

Computational Data Analysis

Machine Learning

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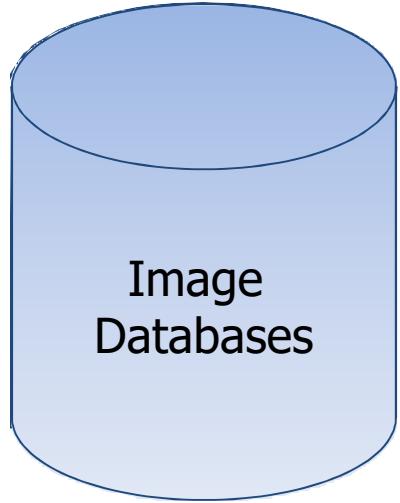
Associate Professor

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Engineering

Clustering

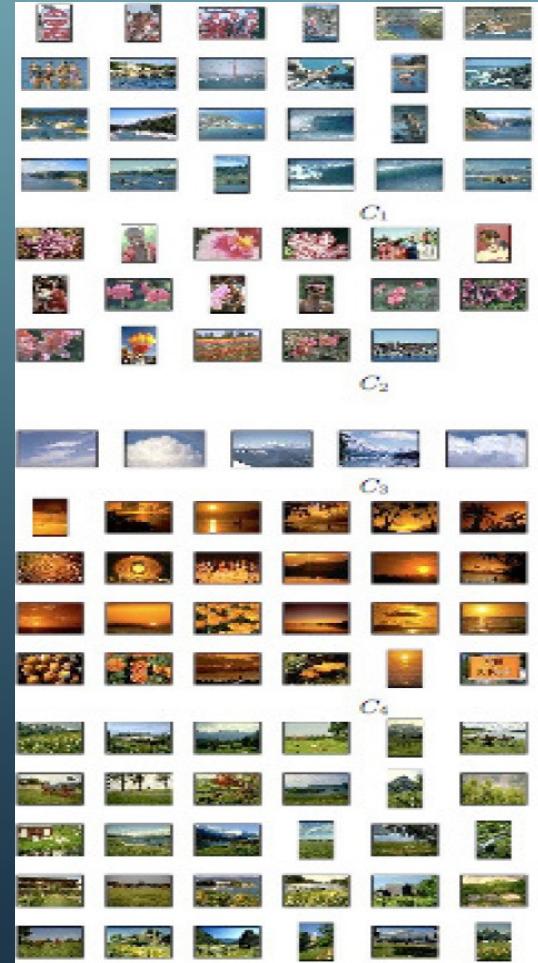


Cluster images



Goal of clustering:

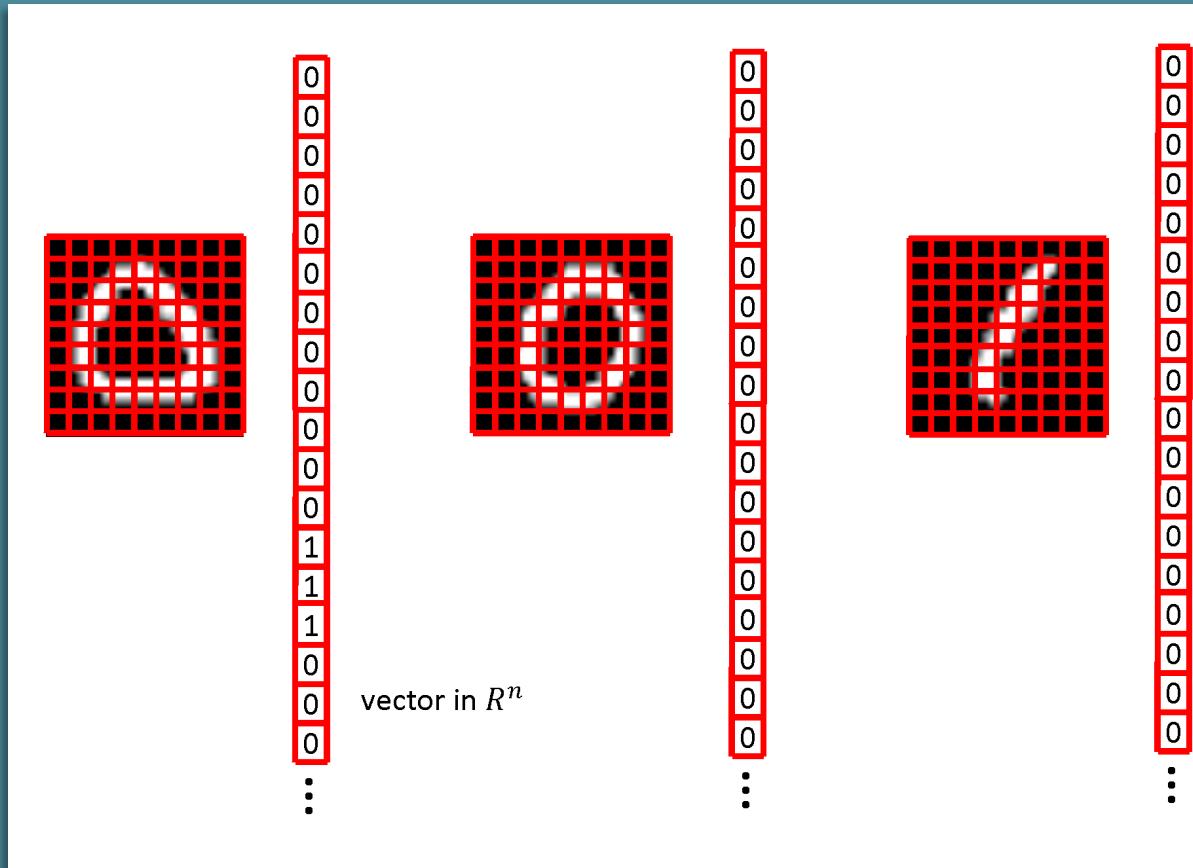
Divide object into groups, and objects within a group are more similar than those outside the group



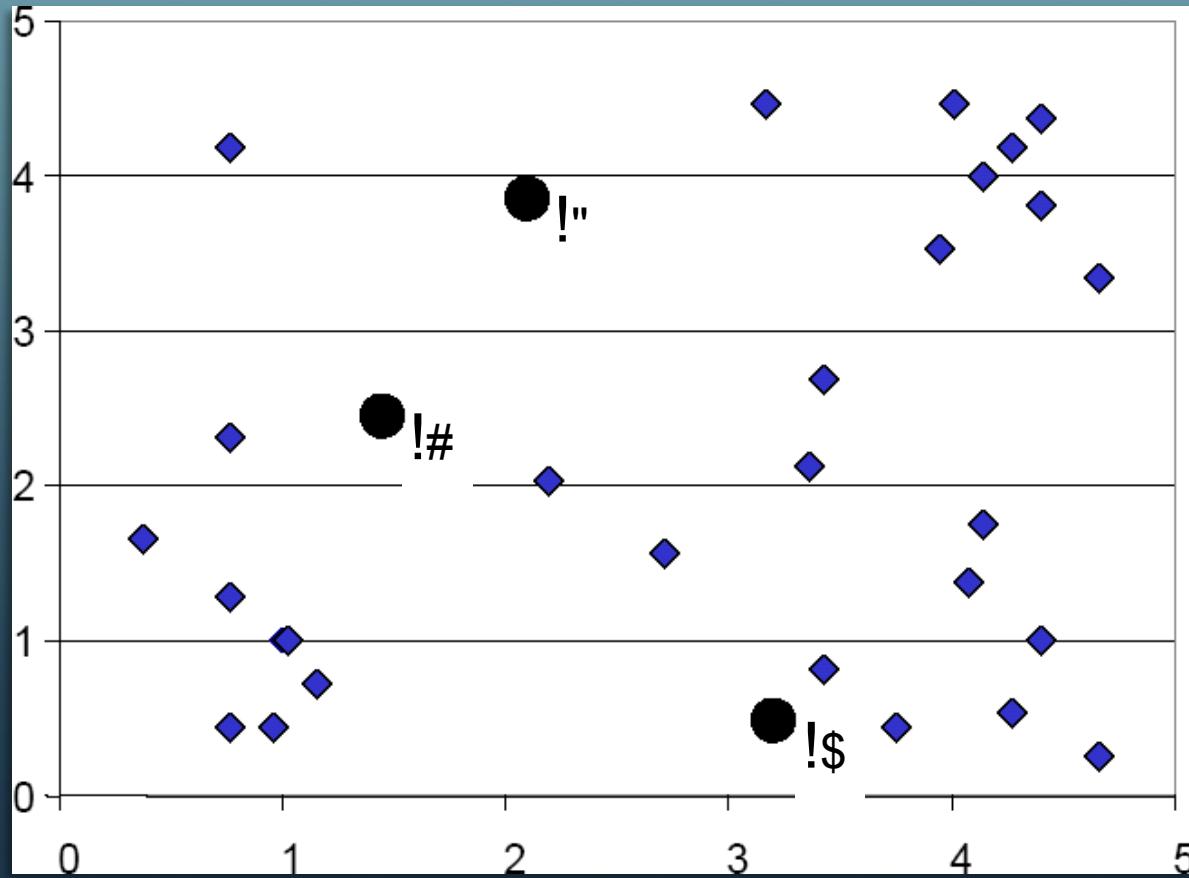
Cluster handwritten digits

72104149590690159784966540740131
34727121174235124463556041957893
74043070291732977627847361369314
17696054992194873974449254767905
85665781016467317182029955156034
465465451447232711818185089250111
09031642361113952945939036557227
12841733887922415987230442419577
28268577918180301994182129759264
15429204002847124027433003196525
12936420711215339786361381051315
56185119462250656372088541140337
61621928619525442838245031773797
19214292049148184598837600302664
85332391268056663882758961841259
19754089910523789406395213136578
22632654897130383193446421825488
40023277087447969098046063548339
33378087170654380963809968685786
02402231975108462479329822927359
18020511376712580371409186774349
19317397691378336128585114431077
07944855408210845040613326726931
46254206217341054311749948402451
16471942415538314568941538032512
83440883317358632613607217142421
79611248177480231310770355276692
83522560829288887493066321322930
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78911691445406223151203812671623
90122089

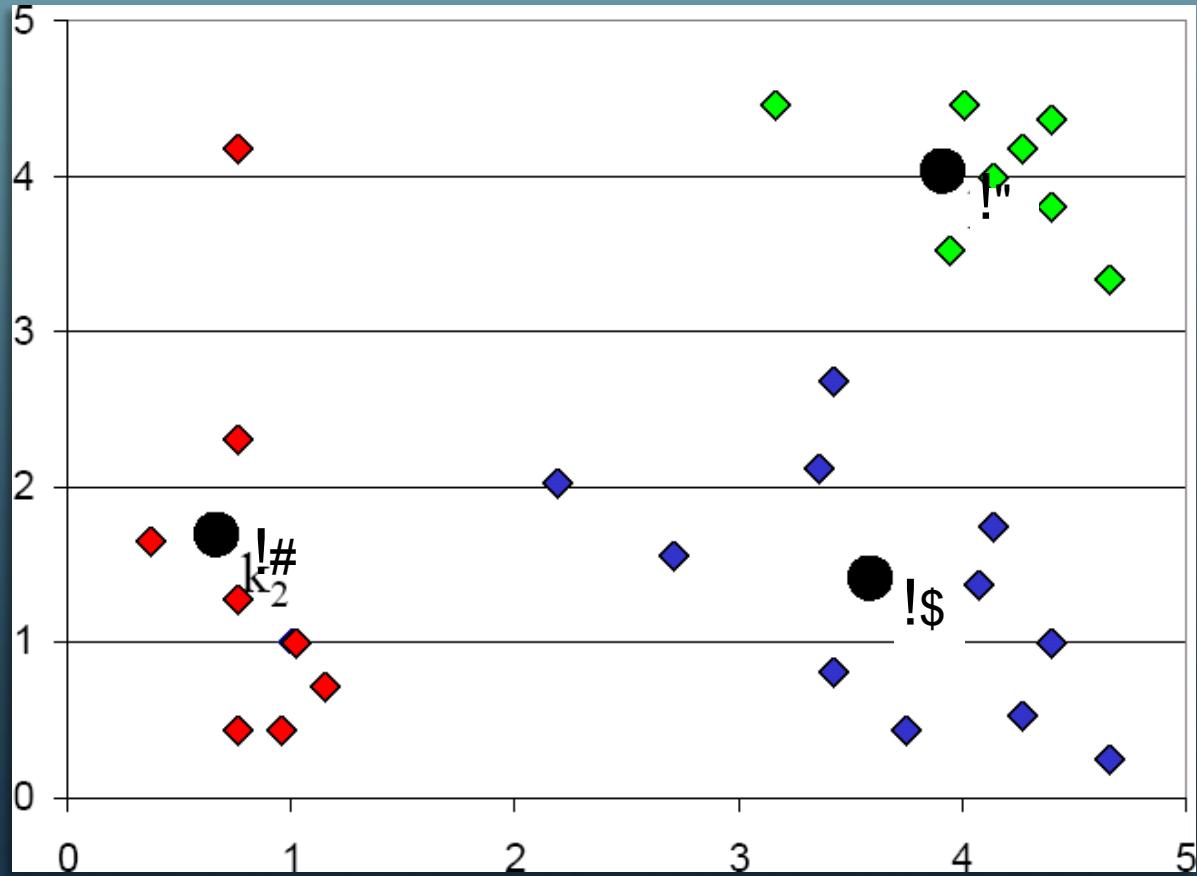
How to represent objects?



Before clustering, a bunch of vectors



After clustering, group assigned



Formal statement and goal of k-means

- Given m data points, $\{x^1, x^2, \dots, x^m\} \in R^n$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^n$
- And assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$

Superscript: index for variables (e.g., sample, cluster index)

Sample size: m

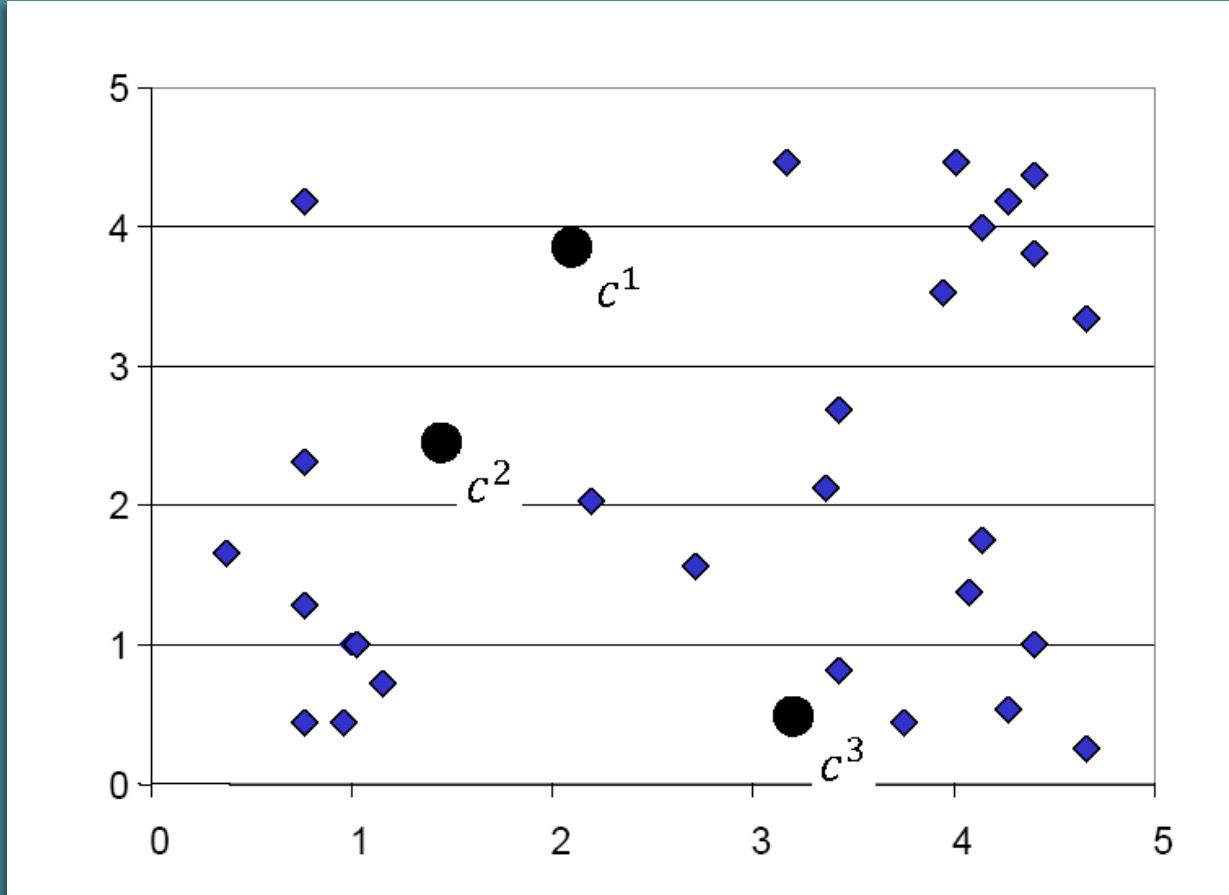
Dimension of each sample: n

number of clusters: k

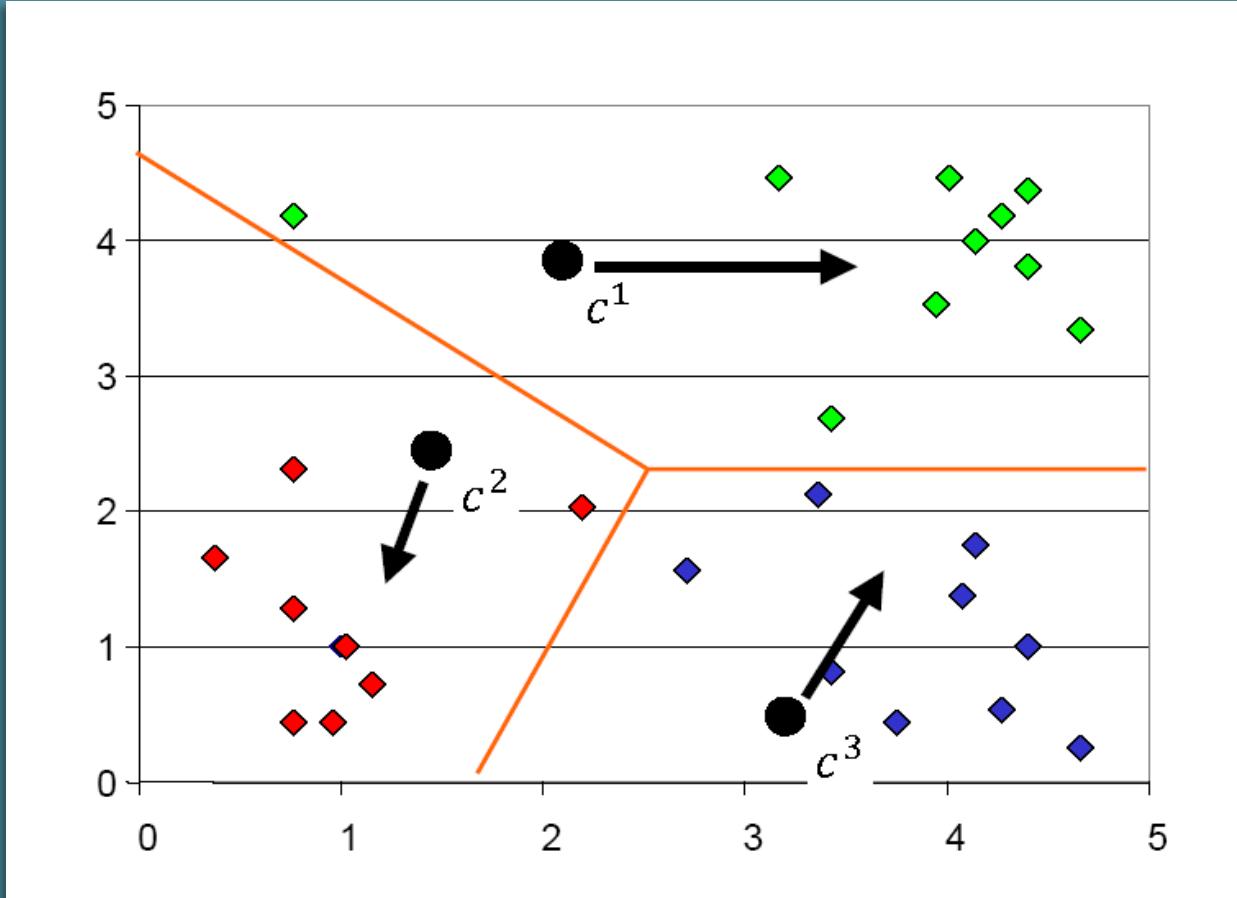
K-means algorithm

- 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**)
$$\pi(i) = \operatorname{argmin}_{j=1,\dots,k} \|x^i - c^j\|^2$$
 - Adjust the cluster centers (**center adjustment**)
$$c^j = \frac{1}{|\{i: \pi(i) = j\}|} \sum_{i: \pi(i)=j} x^i$$
- While any cluster center has been changed

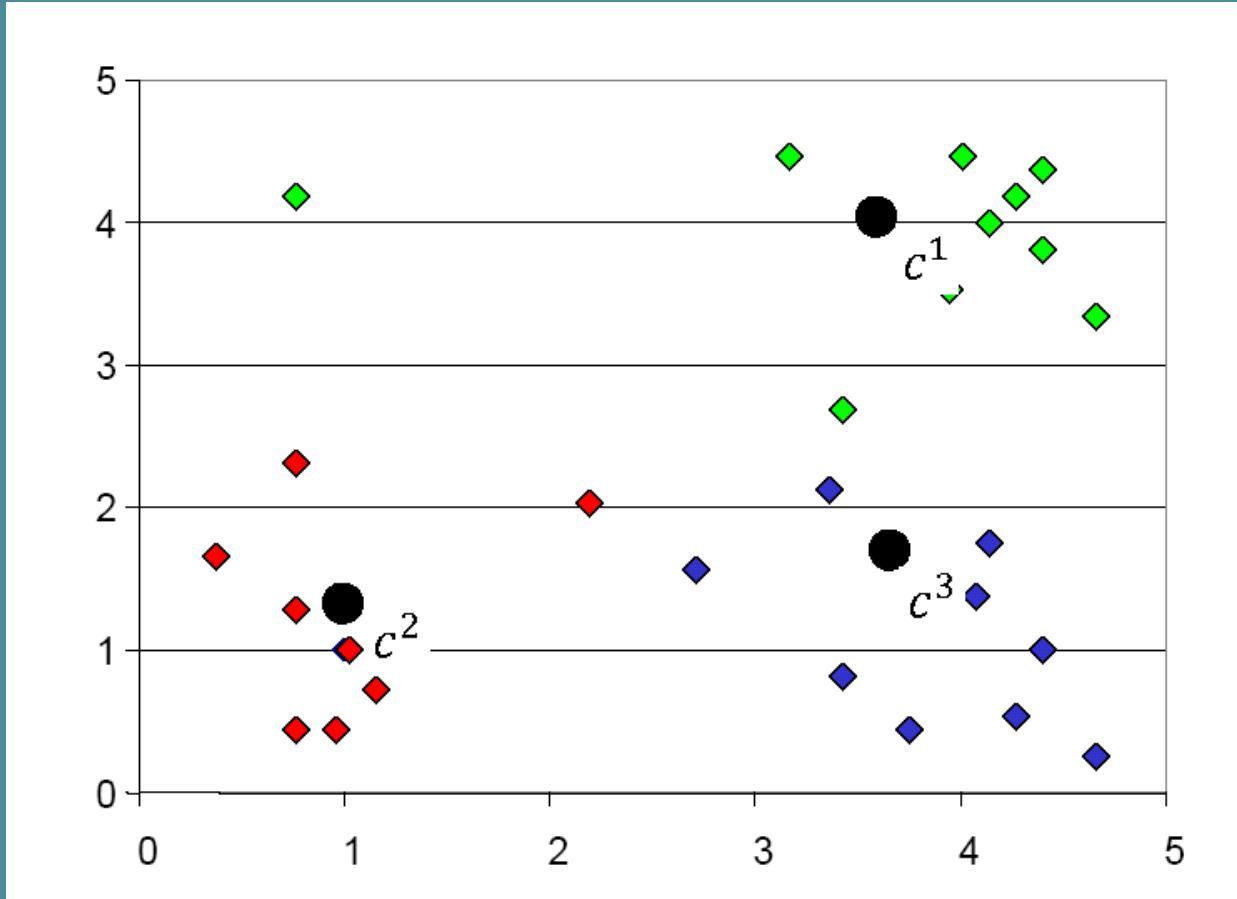
K-means: step 1



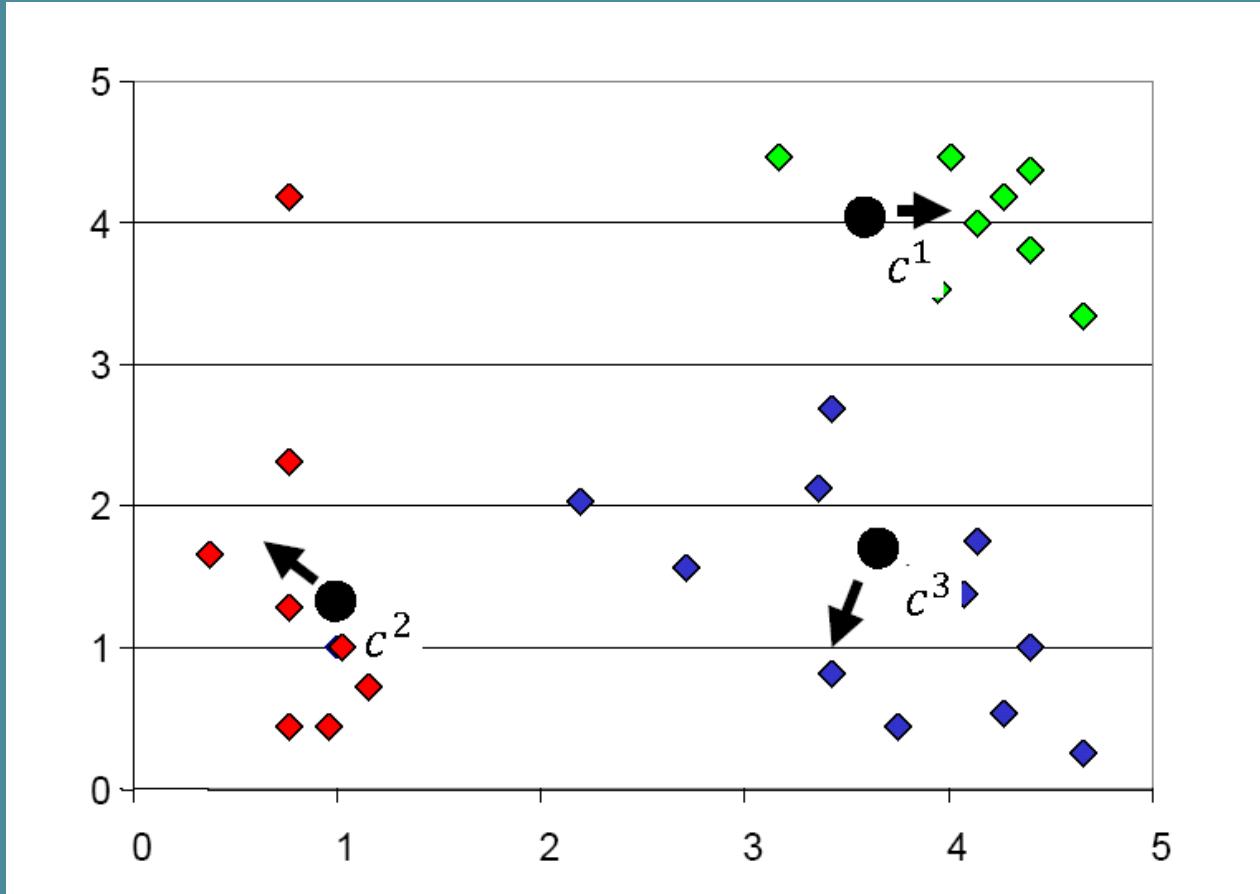
K-means: step 2



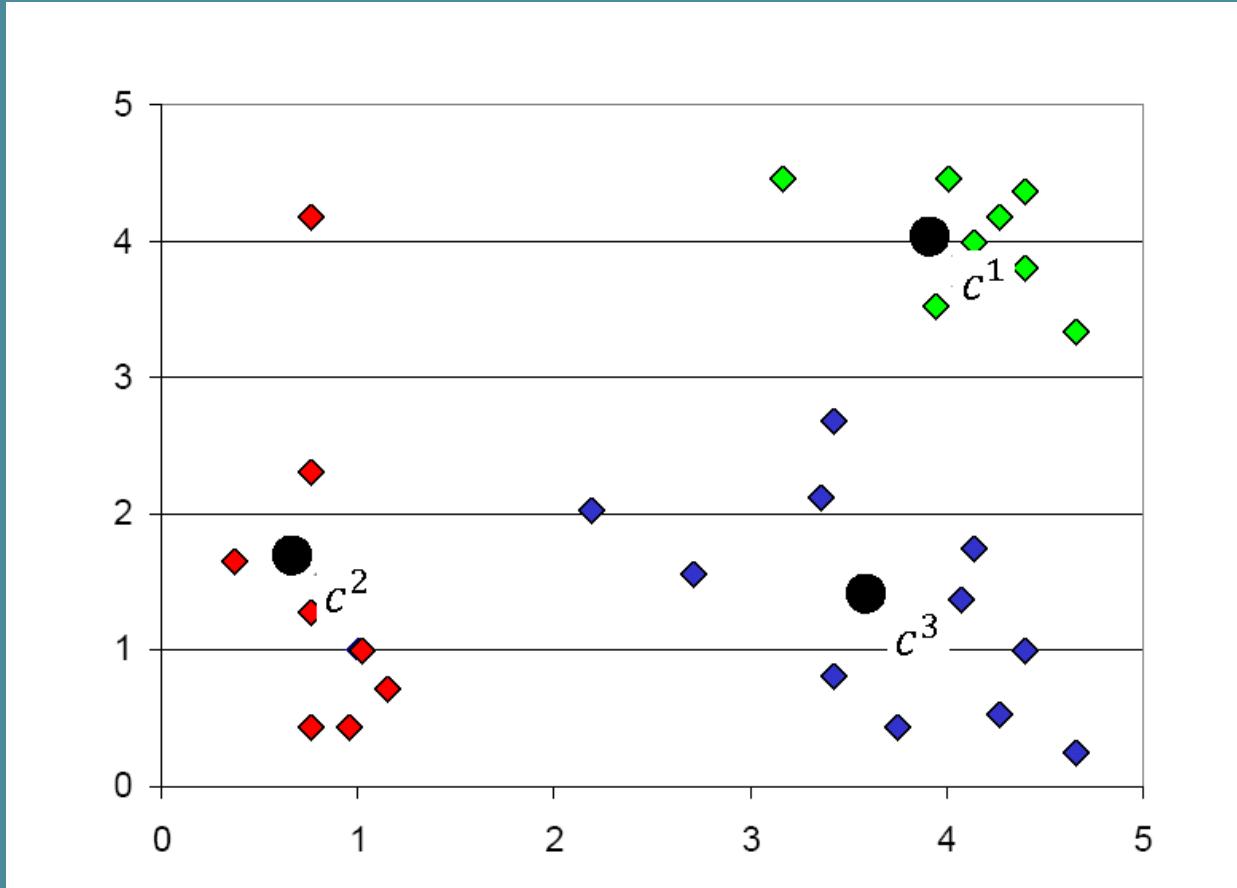
K-means: step 3



K-means: step 4



K-means: step 5



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 k-means objective

- Given m data points, $\{x^1, x^2, \dots, x^m\} \in R^n$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^n$
- 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

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

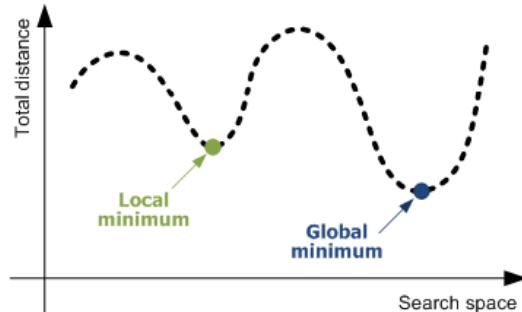
Clustering is NP-hard in general

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

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

NP-hard!

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



Convergence of kmeans algorithm

- Will kmeans objective oscillate?

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

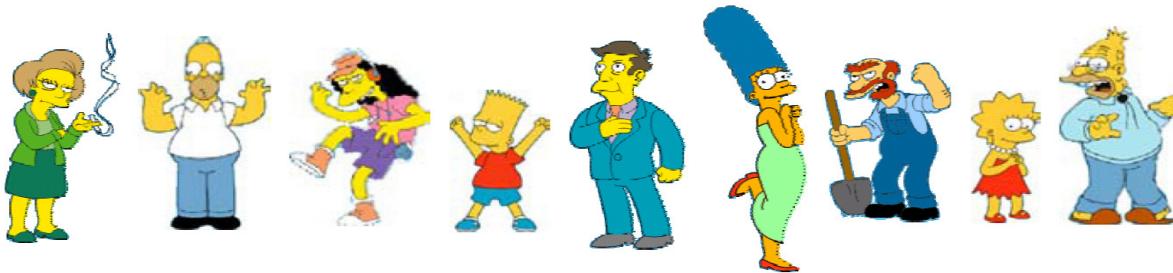
- The minimum value of the objective is finite
- Each iteration of kmeans algorithm decrease the objective
 - Cluster assignment step decreases objective

• $\pi(i) = \operatorname{argmin}_{j=1,\dots,k} \|x^i - c^j\|^2$ for each data point i

- Center adjustment step decreases objective

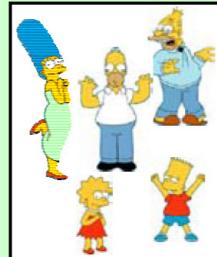
• $c^j = \frac{1}{|\{i:\pi(i)=j\}|} \sum_{i:\pi(i)=j} x^i = \operatorname{argmin}_c \sum_{i:\pi(i)=j} \|x^i - c\|^2$

What else needs to be considered?



What is consider similar/dissimilar?

Clustering is subjective



Simpson's Family



School Employees



Females



Males

You pick your similarity/dissimilarity

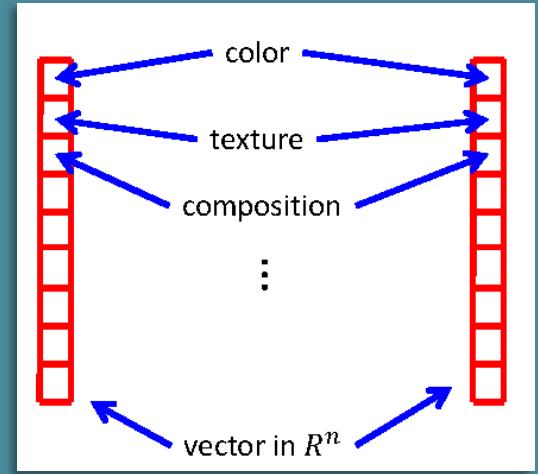


<https://www.paddingtonpups.com.au/tag/similarities-between-owners-and-dogs>

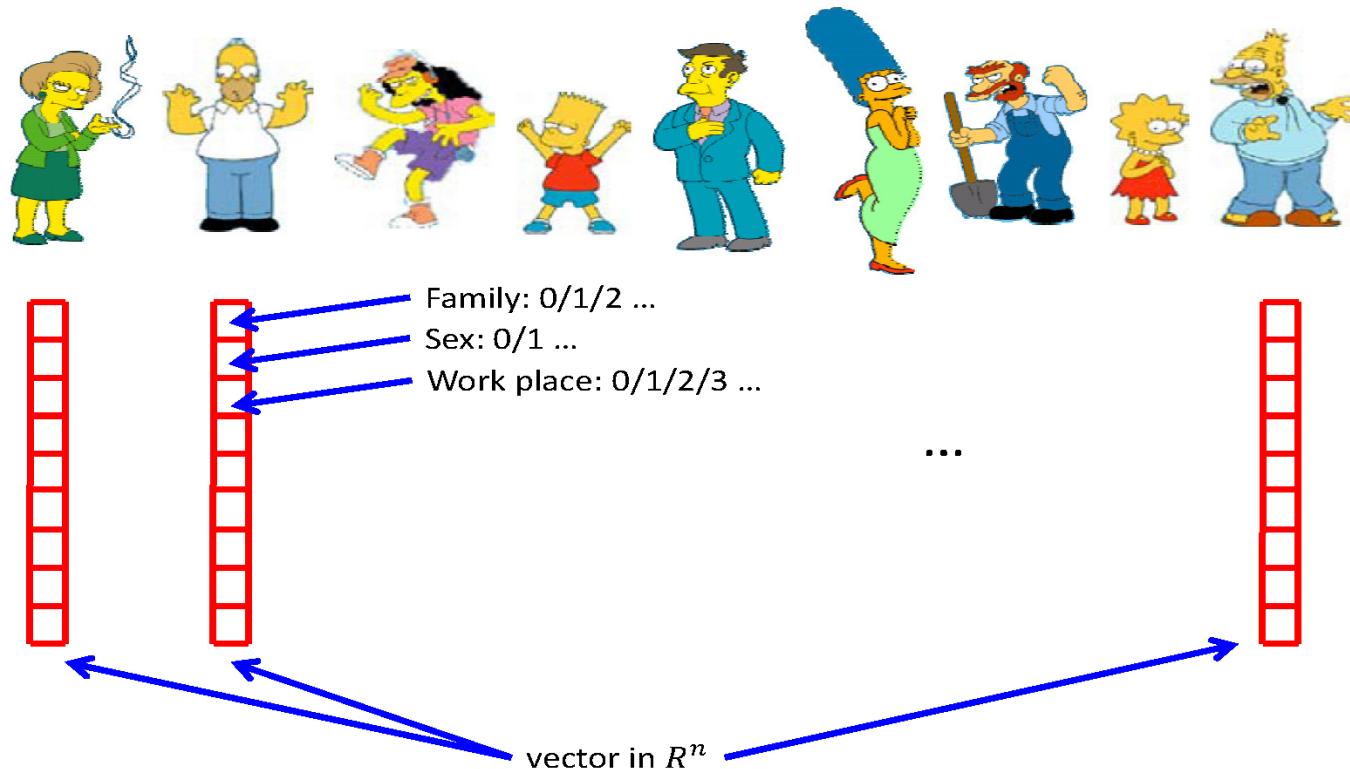
So what is clustering in general?

- 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

Images of different sizes



Objects in real life



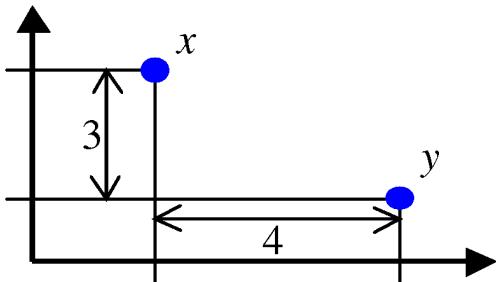
What similarity/dissimilarity function?

- 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^n
 - $x = (x_1, x_2, \dots, x_n)^\top$
 - $y = (y_1, y_2, \dots, y_n)^\top$
- Euclidian distance: $d(x, y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}$
- Minkowski distance: $d(x, y) = \sqrt[p]{\sum_{i=1}^n (x_i - y_i)^p}$
 - Euclidian distance: $p = 2$
 - Manhattan distance: $p = 1, d(x, y) = \sum_{i=1}^n |x_i - y_i|$
 - “inf”-distance: $p = \infty, d(x, y) = \max_{i=1}^n |x_i - y_i|$

Distance example



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

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	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)

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

Generalization of K-means

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

$$\min_{c,\pi} \sum_{i=1}^m d(x^i, c^{\pi(i)})^2$$



NP-hard!

Generalized 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

$$\pi(i) = \operatorname{argmin}_{j=1,\dots,k} d(x^i, c^j)$$

Main difference
from k-means

Adjust the cluster centers

$$c^j = \operatorname{argmin}_{v \in R^n} \sum_{i:\pi(i)=j} d(x^i, v)$$

[A convex optimization problem in many cases.]

While any cluster center has been changed.

