 5) + 1/4 * (8 3) +
1/4 * (6 2) + 1/4 * (7 1) = (5.67 2.67)

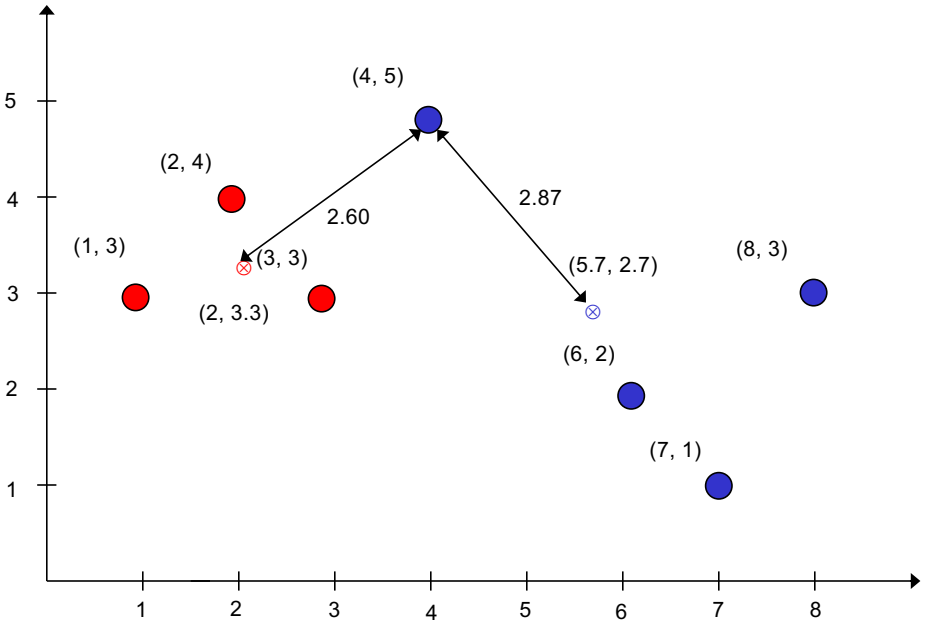
c_2 = 1/3 * (1 3) + 1/3 * (2 4) +
1/3 * (3 3) = (2.00 3.33)



K-means: Example

Now: start next iteration

calculate distances again...

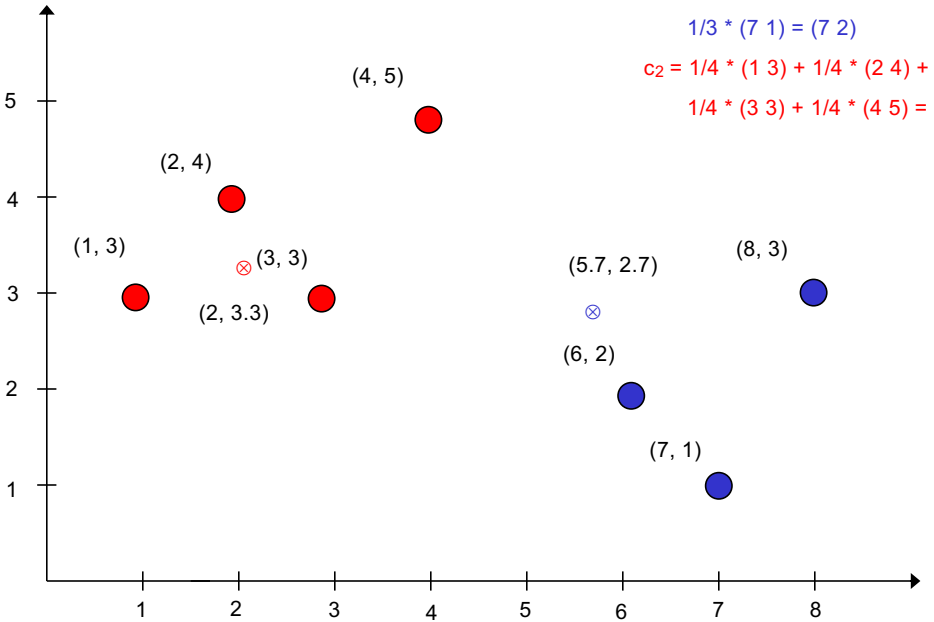


K-means: Example

Now: move cluster centers to be the average of data points.

c_1 = 1/3 * (6 2) + 1/3 * (8 3) +
1/3 * (7 1) = (7 2)

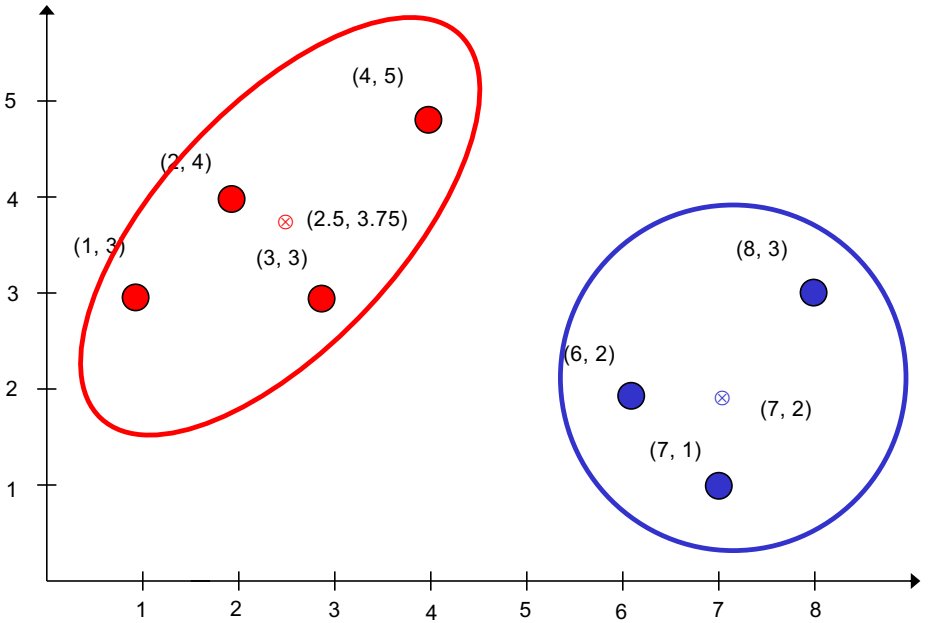
c_2 = 1/4 * (1 3) + 1/4 * (2 4) +
1/4 * (3 3) + 1/4 * (4 5) = (2.5 3.75)



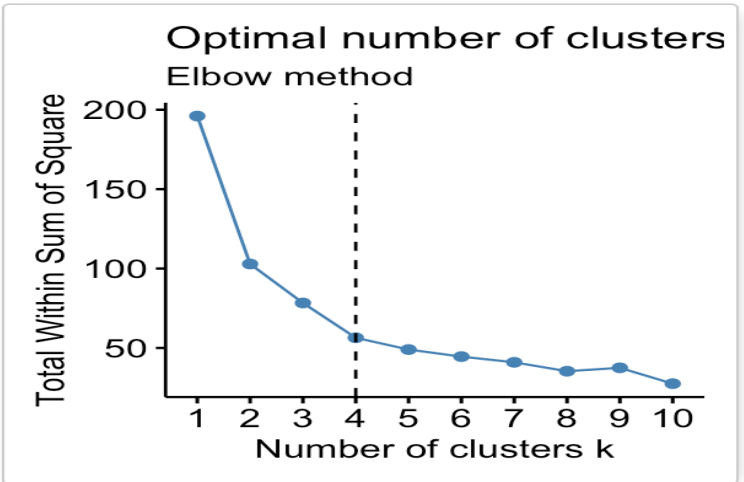
K-means: Example

Now: if we calculate all distances, no data points will change color.

This means, we can stop!



Choosing K



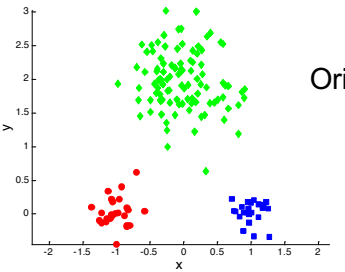
Other methods

Gap Statisitcs: Tibshirani, Robert, Guenther Walther, and Trevor Hastie. "Estimating the number of clusters in a data set via the gap statistic." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 63.2 (2001): 411-423.

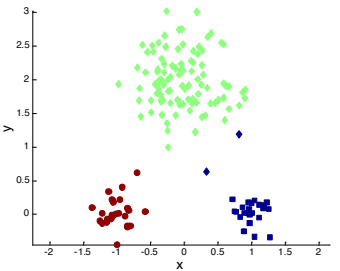
K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O(n * K * d * e)
  - n = number of points, k = number of clusters,
    e = number of iterations, d = number of attributes

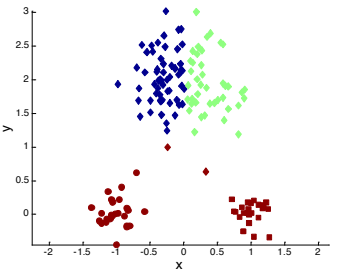
Two different K-means Clusterings



Original Points

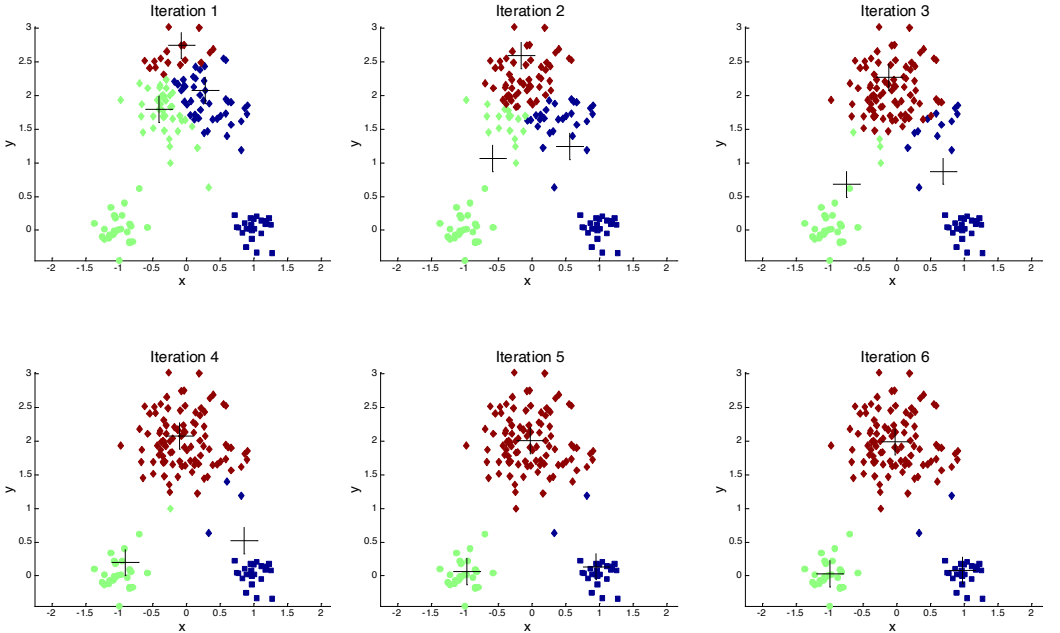


Optimal Clustering

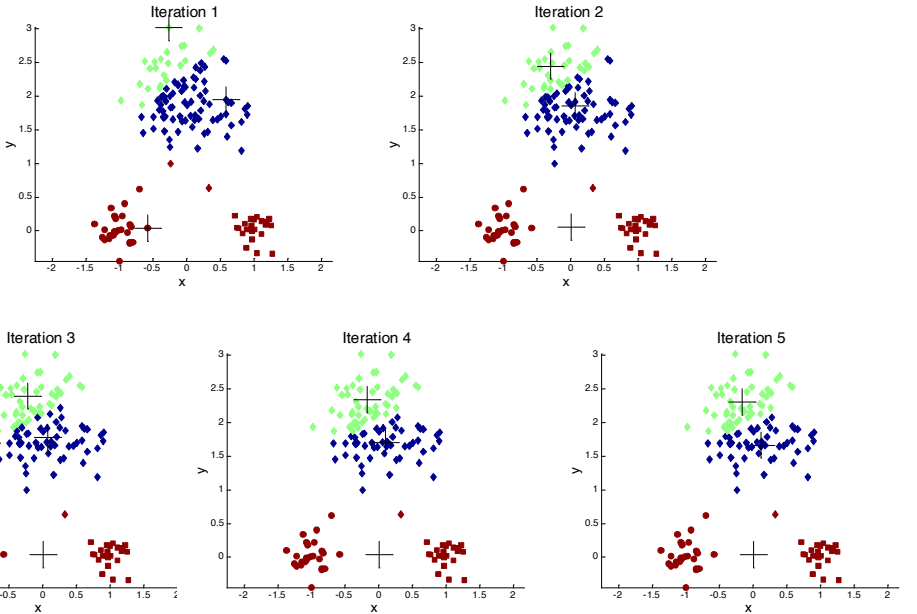


Sub-optimal Clustering

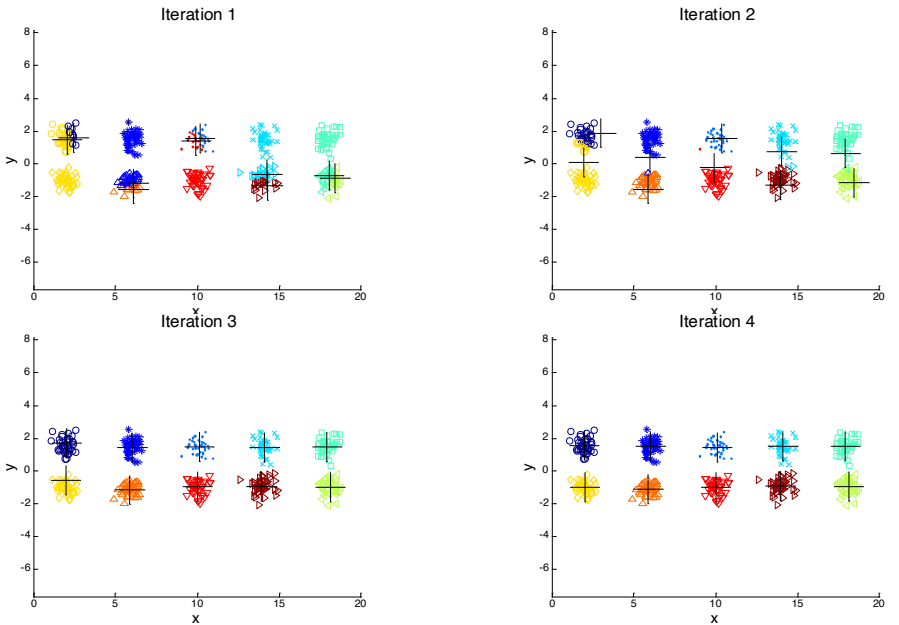
Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids …

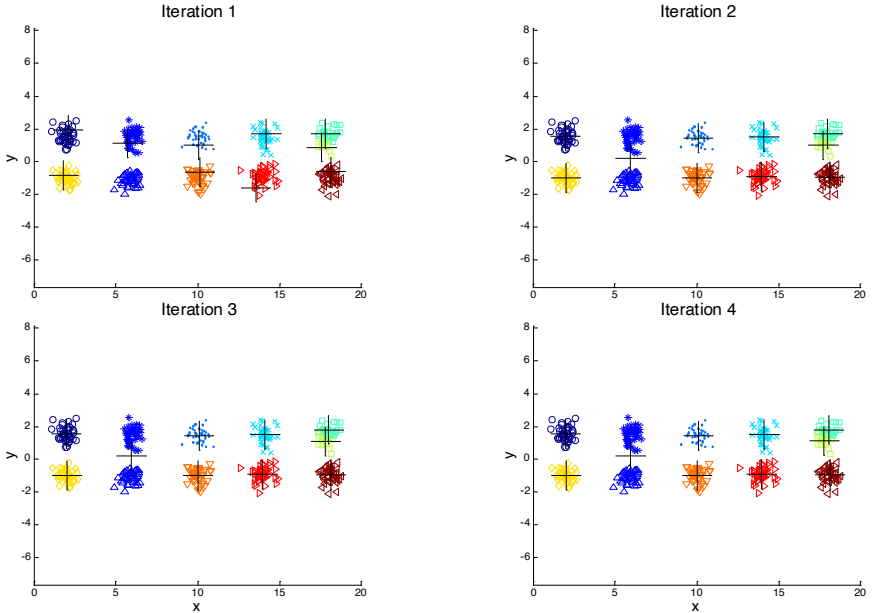


10 Clusters Example



Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



Starting with some pairs of clusters having three initial centroids, while other have only one.

Picking the initialization cluster centers: a significant issue

Sum square error (alternate formula)

$$\varphi(\mathbb{C}) = \sum_{x \in X} min_{c \epsilon \mathbb{C}} d(x, c)^2$$

Interpret $\mathbb{C}$ is the set of centroids. The clustering is uniquely determined from $\mathbb{C}$

φ_{opt} is the minimum value $\varphi(\mathbb{C})$ can attain

- It is the speed and simplicity of the k-means method that make it appealing, not its accuracy. Indeed, there are many natural examples for which the algorithm generates arbitrarily bad clustering (i.e., $\frac{\varphi}{\varphi_{opt}}$ is unbounded even when n and k are fixed). This does not rely on an adversarial placement of the starting centers, and in particular, it can hold with high probability if the centers are chosen uniformly at random from the data points.

Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Bisecting K-means
  - Not as susceptible to initialization issues

Furthest first

- Pick first center to be the mean of the data
- For the subsequent centers iteratively pick the point whose distance to its closest cluster is largest.

$$c_{j+1} \leftarrow argmax_{x \in \mathcal{X}} \; min_{c \epsilon C_j} d(x, c)$$
$$C_{j+1} \leftarrow C_j \cup \{c_{j+1}\}$$

Problem: Outliers get chosen as centers.

C_j is the set of centroids at j^{th} step.

K-Means ++

1a. Take one center c_1, chosen uniformly at random from $\mathcal{X}$.

1b. Take a new center c_i, choosing $x \in \mathcal{X}$ with probability $\frac{D(x)^2}{\sum_{x \in \mathcal{X}} D(x)^2}$.

1c. Repeat Step 1b. until we have taken k centers altogether.

2-4. Proceed as with the standard `k-means` algorithm.

$D(x)$ is the distance of x to it's closest cluster centroid.

Theorem 3.1. *If $\mathcal{C}$ is constructed with* `k-means++`*, then the corresponding potential function ϕ satisfies, $E[\phi] \leq 8(\ln k + 2)\phi_{\text{OPT}}$.*

	Average ϕ		Minimum ϕ		Average T	
k	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	135512	126433	119201	111611	0.14	0.13
25	48050.5	15.8313	25734.6	15.8313	1.69	0.26
50	5466.02	14.76	14.79	14.73	3.79	4.21

Table 2: Experimental results on the *Norm-25* dataset (n = 10000, d = 15)

	Average ϕ		Minimum ϕ		Average T	
k	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	7553.5	6151.2	6139.45	5631.99	0.12	0.05
25	3626.1	2064.9	2568.2	1988.76	0.19	0.09
50	2004.2	1133.7	1344	1088	0.27	0.17

Table 3: Experimental results on the *Cloud* dataset (n = 1024, d = 10)

	Average ϕ		Minimum ϕ		Average T	
k	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	$3.45 \cdot 10^8$	$2.31 \cdot 10^7$	$3.25 \cdot 10^8$	$1.79 \cdot 10^7$	107.5	64.04
25	$3.15 \cdot 10^8$	$2.53 \cdot 10^6$	$3.1 \cdot 10^8$	$2.06 \cdot 10^6$	421.5	313.65
50	$3.08 \cdot 10^8$	$4.67 \cdot 10^5$	$3.08 \cdot 10^8$	$3.98 \cdot 10^5$	766.2	282.9

Table 4: Experimental results on the *Intrusion* dataset (n = 494019, d = 35)

K-means Recap

In general, can be more abstract spaces such as space of trees, graphs or functions

- Given a dataset, $\mathcal{X} \subseteq \mathbb{R}^d$ and number of clusters k, find a clustering $\mathbb{C} \subseteq \mathbb{R}^d$ such that the Sum Square Distance (aka potential) is minimized.

Sum Square Distance

$$\varphi(\mathbb{C}) = \sum_{x \in \mathcal{X}} min_{c \in \mathbb{C}} d(x, c)^2$$

$\mathbb{C}$ is the set of centroids. The clustering is uniquely determined from the centroids.

Loyd's Algorithm

- Start with random assignments of k centroids
- Iteratively,
  - Assign each point $x \in \mathcal{X}$ to the closest center $c \epsilon \mathbb{C}$
  - Re-compute the centroids based on the cluster assignment.

$n = |\mathcal{X}|$

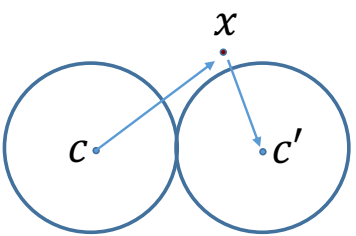
$O(nkd)$

$O(nkd)$ per iteration is prohibitive for large dimension!

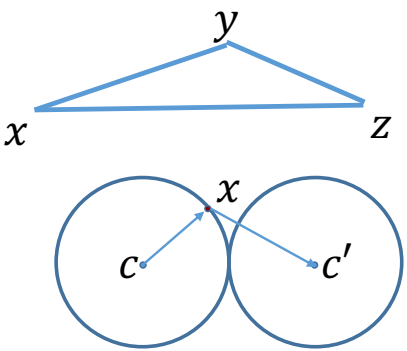
Core ideas for cutting on distance computation

Exploit the triangle inequality

$$d(x,z) \leq d(x,y) + d(y,z)$$



If $d(x,c) \geq \frac{d(c,c')}{2}$ then $d(x,c) \leq d(x,c')$ not guaranteed



If $d(x,c) \leq \frac{d(c,c')}{2}$ then $d(x,c) \leq d(x,c')$ is guaranteed

Upper bound for $d(x,c)$

Also true when $d(x,c) \leq u \leq \frac{d(c,c')}{2}$

Elkan's accelerated K-means

Distance computation: vector operation
Inequality: scalar operation

Requires computation of pairwise distances between the centroids beforehand
$O(k^2)$ distances computes

Pruning principle:

i^{th} point is assigned to the right cluster if $u(i) \leq s(a(i))$. No distance involving the i^{th} point needs to be computed.

i^{th} point cannot be assigned to j^{th} cluster if $u(i) \leq l(i,j)$ or $u(i) \leq$ half the distance between $c(a(i))$ and $c(j)$. The distance between the i^{th} point and the j^{th} centroid need not be computed.

$a(i)$: index of the cluster assigned to the i^{th} point.

$l(i,j)$: lower bound of the distance of the i^{th} point to the j^{th} cluster centroid, matrix ($n \times k$ dimensional).

$u(i)$: upper bound of distance of the i^{th} point to the currently assigned cluster centroid, vector (n dimensional).

$c(j)$: j^{th} cluster centroid,

$s(j)$: half the distance between j^{th} centroid and its closest centroid

Bounding the distance of x from center after the center moves from c to c^*

Distance computation: vector operation

Upper and lower bound: scalar operation

Lower bound

$$d(x,c^*) \geq \max\big(0, d(x,c) - d(c,c^*)\big)$$
$$\geq \max\big(0, l - d(c,c^*)\big)$$
$$= l^*$$

Lower bound for $d(x,c)$

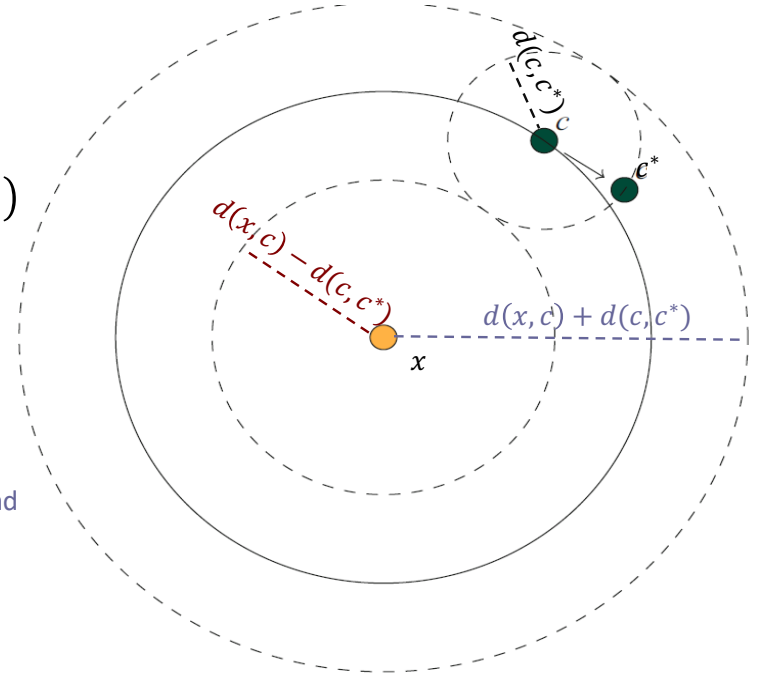
Lower bound for $d(x,c^*)$

Upper bound

$$d(x,c^*) \leq d(x,c) + d(c,c^*)$$
$$\leq u + d(c,c^*)$$
$$= u^*$$

Upper bound for $d(x,c)$

Upper bound for $d(x,c^*)$



Algorithm 3 Elkan's algorithm—using k lower bounds per point and k^2 center-center distances

```
procedure ELKAN(X, C)
    a(i) ← 1, u(i) ← ∞, ∀i ∈ N {Initialize invalid bounds, all in one cluster.}
    ℓ(i, j) ← 0, ∀i ∈ N, j ∈ K
    while not converged do
5:      compute ‖c(j) − c(j′)‖, ∀ j, j′ ∈ K
        compute s(j) ← min_{j′≠j} ‖c(j) − c(j′)‖/2, ∀ j ∈ K
        for all i ∈ N do
            if u(i) ≤ s(a(i)) then continue with next i
            r ← True
10:         for all j ∈ K do
                z ← max(ℓ(i, j), ‖c(a(i)) − c(j)‖/2)
                if j = a(i) or u(i) ≤ z then continue with next j
                if r then
                    u(i) ← ‖x(i) − c(a(i))‖
15:                 r ← False
                    if u(i) ≤ z then continue with next j
                ℓ(i, j) ← ‖x(i) − c(j)‖
                if ℓ(i, j) < u(i) then a(i) ← j
        for all j ∈ K do {Move the centers and track their movement}
20:         move c(j) to its new location
            let δ(j) be the distance moved by c(j)
        for all i ∈ N do {Update the upper and lower distance bounds}
            u(i) ← u(i) + δ(a(i))
            for all j ∈ K do
25:             ℓ(i, j) ← ℓ(i, j) − δ(j)
```

r: tells if the upper bound needs to be tightened.

Both upper bound and the lower bound are tight on this step.

$\max(0, l(i,j) - \delta(j))$

Limitations of Elkan

- Updating the l matrix takes $O(nke)$, even though time spent computing distances is reduced to $O(nd)$ from $O(nkde)$ empirically (not in worst case);
- Storing the l matrix ($n \times k$ dimension) can be a bottleneck for large k.
- Each iteration spent $O(k^2 d)$ time computing between centroid distances.

n: dataset size
k: number of clusters
d: number of dimensions
e: number of iterations

Results for Elkan

		$k = 3$	$k = 20$	$k = 100$
birch	iterations	17	38	56
	standard	5.100e+06	7.600e+07	5.600e+08
	fast	4.495e+05	1.085e+06	1.597e+06
	speedup	11.3	70.0	351
covtype	iterations	18	256	152
	standard	8.100e+06	7.680e+08	2.280e+09
	fast	9.416e+05	7.147e+06	7.353e+06
	speedup	8.60	107	310
kddcup	iterations	34	100	325
	standard	9.732e+06	1.908e+08	3.101e+09
	fast	6.179e+05	3.812e+06	1.005e+07
	speedup	15.4	50.1	309
mnist50	iterations	38	178	217
	standard	6.840e+06	2.136e+08	1.302e+09
	fast	1.573e+06	9.353e+06	3.159e+07
	speedup	4.35	22.8	41.2
mnist784	iterations	63	60	165
	standard	1.134e+07	7.200e+07	9.900e+08
	fast	1.625e+06	7.396e+06	3.055e+07
	speedup	6.98	9.73	32.4
random	iterations	52	33	18
	standard	1.560e+06	6.600e+06	1.800e+07
	fast	1.040e+06	3.020e+06	5.348e+06
	speedup	1.50	2.19	3.37

name	cardinality	dimensionality	description
birch	100000	2	10 by 10 grid of Gaussian clusters, DS1 in (Zhang et al., 1996)
covtype	150000	54	remote soil cover measurements, after (Moore, 2000)
kddcup	95413	56	KDD Cup 1998 data, un-normalized
mnist50	60000	50	random projection of NIST handwritten digit training data
mnist784	60000	784	original NIST handwritten digit training data
random	10000	1000	uniform random data

Table 2. Rows labeled "standard" and "fast" give the number of distance calculations performed by the unaccelerated k-means algorithm and by the new algorithm. Rows labeled "speedup" show how many times faster the new algorithm is, when the unit of measurement is distance calculations.

Hamerly's accelerated K-means

Main difference from Elkan:
$l(i)$ instead of $l(i,j)$.

Maintains one lower bound per point instead of k.

$l(i)$: lower bound of the distance of the i^{th} point to the second closest centroid

Pruning principle:

i^{th} point is assigned to the right cluster if $u(i) \leq s\big(a(i)\big)$ or $u(i) \leq l(i)$. No distance involving the i^{th} point needs to be computed.

Tradeoff

$O(n)$ instead of $O(n \times k)$

- Less memory for storing lower bounds.
- Fewer computations for updating lower bounds.
- However, there is less pruning and consequently more distance computation.

Algorithm 4 Hamerly's algorithm—using 1 lower bound per point

procedure HAMERLY(X, C)
  $a(i) \leftarrow 1, u(i) \leftarrow \infty, \ell(i) \leftarrow 0, \forall i \in N$ {Initialize invalid bounds, all in one cluster.}
  while not converged **do**
    compute $s(j) \leftarrow \min_{j' \neq j} \|c(j) - c(j')\|/2, \forall j \in K$
    for all $i \in N$ **do**
      $z \leftarrow \max(\ell(i), s(a(i)))$
      if $u(i) \leq z$ **then** continue with next i
      $u(i) \leftarrow \|x(i) - c(a(i))\|$ {Tighten the upper bound}
      if $u(i) \leq z$ **then** continue with next i
      Find $c(j)$ and $c(j')$, the two closest centers to $x(i)$, as well as the distances to each.
      if $j \neq a(i)$ **then**
        $a(i) \leftarrow j$
        $u(i) \leftarrow \|x(i) - c(a(i))\|$
      $\ell(i) \leftarrow \|x(i) - c(j')\|$
    for all $j \in K$ **do** {Move the centers and track their movement}
      move $c(j)$ to its new location
      let $\delta(j)$ be the distance moved by $c(j)$
    $\delta' \leftarrow \max_{j \in K} \delta(j)$
    for all $i \in N$ **do** {Update the upper and lower distance bounds}
      $u(i) \leftarrow u(i) + \delta(a(i))$
      $\ell(i) \leftarrow \max(0, l(i) - \delta')$

$l(i)$ by definition is also a lower bound to the distances to other centers, except the closest one.

δ' ensures that if the second closest cluster changes the lower bound is still valid.

Table 1: This table gives the overhead (in time and memory) for each examined algorithm. Each entry represents the asymptotic overhead spent by that algorithm *beyond* Lloyd's algorithm. The initialization time (column 2) is extra time needed to allocate memory and create data structures. Time/iteration is the extra time spent during each k-means iteration, and memory accounts for all extra memory used.

	init. time	time/iteration	memory
k-d tree	$nd + n\log(n)$	-	nd
elkan	$ndk + dk^2$	dk^2	$nk + k^2$
hamerly	ndk	dk^2	n

Some considerations

- Effect of data distribution
  - More clustered data, more pruning
  - More uniform data, less pruning

Dataset		Total user CPU Seconds (User CPU seconds per iteration)							
		$k = 3$		$k = 20$		$k = 100$		$k = 500$	
uniform random	iterations	44		227		298		710	
$n = 1250000$	lloyd	4.0	(0.058)	61.4	(0.264)	320.2	(1.070)	3486.9	(4.909)
$d = 2$	kd-tree	3.5	(**0.006**)	**11.8**	(**0.035**)	34.6	(0.102)	338.8	(0.471)
	elkan	7.2	(0.133)	75.2	(0.325)	353.1	(1.180)	2771.8	(3.902)
	hamerly	**2.7**	(0.031)	14.6	(0.058)	**28.2**	(**0.090**)	**204.2**	(**0.286**)
uniform random	iterations	121		353		312		1405	
$n = 1250000$	lloyd	21.8	(0.134)	178.9	(0.491)	660.7	(2.100)	13854.4	(9.857)
$d = 8$	kd-tree	117.5	(0.886)	622.6	(1.740)	2390.8	(7.633)	46731.5	(33.254)
	elkan	14.1	(0.071)	130.6	(0.354)	591.8	(1.879)	11827.9	(8.414)
	hamerly	**10.9**	(**0.045**)	**40.4**	(**0.099**)	**169.8**	(**0.527**)	**1395.6**	(**0.989**)
uniform random	iterations	137		4120		2096		2408	
$n = 1250000$	lloyd	66.4	(0.323)	5479.5	(1.325)	12543.8	(5.974)	68967.3	(28.632)
$d = 32$	kd-tree	208.4	(1.324)	29719.6	(7.207)	74181.3	(35.380)	425513.0	(176.697)
	elkan	48.1	(0.189)	1370.1	(0.327)	2624.9	(1.242)	14245.9	(5.907)
	hamerly	**46.9**	(**0.180**)	**446.4**	(**0.103**)	**1238.9**	(**0.581**)	**9886.9**	(**4.097**)
birch	iterations	52		179		110		99	
$n = 100000$	lloyd	0.53	(0.004)	4.60	(0.024)	11.80	(0.104)	48.87	(0.490)
$d = 2$	kd-tree	**0.41**	(<**0.001**)	0.96	(**0.003**)	2.67	(0.021)	17.68	(0.173)
	elkan	0.58	(0.005)	4.35	(0.023)	11.80	(0.104)	54.28	(0.545)
	hamerly	0.44	(0.002)	**0.90**	(**0.003**)	**1.86**	(**0.014**)	**7.81**	(**0.075**)
covtype	iterations	19		204		320		111	
$n = 150000$	lloyd	3.52	(0.048)	48.02	(0.222)	322.25	(0.999)	564.05	(5.058)
$d = 54$	kd-tree	6.65	(0.205)	266.65	(1.293)	2014.03	(6.285)	3303.27	(29.734)
	elkan	3.07	(0.022)	11.58	(0.044)	70.45	(0.212)	**152.15**	(**1.347**)
	hamerly	**2.95**	(**0.019**)	**7.40**	(**0.024**)	**42.83**	(**0.126**)	169.53	(1.505)
kddcup	iterations	39		55		169		142	
$n = 95412$	lloyd	4.74	(0.032)	12.35	(0.159)	116.63	(0.669)	464.22	(3.244)
$d = 56$	kd-tree	9.68	(0.156)	58.55	(0.996)	839.31	(4.945)	3349.47	(23.562)
	elkan	4.13	(0.012)	6.24	(0.049)	32.27	(0.169)	**132.39**	(**0.907**)
	hamerly	**3.95**	(**0.011**)	**5.87**	(**0.042**)	**28.39**	(**0.147**)	197.26	(1.364)
mnist50	iterations	37		249		190		81	
$n = 60000$	lloyd	2.92	(0.018)	23.18	(0.084)	75.82	(0.387)	162.09	(1.974)
$d = 50$	kd-tree	4.90	(0.069)	100.09	(0.393)	371.57	(1.943)	794.51	(9.780)
	elkan	2.42	(0.005)	7.02	(0.019)	**21.58**	(**0.101**)	**55.61**	(**0.660**)
	hamerly	**2.41**	(**0.004**)	**4.54**	(**0.009**)	21.95	(0.104)	77.34	(0.928)

Table 3: These results show the fraction of times that each algorithm was able to skip the innermost loop on data of different dimensions (values closer to 1 are better). These results are averaged over runs using k = 3, 20, 100, and 500 (one run for each k). The randX datasets are uniform random hypercube data with X dimensions.

dataset	rand2	rand8	rand32	rand128
elkan	0.56	0.01	0.00	0.00
hamerly	0.97	0.88	0.91	0.83
dataset	birch	covtype	kddcup	mnist50
elkan	0.52	0.34	0.18	0.22
hamerly	0.94	0.89	0.82	0.82

Memory requirements

Dataset	Algorithm	Megabytes k=3	k=20	k=100	k=500
uniform	lloyd	7.5	7.5	7.5	7.5
random	kd-tree	32.1	32.1	32.1	32.1
n=1.25M	elkan	19.8	60.3	251.0	1205.2
d=2	hamerly	14.7	14.7	14.7	14.7
uniform	lloyd	21.9	21.9	21.9	21.9
random	kd-tree	54.8	54.8	54.8	54.8
n=1.25M	elkan	34.1	74.6	265.3	1219.5
d=8	hamerly	29.0	29.0	29.0	29.0
uniform	lloyd	79.1	79.1	79.1	79.1
random	kd-tree	145.2	145.2	145.2	145.3
n=1.25M	elkan	91.3	131.8	322.6	1276.8
d=32	hamerly	86.2	86.2	86.2	86.3
birch	lloyd	1.4	1.1	1.1	1.3
n=100K	kd-tree	2.9	2.9	2.8	2.7
d=2	elkan	2.1	5.2	20.6	97.3
	hamerly	1.5	1.7	1.6	1.5
covtype	lloyd	16.2	16.2	16.1	16.4
n=150K	kd-tree	27.2	27.2	27.2	27.3
d=54	elkan	17.4	22.5	45.3	160.4
	hamerly	17.0	17.0	16.8	17.2
kddcup	lloyd	10.9	10.8	11.1	11.2
n=95412	kd-tree	18.8	18.9	19.1	19.0
d=56	elkan	11.9	15.1	29.6	103.1
	hamerly	11.6	11.6	11.3	11.7
mnist50	lloyd	6.3	6.6	6.4	6.8
n=60K	kd-tree	10.5	10.4	10.6	10.7
d=50	elkan	7.0	9.1	18.4	64.8
	hamerly	6.9	6.9	6.9	6.8

Summary

- For moderate d (< 50) and k (< 100), Hamerly is well-suited (has smaller time and memory footprint).
- Large d (greater than 50), Elkan might be better (has smaller time footprint, in spite of large memory requirements).