Lecture 06
Clustering Analysis and K-Means

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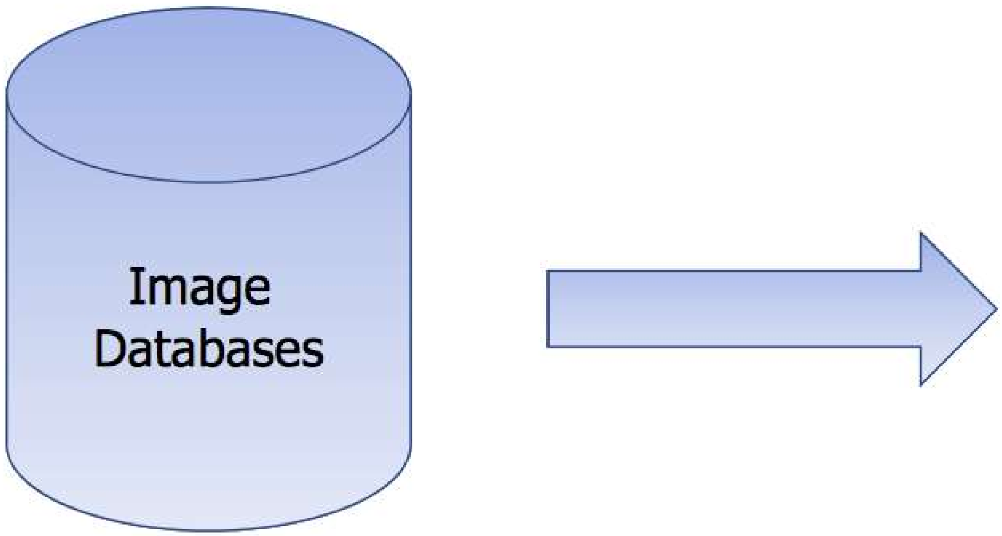
Some of the slides are according to Chao Zhang, and Le Song.

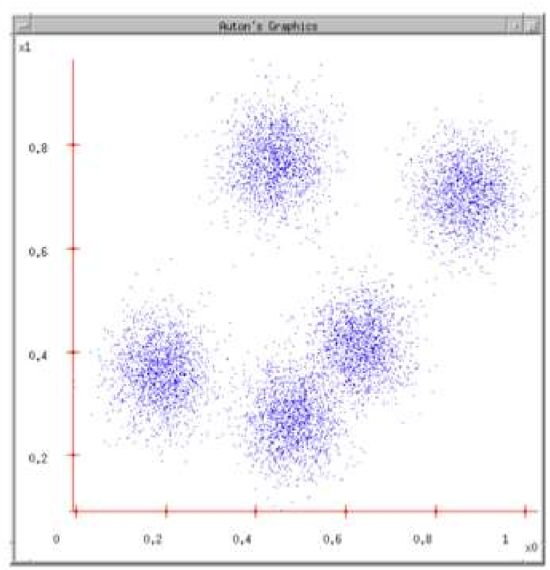
Outline

- Clustering
- Distance Function
- K-Means Algorithm
- Analysis of K-Means

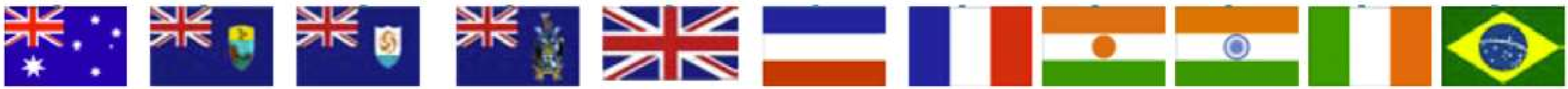
Clustering Images



Goal of clustering:
Divide object into groups, and objects within a group are more similar than those outside the group



Clustering Other Objects



Australia | St. Helena & Dependencies | Anguilla | South Georgia & South Sandwich Islands | U.K. | Serbia & Montenegro | France | Niger | India | Ireland | Brazil

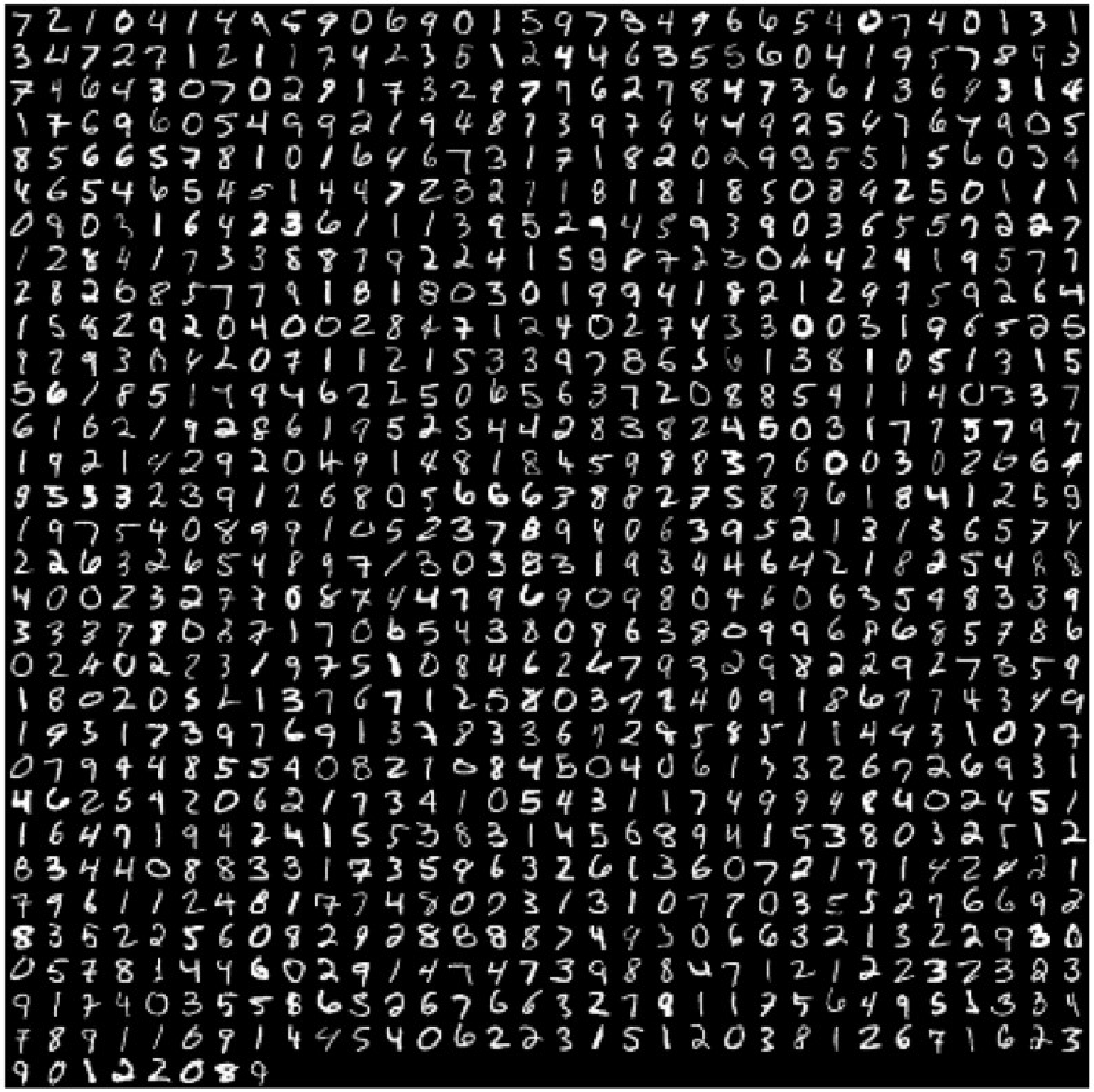
Piotr Belarusian
Pyotr Azerbaijani
Petros Greek
Pietro Italian
Pedro Portuguese
Pierre French
Piero Italian
Peter Dutch
Peder Danish
Peka Couldn't find it – Finish?
Peadar Irish

Linguistic Similarity

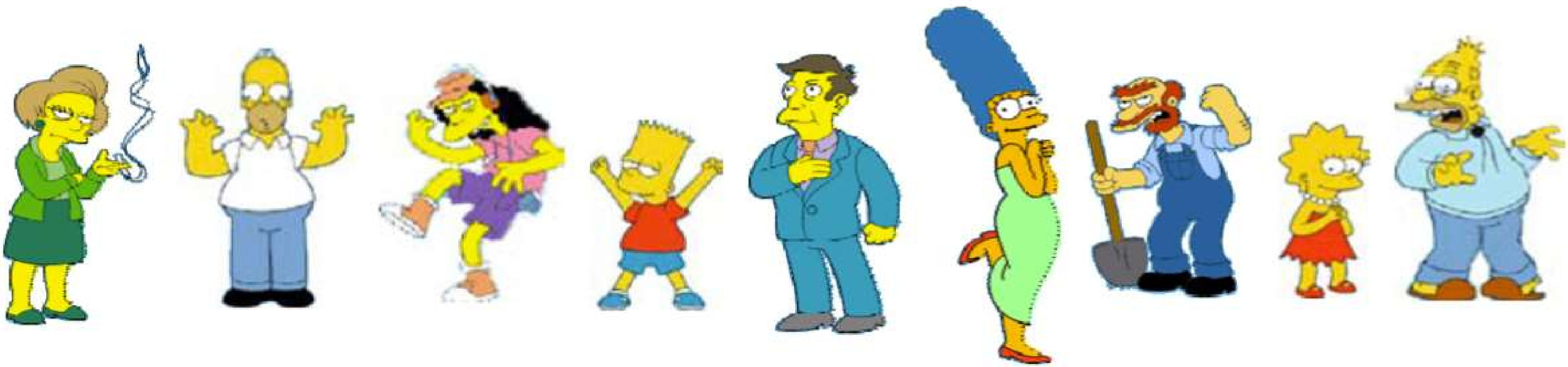
Clustering Hand Digits

0 1 2 3 4 5 6 7 8 9

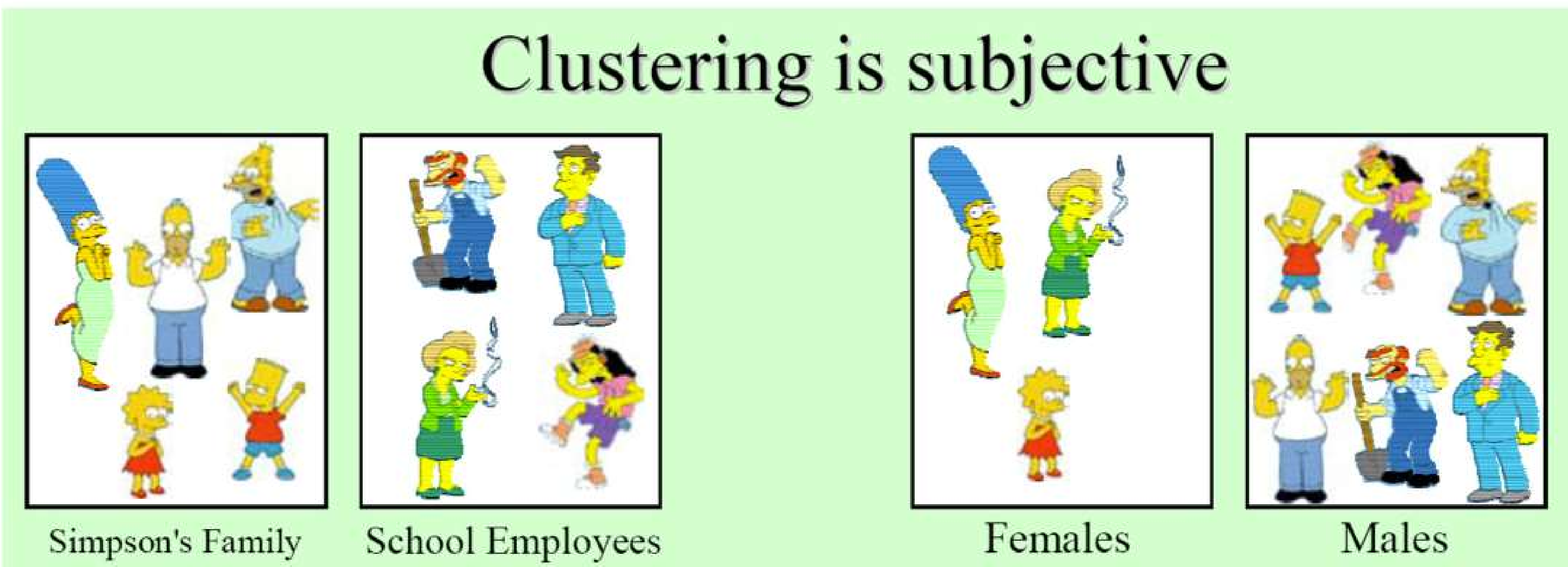
1 1



Clustering is Subjective



What is consider similar/dissimilar?



Are they similar or not?

So What is Clustering in General?

- You pick your similarity/dissimilarity function
- The algorithm figures out the grouping of objects based on the chosen similarity/dissimilarity function
  - Points within a cluster is similar
  - Points across clusters are not so similar
- Issues for clustering
  - How to represent objects? (Vector space? Normalization?)
  - What is a similarity/dissimilarity function for your data?
  - What are the algorithm steps?

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Properties of Similarity Function

- Desired properties of dissimilarity function
  - Symmetry: $d(x,y) = d(y,x)$
    - *Otherwise you could claim "Alex looks like Bob, but Bob looks nothing like Alex"*
  - Positive separability: $d(x,y) = 0$, if and only if $x = y$
    - *Otherwise there are objects that are different, but you cannot tell apart*
  - Triangular inequality: $d(x,y) \le d(x,z) + d(z,y)$
    - *Otherwise you could claim "Alex is very like Bob, and Alex is very like Carl, but Bob is very unlike Carl"*

Distance Functions for Vectors

- Suppose two data points, both in R^d
  - $x = (x_1, x_2, \ldots, x_d)^T$
  - $y = (y_1, y_2, \ldots, y_d)^T$

- Euclidian distance: $d(x,y) = \sqrt{\sum_{i=1}^{d}(x_i - y_i)^2}$

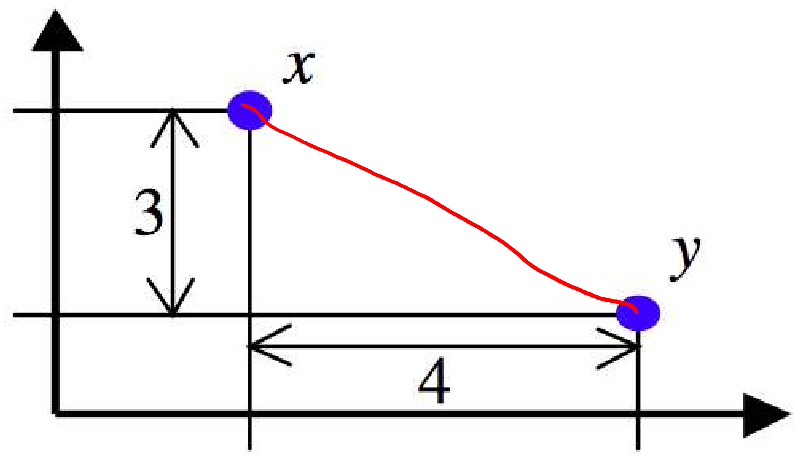
- Minkowski distance: $d(x,y) = \sqrt[p]{\sum_{i=1}^{d}(x_i - y_i)^p}$

  - Euclidian distance: $p = 2$

  - Manhattan distance: $p = 1, d(x,y) = \sum_{i=1}^{d}|x_i - y_i|$

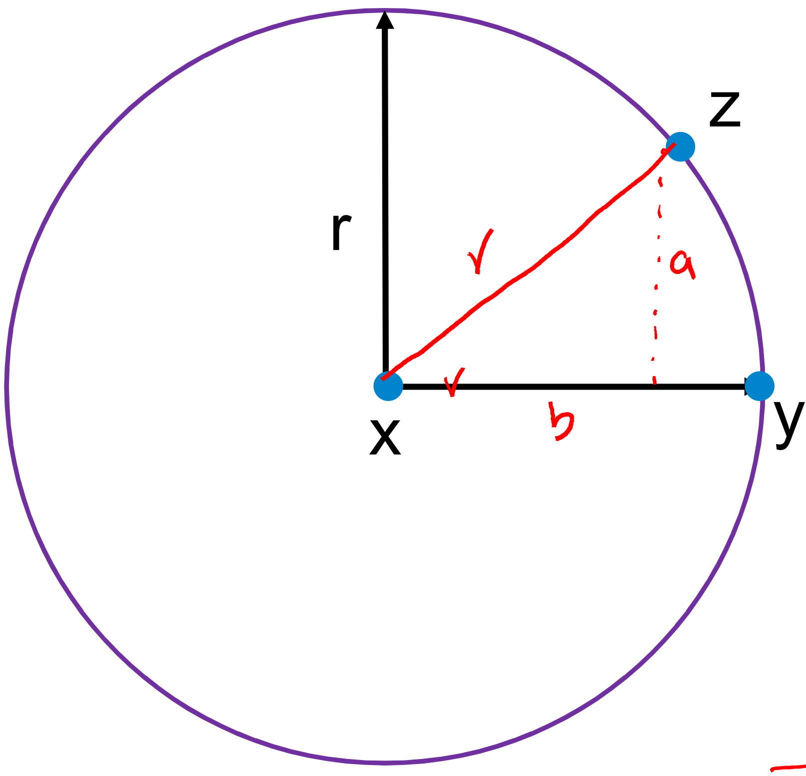
  - "inf"-distance: $p = \infty, d(x,y) = \max_{i=1}^{d}|x_i - y_i|$

Example



- Euclidian distance: $\sqrt{4^2 + 3^2} = 5$
- Manhattan distance: $4 + 3 = 7$
- "inf"-distance: $max\{4,3\} = 4$

Some problems with Euclidean distance



$$d = \sqrt{(x_1-y_1)^2 + (x_2-y_2)^2 + \cdots}$$

hyper sphere

r $\qquad$ $a+b$

d(x,y) and d(x,z) ?

Curse of dimensionality

Hamming Distance

- Manhattan distance is also called *Hamming distance* when all features are binary
  - Count the number of difference between two binary vectors
  - Example, $x, y \in \{0,1\}^{17}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
x	0	1	1	0	0	1	0	0	1	0	0	1	1	1	0	0	1
y	0	1	1	1	0	0	0	0	1	1	1	1	1	1	0	1	1

$$|x-y| \longrightarrow d(x,y) = 5$$

Edit Distance

- Transform one of the objects into the other, and measure how much effort it takes

x	I	N	T	E	*	N	T	I	O	N
y	*	E	X	E	C	U	T	I	O	N
	d	s	s		i	s				

d: deletion (cost 5)
s: substitution (cost 1)
i: insertion (cost 2)

$$d(x, y) = 5 \times 1 + 3 \times 1 + 1 \times 2 = 10$$

$X = \text{I N T E N T I O N}$

$Y = \text{I N S E R T I O N}$

$\quad\quad\quad\;\; \downarrow \quad\;\; \downarrow$

$\quad\quad\quad\;\; s \quad\;\;\; s$

$d(x,y) = 2$

d: deletion (cost 5)
s: substitution (cost 1)
i: insertion (cost 2)

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Results of K-Means Clustering:

Image

Clusters on intensity

Clusters on color

K-means clustering using intensity alone and color alone

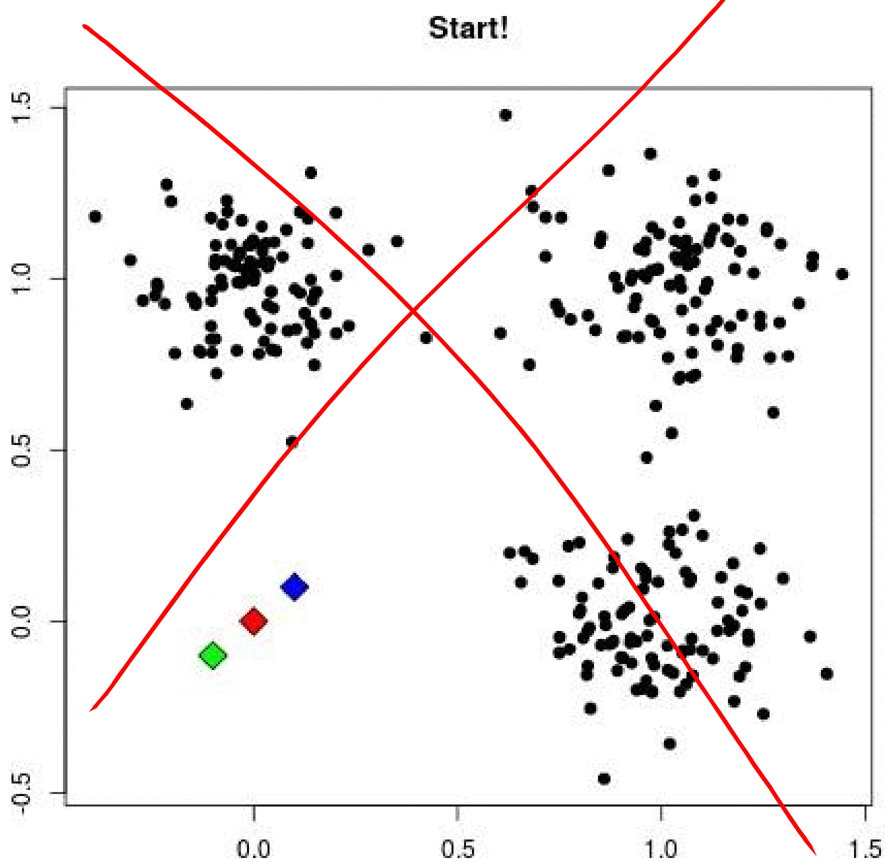
Image

Clusters on color

K-means using color alone, 11 segments (clusters)

* Pictures from Mean Shift: A Robust Approach toward Feature Space Analysis, by D. Comaniciu and P. Meer http://www.caip.rutgers.edu/~comanici/MSPAMI/msPamiResults.html

K-Means Algorithm



$X_1 = \{x^{(1)}, x^{(2)}$

orange blue green

X_1

X_2

X_{100}

100×3

[Visualizing K-Means Clustering]

K-Means Algorithm

- Initialize k cluster centers, $\{c^1, c^2, \ldots, c^k\}$, randomly

- Do

Expectation

  - Decide the cluster memberships of each data point, x^i, by assigning it to the nearest cluster center (cluster assignment)

$$\pi(i) = argmin_{j=1,\ldots,k} \left\|x^i - c^j\right\|^2$$

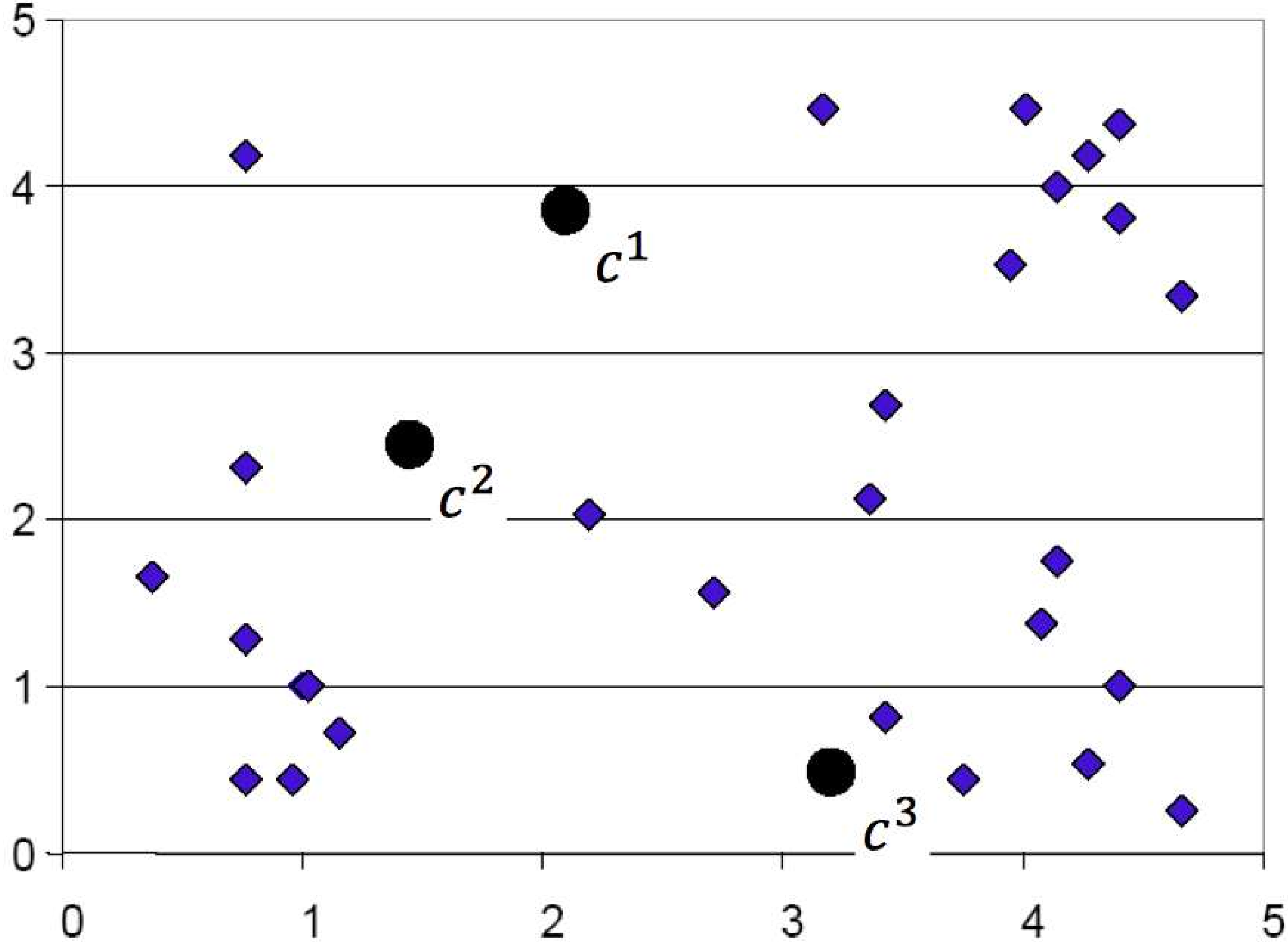
  - Adjust the cluster centers (center adjustment)

Maximization

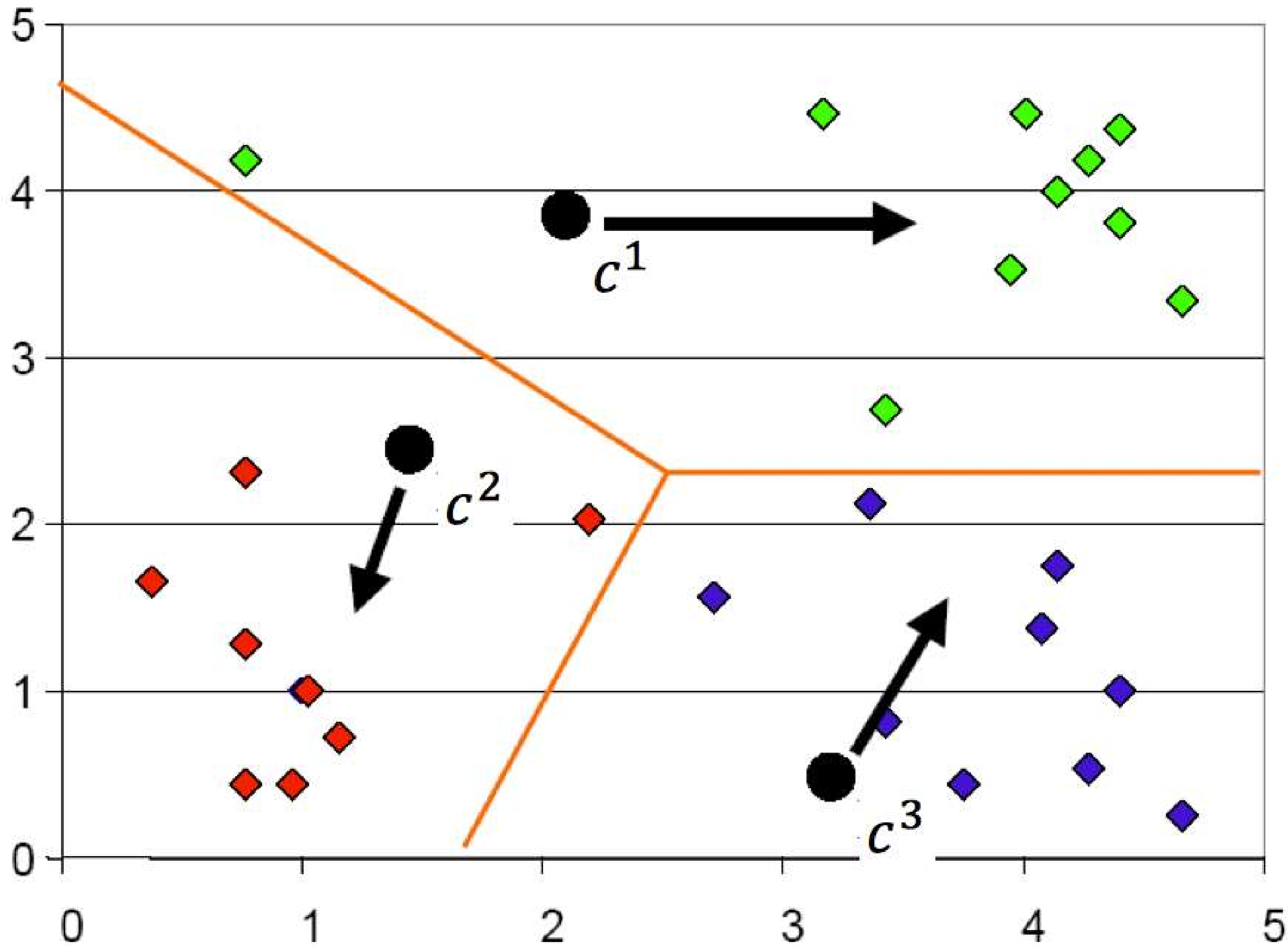
$$c^j = \frac{1}{|\{i: \pi(i) = j\}|} \sum_{i:\pi(i)=j} x^i$$

- While any cluster center has been changed

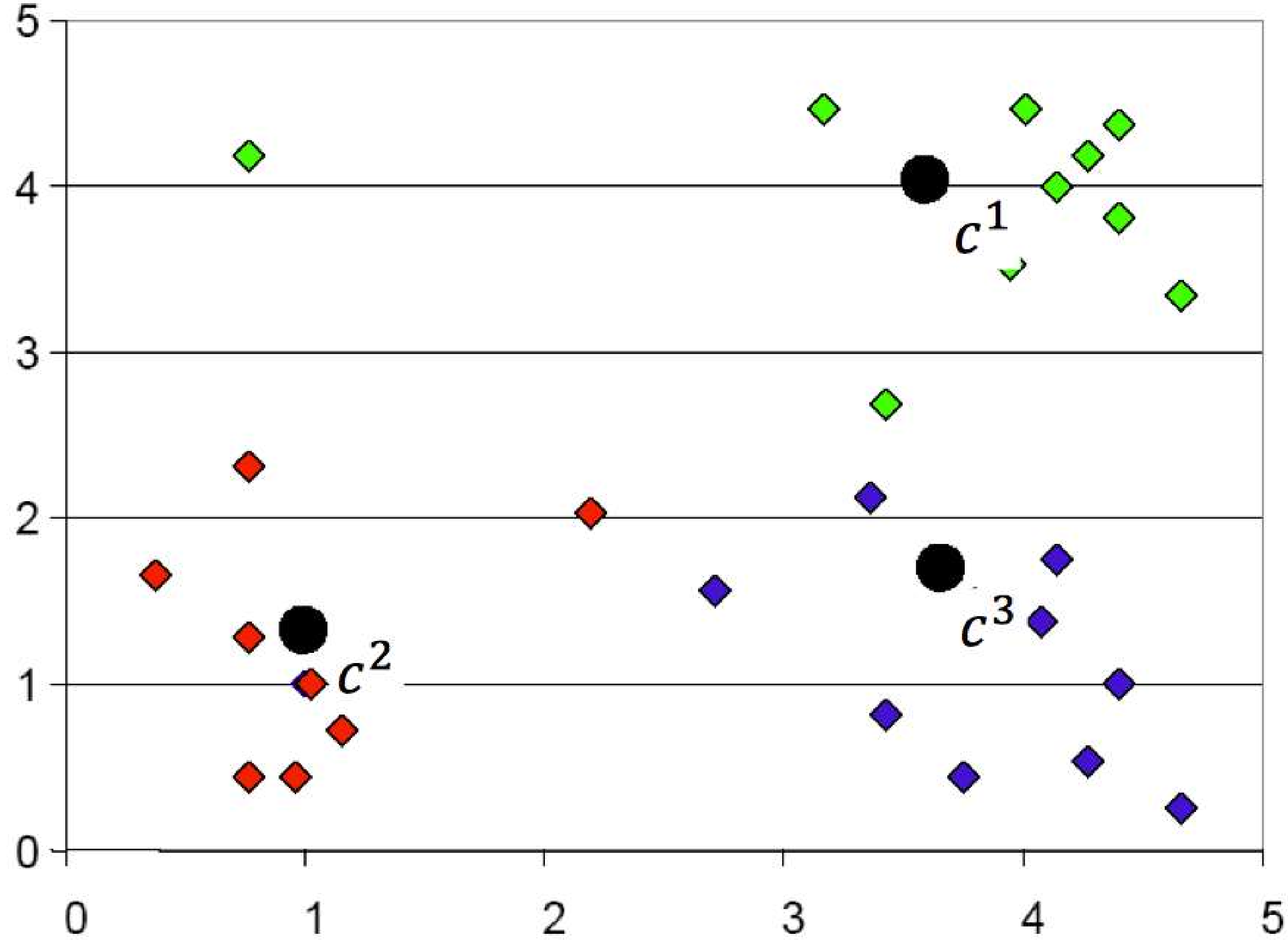
K-Means: Step 1



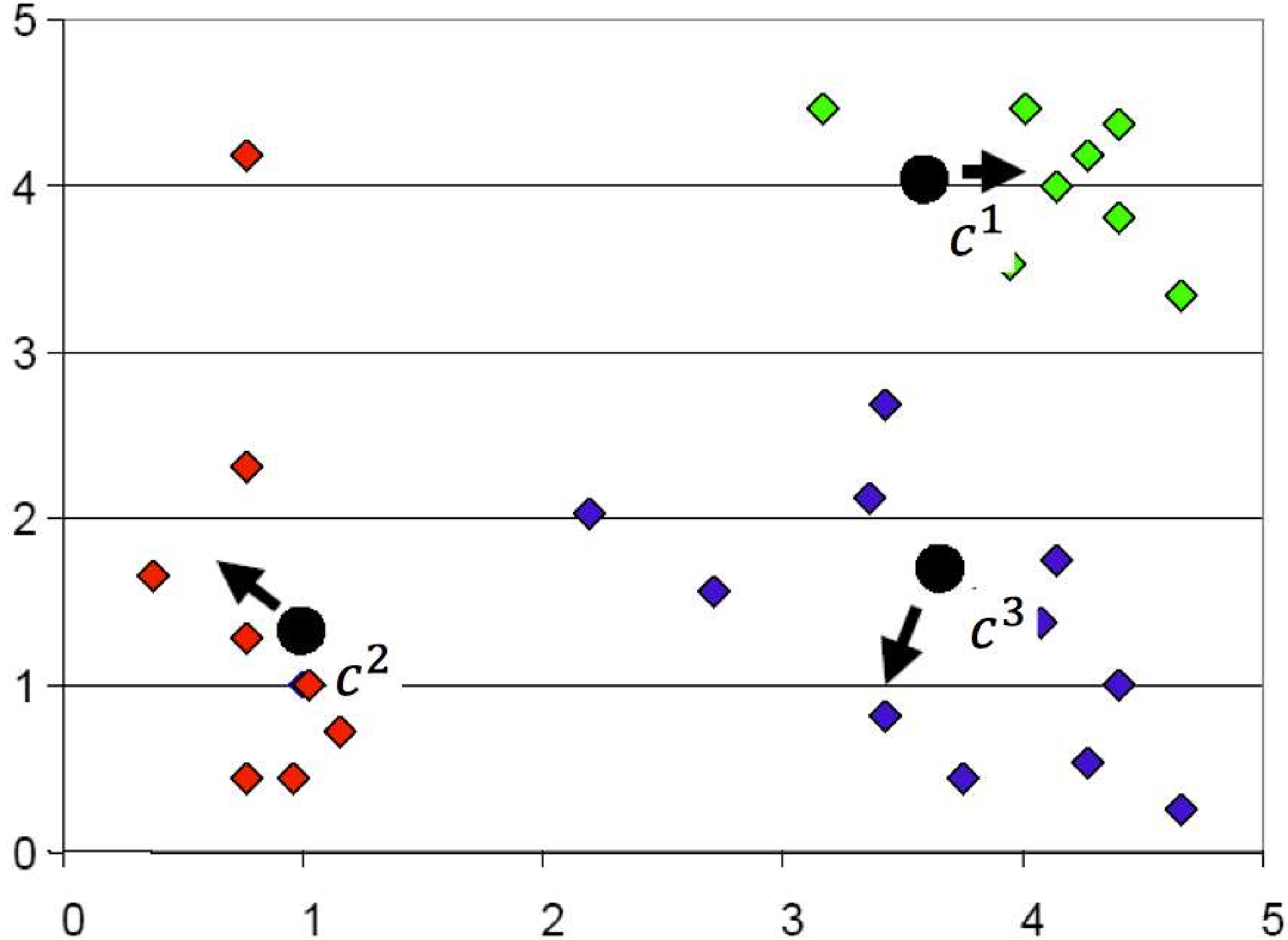
K-Means: Step 2



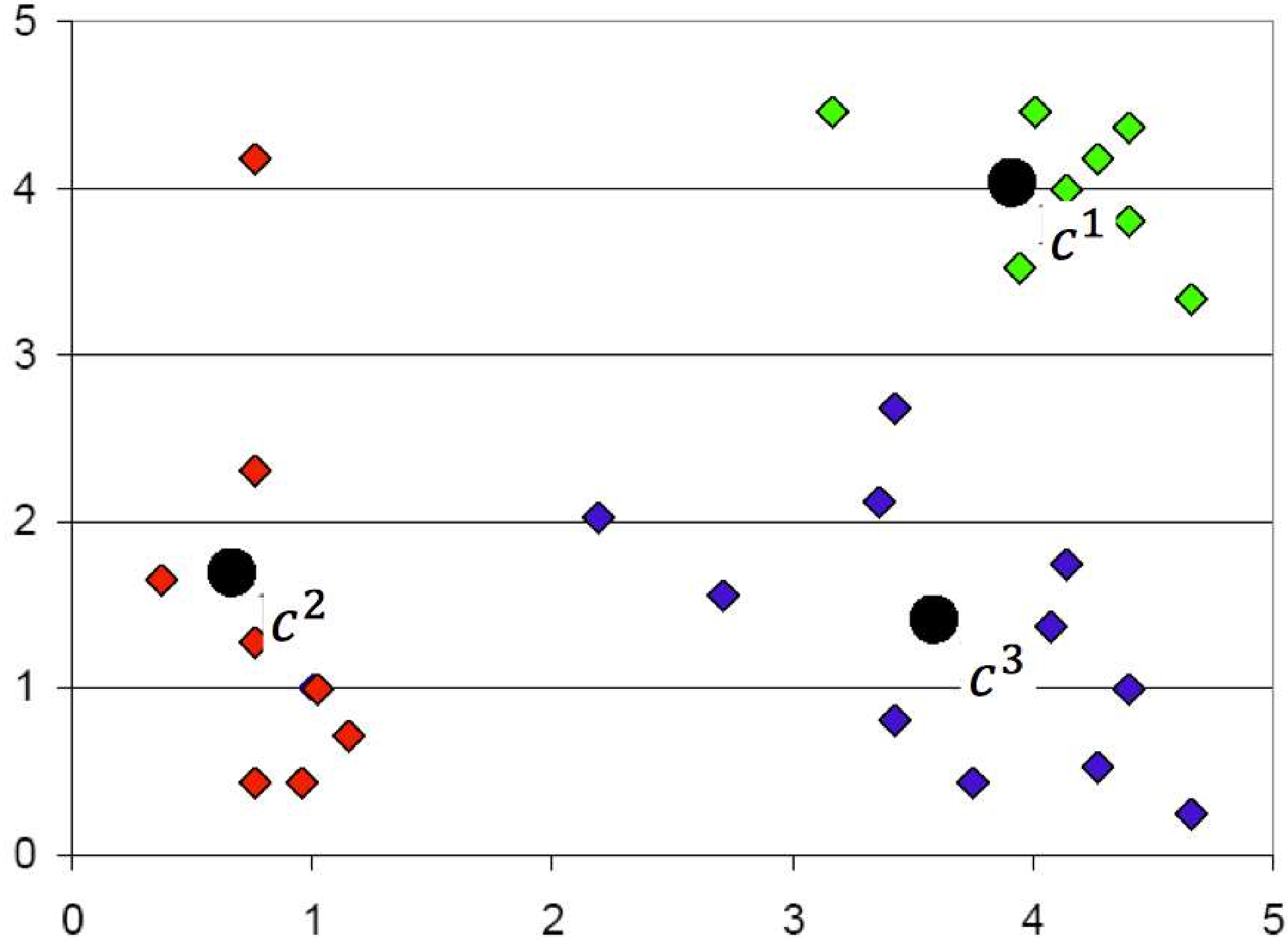
K-Means: Step 3



K-Means: Step 4



K-Means: Step 5



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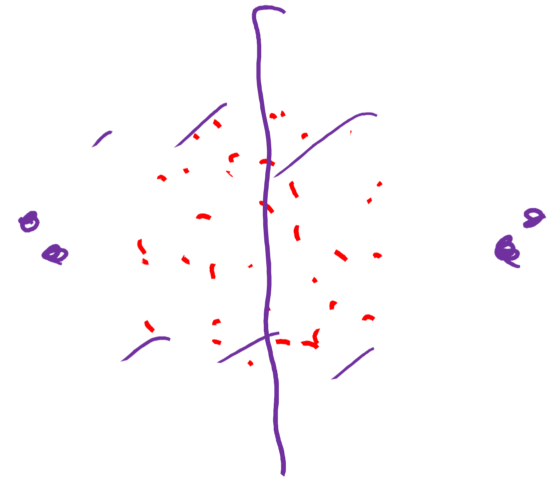
Questions

- Will different initialization lead to different results?
  - Yes
  - No
  - Sometimes



- Will the algorithm always stop after some iteration?
  - Yes
  - No (we have to set a maximum number of iterations)
  - Sometimes

Formal Statement of the Clustering Problem

- Given n data points, $\{x^1, x^2, \dots x^n\} \in R^d$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^d$
- And assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$
- Such that the averaged square distances from each data point to its respective cluster center is small

$$\min_{c,\pi} \frac{1}{n} \sum_{i=1}^{n} \left\| x^i - c^{\pi(i)} \right\|^2$$

Clustering is NP-Hard

- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^d$, and assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$, to minimize

$$\min_{c,\pi} \frac{1}{n} \sum_{i=1}^{n} \left\| x^i - c^{\pi(i)} \right\|^2$$

- A search problem over the space of discrete assignments
  - For all n data point together, there are k^n possibility
  - The cluster assignment determines cluster centers, and vice versa

- For all n data point together, there are k^n possibility

X = {A,B,C}

n=3 (data points)

k=2 clusters of two members

Cluster 1	Cluster 2
A, B	C
C	A, B
A, C	B
B, C	A
B	A, C
A, B, C { }	{ } A, B, C

Convergence of K-Means

- Will kmeans objective oscillate?

$$\frac{1}{n}\sum_{i=1}^{n}\left\|x^i - c^{\pi(i)}\right\|^2$$

- The minimum value of the objective is finite

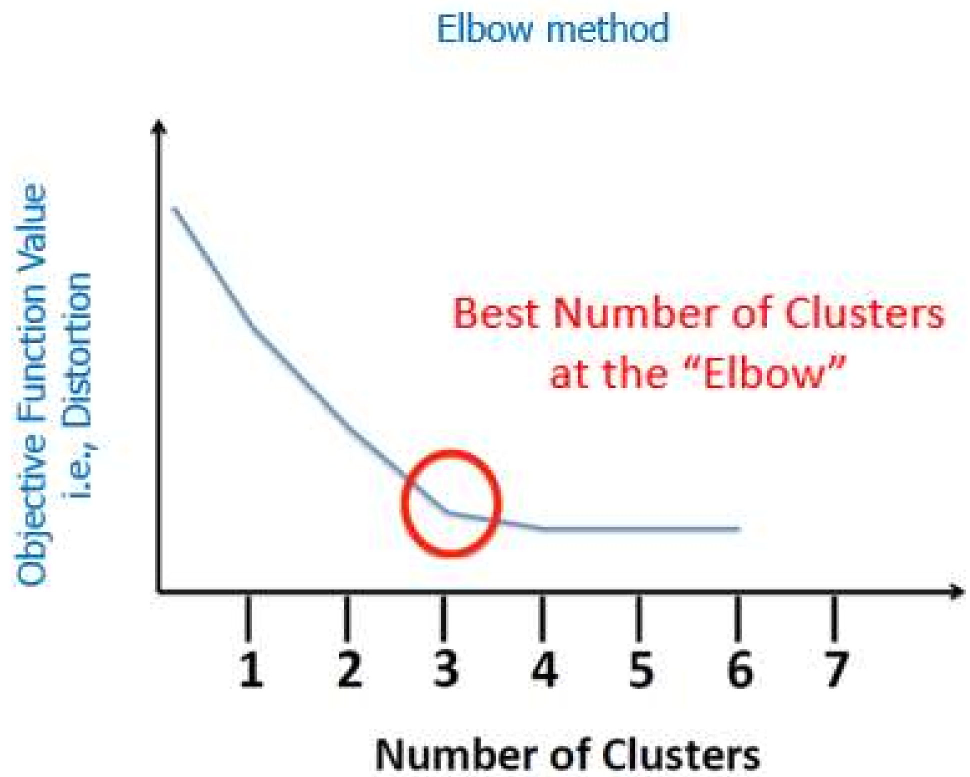
- Each iteration of kmeans algorithm decrease the objective
  - Cluster assignment step decreases objective
    - $\pi(i) = argmin_{j=1,\dots,k} \left\|x^i - c^j\right\|^2$ for each data point i
  - Center adjustment step decreases objective
    - $c^j = \frac{1}{|\{i:\pi(i)=j\}|}\sum_{i:\pi(i)=j} x^i = argmin_c \sum_{i:\pi(i)=j}\left\|x^i - c\right\|^2$

Time Complexity

- Assume computing distance between two instances is O(d) where m is the dimensionality of the vectors.
- Reassigning clusters for all datapoints:
  - O(kn) distance computations (when there is one feature)
  - O(knd) (when there is d features)
- Computing centroids: Each instance vector gets added once to some centroid (Finding centroid for each feature): O(nd).
- Assume these two steps are each done once for I iterations: O(Iknd).

Slide credit: Ray Mooney.

How to Choose K?



Distortion score: computing the sum of squared distances from each point to its assigned center

Image credit: Dileka Madushan.