Clustering Analysis and K-Means

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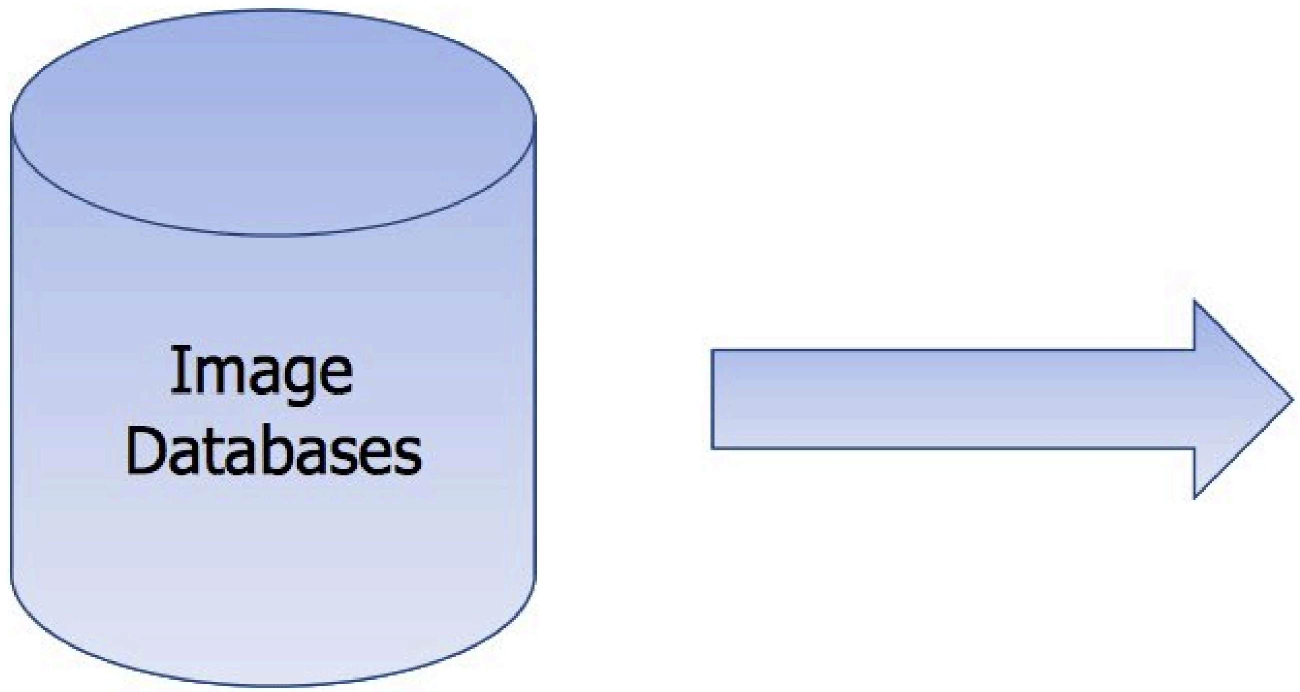
Some of the slides are inspired based on slides from Chao Zhang, and Le Song.

60+ hours on 16 GPU nvidia CUDA cluster.

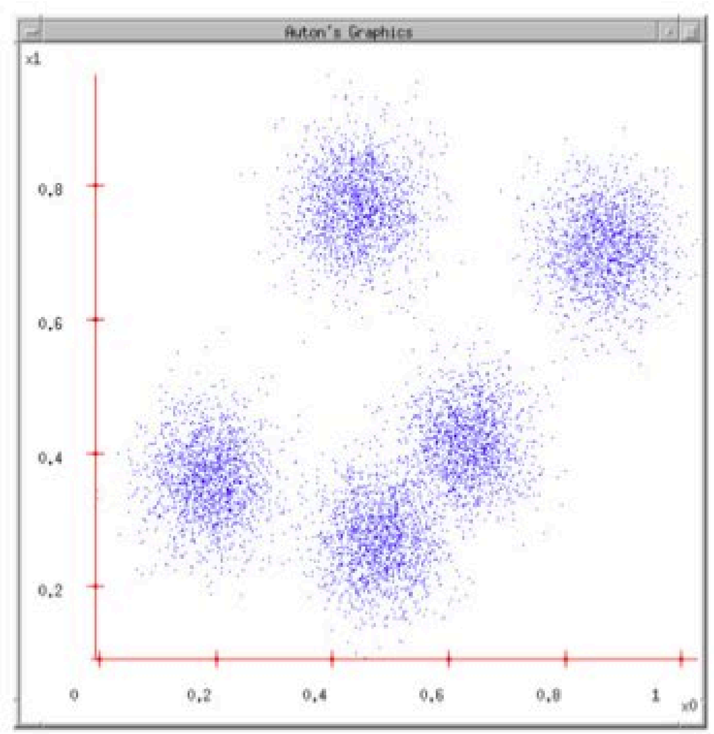
Outline

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

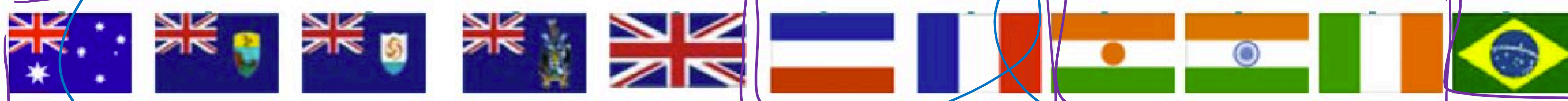
Clustering Images



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

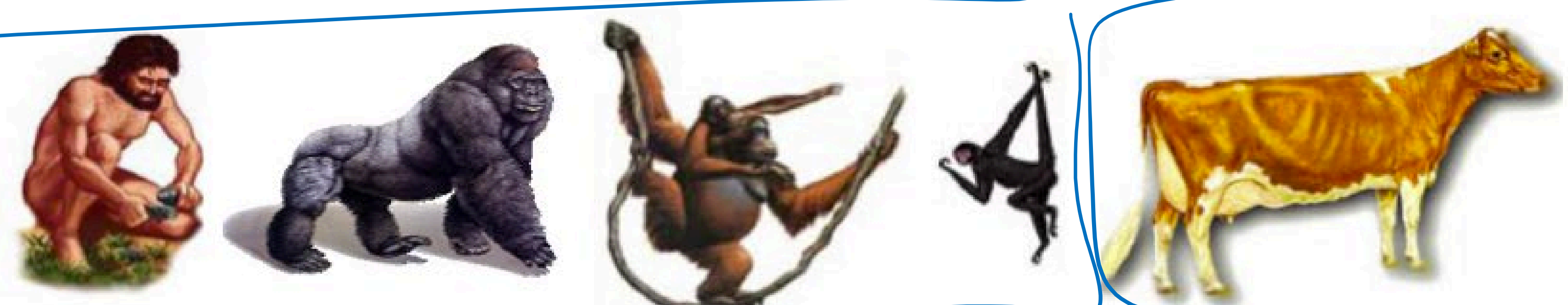


Clustering Other Objects



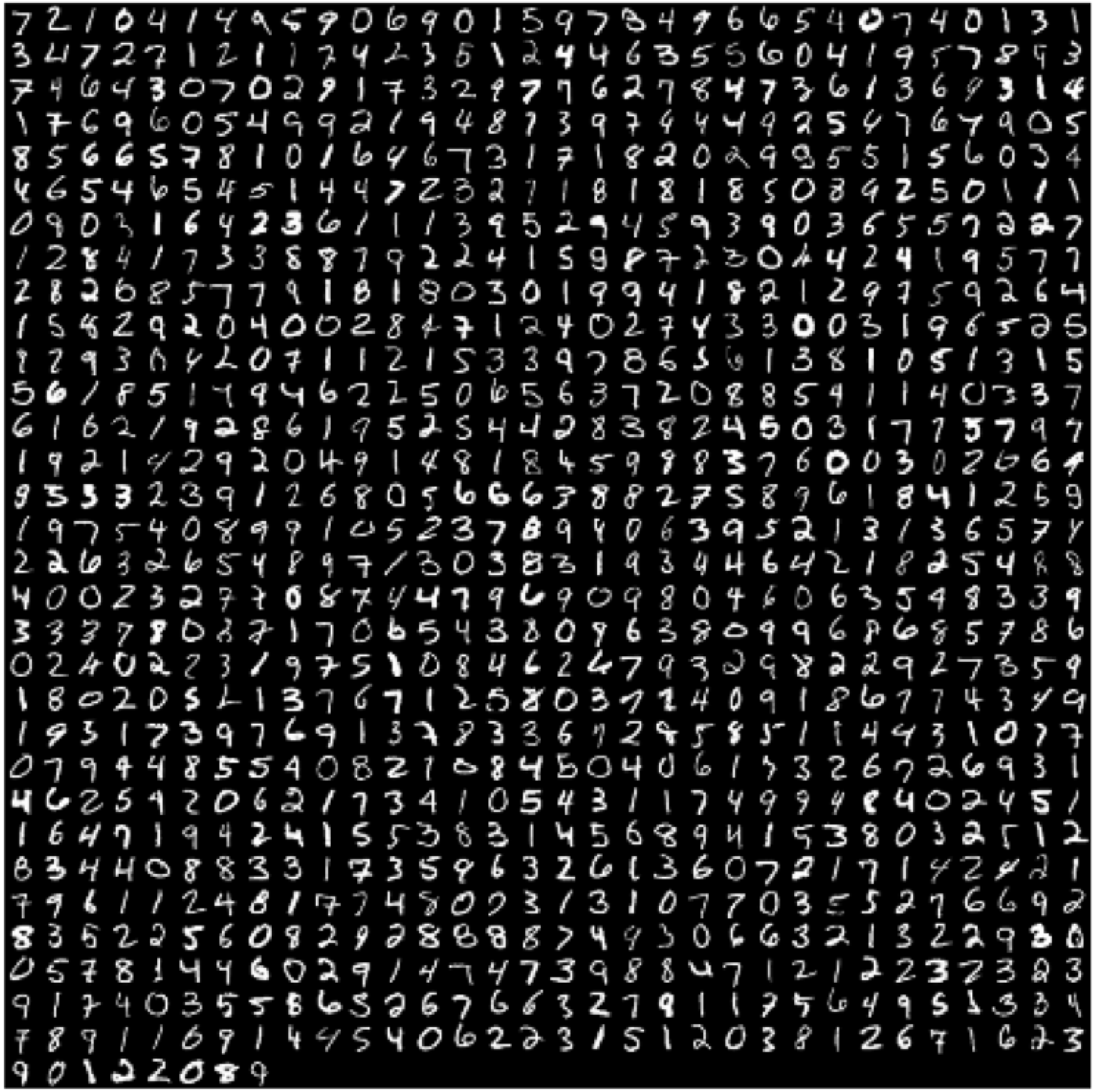
Piotr Belarusian
Pyotr Azerbaijani
Petros Greek
Pietro Italian
Pedro Portuguese
Pierre French
Piero Italian
Peter Dutch
Peder Danish
Peka Couldn't find it – Finish?
Peadar Irish

Linguistic Similarity

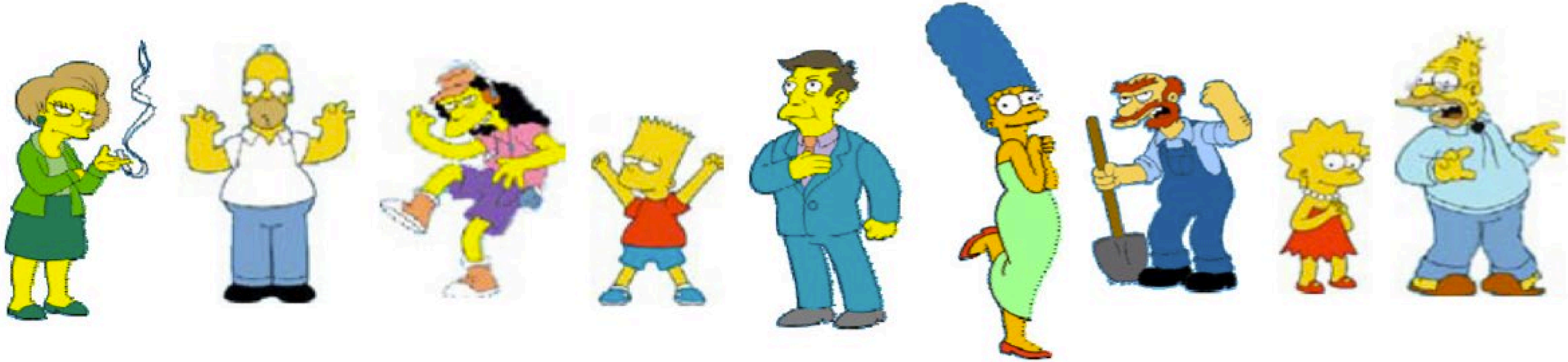


Clustering Hand Digits

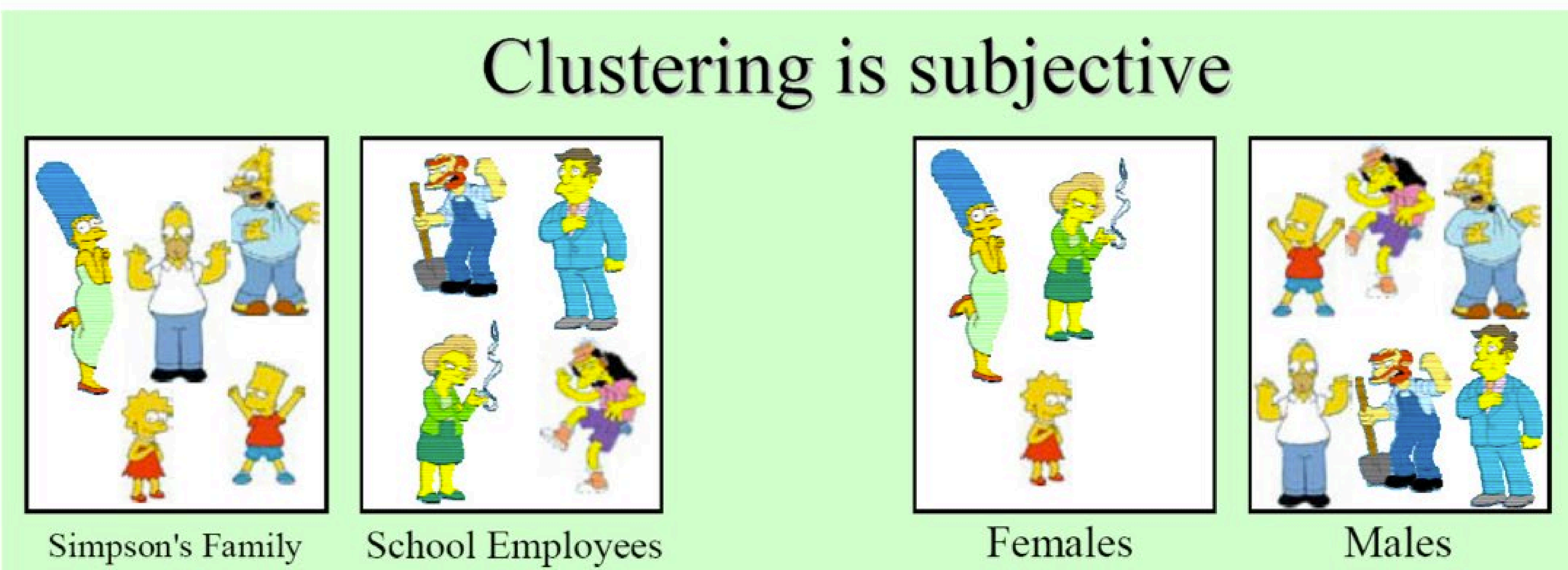
0 1 2 3 4 5 6 7 8 9



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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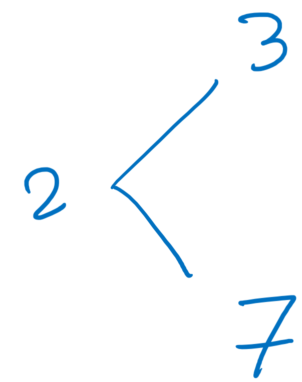


Properties of Similarity Function

- 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: $d(x, y) \leq d(x, z) + d(z, y)$
    - *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
  - $x = (x_1, x_2, \dots, x_d)$
  - $y = (y_1, y_2, \dots, y_d)$

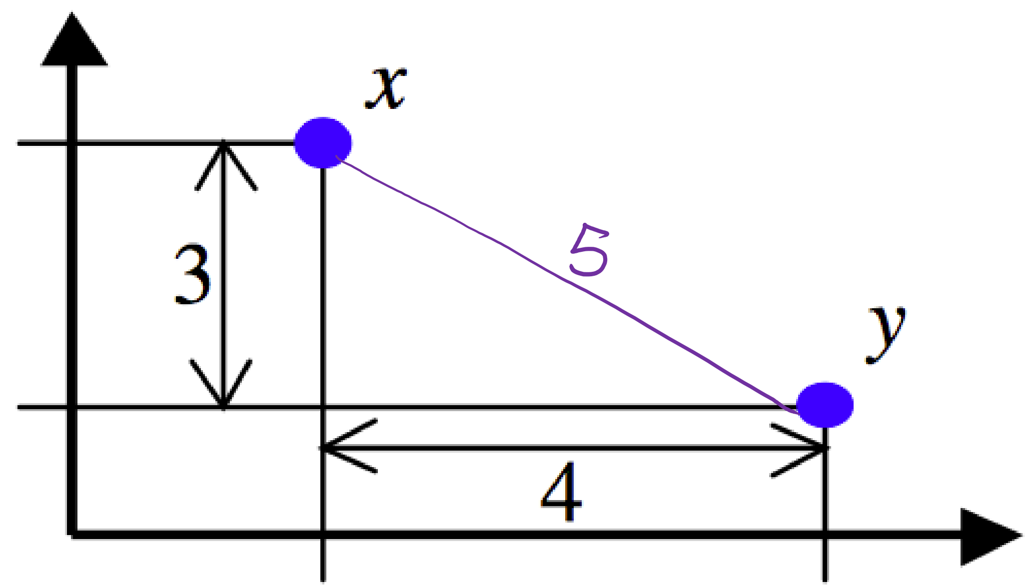
datapoint
sample

$X = \begin{array}{c} 1 \quad 2 \quad \cdots \quad d \\ \begin{bmatrix} \quad & \quad & \quad \\ & & \\ & & \end{bmatrix} \end{array}$ $n \times d$

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

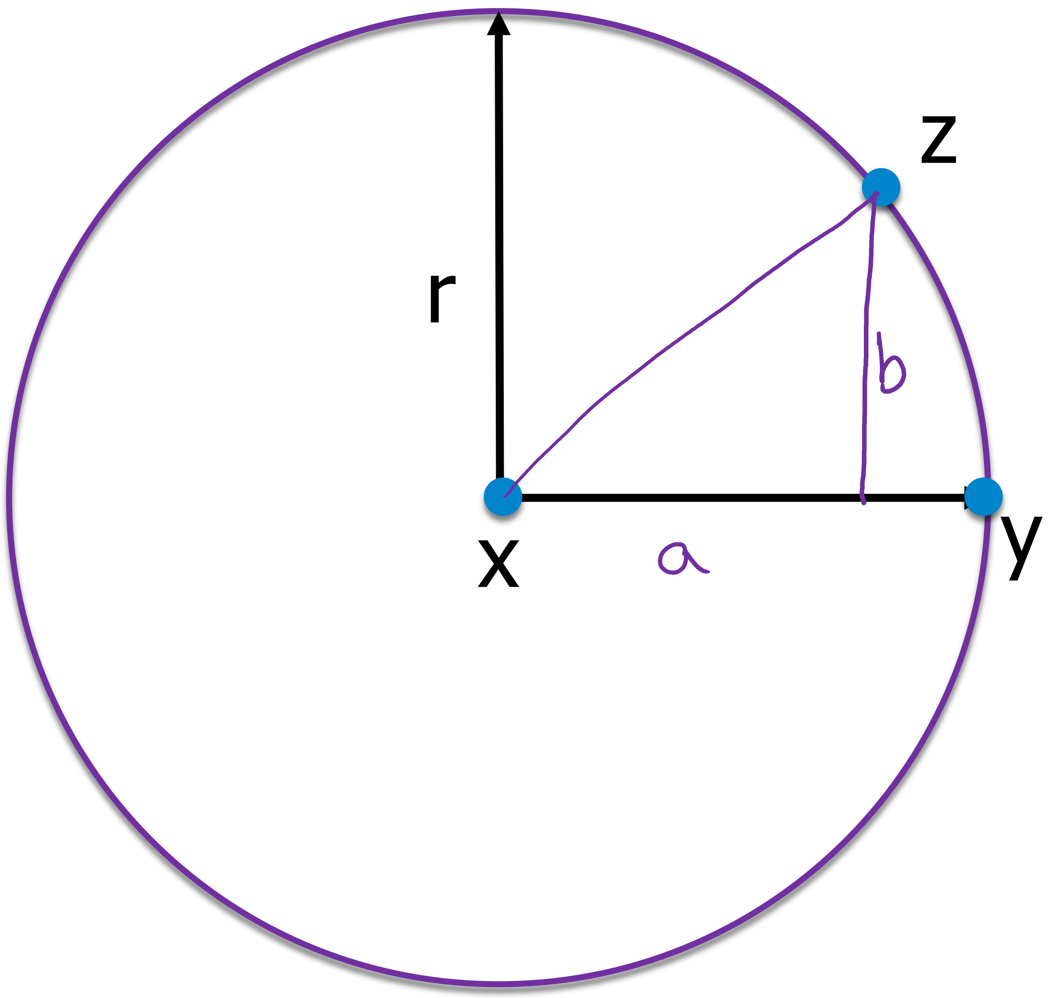
- Minkowski distance: $d(x, y) = \sqrt[p]{\sum_{i=1}^{d} (x_i - y_i)^p}$
  - Euclidean distance: $p = 2$
  - Manhattan distance: $p = 1, d(x, y) = \sum_{i=1}^{d} |x_i - y_i|$
  - "inf"-distance: $p = \infty, d(x, y) = \max_{i=1}^{d} |x_i - y_i|$

Example

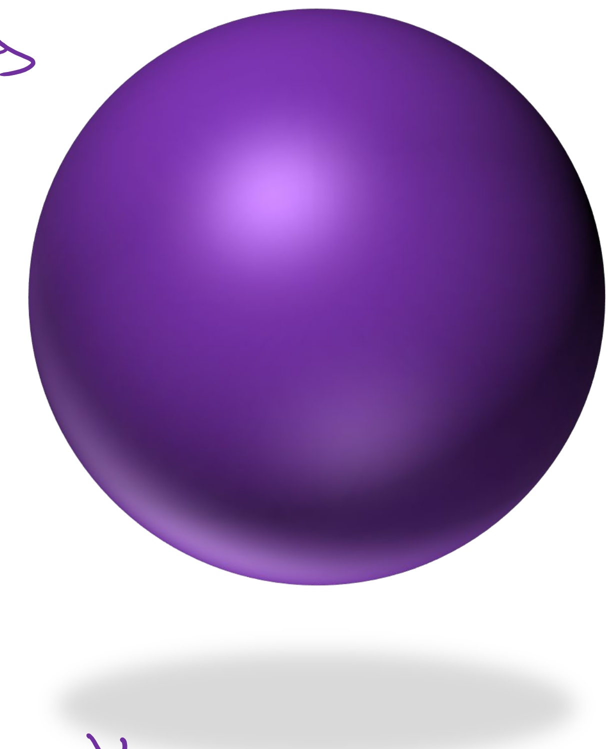


- Euclidean distance: $\sqrt{4^2 + 3^2} = 5$
- Manhattan distance: $4 + 3 = 7$
- “inf”-distance: $max\{4,3\} = 4$

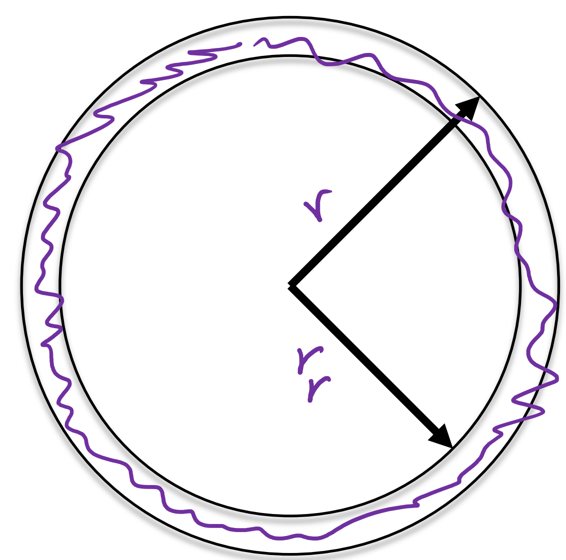
Some problems with Euclidean distance



$V_{total} = \frac{4}{3}\pi r^{3} = cr^{d}$



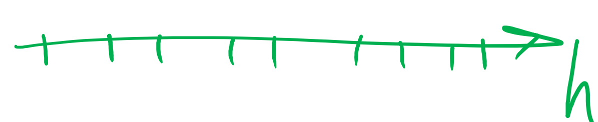
$V_{shell} = cr^{d} - cr_r^{d}$

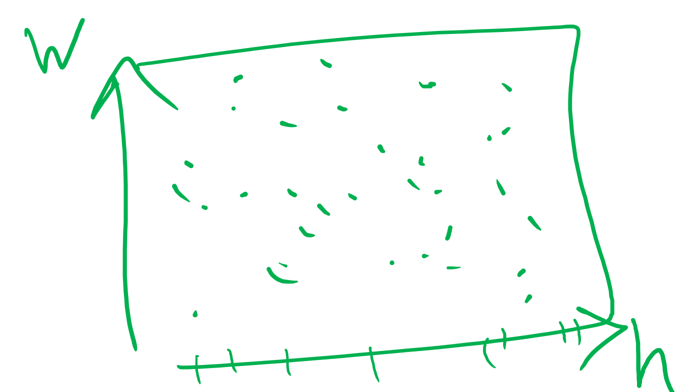


$\frac{V_{shell}}{V_{total}} = 1 - \left(\underbrace{\frac{r_r}{r}}_{0< \quad <1}\right)^{d}$

$V_{shell} \approx V_{Total} \quad d \to \infty$

$\underbrace{d(x,y)}_{r}$ and $\underbrace{d(x,z)}_{r}$?





p=1 manhattan ⇒ $\underbrace{d(x,y)}_{r}$ $\underbrace{d(x,z)}_{a+b}$

[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

$$d(x, y) = 5$$

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	I	N	T	E	N	T	I	O	N
y	I	N	S	E	R	T	I	O	N
	x	x	s	x	s	x	x	x	x

$d(x, y) = 2$

word2vec → by Google

Glove → by Stanford

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

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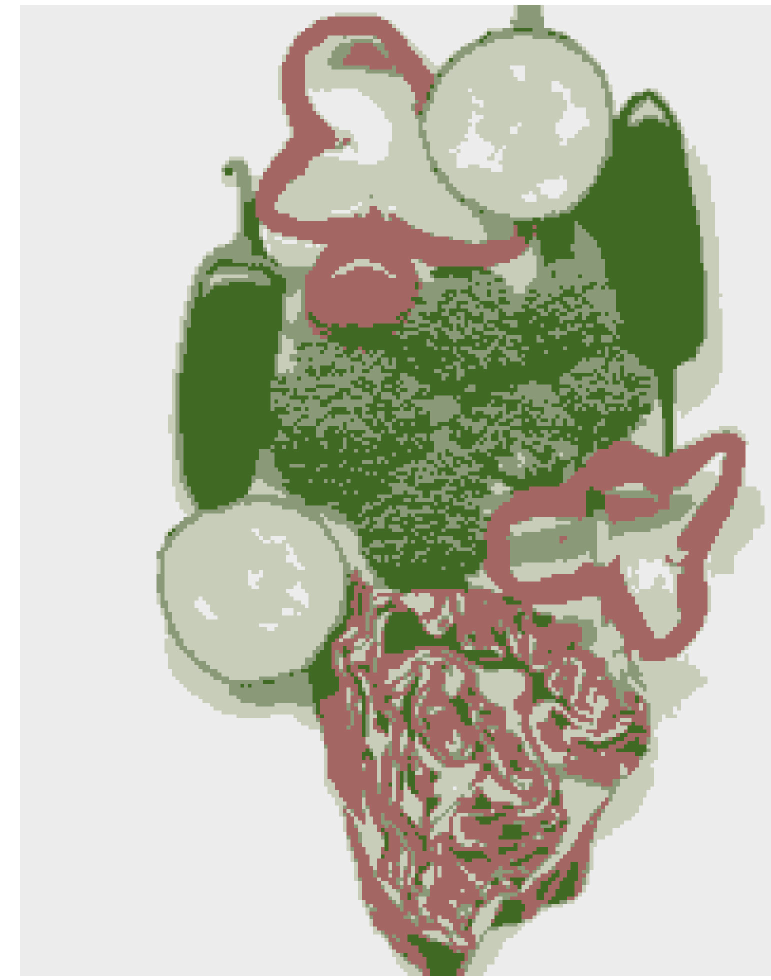
Results of K-Means Clustering:

Image

Clusters on intensity



Clusters on color

K-means clustering using intensity alone and color alone

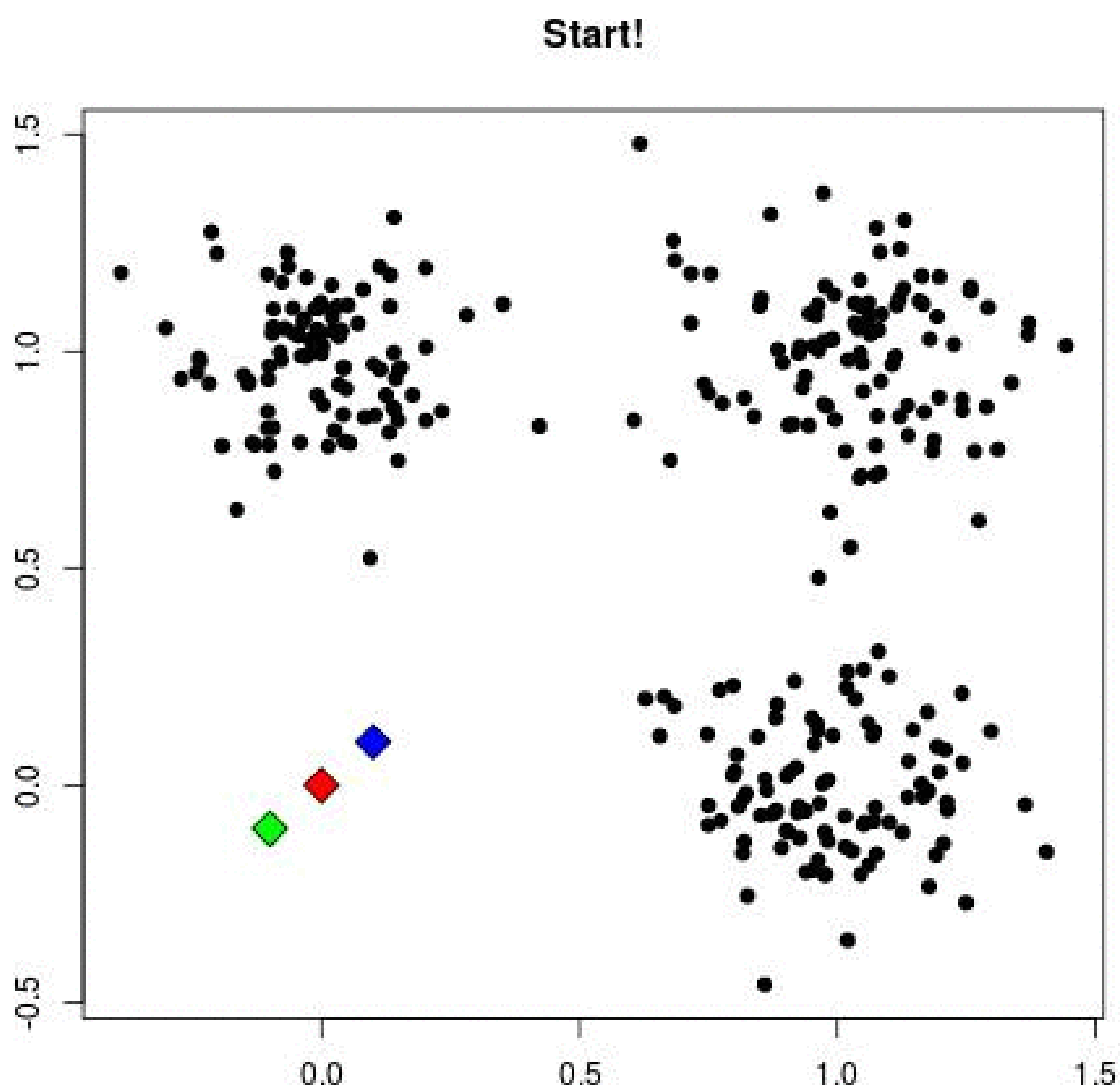
Image

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 [h w]

[h w]

k_1 k_2 k_3

x_1

x_2

x_{100}

$n \times k$

$\Rightarrow$

min(k_1, k_2, k_3)

$n \times 1$

[Visualizing K-Means Clustering]()

K-Means Algorithm

- Initialize k cluster centers, $\{c_1, c_2, \dots, c_k\}$, randomly
- Do
  - Decide the cluster memberships of each data point, x_i by assigning it to the nearest cluster center (cluster assignment)

$$\pi(i) = argmin_{j=1,\dots,k} \quad \left\|x_i - c_j\right\|^2$$

Expectation

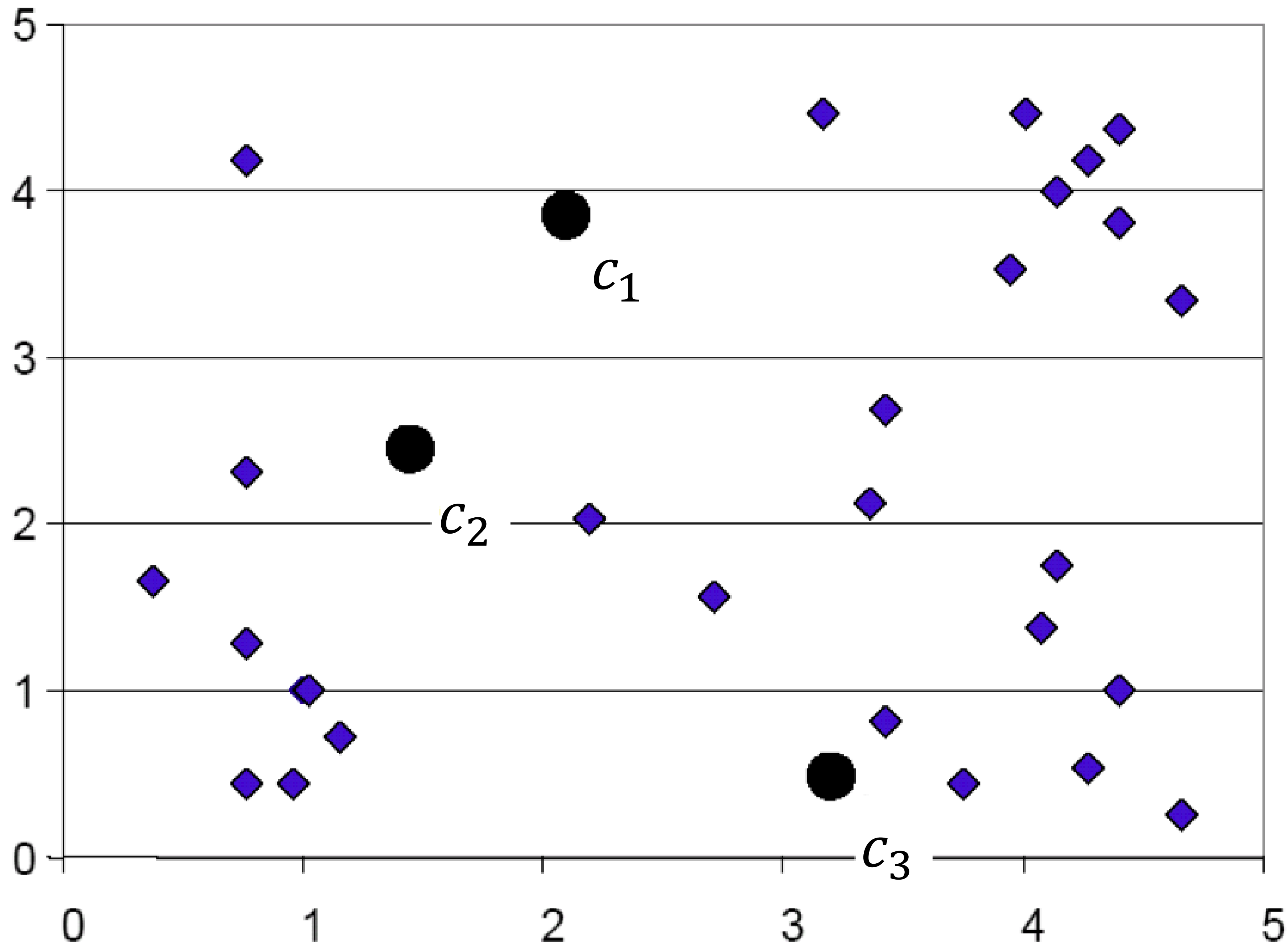
  - Adjust the cluster centers (center adjustment)

$$c_j = \frac{1}{|\{i: \pi(i) = j\}|} \sum_{i:\pi(i)} x_i$$

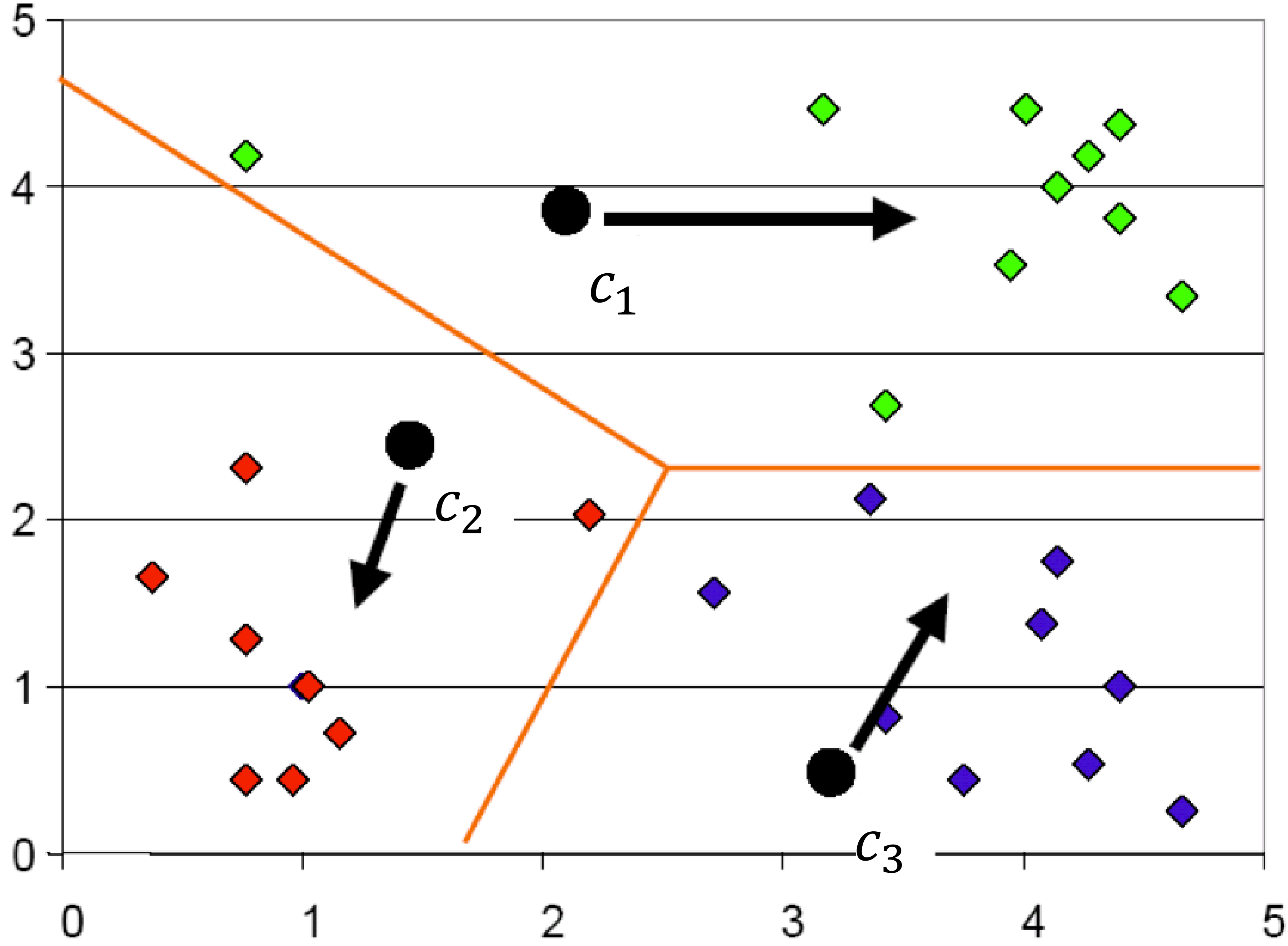
Maximization

- While any cluster center has been changed

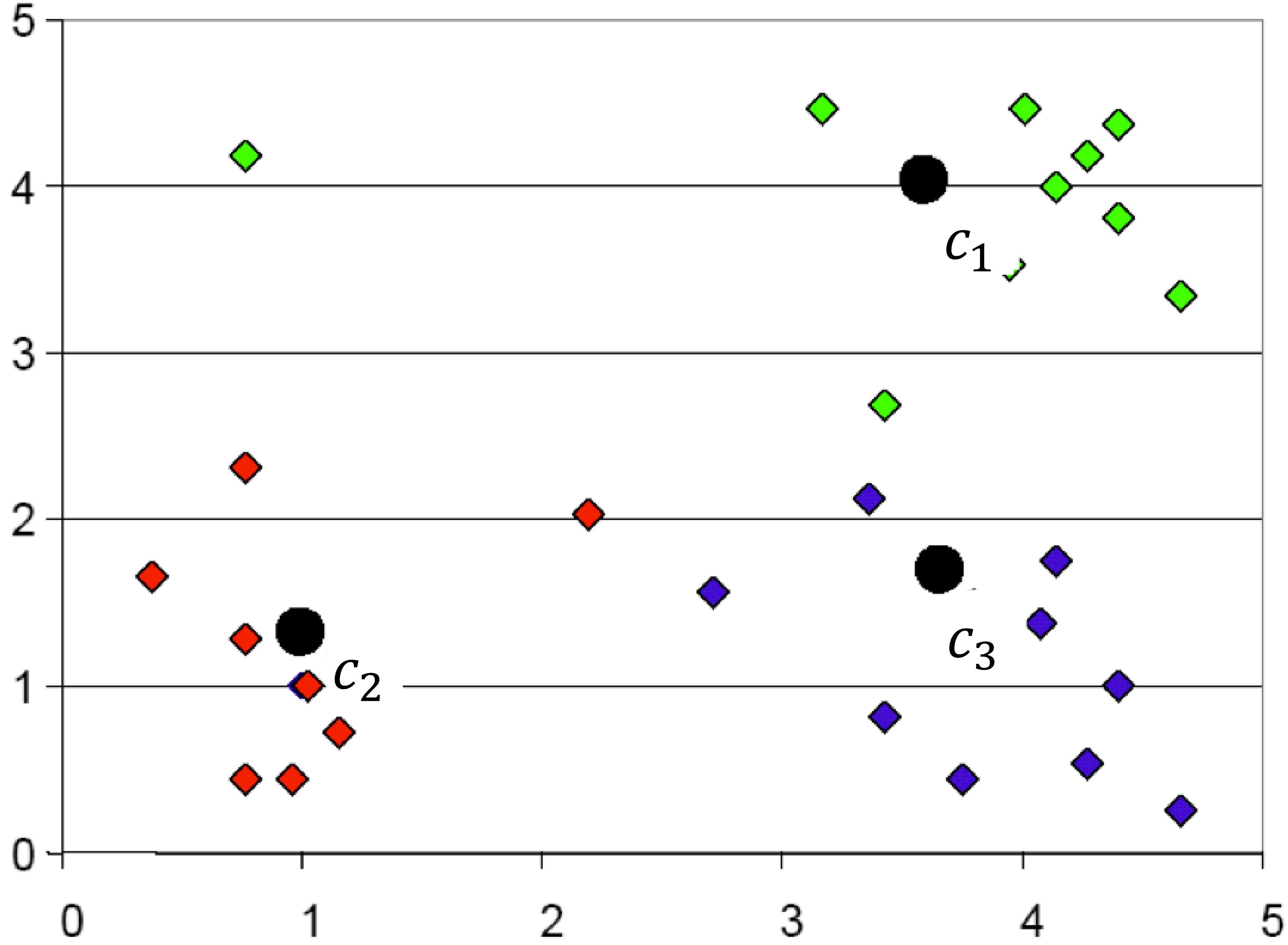
K-Means: Step 1



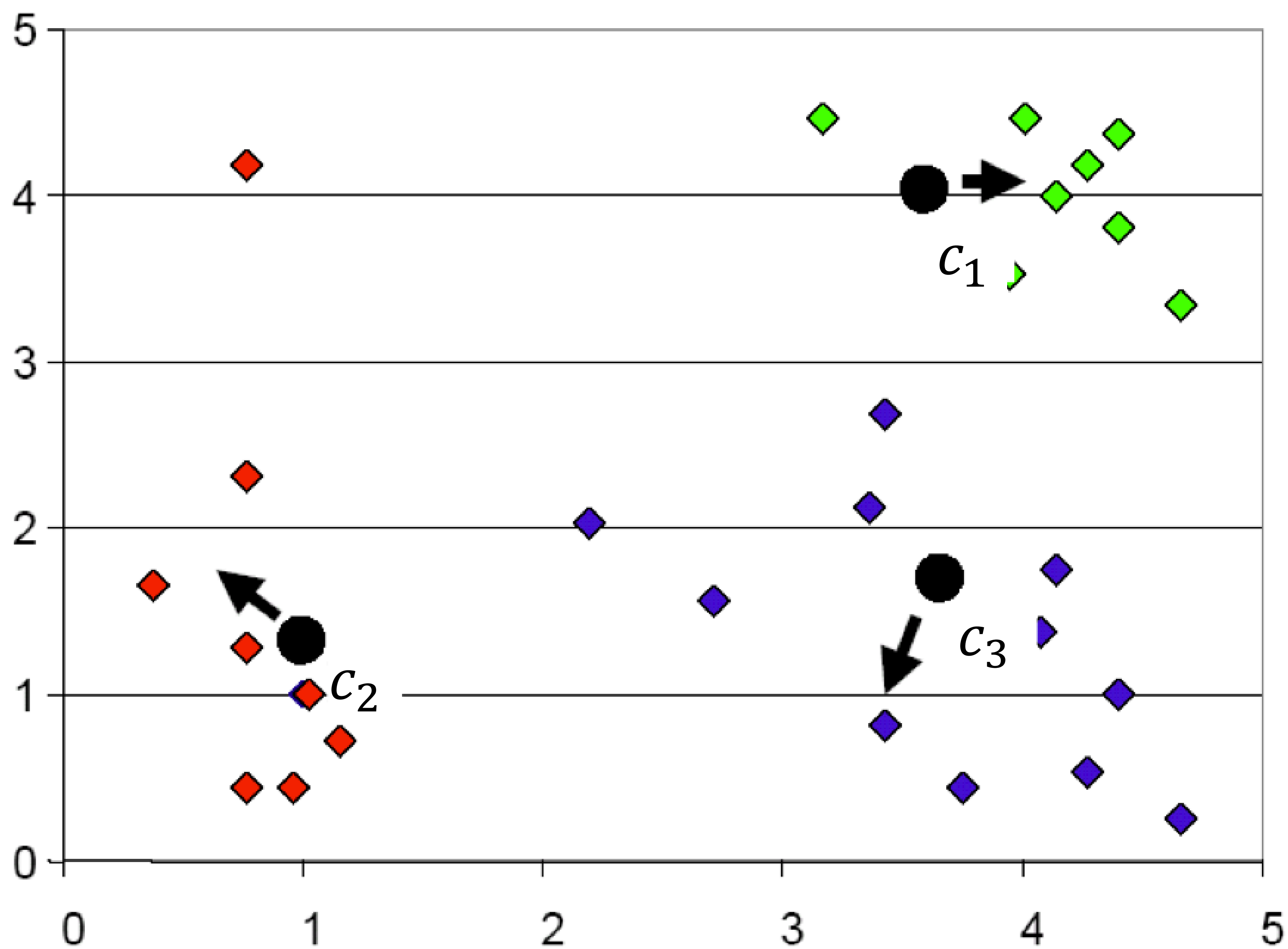
K-Means: Step 2



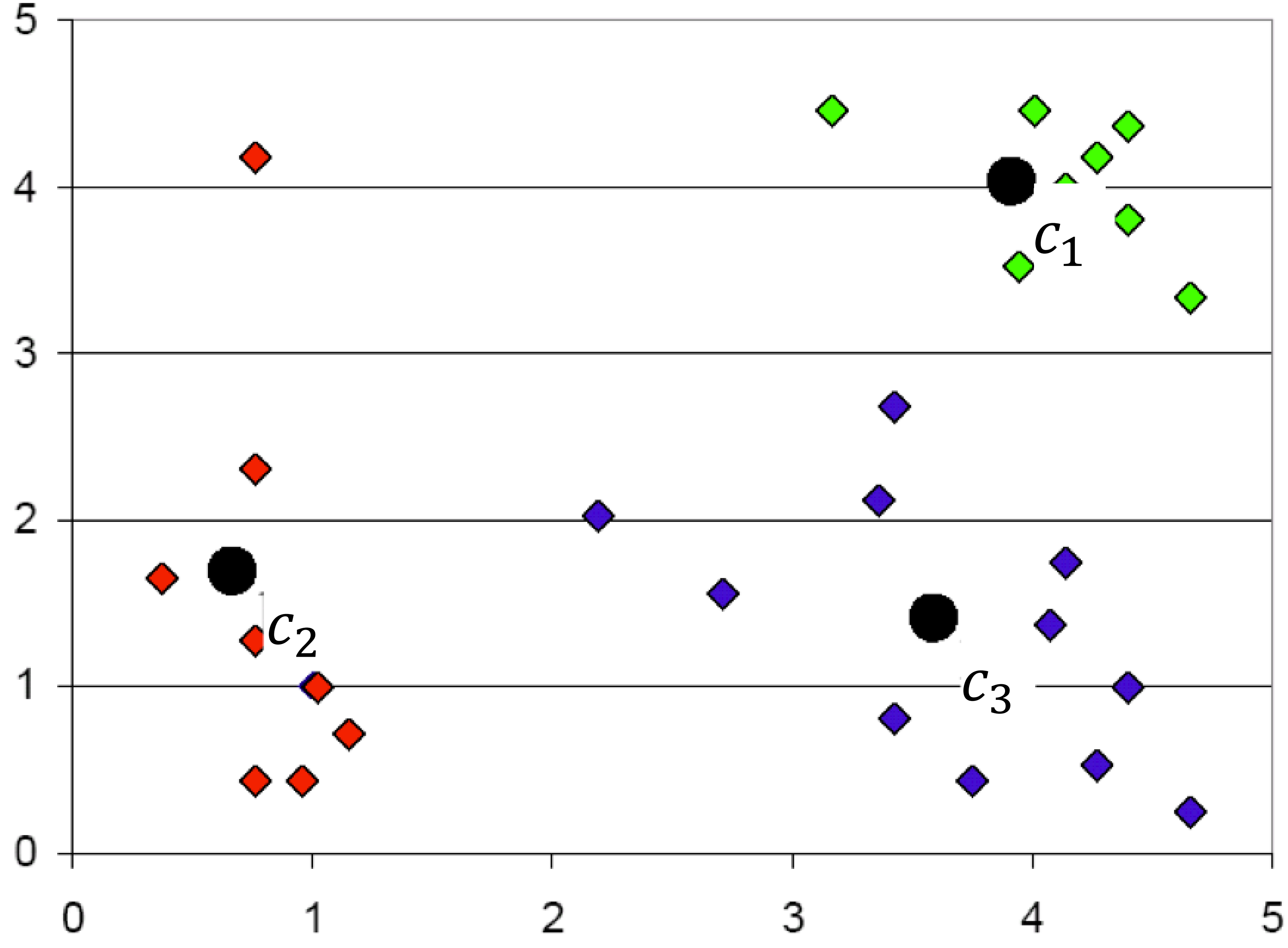
K-Means: Step 3



K-Means: Step 4



K-Means: Step 5



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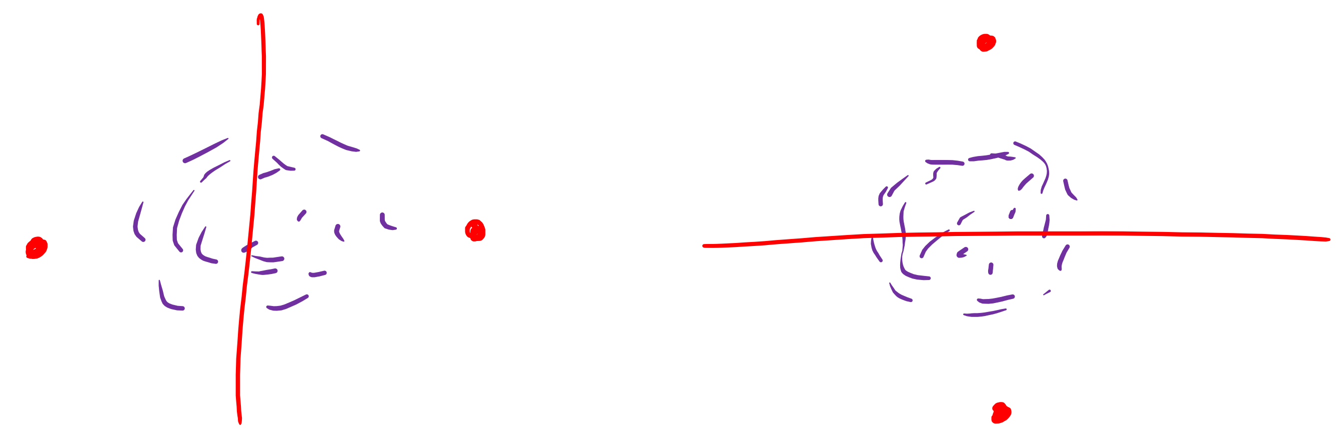
Questions

- 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, $\{x_1, x_2, \ldots, x_n\}$ $x \in R^d$
- Find k cluster centers, $\{c_1, c_2, \ldots, c_k\}$ $c \in R^d$
- And assign each datapoint i to one cluster, $\pi(i) \in \{1, \ldots, k\}$
- Such that the averaged square distances from each datapoint to its respective cluster center is small

distortion

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

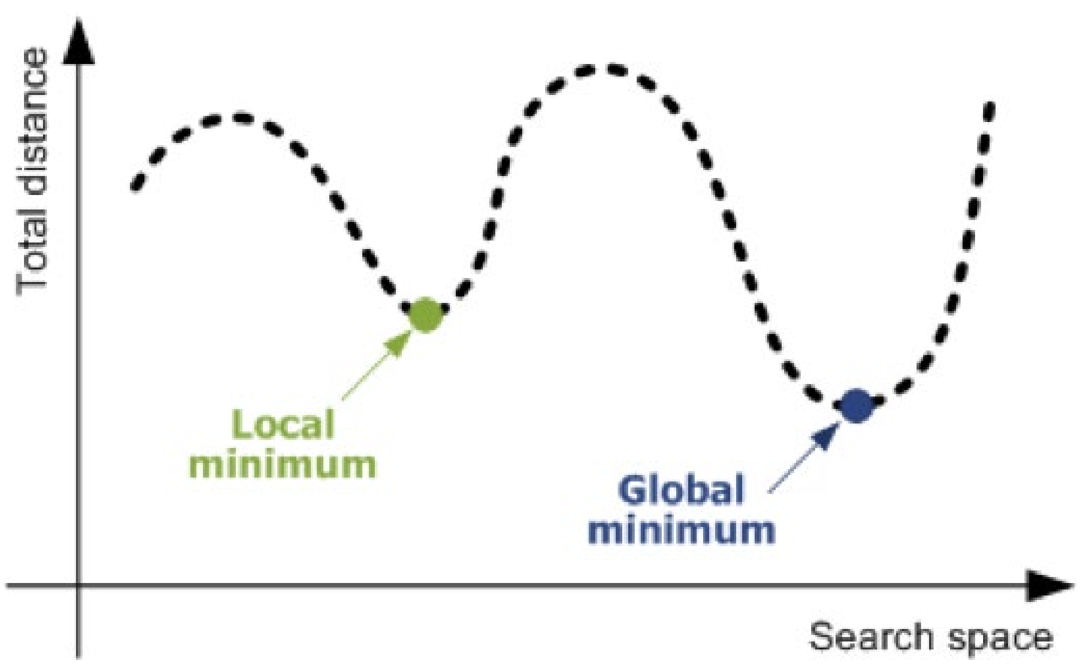
Clustering is [NP-Hard]

- Find k cluster centers, $\{c_1, c_2, \dots, c_k\}$ $c \in R^d$, and assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$, to minimize

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

NP-hard!

- 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

$2^3 = 8$

$X = \{A,B,C\}$

n=3 (data points)

k=2 clusters of two members

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

Convergence of K-Means

- Will kmeans objective oscillate?

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

- The minimum value of the objective is finite

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

Time Complexity

- Assume computing distance between two instances is O(d) where d is the dimensionality of the vectors.

$X_1 = [1 \quad 2 \quad 3 \quad \ldots]d$

$X_2 = [2 \quad 3 \quad 4 \quad \ldots]d$

$d(X_1, X_2) = \sqrt{(1-2)^2 + (2-3)^2 + \ldots}$

$O(d)$

$\downarrow$

$O(nd)$

$\downarrow$

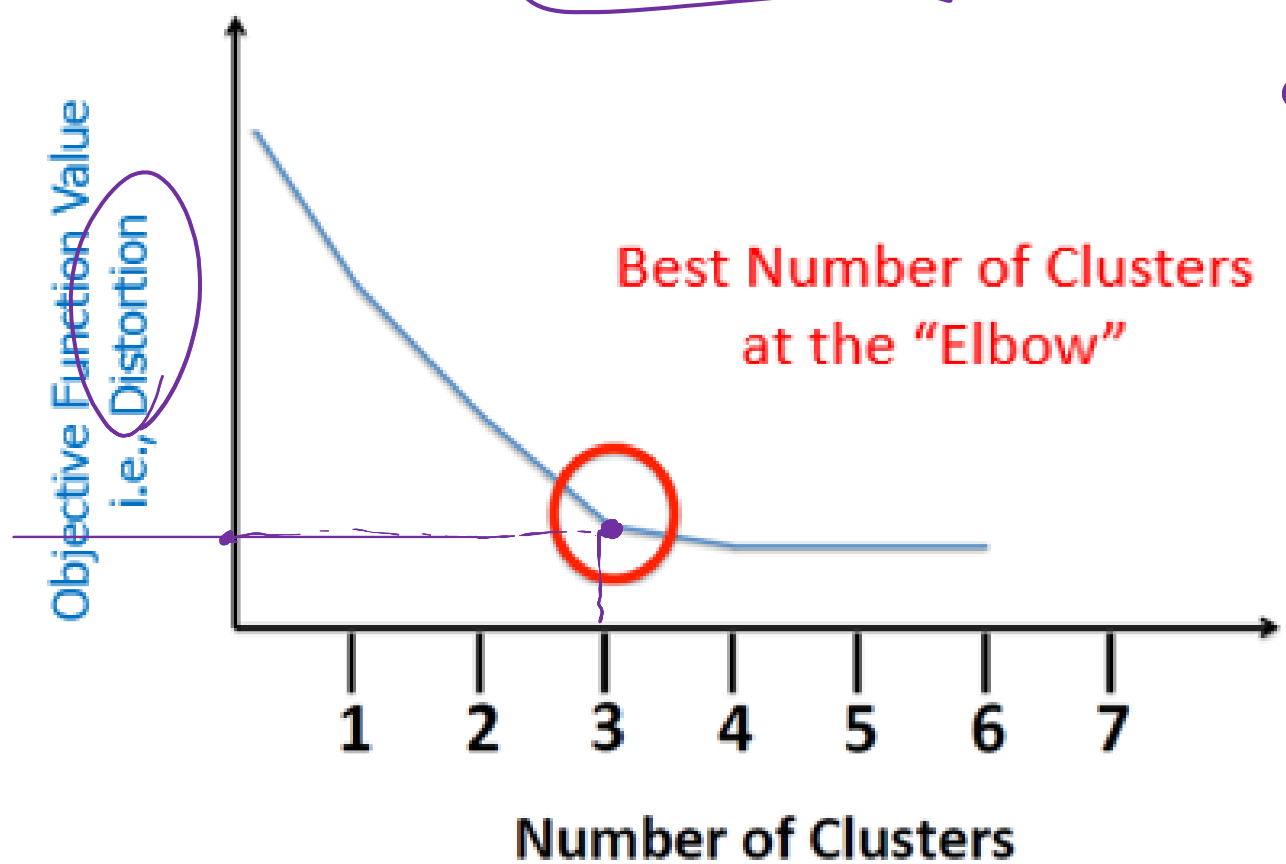
$O(knd)$

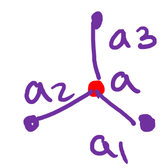
$O(Iknd)$

- 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).

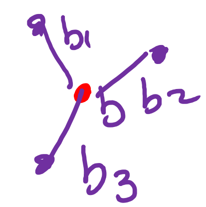
How to Choose K?

Elbow method

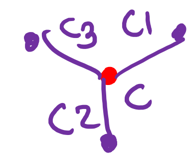




$a_1+a_2+a_3=A$

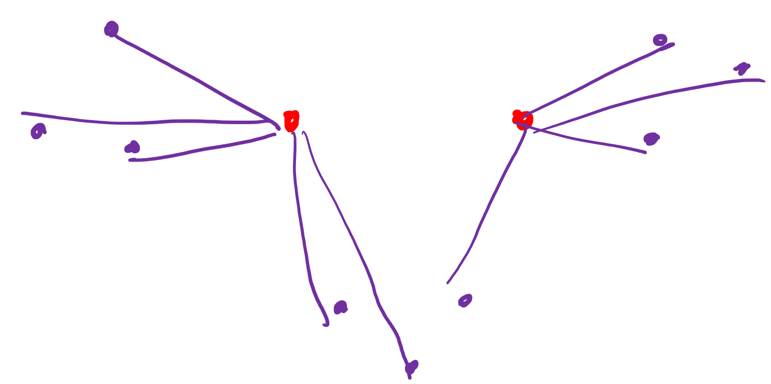


$b_1+b_2+b_3=B$



$c_1+c_2+c_3=C$

Distortion $= A+B+C$



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

Image credit: Dileka Madushan.